



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 03:43 am BST

PDB ID : 2WSC / pdb\_00002wsc  
Title : Improved Model of Plant Photosystem I  
Authors : Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.  
Deposited on : 2009-09-04  
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

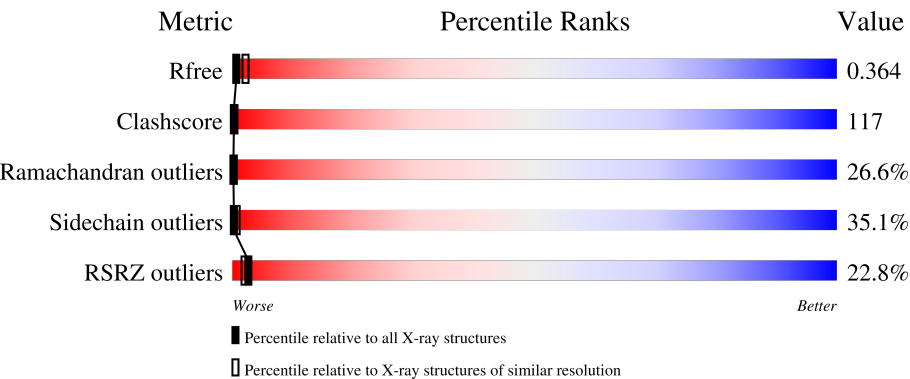
MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	241	<div><div>36%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>30%25%11%.32%</div></div>
2	2	269	<div><div>22%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>24%30%10%.35%</div></div>
3	3	276	<div><div>30%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>16%21%16%6%41%</div></div>
4	4	251	<div><div>23%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>22%27%14%.34%</div></div>
5	A	758	<div><div>19%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>6%48%34%9%. </div></div>

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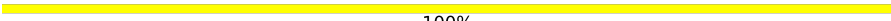


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Mol	Chain	Length	Quality of chain
6	B	734	
7	C	81	
8	D	212	
9	E	143	
10	F	231	
11	G	167	
12	H	144	
13	I	40	
14	J	44	
15	K	131	
16	L	216	
17	N	170	
18	R	53	
19	M	2	
19	O	2	
19	P	2	
19	Q	2	
19	S	2	
19	T	2	
19	U	2	
19	V	2	
19	W	2	
19	X	2	
19	Y	2	
19	Z	2	

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Mol	Chain	Length	Quality of chain
19	a	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	GLC	M	1	-	-	X	-
19	FRU	M	2	X	-	X	-
19	FRU	O	2	X	-	X	-
19	FRU	P	2	X	-	-	-
19	GLC	Q	1	-	-	X	-
19	FRU	Q	2	X	-	X	-
19	FRU	S	2	X	-	-	-
19	GLC	T	1	-	-	X	-
19	FRU	T	2	X	-	X	-
19	GLC	U	1	-	-	X	-
19	FRU	U	2	X	-	X	-
19	FRU	V	2	X	-	-	-
19	GLC	W	1	-	-	X	-
19	FRU	W	2	X	-	X	-
19	GLC	X	1	-	-	X	-
19	FRU	X	2	X	-	X	-
19	FRU	Y	2	X	-	-	-
19	GLC	Z	1	-	-	X	-
19	FRU	Z	2	X	-	X	-
19	FRU	a	2	X	-	-	-
20	CLA	1	1187	X	-	-	-
20	CLA	1	1188	X	-	-	-
20	CLA	1	1189	X	-	-	-
20	CLA	1	1190	X	-	-	-
20	CLA	1	1191	X	-	-	-
20	CLA	1	1192	X	-	-	-
20	CLA	1	1193	X	-	-	-
20	CLA	1	1194	X	-	-	-
20	CLA	1	1195	X	-	-	-
20	CLA	1	1196	X	-	-	-
20	CLA	1	1197	X	-	-	-
20	CLA	1	1198	X	-	-	-
20	CLA	1	1199	X	-	-	-
20	CLA	1	1200	X	-	-	-
20	CLA	1	1201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	1212	X	-	-	-
20	CLA	2	1213	X	-	-	-
20	CLA	2	1214	X	-	-	-
20	CLA	2	1215	X	-	X	-
20	CLA	2	1216	X	-	-	-
20	CLA	2	1217	X	-	-	-
20	CLA	2	1218	X	-	-	-
20	CLA	2	1219	X	-	-	-
20	CLA	2	1220	X	-	X	-
20	CLA	2	1221	X	-	-	-
20	CLA	2	1222	X	-	-	-
20	CLA	2	1223	X	-	-	-
20	CLA	2	1224	X	-	-	-
20	CLA	2	1227	X	-	-	-
20	CLA	2	2010	X	-	-	-
20	CLA	3	1212	X	-	-	-
20	CLA	3	1213	X	-	-	-
20	CLA	3	1214	X	-	-	-
20	CLA	3	1215	X	-	-	-
20	CLA	3	1216	X	-	-	-
20	CLA	3	1217	X	-	-	-
20	CLA	3	1218	X	-	X	-
20	CLA	3	1219	X	-	-	-
20	CLA	3	3001	X	-	-	-
20	CLA	3	3002	X	-	-	-
20	CLA	3	3007	X	-	-	-
20	CLA	3	3008	X	-	-	-
20	CLA	3	3011	X	-	-	-
20	CLA	3	3014	X	-	-	-
20	CLA	3	3015	X	-	-	-
20	CLA	4	1196	X	-	X	-
20	CLA	4	1197	X	-	-	-
20	CLA	4	1198	X	-	X	-
20	CLA	4	1199	X	-	X	-
20	CLA	4	1200	X	-	-	-
20	CLA	4	1201	X	-	X	-
20	CLA	4	1202	X	-	-	-
20	CLA	4	1203	X	-	-	-
20	CLA	4	1204	X	-	-	-
20	CLA	4	1205	X	-	-	-
20	CLA	4	1206	X	-	-	-
20	CLA	4	1207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	4	1208	X	-	-	-
20	CLA	4	1209	X	-	-	-
20	CLA	4	4003	X	-	-	-
20	CLA	4	4007	X	-	-	-
20	CLA	4	4014	X	-	-	-
20	CLA	A	1759	X	-	-	-
20	CLA	A	1760	X	-	X	-
20	CLA	A	1761	X	-	X	-
20	CLA	A	1762	X	-	-	-
20	CLA	A	1763	X	-	X	-
20	CLA	A	1764	X	-	X	-
20	CLA	A	1765	X	-	X	-
20	CLA	A	1766	X	-	-	-
20	CLA	A	1767	X	-	X	-
20	CLA	A	1768	X	-	-	-
20	CLA	A	1769	X	-	X	-
20	CLA	A	1770	X	-	X	-
20	CLA	A	1771	X	-	-	-
20	CLA	A	1772	X	-	X	-
20	CLA	A	1773	X	-	-	-
20	CLA	A	1774	X	-	X	-
20	CLA	A	1775	X	-	-	-
20	CLA	A	1776	X	-	X	-
20	CLA	A	1777	X	-	-	-
20	CLA	A	1778	X	-	-	-
20	CLA	A	1779	X	-	X	-
20	CLA	A	1780	X	-	-	-
20	CLA	A	1781	X	-	X	-
20	CLA	A	1782	X	-	X	-
20	CLA	A	1783	X	-	X	-
20	CLA	A	1784	X	-	-	-
20	CLA	A	1785	X	-	-	-
20	CLA	A	1786	X	-	-	-
20	CLA	A	1787	X	-	X	-
20	CLA	A	1788	X	-	X	-
20	CLA	A	1789	X	-	-	-
20	CLA	A	1790	X	-	-	-
20	CLA	A	1791	X	-	X	-
20	CLA	A	1792	X	-	X	-
20	CLA	A	1793	X	-	X	-
20	CLA	A	1794	X	-	X	-
20	CLA	A	1795	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	1796	X	-	X	-
20	CLA	A	1797	X	-	X	-
20	CLA	A	1798	X	-	X	-
20	CLA	A	1799	X	-	-	-
20	CLA	A	1800	X	-	X	-
20	CLA	A	1801	X	-	-	-
20	CLA	A	1811	X	-	-	-
20	CLA	A	1812	X	-	X	-
20	CLA	A	1813	X	-	X	-
20	CLA	A	1815	X	-	-	-
20	CLA	A	1816	X	-	X	-
20	CLA	A	1817	X	-	-	-
20	CLA	B	1735	X	-	X	-
20	CLA	B	1736	X	-	-	-
20	CLA	B	1737	X	-	X	-
20	CLA	B	1738	X	-	-	-
20	CLA	B	1739	X	-	X	-
20	CLA	B	1740	X	-	-	-
20	CLA	B	1741	X	-	-	-
20	CLA	B	1742	X	-	-	-
20	CLA	B	1743	X	-	X	-
20	CLA	B	1744	X	-	-	-
20	CLA	B	1745	X	-	-	-
20	CLA	B	1746	X	-	X	-
20	CLA	B	1747	X	-	X	-
20	CLA	B	1748	X	-	-	-
20	CLA	B	1749	X	-	-	-
20	CLA	B	1750	X	-	-	-
20	CLA	B	1751	X	-	-	-
20	CLA	B	1752	X	-	-	-
20	CLA	B	1753	X	-	X	-
20	CLA	B	1754	X	-	X	-
20	CLA	B	1755	X	-	X	-
20	CLA	B	1756	X	-	X	-
20	CLA	B	1757	X	-	X	-
20	CLA	B	1758	X	-	X	-
20	CLA	B	1759	X	-	X	-
20	CLA	B	1760	X	-	-	-
20	CLA	B	1761	X	-	-	-
20	CLA	B	1762	X	-	X	-
20	CLA	B	1763	X	-	-	-
20	CLA	B	1764	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	1765	X	-	-	-
20	CLA	B	1766	X	-	-	-
20	CLA	B	1767	X	-	-	-
20	CLA	B	1768	X	-	X	-
20	CLA	B	1769	X	-	X	-
20	CLA	B	1770	X	-	X	-
20	CLA	B	1771	X	-	X	-
20	CLA	B	1772	X	-	-	-
20	CLA	B	1785	X	-	X	-
20	CLA	B	1786	X	-	X	-
20	CLA	B	1787	X	-	X	-
20	CLA	F	1155	X	-	-	-
20	CLA	F	1156	X	-	-	-
20	CLA	F	1157	X	-	-	-
20	CLA	G	1099	X	-	-	-
20	CLA	H	1079	X	-	-	-
20	CLA	I	1031	X	-	-	-
20	CLA	I	1033	X	-	-	-
20	CLA	J	1043	X	-	X	-
20	CLA	J	1044	X	-	X	-
20	CLA	J	1045	X	-	X	-
20	CLA	J	1046	X	-	-	-
20	CLA	K	1085	X	-	X	-
20	CLA	K	1142	X	-	X	-
20	CLA	K	1146	X	-	-	-
20	CLA	K	3009	X	-	-	-
20	CLA	L	1166	X	-	-	-
20	CLA	L	1167	X	-	-	-
20	CLA	L	1168	X	-	-	-
20	CLA	L	1505	X	-	-	-
20	CLA	R	1054	X	-	-	-
20	CLA	R	1055	X	-	-	-
21	LMU	A	7016	-	-	X	-
21	LMU	A	7020	-	-	X	-
21	LMU	A	7021	-	-	X	-
21	LMU	A	7023	-	-	X	-
21	LMU	A	7026	-	-	X	-
21	LMU	A	7032	-	-	X	-
21	LMU	A	7037	-	-	X	-
21	LMU	A	7042	-	-	X	-
21	LMU	R	1057	X	-	-	-
22	BCR	3	1220	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	BCR	A	1803	-	-	X	-
22	BCR	A	1804	-	-	X	-
22	BCR	A	1805	-	-	X	-
22	BCR	A	1806	-	-	X	-
22	BCR	A	1807	-	-	X	-
22	BCR	A	1808	-	-	X	-
22	BCR	B	1777	-	-	X	-
22	BCR	B	1778	-	-	X	-
22	BCR	B	1779	-	-	X	-
22	BCR	B	1780	-	-	X	-
22	BCR	I	1032	-	-	X	-
22	BCR	L	1169	-	-	X	-
23	PQN	A	1802	X	-	-	-
23	PQN	B	1773	X	-	X	-
24	LMG	B	1783	-	-	X	-
25	SF4	B	1784	-	-	X	-
25	SF4	C	1082	-	-	X	-
25	SF4	C	1083	-	-	X	-

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 36379 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	165	Total	C	N	O	S	0	0	0
			1264	822	208	230	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	conflict	UNP Q9C5R7
1	-1	ARG	LYS	conflict	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	176	Total	C	N	O	S	0	0	0
			1374	899	226	245	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	insertion	UNP Q41038
2	?	-	GLY	deletion	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	162	Total	C	N	O	S	0	0	0
			1254	826	203	220	5			

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	166	Total	C	N	O	S	0	0	0
			1319	861	219	236	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	deletion	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	730	Total	C	N	O	S	0	0	0
			5745	3766	974	987	18			

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5848	3843	997	995	13			

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	conflict	UNP P12353
D	-50	PRO	GLN	conflict	UNP P12353
D	-44	ARG	PRO	conflict	UNP P12353
D	-34	GLU	ASP	conflict	UNP P12353
D	-11	LEU	HIS	conflict	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	conflict	UNP P12353
D	12	THR	PRO	conflict	UNP P12353
D	14	ALA	GLY	conflict	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	65	Total	C	N	O	0	0	0
			520	332	93	95			

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	S	0	0	0
			740	481	120	137	2			

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	69	Total	C	N	O	0	0	0
			529	344	82	103			

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	ILE	LEU	conflict	UNP P36886

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	161	Total	C	N	O	S	0	0	0
			1203	791	193	214	5			

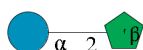
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

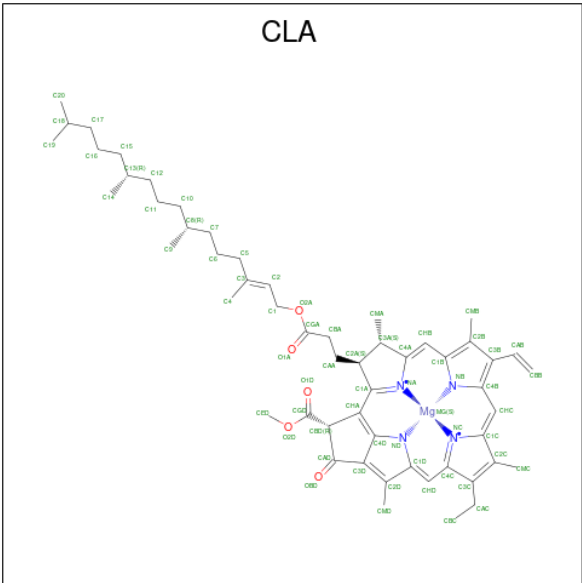
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
19	M	2	Total	C	O	0	0	0
			22	12	10			
19	O	2	Total	C	O	0	0	0
			23	12	11			
19	P	2	Total	C	O	0	0	0
			23	12	11			
19	Q	2	Total	C	O	0	0	0
			23	12	11			
19	S	2	Total	C	O	0	0	0
			23	12	11			
19	T	2	Total	C	O	0	0	0
			23	12	11			
19	U	2	Total	C	O	0	0	0
			23	12	11			
19	V	2	Total	C	O	0	0	0
			23	12	11			
19	W	2	Total	C	O	0	0	0
			23	12	11			
19	X	2	Total	C	O	0	0	0
			23	12	11			
19	Y	2	Total	C	O	0	0	0
			23	12	11			
19	Z	2	Total	C	O	0	0	0
			23	12	11			
19	a	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	2	1	Total 25	C 20	Mg 1	N 4	0	0
20	2	1	Total 56	C 46	Mg 1	N 4 O 5	0	0
20	2	1	Total 25	C 20	Mg 1	N 4	0	0
20	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
20	2	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
20	2	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
20	2	1	Total 25	C 20	Mg 1	N 4	0	0
20	2	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
20	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 25	C 20	Mg 1	N 4	0	0
20	3	1	Total 42	C 34	Mg 1	N 4 O 3	0	0
20	3	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
20	3	1	Total 65	C 55	Mg 1	N 4 O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	3	1	Total 25	C 20	Mg 1	N 4		0	0
20	3	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	4	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
20	4	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	4	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 36	C 30	Mg 1	N 4	O 1	0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	4	1	Total 25	C 20	Mg 1	N 4		0	0
20	4	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
20	4	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
20	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
20	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
20	B	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	B	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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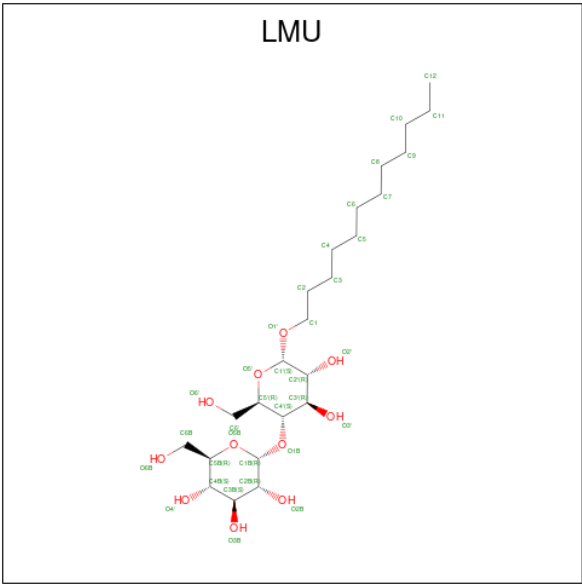
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	I	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	J	1	Total	C	Mg	N		0	0
			25	20	1	4			
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	3	1	Total	C	O	0	0
			35	24	11		
21	4	1	Total	C	O	0	0
			35	24	11		

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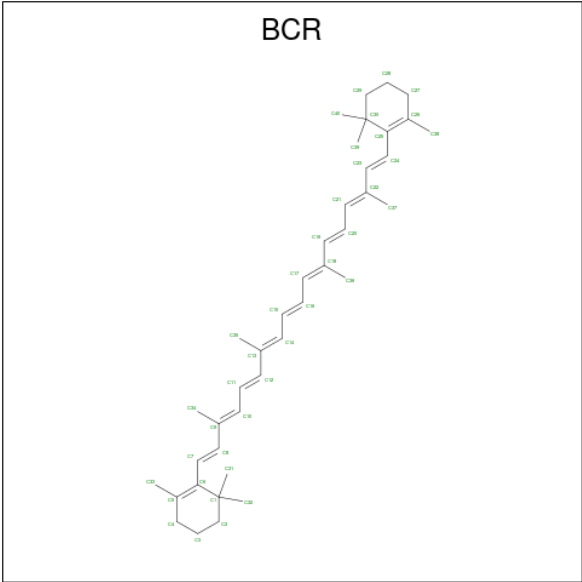
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			34	23	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			34	23	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	A	1	Total	C	O	0	0
			35	24	11		
21	B	1	Total	C	O	0	0
			25	14	11		
21	K	1	Total	C	O	0	0
			35	24	11		
21	L	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		
21	R	1	Total	C	O	0	0
			35	24	11		

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	3	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0

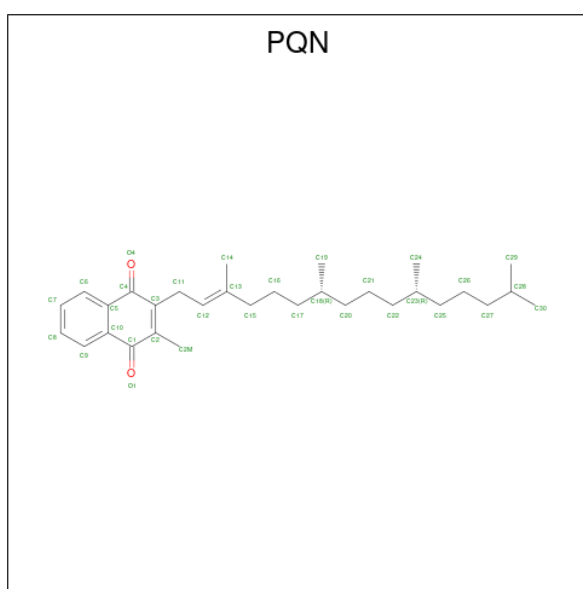
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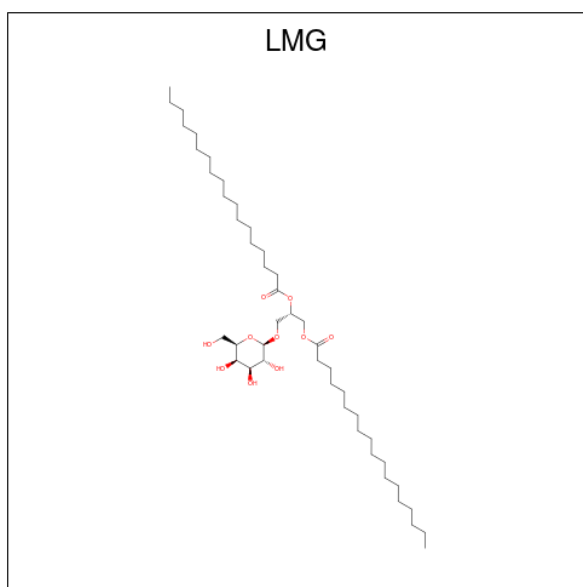
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



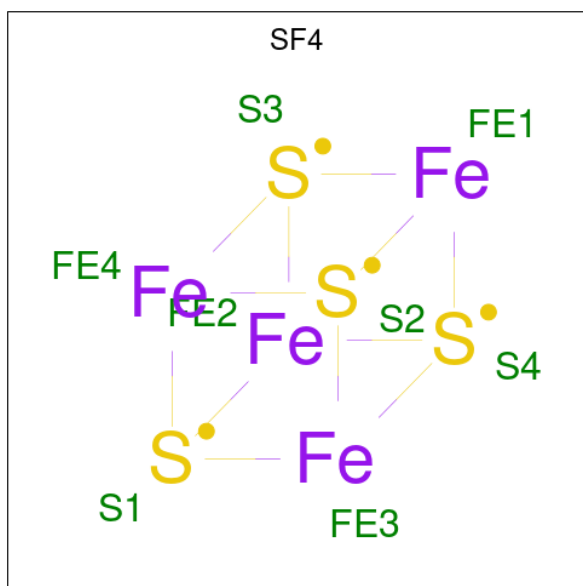
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		
25	C	1	Total	Fe	S	0	0
			8	4	4		

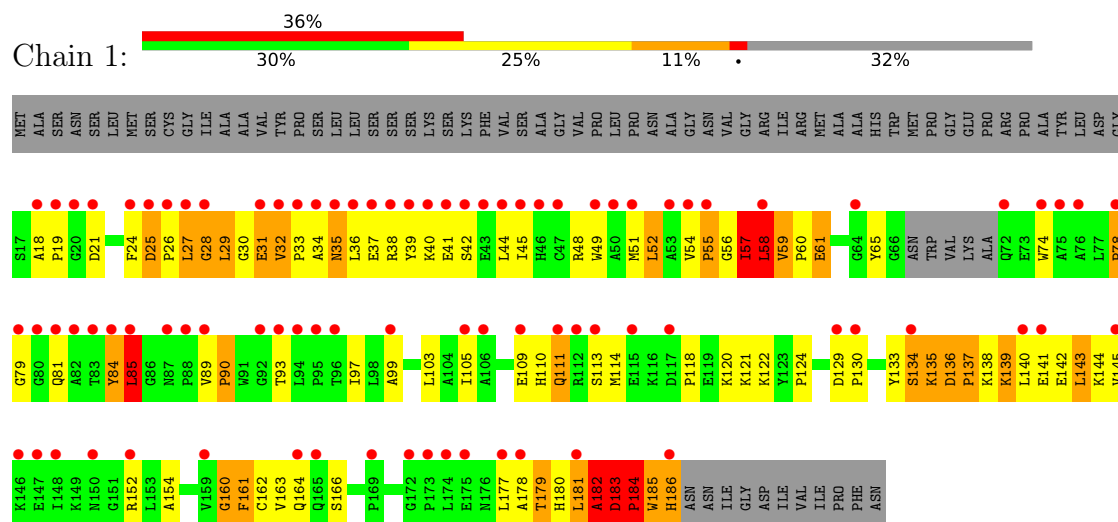
- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			23	12	11		

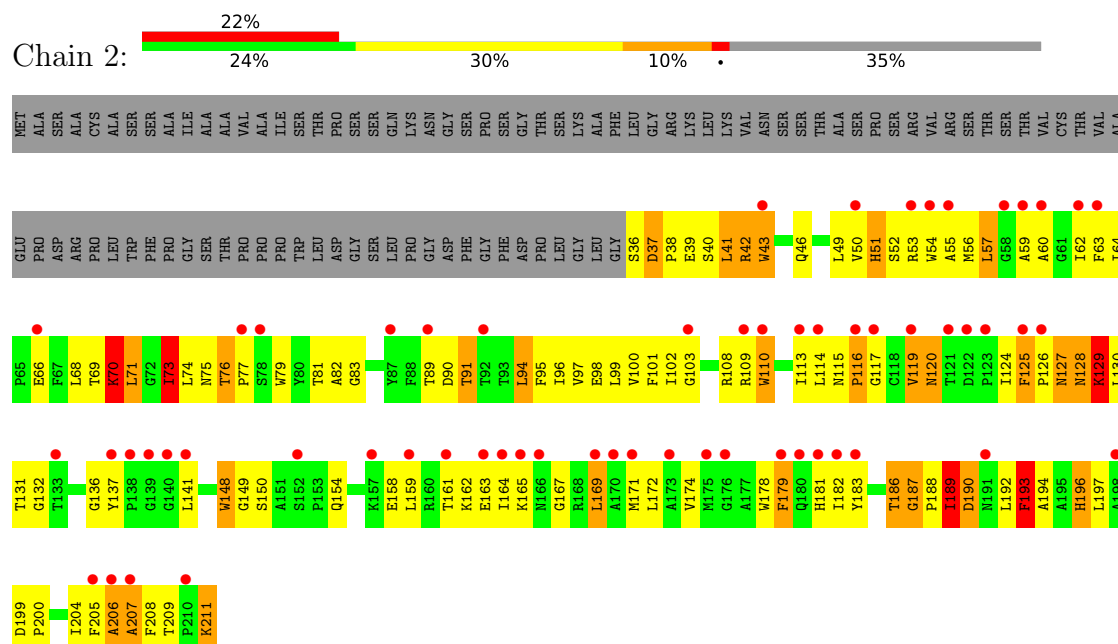
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

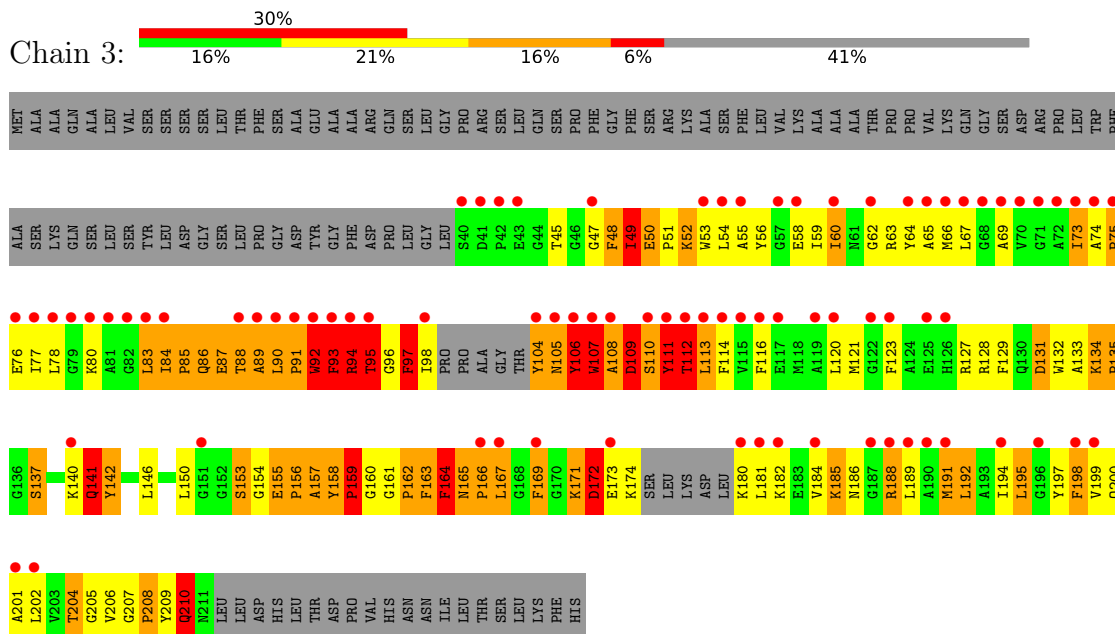
#### • Molecule 1: AT3G54890



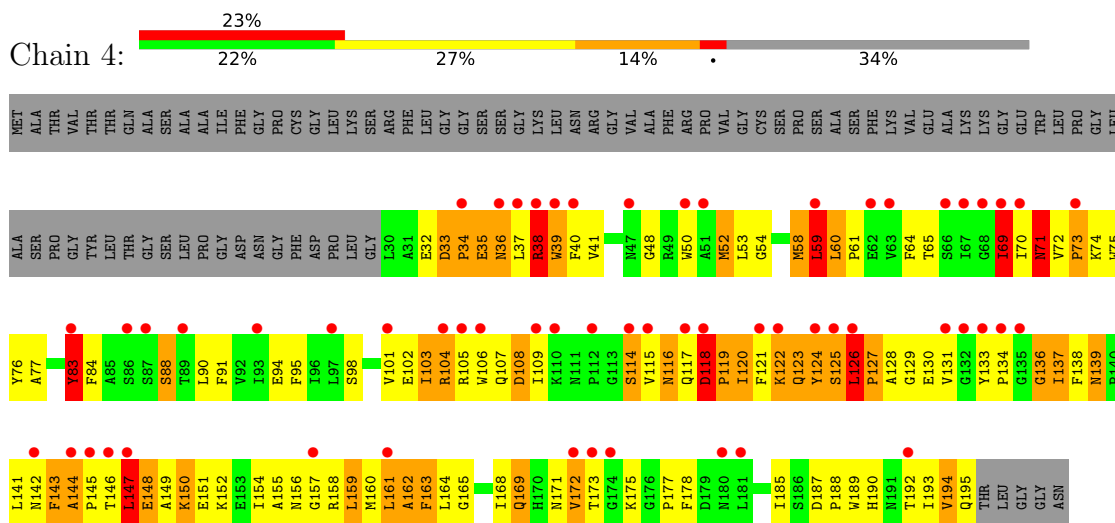
#### • Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I



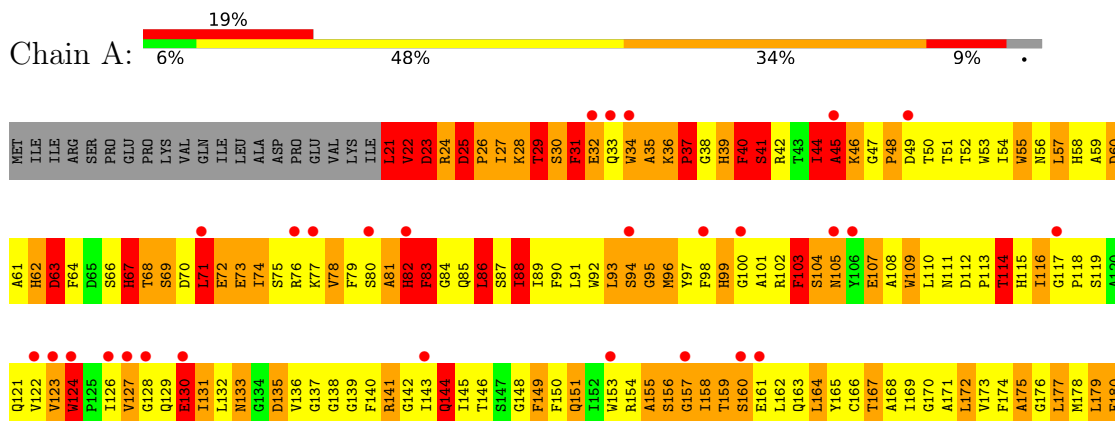
- Molecule 3: LHCA3

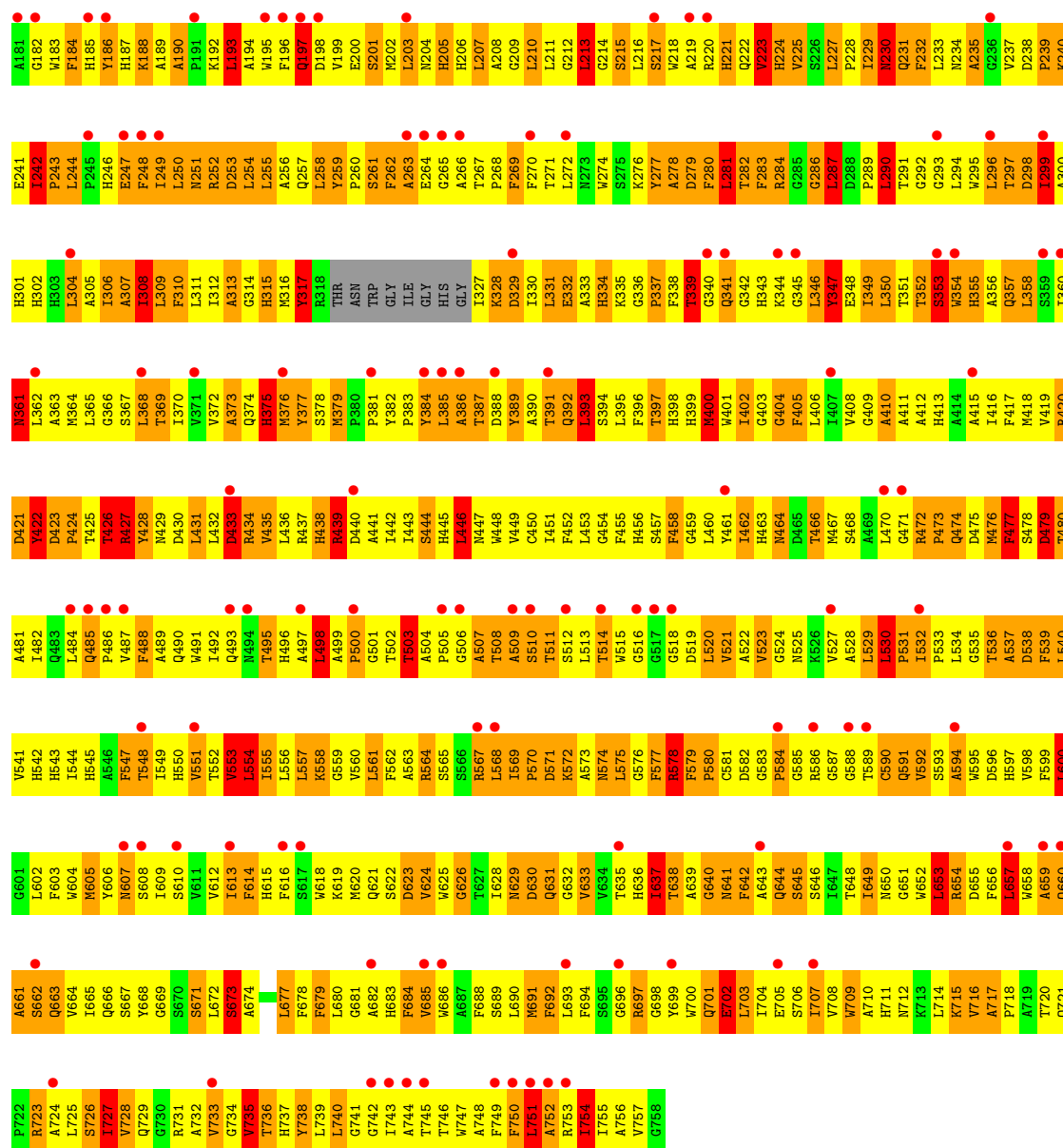


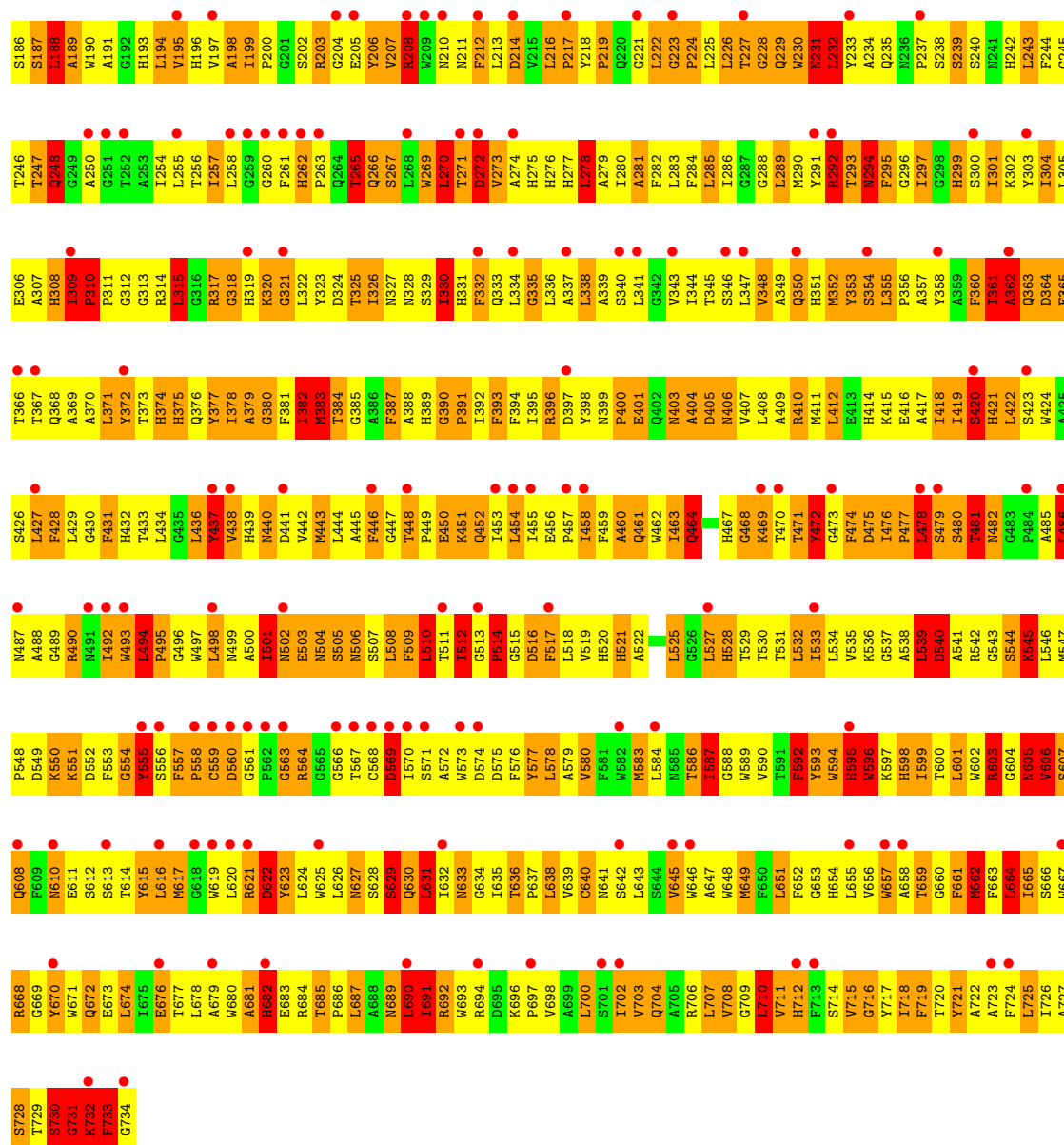
- Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC



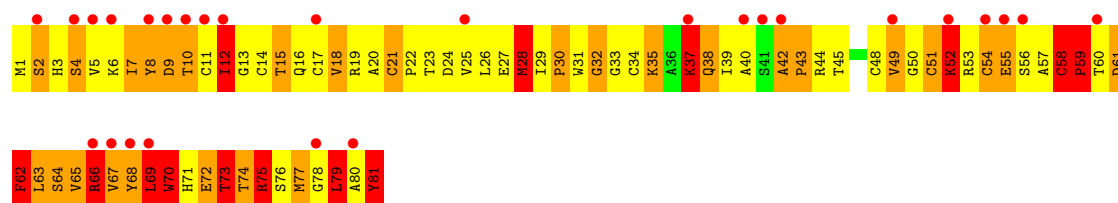
- Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1





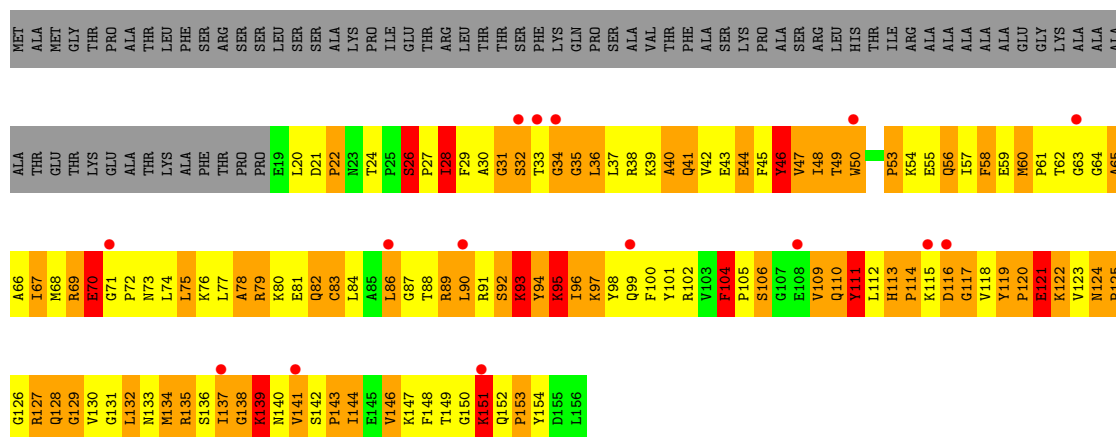


● Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER

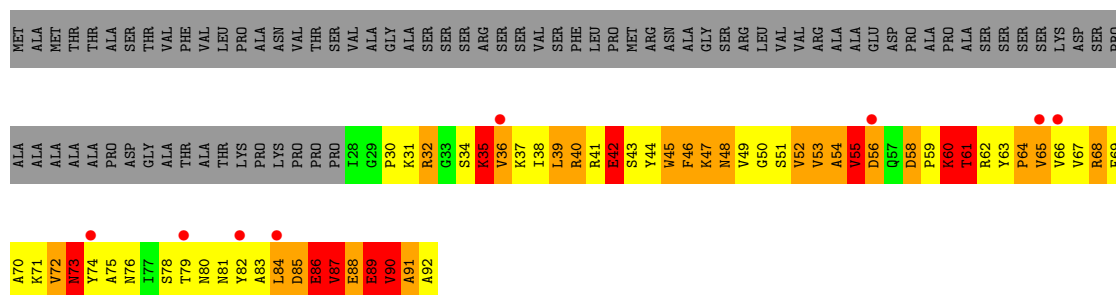
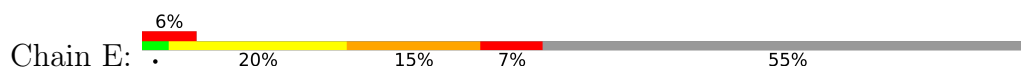


● Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC

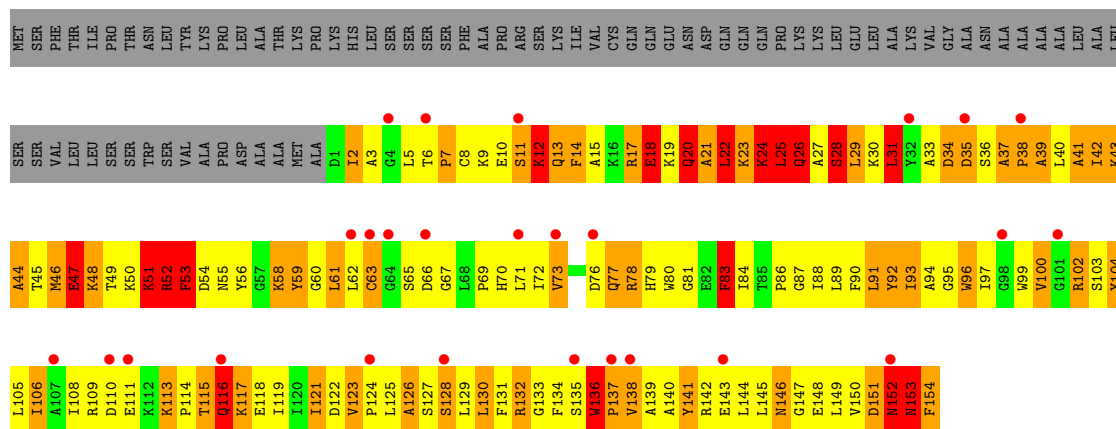




• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC



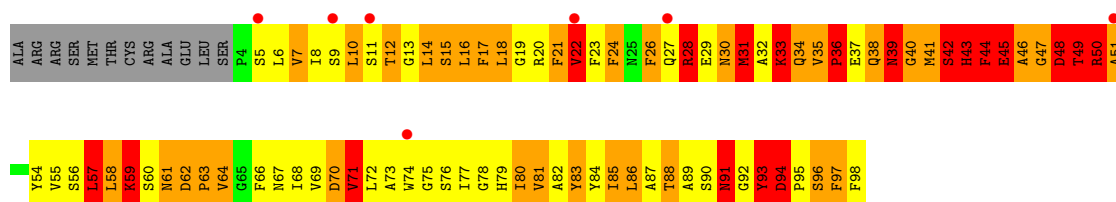
• Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC



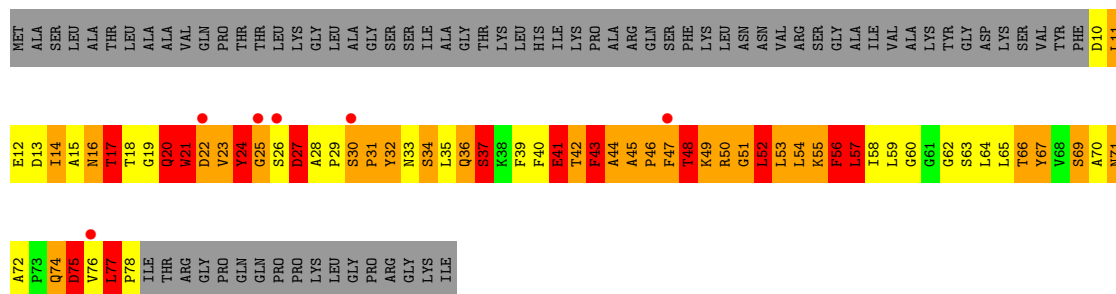
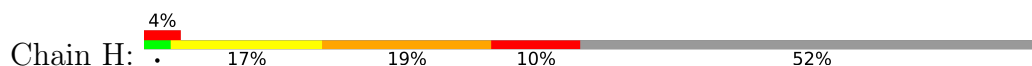
• Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC



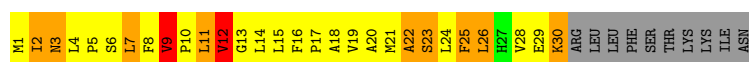




• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC



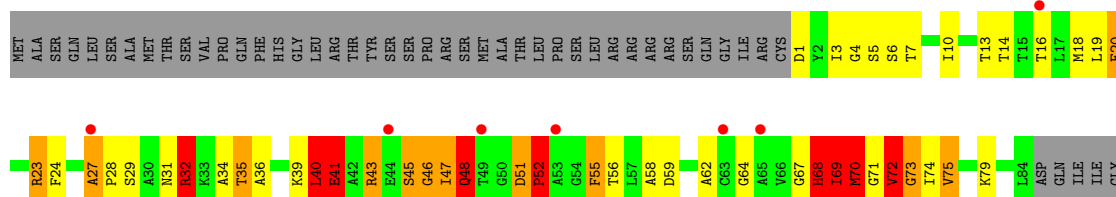
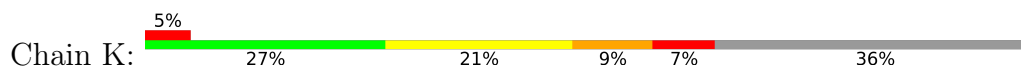
• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII



• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

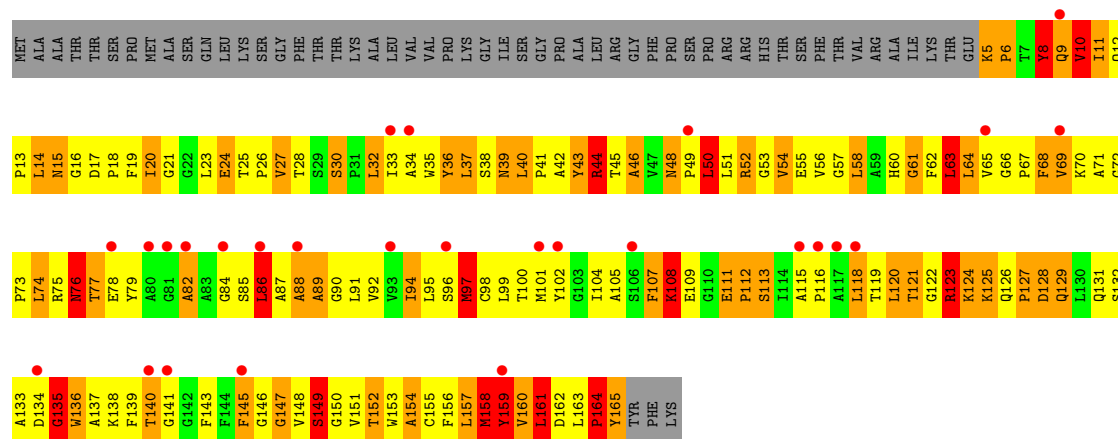


• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

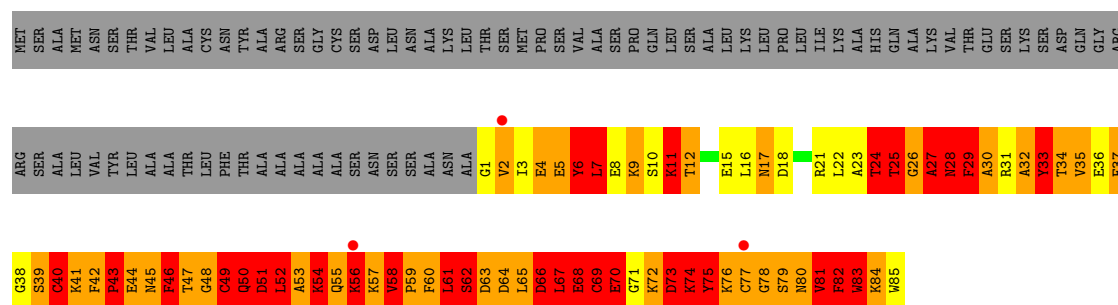
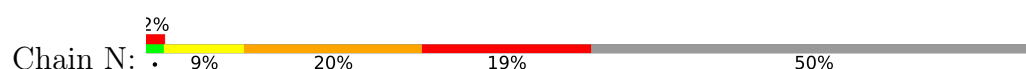


• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

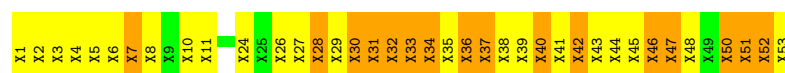




• Molecule 17: PHOTOSYSTEM I-N SUBUNIT



• Molecule 18: PHOTOSYSTEM I-N SUBUNIT



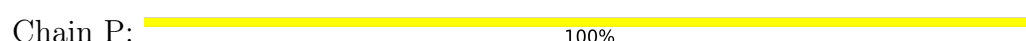
• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q:  100%GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain S:  50% 50%GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain T:  100%GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain U:  100%GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain V:  100%GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain W:  100%GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain X:  100%GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Y:  100%

GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Z:  100%

GLC1  
FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain a:  100%

GLC1  
FRU2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.3 (30.00-3.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.363 , 0.366 0.359 , 0.364	Depositor DCC
$R_{free}$ test set	4345 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.5	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.13 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	36379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, SF4, FRU, BCR, CLA, GLC, LMG, PQN, LMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.48	0/1303	0.72	3/1774 (0.2%)
2	2	0.45	0/1420	0.71	0/1943
3	3	0.87	6/1292 (0.5%)	0.96	3/1743 (0.2%)
4	4	0.49	0/1359	0.75	2/1851 (0.1%)
5	A	0.95	3/5938 (0.1%)	1.04	11/8104 (0.1%)
6	B	0.95	2/6058 (0.0%)	1.02	14/8278 (0.2%)
7	C	1.43	7/632 (1.1%)	1.33	4/856 (0.5%)
8	D	1.10	0/1122	1.05	0/1514
9	E	1.15	0/530	1.17	2/718 (0.3%)
10	F	1.10	1/1250 (0.1%)	1.07	2/1687 (0.1%)
11	G	1.07	0/760	1.28	9/1031 (0.9%)
12	H	1.16	0/543	1.19	3/741 (0.4%)
13	I	1.00	0/235	0.97	0/320
14	J	1.02	0/349	1.09	1/475 (0.2%)
15	K	0.55	0/599	0.83	1/810 (0.1%)
16	L	1.08	0/1238	1.10	5/1691 (0.3%)
17	N	1.23	1/699 (0.1%)	1.33	7/936 (0.7%)
All	All	0.94	20/25327 (0.1%)	1.02	67/34472 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
2	2	0	1
3	3	0	19
5	A	0	28
6	B	0	20
7	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	0	6
9	E	0	6
10	F	0	12
11	G	1	16
12	H	0	9
15	K	0	2
16	L	0	3
17	N	0	21
18	R	0	17
All	All	1	166

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	92	TRP	CB-CG	16.88	1.80	1.50
3	3	93	PHE	CE1-CZ	8.69	1.53	1.37
6	B	640	CYS	CB-SG	7.67	1.95	1.82
7	C	72	GLU	CD-OE1	-7.43	1.17	1.25
3	3	93	PHE	CD2-CE2	7.38	1.54	1.39
5	A	317	TYR	C-N	-7.34	1.17	1.34
7	C	58	CYS	CB-SG	6.76	1.93	1.82
3	3	93	PHE	CE2-CZ	6.63	1.50	1.37
7	C	72	GLU	CG-CD	-6.59	1.42	1.51
7	C	72	GLU	CD-OE2	-6.30	1.18	1.25
17	N	70	GLU	CB-CG	6.07	1.63	1.52
7	C	81	TYR	CE1-CZ	-5.97	1.30	1.38
10	F	47	GLU	CG-CD	5.72	1.60	1.51
7	C	54	CYS	CB-SG	-5.66	1.72	1.81
3	3	93	PHE	CD1-CE1	5.41	1.50	1.39
7	C	81	TYR	CD2-CE2	-5.39	1.31	1.39
6	B	401	GLU	CG-CD	5.25	1.59	1.51
3	3	92	TRP	CG-CD1	5.14	1.44	1.36
5	A	702	GLU	CG-CD	5.11	1.59	1.51
5	A	32	GLU	CG-CD	5.03	1.59	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	732	LYS	N-CA-C	-8.11	89.10	111.00
5	A	93	LEU	CA-CB-CG	8.06	133.84	115.30
5	A	530	LEU	CA-CB-CG	7.27	132.02	115.30
6	B	486	LEU	CA-CB-CG	7.27	132.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	315	LEU	CA-CB-CG	7.21	131.88	115.30
16	L	86	LEU	CA-CB-CG	7.18	131.82	115.30
17	N	33	TYR	N-CA-C	-7.15	91.70	111.00
5	A	540	LEU	CA-CB-CG	7.08	131.59	115.30
11	G	16	LEU	CA-CB-CG	7.00	131.40	115.30
5	A	554	LEU	CA-CB-CG	6.93	131.24	115.30
6	B	710	LEU	N-CA-C	-6.87	92.46	111.00
15	K	46	GLY	N-CA-C	-6.80	96.11	113.10
10	F	22	LEU	CB-CG-CD1	-6.55	99.87	111.00
4	4	147	LEU	CA-CB-CG	6.54	130.34	115.30
3	3	93	PHE	N-CA-CB	-6.42	99.05	110.60
5	A	271	THR	N-CA-C	-6.37	93.79	111.00
9	E	90	VAL	N-CA-C	-6.37	93.81	111.00
11	G	43	HIS	N-CA-C	-6.33	93.91	111.00
17	N	24	THR	N-CA-C	-6.29	94.03	111.00
7	C	79	LEU	CA-CB-CG	6.24	129.65	115.30
3	3	95	THR	N-CA-C	6.24	127.84	111.00
16	L	135	GLY	N-CA-C	-6.16	97.69	113.10
6	B	338	LEU	CA-CB-CG	6.15	129.45	115.30
1	1	183	ASP	C-N-CD	-6.14	107.10	120.60
6	B	494	LEU	CA-CB-CG	6.09	129.30	115.30
1	1	183	ASP	N-CA-C	6.08	127.42	111.00
17	N	27	ALA	N-CA-C	-6.06	94.63	111.00
11	G	91	ASN	N-CA-C	6.05	127.33	111.00
11	G	44	PHE	N-CA-C	-6.04	94.68	111.00
14	J	35	ASP	N-CA-C	6.04	127.30	111.00
7	C	69	LEU	CA-CB-CG	6.02	129.14	115.30
4	4	161	LEU	CA-CB-CG	5.93	128.93	115.30
6	B	194	LEU	CB-CG-CD1	-5.86	101.03	111.00
11	G	57	LEU	CA-CB-CG	5.79	128.62	115.30
11	G	51	ALA	N-CA-C	5.75	126.52	111.00
5	A	350	LEU	CA-CB-CG	-5.71	102.17	115.30
7	C	79	LEU	CB-CG-CD2	5.65	120.61	111.00
6	B	380	GLY	N-CA-C	-5.65	98.98	113.10
16	L	159	TYR	CA-CB-CG	5.63	124.10	113.40
12	H	27	ASP	N-CA-C	-5.63	95.81	111.00
17	N	62	SER	N-CA-C	-5.60	95.89	111.00
17	N	31	ARG	N-CA-C	-5.54	96.04	111.00
5	A	653	LEU	CA-CB-CG	5.50	127.94	115.30
6	B	104	PHE	N-CA-C	-5.47	96.23	111.00
7	C	75	ARG	CA-CB-CG	5.45	125.40	113.40
6	B	478	LEU	CA-CB-CG	5.44	127.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	60	LYS	N-CA-C	5.43	125.65	111.00
17	N	74	LYS	N-CA-C	5.41	125.61	111.00
5	A	626	GLY	N-CA-C	-5.35	99.72	113.10
17	N	6	TYR	N-CA-C	-5.34	96.58	111.00
6	B	289	LEU	CA-CB-CG	5.32	127.53	115.30
6	B	631	LEU	CA-CB-CG	5.28	127.44	115.30
12	H	52	LEU	N-CA-C	5.21	125.08	111.00
16	L	50	LEU	CA-CB-CG	5.19	127.23	115.30
12	H	57	LEU	CA-CB-CG	5.18	127.22	115.30
5	A	287	LEU	CA-CB-CG	5.18	127.20	115.30
5	A	385	LEU	CA-CB-CG	5.17	127.19	115.30
11	G	14	LEU	CA-CB-CG	-5.16	103.44	115.30
5	A	600	LEU	CA-CB-CG	5.12	127.07	115.30
16	L	158	MET	N-CA-C	-5.08	97.29	111.00
3	3	111	TYR	CA-CB-CG	5.07	123.04	113.40
6	B	72	GLY	N-CA-C	-5.07	100.44	113.10
10	F	59	TYR	CB-CA-C	-5.06	100.28	110.40
11	G	21	PHE	N-CA-C	5.05	124.64	111.00
6	B	596	TRP	N-CA-C	-5.04	97.38	111.00
11	G	16	LEU	N-CA-C	-5.04	97.40	111.00
1	1	85	LEU	CA-CB-CG	5.02	126.85	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	21	PHE	CA

All (166) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	182	ALA	Peptide
1	1	183	ASP	Peptide
1	1	184	PRO	Peptide
2	2	120	ASN	Peptide
3	3	104	TYR	Peptide
3	3	105	ASN	Peptide
3	3	106	TYR	Peptide
3	3	107	TRP	Peptide
3	3	109	ASP	Peptide
3	3	111	TYR	Peptide
3	3	112	THR	Peptide
3	3	155	GLU	Peptide

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Mol	Chain	Res	Type	Group
3	3	159	PRO	Peptide
3	3	169	PHE	Peptide
3	3	172	ASP	Peptide
3	3	49	ILE	Peptide
3	3	87	GLU	Peptide
3	3	89	ALA	Peptide
3	3	91	PRO	Peptide
3	3	92	TRP	Peptide
3	3	93	PHE	Peptide
3	3	94	ARG	Peptide
3	3	95	THR	Peptide
5	A	103	PHE	Peptide
5	A	117	GLY	Peptide
5	A	123	VAL	Peptide
5	A	197	GLN	Peptide
5	A	199	VAL	Peptide
5	A	201	SER	Peptide
5	A	21	LEU	Peptide
5	A	22	VAL	Peptide
5	A	23	ASP	Peptide
5	A	240	LYS	Peptide
5	A	242	ILE	Peptide
5	A	25	ASP	Peptide
5	A	27	ILE	Peptide
5	A	29	THR	Peptide
5	A	315	HIS	Peptide
5	A	347	TYR	Peptide
5	A	37	PRO	Peptide
5	A	393	LEU	Peptide
5	A	41	SER	Peptide
5	A	427	ARG	Peptide
5	A	44	ILE	Peptide
5	A	45	ALA	Peptide
5	A	482	ILE	Peptide
5	A	55	TRP	Peptide
5	A	551	VAL	Peptide
5	A	573	ALA	Peptide
5	A	67	HIS	Peptide
5	A	81	ALA	Peptide
6	B	104	PHE	Peptide
6	B	126	THR	Peptide
6	B	232	LEU	Peptide

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Mol	Chain	Res	Type	Group
6	B	265	THR	Peptide
6	B	304	ILE	Peptide
6	B	310	PRO	Peptide
6	B	362	ALA	Peptide
6	B	377	TYR	Peptide
6	B	390	GLY	Peptide
6	B	404	ALA	Peptide
6	B	481	THR	Peptide
6	B	510	LEU	Peptide
6	B	563	GLY	Peptide
6	B	595	HIS	Peptide
6	B	622	ASP	Peptide
6	B	728	SER	Peptide
6	B	730	SER	Peptide
6	B	731	GLY	Peptide
6	B	732	LYS	Peptide
6	B	99	PRO	Peptide
7	C	42	ALA	Peptide
7	C	51	CYS	Peptide
7	C	79	LEU	Peptide
8	D	104	PHE	Peptide
8	D	111	TYR	Peptide
8	D	113	HIS	Peptide
8	D	117	GLY	Peptide
8	D	141	VAL	Peptide
8	D	90	LEU	Peptide
9	E	59	PRO	Peptide
9	E	85	ASP	Peptide
9	E	86	GLU	Peptide
9	E	87	VAL	Peptide
9	E	88	GLU	Peptide
9	E	89	GLU	Peptide
10	F	136	TRP	Peptide
10	F	148	GLU	Peptide
10	F	18	GLU	Peptide
10	F	20	GLN	Peptide
10	F	22	LEU	Peptide
10	F	24	LYS	Peptide
10	F	26	GLN	Peptide
10	F	28	SER	Peptide
10	F	31	LEU	Peptide
10	F	41	ALA	Peptide

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Mol	Chain	Res	Type	Group
10	F	51	LYS	Peptide
10	F	56	TYR	Peptide
11	G	15	SER	Peptide
11	G	22	VAL	Peptide
11	G	26	PHE	Peptide
11	G	36	PRO	Peptide
11	G	39	ASN	Peptide
11	G	40	GLY	Peptide
11	G	42	SER	Peptide
11	G	43	HIS	Peptide
11	G	44	PHE	Peptide
11	G	45	GLU	Peptide
11	G	47	GLY	Peptide
11	G	48	ASP	Peptide
11	G	49	THR	Peptide
11	G	50	ARG	Peptide
11	G	90	SER	Peptide
11	G	94	ASP	Peptide
12	H	12	GLU	Peptide
12	H	20	GLN	Peptide
12	H	21	TRP	Peptide
12	H	22	ASP	Peptide
12	H	25	GLY	Peptide
12	H	27	ASP	Peptide
12	H	43	PHE	Peptide
12	H	48	THR	Peptide
12	H	51	GLY	Peptide
15	K	45	SER	Peptide
15	K	46	GLY	Peptide
16	L	157	LEU	Mainchain
16	L	160	VAL	Peptide
16	L	82	ALA	Peptide
17	N	12	THR	Peptide
17	N	15	GLU	Peptide
17	N	17	ASN	Peptide
17	N	23	ALA	Peptide
17	N	26	GLY	Peptide
17	N	28	ASN	Peptide
17	N	29	PHE	Peptide
17	N	30	ALA	Peptide
17	N	32	ALA	Peptide
17	N	43	PRO	Peptide

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Mol	Chain	Res	Type	Group
17	N	44	GLU	Peptide
17	N	46	PHE	Peptide
17	N	52	LEU	Peptide
17	N	53	ALA	Peptide
17	N	54	LYS	Peptide
17	N	56	LYS	Peptide
17	N	67	LEU	Peptide
17	N	7	LEU	Peptide
17	N	70	GLU	Peptide
17	N	73	ASP	Peptide
17	N	75	TYR	Peptide
18	R	28	UNK	Peptide
18	R	30	UNK	Peptide
18	R	31	UNK	Peptide
18	R	32	UNK	Peptide
18	R	33	UNK	Peptide
18	R	34	UNK	Peptide
18	R	36	UNK	Peptide
18	R	37	UNK	Peptide
18	R	40	UNK	Peptide
18	R	42	UNK	Peptide
18	R	46	UNK	Peptide
18	R	47	UNK	Peptide
18	R	48	UNK	Peptide
18	R	50	UNK	Peptide
18	R	51	UNK	Peptide
18	R	52	UNK	Peptide
18	R	7	UNK	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1264	0	1230	91	1
2	2	1374	0	1329	142	0
3	3	1254	0	1221	333	1
4	4	1319	0	1283	201	13
5	A	5745	0	5595	1661	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5848	0	5655	1449	1
7	C	619	0	608	236	0
8	D	1095	0	1112	226	0
9	E	520	0	528	150	0
10	F	1221	0	1246	289	0
11	G	740	0	709	297	7
12	H	529	0	514	117	0
13	I	229	0	252	58	0
14	J	338	0	340	80	0
15	K	593	0	619	65	1
16	L	1203	0	1213	326	13
17	N	685	0	671	448	7
18	R	265	0	67	77	0
19	M	22	0	18	11	0
19	O	23	0	21	14	0
19	P	23	0	21	0	0
19	Q	23	0	21	11	0
19	S	23	0	20	1	0
19	T	23	0	21	8	0
19	U	23	0	21	9	0
19	V	23	0	21	3	0
19	W	23	0	21	17	0
19	X	23	0	21	7	0
19	Y	23	0	21	1	0
19	Z	23	0	20	20	0
19	a	23	0	19	0	0
20	1	644	0	429	113	2
20	2	658	0	480	160	0
20	3	548	0	326	115	0
20	4	699	0	454	157	0
20	A	2777	0	2599	1120	1
20	B	2372	0	2285	808	0
20	F	130	0	86	27	0
20	G	51	0	40	6	0
20	H	65	0	71	19	0
20	I	115	0	106	26	0
20	J	202	0	169	99	0
20	K	210	0	177	44	2
20	L	202	0	158	40	0
20	R	122	0	123	17	0
21	1	70	0	92	15	0
21	2	105	0	138	15	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	3	35	0	46	3	0
21	4	35	0	46	0	0
21	A	1153	0	1505	397	0
21	B	25	0	23	1	0
21	K	35	0	45	6	0
21	L	35	0	46	3	0
21	R	70	0	91	24	0
22	3	40	0	54	21	0
22	A	240	0	323	250	0
22	B	320	0	432	225	0
22	I	40	0	54	47	0
22	L	80	0	105	61	0
23	A	33	0	46	12	0
23	B	33	0	46	33	0
24	B	49	0	71	30	0
25	B	8	0	0	18	0
25	C	16	0	0	9	0
26	B	23	0	0	2	0
All	All	36379	0	35124	8371	25

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 117.

All (8371) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:160:MET:SD	20:4:1201:CLA:HBB1	1.28	1.66
20:A:1776:CLA:H92	22:A:1805:BCR:C37	1.17	1.58
6:B:25:ILE:HG21	22:L:1169:BCR:C29	1.11	1.58
5:A:51:THR:HG21	20:A:1795:CLA:CBB	1.24	1.57
21:A:7036:LMU:H82	21:A:7036:LMU:C2	1.34	1.57
21:A:7042:LMU:H22	21:A:7042:LMU:C7	1.33	1.56
16:L:163:LEU:CD2	16:L:164:PRO:HD2	1.34	1.56
20:1:1191:CLA:CAB	20:1:1197:CLA:HBC2	1.32	1.55
3:3:132:TRP:CZ3	3:3:155:GLU:HG2	1.37	1.55
23:B:1773:PQN:C19	22:B:1780:BCR:H10C	1.33	1.55
3:3:64:TYR:HB3	20:3:1218:CLA:C4	1.34	1.54
3:3:132:TRP:CH2	3:3:155:GLU:CD	1.76	1.54
20:A:1772:CLA:H2A	20:A:1772:CLA:CED	1.33	1.54
23:B:1773:PQN:H162	22:B:1780:BCR:C33	1.29	1.53
20:A:1776:CLA:C9	22:A:1805:BCR:H373	1.33	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:3008:CLA:HBA2	20:3:3008:CLA:CBD	1.34	1.52
20:A:1779:CLA:C4C	22:A:1805:BCR:H19C	1.32	1.52
20:A:1816:CLA:HED1	20:A:1816:CLA:C2	1.29	1.52
18:R:32:UNK:CB	18:R:33:UNK:CB	1.85	1.51
21:A:7023:LMU:H91	21:A:7023:LMU:C2	1.41	1.50
11:G:45:GLU:CG	11:G:49:THR:HG23	1.38	1.50
20:2:1220:CLA:HBD	20:2:1220:CLA:CGA	1.35	1.50
17:N:45:ASN:ND2	17:N:54:LYS:HG2	1.24	1.50
17:N:62:SER:HB3	17:N:66:ASP:CB	1.41	1.49
5:A:328:LYS:CE	5:A:332:GLU:HG3	1.40	1.49
3:3:132:TRP:CZ3	3:3:155:GLU:CG	1.91	1.49
6:B:732:LYS:HG2	6:B:733:PHE:C	1.23	1.48
6:B:732:LYS:CG	6:B:734:GLY:N	1.75	1.47
21:A:7016:LMU:H81	21:A:7016:LMU:C2	1.44	1.46
21:A:7042:LMU:C6'	21:A:7042:LMU:H32	1.41	1.46
6:B:25:ILE:CG2	22:L:1169:BCR:C29	1.95	1.45
4:4:107:GLN:CA	20:4:1196:CLA:HMA3	1.47	1.44
20:4:1198:CLA:HAA2	20:4:1198:CLA:CED	1.46	1.44
20:A:1816:CLA:HAA1	20:A:1816:CLA:CGD	1.45	1.44
7:C:14:CYS:HA	7:C:17:CYS:SG	1.56	1.43
20:2:1220:CLA:C4	3:3:140:LYS:HG2	1.45	1.43
20:J:1043:CLA:HED3	20:J:1043:CLA:C1A	1.47	1.42
16:L:161:LEU:HD12	16:L:162:ASP:N	1.24	1.42
17:N:45:ASN:HD22	17:N:54:LYS:CG	1.28	1.41
11:G:48:ASP:CB	11:G:49:THR:HG22	1.47	1.41
20:2:1220:CLA:H41	3:3:140:LYS:CD	1.51	1.41
5:A:744:ALA:CB	22:A:1807:BCR:H391	1.51	1.40
3:3:74:ALA:HA	20:3:1215:CLA:C3D	1.51	1.40
11:G:93:TYR:HA	11:G:94:ASP:CB	1.43	1.40
17:N:48:GLY:HA2	17:N:49:CYS:SG	1.62	1.40
6:B:732:LYS:CG	6:B:733:PHE:C	1.83	1.40
20:A:1796:CLA:H141	22:A:1807:BCR:C2	1.51	1.39
20:A:1816:CLA:CED	20:A:1816:CLA:H2	1.51	1.39
20:B:1768:CLA:H152	22:B:1779:BCR:C31	1.52	1.39
5:A:21:LEU:CA	5:A:22:VAL:HB	1.47	1.39
20:A:1779:CLA:CHD	22:A:1805:BCR:H19C	1.52	1.39
20:K:1085:CLA:HMB2	20:K:1142:CLA:CED	1.49	1.39
17:N:61:LEU:HD11	17:N:63:ASP:C	1.40	1.39
20:J:1044:CLA:H41	20:J:1044:CLA:C7	1.49	1.38
3:3:132:TRP:CH2	3:3:155:GLU:OE2	1.68	1.38
17:N:58:VAL:HB	17:N:59:PRO:CD	1.47	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:732:LYS:HB3	6:B:733:PHE:CA	1.49	1.37
20:4:1201:CLA:HMA2	20:4:1201:CLA:CBA	1.54	1.37
3:3:205:GLY:N	5:A:252:ARG:HH22	1.16	1.36
5:A:368:LEU:HD21	20:A:1774:CLA:C9	1.55	1.36
17:N:45:ASN:ND2	17:N:54:LYS:CG	1.82	1.36
17:N:62:SER:HB3	17:N:66:ASP:CG	1.46	1.36
17:N:72:LYS:HG3	17:N:74:LYS:CB	1.56	1.36
20:A:1770:CLA:C4B	22:A:1803:BCR:H19C	1.56	1.36
20:A:1783:CLA:H203	22:A:1808:BCR:C17	1.54	1.36
4:4:160:MET:CE	20:4:1201:CLA:CBB	2.02	1.35
20:A:1763:CLA:C3B	22:A:1808:BCR:H331	1.53	1.35
5:A:316:MET:HG2	5:A:317:TYR:CD1	1.62	1.35
7:C:54:CYS:HB2	25:C:1082:SF4:S1	1.67	1.35
17:N:72:LYS:HB3	17:N:73:ASP:CA	1.48	1.35
21:A:7037:LMU:C7	21:A:7037:LMU:H32	1.51	1.35
9:E:52:VAL:O	9:E:53:VAL:CG2	1.75	1.35
5:A:23:ASP:HB2	5:A:24:ARG:NE	1.42	1.34
21:A:7033:LMU:H3'	21:A:7033:LMU:C6B	1.55	1.34
4:4:160:MET:SD	20:4:1201:CLA:CBB	2.14	1.34
17:N:47:THR:HG21	17:N:54:LYS:NZ	1.37	1.34
17:N:61:LEU:HD11	17:N:63:ASP:CA	1.56	1.34
4:4:119:PRO:HG3	20:4:1206:CLA:C2D	1.56	1.33
5:A:567:ARG:NH1	8:D:35:GLY:HA2	1.43	1.33
20:B:1753:CLA:HMC1	20:B:1753:CLA:CBC	1.58	1.33
16:L:163:LEU:HD13	16:L:164:PRO:CB	1.57	1.33
5:A:453:LEU:CD2	20:A:1793:CLA:HBB2	1.57	1.33
20:B:1742:CLA:HAC2	20:B:1743:CLA:CBB	1.54	1.33
21:K:1086:LMU:C4	21:K:1086:LMU:H81	1.47	1.33
5:A:51:THR:CG2	20:A:1795:CLA:CBB	2.05	1.32
20:J:1044:CLA:C4	20:J:1044:CLA:H72	1.58	1.32
9:E:52:VAL:O	9:E:53:VAL:HG23	1.24	1.32
11:G:6:LEU:HB3	11:G:9:SER:CB	1.59	1.32
5:A:51:THR:CG2	20:A:1795:CLA:HBB2	1.60	1.32
5:A:269:PHE:CE1	15:K:14:THR:HG21	1.65	1.32
20:1:1187:CLA:HBC3	20:1:1187:CLA:CMC	1.46	1.32
20:4:1198:CLA:H151	20:4:1198:CLA:C20	1.59	1.31
21:A:7036:LMU:H31	21:A:7036:LMU:C7	1.45	1.31
4:4:107:GLN:CA	20:4:1196:CLA:CMA	2.09	1.31
4:4:107:GLN:HA	20:4:1196:CLA:CMA	1.61	1.31
10:F:24:LYS:HE2	10:F:24:LYS:CA	1.49	1.31
20:2:1220:CLA:H92	20:2:1220:CLA:C5	1.53	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1220:CLA:H52	20:2:1220:CLA:C9	1.52	1.31
5:A:452:PHE:CE1	20:A:1793:CLA:HBB1	1.64	1.31
20:J:1045:CLA:HHD	20:J:1045:CLA:CBC	1.57	1.31
20:3:3008:CLA:HBA2	20:3:3008:CLA:CGD	1.61	1.31
21:A:7032:LMU:H31	21:A:7032:LMU:C2B	1.60	1.30
17:N:66:ASP:C	17:N:67:LEU:HD12	1.50	1.30
21:A:7023:LMU:H82	21:A:7023:LMU:C3	1.61	1.29
20:B:1768:CLA:H93	20:B:1768:CLA:CBB	1.61	1.29
20:A:1816:CLA:HED1	20:A:1816:CLA:C1	1.62	1.29
20:A:1816:CLA:HHD	20:A:1816:CLA:CBC	1.62	1.29
11:G:6:LEU:CB	11:G:9:SER:HB3	1.60	1.28
20:2:1220:CLA:C4	3:3:140:LYS:CG	2.12	1.28
21:A:7023:LMU:H21	21:A:7023:LMU:C9	1.60	1.28
23:B:1773:PQN:C16	22:B:1780:BCR:C33	2.11	1.28
20:J:1044:CLA:O1D	20:J:1045:CLA:C9	1.80	1.28
22:3:1220:BCR:H23C	22:3:1220:BCR:C39	1.55	1.28
5:A:744:ALA:HB2	22:A:1807:BCR:C39	1.61	1.28
22:A:1804:BCR:H23C	22:A:1804:BCR:C40	1.60	1.28
20:4:4014:CLA:HED2	20:4:4014:CLA:C2A	1.62	1.28
20:A:1763:CLA:C3B	22:A:1808:BCR:C33	2.10	1.28
20:A:1779:CLA:CBB	22:A:1805:BCR:C35	2.10	1.27
12:H:20:GLN:HB3	12:H:22:ASP:CB	1.63	1.27
17:N:65:LEU:C	17:N:65:LEU:HD23	1.52	1.27
3:3:132:TRP:CH2	3:3:155:GLU:CG	2.12	1.27
20:A:1770:CLA:C3B	22:A:1803:BCR:H19C	1.63	1.27
6:B:732:LYS:CB	6:B:733:PHE:HA	1.63	1.27
21:A:7037:LMU:C3	21:A:7037:LMU:H72	1.55	1.27
11:G:45:GLU:CG	11:G:49:THR:CG2	2.10	1.27
5:A:331:LEU:CD2	5:A:343:HIS:O	1.82	1.27
20:A:1781:CLA:HED1	20:A:1782:CLA:C2D	1.65	1.27
17:N:67:LEU:HB2	17:N:68:GLU:CG	1.65	1.27
21:A:7023:LMU:C9	21:A:7023:LMU:H41	1.64	1.26
20:3:1219:CLA:H142	20:3:1219:CLA:C10	1.65	1.26
21:A:7020:LMU:C5B	21:A:7020:LMU:H6E	1.64	1.26
11:G:93:TYR:CA	11:G:94:ASP:HB2	1.64	1.26
17:N:41:LYS:HB2	17:N:42:PHE:CB	1.65	1.26
17:N:45:ASN:ND2	17:N:54:LYS:CB	1.99	1.26
5:A:79:PHE:CE2	5:A:185:HIS:CD2	2.24	1.26
21:A:7036:LMU:H82	21:A:7036:LMU:C3	1.64	1.26
17:N:67:LEU:CB	17:N:68:GLU:HG2	1.66	1.26
20:4:4014:CLA:H2A	20:4:4014:CLA:CED	1.66	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:72:LYS:CG	17:N:74:LYS:HG3	1.66	1.25
7:C:17:CYS:HB2	7:C:58:CYS:SG	1.77	1.25
20:2:1212:CLA:H42	20:2:1212:CLA:O1A	1.37	1.25
20:2:1220:CLA:H41	3:3:140:LYS:CG	1.67	1.25
20:4:1201:CLA:HAA2	20:4:1201:CLA:CGD	1.67	1.25
7:C:62:PHE:CE2	9:E:42:GLU:OE1	1.90	1.25
12:H:25:GLY:CA	12:H:27:ASP:H	1.49	1.24
20:A:1776:CLA:CMD	20:A:1778:CLA:HBB2	1.67	1.24
21:A:7039:LMU:H3'	21:A:7039:LMU:C6B	1.66	1.24
6:B:25:ILE:CG2	22:L:1169:BCR:C28	2.14	1.24
4:4:151:GLU:O	4:4:154:ILE:HG12	1.36	1.24
22:B:1779:BCR:H321	22:B:1779:BCR:C8	1.55	1.24
12:H:20:GLN:CB	12:H:22:ASP:HB3	1.65	1.24
20:1:1187:CLA:HMC1	20:1:1187:CLA:CBC	1.64	1.24
22:I:1032:BCR:HC8	22:I:1032:BCR:C31	1.62	1.24
21:A:7042:LMU:H71	21:A:7042:LMU:C2	1.68	1.23
20:J:1045:CLA:CAD	20:J:1045:CLA:HED3	1.67	1.23
21:A:7042:LMU:H22	21:A:7042:LMU:C6	1.58	1.23
6:B:732:LYS:CB	6:B:733:PHE:CA	2.14	1.23
3:3:74:ALA:HA	20:3:1215:CLA:C4D	1.69	1.23
21:A:7016:LMU:H81	21:A:7016:LMU:C3	1.69	1.23
14:J:31:ARG:HH22	20:J:1043:CLA:C4B	1.50	1.23
4:4:106:TRP:CD1	20:4:1196:CLA:HED3	1.74	1.23
20:K:1085:CLA:O1A	20:K:1085:CLA:H3A	1.38	1.23
20:A:1783:CLA:C20	22:A:1808:BCR:H17C	1.68	1.23
13:I:11:LEU:CD1	22:I:1032:BCR:H10C	1.69	1.23
21:A:7032:LMU:H31	21:A:7032:LMU:C1B	1.67	1.22
6:B:25:ILE:CG2	22:L:1169:BCR:H292	1.60	1.22
21:K:1086:LMU:H42	21:K:1086:LMU:C8	1.67	1.22
2:2:120:ASN:CB	14:J:5:LYS:HD2	1.68	1.22
5:A:81:ALA:CB	20:A:1760:CLA:HMA1	1.68	1.22
7:C:7:ILE:O	7:C:8:TYR:O	1.55	1.22
20:4:1198:CLA:HED3	20:4:1198:CLA:CAA	1.70	1.22
20:A:1772:CLA:HMC1	20:A:1772:CLA:CBC	1.70	1.22
20:A:1816:CLA:C2	20:A:1816:CLA:CED	2.13	1.22
6:B:517:PHE:CD2	6:B:517:PHE:O	1.93	1.22
6:B:732:LYS:HG2	6:B:734:GLY:N	0.90	1.22
5:A:328:LYS:CG	5:A:332:GLU:HB2	1.70	1.22
5:A:342:GLY:CA	5:A:430:ASP:HB2	1.70	1.22
21:A:7020:LMU:H5B	21:A:7020:LMU:C6'	1.69	1.22
6:B:25:ILE:CG2	22:L:1169:BCR:H282	1.68	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1755:CLA:HBB1	20:B:1769:CLA:CMB	1.70	1.22
3:3:84:ILE:HB	20:A:1798:CLA:O1A	1.40	1.21
21:A:7023:LMU:H2B	21:A:7023:LMU:C6B	1.65	1.21
16:L:163:LEU:HD13	16:L:164:PRO:CD	1.69	1.21
21:A:7022:LMU:H2'	21:A:7022:LMU:C2	1.66	1.21
20:2:1220:CLA:H61	3:3:140:LYS:CD	1.69	1.21
20:A:1779:CLA:CBB	22:A:1805:BCR:H351	1.70	1.21
17:N:57:LYS:CG	17:N:58:VAL:H	1.52	1.21
5:A:81:ALA:CB	20:A:1760:CLA:CMA	2.18	1.21
5:A:331:LEU:HD11	5:A:346:LEU:CB	1.69	1.21
20:A:1781:CLA:HED1	20:A:1782:CLA:C3D	1.70	1.21
9:E:86:GLU:HG3	9:E:87:VAL:N	1.49	1.21
19:V:1:GLC:O2	19:V:2:FRU:H3	1.39	1.21
16:L:161:LEU:HD12	16:L:161:LEU:C	1.51	1.21
20:R:1054:CLA:HED3	20:R:1054:CLA:C1A	1.69	1.21
16:L:164:PRO:HB3	16:L:165:TYR:CE2	1.75	1.20
17:N:45:ASN:ND2	17:N:54:LYS:HB2	1.53	1.20
3:3:48:PHE:CD2	3:3:49:ILE:HG22	1.74	1.20
20:A:1781:CLA:HED2	20:A:1782:CLA:CAD	1.71	1.20
21:A:7036:LMU:C8	21:A:7036:LMU:H22	1.71	1.20
21:A:7043:LMU:C6	21:A:7043:LMU:H102	1.69	1.20
20:4:1201:CLA:HBA1	20:4:1201:CLA:CMA	1.55	1.20
5:A:76:ARG:NH1	5:A:192:LYS:HG2	1.57	1.20
17:N:70:GLU:OE2	17:N:72:LYS:O	1.58	1.20
3:3:205:GLY:H	5:A:252:ARG:NH2	1.39	1.20
6:B:25:ILE:HG21	22:L:1169:BCR:C28	1.68	1.20
16:L:163:LEU:HD13	16:L:164:PRO:CG	1.72	1.20
4:4:33:ASP:HB3	4:4:34:PRO:HD2	1.23	1.19
21:A:7016:LMU:C9	21:A:7016:LMU:H32	1.72	1.19
11:G:46:ALA:N	11:G:48:ASP:HB3	1.56	1.19
5:A:541:VAL:HG11	5:A:615:HIS:CD2	1.77	1.19
6:B:403:ASN:O	6:B:406:ASN:CB	1.90	1.19
11:G:45:GLU:HG2	11:G:49:THR:HG23	1.19	1.19
16:L:164:PRO:HB3	16:L:165:TYR:CD2	1.78	1.19
17:N:61:LEU:HD12	17:N:62:SER:C	1.63	1.19
20:1:1198:CLA:H52	20:1:1198:CLA:C10	1.72	1.19
22:3:1220:BCR:H393	22:3:1220:BCR:C23	1.67	1.19
20:4:1196:CLA:HHD	20:4:1196:CLA:CBC	1.73	1.19
21:A:7021:LMU:C1'	21:A:7021:LMU:H31	1.67	1.19
6:B:120:VAL:HA	6:B:123:TRP:CD1	1.76	1.19
6:B:293:THR:O	11:G:38:GLN:OE1	1.56	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:41:UNK:CB	18:R:42:UNK:HA	1.70	1.19
20:B:1753:CLA:H43	20:B:1753:CLA:C1A	1.72	1.19
17:N:48:GLY:CA	17:N:49:CYS:SG	2.30	1.18
5:A:81:ALA:HB2	20:A:1760:CLA:CMA	1.71	1.18
5:A:702:GLU:OE2	6:B:550:LYS:NZ	1.76	1.18
22:B:1779:BCR:C27	22:B:1779:BCR:H403	1.52	1.18
18:R:52:UNK:HA	18:R:53:UNK:CB	1.68	1.18
20:1:1197:CLA:HED2	20:1:1197:CLA:CAD	1.67	1.18
21:A:7039:LMU:H6'2	21:A:7039:LMU:C3'	1.74	1.18
20:B:1768:CLA:C15	22:B:1779:BCR:C31	2.20	1.18
15:K:68:HIS:O	15:K:70:MET:HB2	1.41	1.18
17:N:79:SER:HA	17:N:80:ASN:O	1.39	1.18
20:3:1219:CLA:HMC1	20:3:1219:CLA:HBC3	1.22	1.18
5:A:331:LEU:HD23	5:A:331:LEU:O	1.42	1.18
17:N:57:LYS:HG3	17:N:58:VAL:N	1.44	1.18
3:3:132:TRP:CZ3	3:3:155:GLU:CD	2.06	1.18
5:A:51:THR:CB	20:A:1795:CLA:HBB2	1.70	1.18
5:A:342:GLY:HA3	5:A:430:ASP:CB	1.74	1.18
20:A:1801:CLA:HMA3	16:L:27:VAL:HA	1.24	1.18
16:L:163:LEU:HD22	16:L:164:PRO:CD	1.72	1.18
4:4:107:GLN:C	20:4:1196:CLA:CMA	2.13	1.17
5:A:27:ILE:O	5:A:28:LYS:HG3	1.41	1.17
22:A:1807:BCR:C31	20:A:1813:CLA:C14	2.21	1.17
20:1:1198:CLA:HBC3	20:1:1198:CLA:CHD	1.74	1.17
10:F:24:LYS:HE2	10:F:24:LYS:N	1.57	1.17
20:J:1044:CLA:O1D	20:J:1045:CLA:H91	1.45	1.17
3:3:87:GLU:C	22:3:1220:BCR:C38	2.12	1.17
5:A:316:MET:HB3	5:A:317:TYR:CB	1.73	1.17
17:N:41:LYS:CB	17:N:42:PHE:HB3	1.75	1.17
20:3:3008:CLA:HBD	20:3:3008:CLA:CBA	1.75	1.17
20:A:1779:CLA:C4C	22:A:1805:BCR:C19	2.23	1.17
20:B:1753:CLA:HBC3	20:B:1753:CLA:CMC	1.65	1.17
20:B:1768:CLA:C9	20:B:1768:CLA:HBB2	1.75	1.17
3:3:132:TRP:HH2	3:3:155:GLU:CD	1.21	1.16
5:A:79:PHE:CE2	5:A:185:HIS:NE2	2.13	1.16
5:A:590:CYS:SG	25:B:1784:SF4:S1	2.42	1.16
20:A:1781:CLA:HED1	20:A:1782:CLA:CMD	1.75	1.16
20:A:1815:CLA:H61	20:A:1815:CLA:CMA	1.76	1.16
3:3:64:TYR:CB	20:3:1218:CLA:C4	2.21	1.16
3:3:83:LEU:HA	20:A:1798:CLA:H43	1.25	1.16
3:3:132:TRP:HH2	3:3:155:GLU:OE2	0.82	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7026:LMU:O3B	19:Z:2:FRU:H5	1.37	1.16
7:C:1:MET:H2	7:C:3:HIS:N	1.42	1.16
20:J:1044:CLA:CGD	20:J:1045:CLA:H92	1.75	1.16
20:2:1220:CLA:C9	3:3:137:SER:HB2	1.75	1.16
5:A:25:ASP:OD1	5:A:26:PRO:HG3	1.44	1.16
20:A:1781:CLA:H72	20:A:1782:CLA:CED	1.74	1.16
6:B:87:ILE:HA	6:B:115:ASN:HA	1.25	1.16
25:B:1784:SF4:S2	25:B:1784:SF4:S4	2.44	1.16
17:N:72:LYS:CB	17:N:73:ASP:HA	1.74	1.16
20:A:1797:CLA:HMA2	20:A:1797:CLA:C1	1.75	1.16
20:B:1768:CLA:H161	22:B:1779:BCR:H313	1.25	1.16
20:B:1753:CLA:H151	20:B:1753:CLA:C10	1.66	1.16
3:3:110:SER:C	3:3:111:TYR:HD2	1.48	1.15
5:A:304:LEU:HD22	20:A:1772:CLA:HBB2	1.18	1.15
21:A:7022:LMU:H21	21:A:7022:LMU:C2'	1.59	1.15
20:B:1755:CLA:HHD	20:B:1755:CLA:CBC	1.76	1.15
21:A:7016:LMU:H21	21:A:7016:LMU:C8	1.75	1.15
21:A:7043:LMU:C11	21:A:7043:LMU:H71	1.67	1.15
22:I:1032:BCR:HC31	20:I:1033:CLA:HAC2	1.28	1.15
17:N:63:ASP:H	17:N:64:ASP:CB	1.57	1.15
17:N:70:GLU:O	17:N:72:LYS:HD3	1.41	1.15
19:Z:2:FRU:H12	19:Z:2:FRU:C6	1.70	1.15
20:L:1168:CLA:HBC3	20:L:1168:CLA:HHD	1.19	1.15
21:R:1057:LMU:H62	21:R:1057:LMU:H11	1.17	1.15
20:1:1191:CLA:HMC1	20:1:1194:CLA:HHD	1.15	1.15
20:2:1220:CLA:HBD	20:2:1220:CLA:O1A	1.44	1.15
5:A:685:VAL:HG23	20:A:1796:CLA:HBB1	1.27	1.15
11:G:46:ALA:N	11:G:49:THR:HG21	1.59	1.15
5:A:316:MET:CB	5:A:317:TYR:CD1	2.29	1.15
23:B:1773:PQN:C19	22:B:1780:BCR:C10	2.24	1.15
8:D:134:MET:N	8:D:134:MET:SD	2.20	1.15
3:3:92:TRP:HA	3:3:93:PHE:CD1	1.80	1.14
5:A:316:MET:CG	5:A:317:TYR:CD1	2.29	1.14
22:A:1804:BCR:H23C	22:A:1804:BCR:H403	1.28	1.14
7:C:1:MET:CB	7:C:4:SER:OG	1.94	1.14
3:3:74:ALA:HA	20:3:1215:CLA:C2D	1.77	1.14
21:A:7026:LMU:O3B	19:Z:2:FRU:C5	1.78	1.14
6:B:22:TRP:NE1	20:B:1770:CLA:HBB1	1.60	1.14
20:J:1045:CLA:HBD	20:J:1045:CLA:CBA	1.76	1.14
17:N:72:LYS:HG3	17:N:74:LYS:CG	1.77	1.14
21:1:7004:LMU:H12	21:1:7004:LMU:H3'	1.20	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:194:ILE:CD1	20:3:1212:CLA:HMC2	1.75	1.14
20:3:1219:CLA:H142	20:3:1219:CLA:H101	1.23	1.14
21:A:7043:LMU:H62	21:A:7043:LMU:C10	1.76	1.14
6:B:189:ALA:CB	20:B:1758:CLA:H203	1.76	1.14
11:G:33:LYS:HA	11:G:33:LYS:CE	1.68	1.14
17:N:61:LEU:HD12	17:N:61:LEU:C	1.65	1.14
18:R:26:UNK:O	18:R:28:UNK:CB	1.96	1.14
5:A:304:LEU:HD22	20:A:1772:CLA:CBB	1.77	1.14
5:A:316:MET:HB3	5:A:317:TYR:CD1	1.81	1.14
6:B:493:TRP:O	6:B:495:PRO:HD3	1.48	1.14
20:B:1786:CLA:C9	20:B:1787:CLA:H91	1.77	1.14
19:W:2:FRU:H62	19:W:2:FRU:C1	1.75	1.14
20:2:1220:CLA:H61	3:3:140:LYS:HD3	1.17	1.14
5:A:251:ASN:O	5:A:253:ASP:N	1.79	1.14
5:A:711:HIS:CD2	20:A:1795:CLA:HBC1	1.82	1.14
20:A:1781:CLA:C4B	22:A:1806:BCR:H373	1.77	1.14
6:B:672:GLN:HA	6:B:672:GLN:HE21	1.09	1.14
19:W:2:FRU:H62	19:W:2:FRU:H11	1.28	1.14
20:A:1788:CLA:H52	22:B:1780:BCR:H343	1.19	1.13
20:A:1797:CLA:HMA2	20:A:1797:CLA:H12	1.16	1.13
20:B:1751:CLA:HBC2	20:B:1751:CLA:HHD	1.14	1.13
25:B:1784:SF4:S1	25:B:1784:SF4:S3	2.46	1.13
19:O:2:FRU:H62	19:O:2:FRU:C1	1.70	1.13
4:4:104:ARG:HA	4:4:107:GLN:HB2	1.27	1.13
20:A:1781:CLA:HBA2	20:A:1794:CLA:HED1	1.20	1.13
6:B:596:TRP:CH2	6:B:612:SER:O	2.02	1.13
11:G:33:LYS:HA	11:G:33:LYS:HE3	1.26	1.13
22:I:1032:BCR:H313	22:I:1032:BCR:C8	1.75	1.13
5:A:22:VAL:HG12	5:A:23:ASP:H	1.13	1.13
5:A:23:ASP:CA	5:A:24:ARG:HD2	1.78	1.13
21:A:7009:LMU:O3'	21:A:7009:LMU:H5B	1.45	1.13
20:B:1739:CLA:HBB2	20:B:1739:CLA:C9	1.78	1.13
7:C:14:CYS:CA	7:C:17:CYS:SG	2.36	1.13
17:N:61:LEU:HD12	17:N:62:SER:N	1.62	1.13
20:1:1191:CLA:CAB	20:1:1197:CLA:CBC	2.25	1.13
20:1:1197:CLA:HAA2	20:1:1197:CLA:O1D	1.46	1.13
5:A:160:SER:O	5:A:163:GLN:HG2	1.45	1.13
20:A:1779:CLA:CHD	22:A:1805:BCR:C19	2.26	1.13
20:A:1816:CLA:HHD	20:A:1816:CLA:HBC3	1.18	1.13
6:B:403:ASN:O	6:B:406:ASN:HB3	0.97	1.13
20:B:1742:CLA:CAC	20:B:1743:CLA:HBB2	1.78	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:110:SER:O	3:3:111:TYR:HD2	1.31	1.13
22:A:1807:BCR:H313	20:A:1813:CLA:C14	1.77	1.12
6:B:58:PHE:HB2	6:B:146:SER:HB3	1.27	1.12
20:B:1753:CLA:H102	20:B:1753:CLA:C15	1.77	1.12
22:B:1779:BCR:HC8	22:B:1779:BCR:C32	1.66	1.13
12:H:69:SER:HB2	20:H:1079:CLA:H61	1.13	1.13
13:I:7:LEU:CD1	22:I:1032:BCR:H333	1.79	1.12
16:L:164:PRO:CB	16:L:165:TYR:CD2	2.30	1.12
19:X:1:GLC:H5	19:X:2:FRU:O1	1.49	1.12
3:3:64:TYR:HB3	20:3:1218:CLA:H43	1.28	1.12
5:A:435:VAL:O	5:A:438:HIS:O	1.67	1.12
5:A:451:ILE:HD12	20:A:1788:CLA:HED3	1.29	1.12
20:A:1772:CLA:H141	20:A:1772:CLA:H172	1.13	1.12
25:B:1784:SF4:S1	25:B:1784:SF4:S2	2.47	1.12
12:H:25:GLY:HA3	12:H:27:ASP:N	1.62	1.12
20:3:1217:CLA:CHA	20:3:3011:CLA:CBC	2.27	1.12
3:3:158:TYR:HB3	3:3:159:PRO:HD2	1.31	1.12
5:A:24:ARG:HD2	5:A:24:ARG:N	1.64	1.12
5:A:423:ASP:HB3	5:A:424:PRO:HD3	1.20	1.12
21:A:7036:LMU:H31	21:A:7036:LMU:C8	1.79	1.12
17:N:58:VAL:CB	17:N:59:PRO:HD2	1.77	1.12
21:A:7010:LMU:H3'	21:A:7010:LMU:O2B	1.49	1.12
16:L:163:LEU:CD1	16:L:164:PRO:HB2	1.78	1.12
17:N:75:TYR:O	17:N:76:LYS:O	1.68	1.12
20:4:1196:CLA:HHD	20:4:1196:CLA:HBC2	1.23	1.11
20:4:1199:CLA:HAA1	20:F:1157:CLA:H42	1.31	1.11
20:A:1772:CLA:H141	20:A:1772:CLA:C17	1.78	1.11
20:A:1813:CLA:HMD3	6:B:578:LEU:HD23	1.13	1.11
11:G:12:THR:HG22	11:G:72:LEU:HG	1.19	1.11
20:J:1045:CLA:CBD	20:J:1045:CLA:HBA2	1.79	1.11
3:3:84:ILE:HA	20:A:1798:CLA:H51	1.24	1.11
20:A:1791:CLA:HBC2	22:A:1806:BCR:HC31	1.32	1.11
21:A:7033:LMU:H6'2	21:A:7033:LMU:C3'	1.78	1.11
6:B:131:THR:HB	6:B:134:ASP:HB2	1.16	1.11
6:B:608:GLN:HE21	6:B:608:GLN:HA	1.02	1.11
10:F:25:LEU:CD2	10:F:46:MET:HB3	1.80	1.11
20:1:1191:CLA:CMC	20:1:1194:CLA:HHD	1.77	1.11
5:A:472:ARG:HH12	16:L:74:LEU:HG	1.01	1.11
20:A:1781:CLA:CED	20:A:1782:CLA:HMD1	1.80	1.11
20:A:1817:CLA:HBC2	20:A:1817:CLA:HMC1	1.24	1.11
21:A:7030:LMU:C5	21:A:7030:LMU:H91	1.67	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1735:CLA:H101	20:B:1735:CLA:HBB2	1.14	1.11
23:B:1773:PQN:H191	22:B:1780:BCR:C10	1.78	1.11
22:B:1780:BCR:H382	22:B:1780:BCR:H23C	1.21	1.11
25:B:1784:SF4:S1	25:B:1784:SF4:S4	2.47	1.11
10:F:22:LEU:H	10:F:22:LEU:CD1	1.64	1.11
11:G:45:GLU:C	11:G:49:THR:HG21	1.70	1.11
15:K:69:ILE:HG22	15:K:70:MET:H	1.16	1.11
17:N:61:LEU:CD1	17:N:63:ASP:HB2	1.80	1.11
2:2:64:ILE:O	2:2:68:LEU:HB2	1.49	1.11
3:3:52:LYS:O	3:3:56:TYR:CD2	2.03	1.11
3:3:87:GLU:O	22:3:1220:BCR:H381	1.50	1.11
20:4:1199:CLA:HMC1	20:4:1199:CLA:HBC3	1.11	1.11
5:A:76:ARG:CZ	5:A:192:LYS:HG2	1.79	1.11
5:A:425:THR:HG21	8:D:59:GLU:OE2	1.48	1.11
5:A:581:CYS:HB2	5:A:590:CYS:HA	1.23	1.11
5:A:588:GLY:CA	6:B:668:ARG:HD3	1.81	1.11
20:B:1759:CLA:HMC1	20:B:1759:CLA:CBC	1.79	1.11
20:B:1768:CLA:C16	22:B:1779:BCR:H313	1.79	1.11
5:A:316:MET:HB3	5:A:317:TYR:CG	1.85	1.11
21:A:7016:LMU:H22	21:A:7016:LMU:H61	1.26	1.11
20:B:1786:CLA:H93	20:B:1787:CLA:H91	1.16	1.11
7:C:66:ARG:HG2	7:C:66:ARG:HH21	1.16	1.11
2:2:127:ASN:ND2	14:J:2:ARG:HH12	1.47	1.10
3:3:84:ILE:H	20:A:1798:CLA:C4	1.61	1.10
5:A:208:ALA:HA	5:A:310:PHE:O	1.50	1.10
5:A:685:VAL:HG23	20:A:1796:CLA:CBB	1.81	1.10
11:G:42:SER:HB2	11:G:45:GLU:CD	1.71	1.10
17:N:67:LEU:C	17:N:68:GLU:HG3	1.72	1.10
20:2:1220:CLA:CGA	20:2:1220:CLA:CBD	2.29	1.10
5:A:331:LEU:HD21	5:A:343:HIS:O	0.94	1.10
22:A:1803:BCR:H23C	22:A:1803:BCR:H402	1.32	1.10
21:A:7026:LMU:O4'	19:Z:2:FRU:H3	1.38	1.10
21:A:7030:LMU:C5	21:A:7030:LMU:C9	2.30	1.10
21:A:7036:LMU:C3	21:A:7036:LMU:C8	2.29	1.10
6:B:247:THR:CA	6:B:250:ALA:HB2	1.79	1.10
17:N:72:LYS:HG2	17:N:74:LYS:HG3	1.32	1.10
19:Z:2:FRU:H12	19:Z:2:FRU:H61	1.31	1.10
20:1:1198:CLA:H71	20:1:1198:CLA:H41	1.11	1.10
21:A:7016:LMU:H32	21:A:7016:LMU:C8	1.81	1.10
8:D:113:HIS:NE2	8:D:118:VAL:HG11	1.63	1.10
9:E:86:GLU:CG	9:E:87:VAL:H	1.65	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1772:CLA:CED	20:A:1772:CLA:C2A	2.30	1.10
21:A:7016:LMU:C2	21:A:7016:LMU:C8	2.30	1.10
21:A:7023:LMU:H41	21:A:7023:LMU:H92	1.13	1.10
6:B:58:PHE:CB	6:B:146:SER:HB3	1.80	1.10
13:I:7:LEU:HD12	22:I:1032:BCR:C33	1.80	1.10
20:K:1085:CLA:CMB	20:K:1142:CLA:CED	2.30	1.10
17:N:54:LYS:HB3	17:N:57:LYS:HE2	1.22	1.10
20:1:1200:CLA:HMC1	20:1:1200:CLA:CBC	1.80	1.10
20:3:3008:CLA:CGD	20:3:3008:CLA:CBA	2.30	1.10
5:A:23:ASP:CB	5:A:24:ARG:HD2	1.82	1.10
20:A:1760:CLA:H12	20:A:1767:CLA:H61	1.25	1.10
20:A:1770:CLA:HMB2	22:A:1803:BCR:H382	1.34	1.10
21:A:7016:LMU:C3	21:A:7016:LMU:C8	2.29	1.10
21:A:7023:LMU:C4	21:A:7023:LMU:C8	2.30	1.10
21:A:7026:LMU:C8	21:A:7026:LMU:H41	1.80	1.10
18:R:38:UNK:O	18:R:42:UNK:HA	1.48	1.10
19:Q:1:GLC:C1	19:Q:2:FRU:C5	2.29	1.10
5:A:328:LYS:HG2	5:A:332:GLU:HB2	1.31	1.09
5:A:331:LEU:HD11	5:A:346:LEU:HB3	1.23	1.09
20:A:1770:CLA:C4B	22:A:1803:BCR:C19	2.29	1.09
6:B:119:GLY:HA3	20:B:1758:CLA:HED1	1.14	1.09
10:F:22:LEU:N	10:F:22:LEU:HD12	1.52	1.09
22:I:1032:BCR:C4	22:I:1032:BCR:H322	1.61	1.09
16:L:163:LEU:CD1	16:L:164:PRO:CB	2.30	1.09
16:L:163:LEU:CD1	16:L:164:PRO:CG	2.29	1.09
20:4:1198:CLA:CED	20:4:1198:CLA:CAA	2.29	1.09
20:4:4014:CLA:HMC1	20:4:4014:CLA:HBC3	1.22	1.09
5:A:23:ASP:CB	5:A:24:ARG:CD	2.30	1.09
20:A:1771:CLA:HBB1	22:A:1803:BCR:C35	1.81	1.09
21:A:7023:LMU:C9	21:A:7023:LMU:C4	2.30	1.09
21:A:7033:LMU:C6B	21:A:7033:LMU:C3'	2.30	1.09
21:A:7037:LMU:C1	21:A:7037:LMU:C5	2.29	1.09
6:B:103:ALA:O	6:B:104:PHE:HB2	1.48	1.09
22:I:1032:BCR:HC31	20:I:1033:CLA:CAC	1.80	1.09
20:J:1045:CLA:CAD	20:J:1045:CLA:CED	2.30	1.09
17:N:72:LYS:HG3	17:N:74:LYS:CA	1.80	1.09
17:N:72:LYS:CG	17:N:74:LYS:CG	2.31	1.09
20:2:1220:CLA:HBA2	20:2:1220:CLA:CHA	1.63	1.09
3:3:87:GLU:HB2	22:3:1220:BCR:H382	1.34	1.09
5:A:453:LEU:HD23	20:A:1793:CLA:HBB2	1.21	1.09
20:A:1791:CLA:CBC	22:A:1806:BCR:HC31	1.80	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1816:CLA:CED	20:A:1816:CLA:CGA	2.31	1.09
21:A:7023:LMU:C3	21:A:7023:LMU:C8	2.30	1.09
21:A:7039:LMU:C6B	21:A:7039:LMU:C3'	2.29	1.09
10:F:47:GLU:HG3	10:F:51:LYS:HE3	1.16	1.09
20:K:1085:CLA:HMB2	20:K:1142:CLA:HED1	1.18	1.09
16:L:163:LEU:CD1	16:L:164:PRO:CD	2.29	1.09
17:N:72:LYS:CG	17:N:74:LYS:CB	2.31	1.09
18:R:46:UNK:CB	18:R:47:UNK:CB	2.30	1.09
20:R:1055:CLA:HBA2	20:R:1055:CLA:HBD	1.28	1.09
5:A:316:MET:HG2	5:A:317:TYR:CE1	1.88	1.09
20:A:1770:CLA:HHC	22:A:1803:BCR:H17C	1.32	1.09
21:A:7032:LMU:C1B	21:A:7032:LMU:C3	2.29	1.09
8:D:117:GLY:O	8:D:118:VAL:HG23	1.52	1.09
14:J:11:ALA:HB1	14:J:12:PRO:HD2	1.34	1.09
18:R:34:UNK:CB	18:R:35:UNK:CB	2.30	1.09
20:2:1220:CLA:H61	3:3:140:LYS:CE	1.83	1.09
20:4:1201:CLA:HMA2	20:4:1201:CLA:CGA	1.82	1.09
5:A:328:LYS:CE	5:A:332:GLU:CG	2.30	1.09
5:A:335:LYS:HG2	5:A:336:GLY:H	1.12	1.09
20:A:1781:CLA:CED	20:A:1782:CLA:CMD	2.30	1.09
11:G:43:HIS:CA	11:G:44:PHE:HB3	1.81	1.09
16:L:164:PRO:CA	16:L:165:TYR:CE2	2.35	1.09
17:N:62:SER:CB	17:N:66:ASP:CB	2.29	1.09
18:R:41:UNK:CB	18:R:42:UNK:CA	2.30	1.09
20:A:1776:CLA:HMD3	20:A:1778:CLA:HBB2	1.13	1.08
22:A:1805:BCR:H382	22:A:1805:BCR:H23C	1.21	1.08
21:A:7043:LMU:H71	21:A:7043:LMU:H112	1.27	1.08
6:B:22:TRP:HE1	20:B:1770:CLA:CBB	1.65	1.08
20:B:1759:CLA:HMC1	20:B:1759:CLA:HBC2	1.29	1.08
22:B:1777:BCR:H382	22:B:1777:BCR:H23C	1.30	1.08
10:F:102:ARG:HG2	10:F:106:ILE:HD11	1.12	1.08
16:L:164:PRO:CB	16:L:165:TYR:CE2	2.35	1.08
3:3:107:TRP:CD1	3:3:108:ALA:N	2.21	1.08
4:4:107:GLN:CB	20:4:1196:CLA:HMA3	1.84	1.08
20:A:1788:CLA:H161	22:L:1169:BCR:H361	1.32	1.08
21:A:7032:LMU:H3'	21:A:7032:LMU:O5B	1.35	1.08
6:B:293:THR:C	11:G:38:GLN:OE1	1.68	1.08
20:1:1197:CLA:CAD	20:1:1197:CLA:CED	2.32	1.08
4:4:38:ARG:HH11	4:4:38:ARG:HG3	1.14	1.08
20:A:1781:CLA:CED	20:A:1782:CLA:CAD	2.30	1.08
21:A:7042:LMU:H6D	21:A:7042:LMU:C3	1.82	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:48:ASP:CB	11:G:49:THR:CG2	2.30	1.08
20:J:1044:CLA:C10	20:J:1044:CLA:H152	1.55	1.08
16:L:163:LEU:HD13	16:L:164:PRO:N	1.67	1.08
5:A:51:THR:HG21	20:A:1795:CLA:HBB1	1.17	1.08
5:A:365:LEU:HD23	20:A:1761:CLA:HED3	1.29	1.08
5:A:402:ILE:HG13	20:A:1784:CLA:HBB2	1.32	1.08
20:A:1797:CLA:HBC3	20:A:1797:CLA:HHD	1.31	1.08
20:A:1816:CLA:CGD	20:A:1816:CLA:CAA	2.30	1.08
21:A:7042:LMU:C6'	21:A:7042:LMU:C3	2.30	1.08
21:A:7036:LMU:C7	21:A:7036:LMU:C3	2.29	1.08
20:B:1755:CLA:HBB1	20:B:1769:CLA:HMB3	1.29	1.08
10:F:23:LYS:HB2	10:F:24:LYS:HZ1	1.17	1.08
20:K:1146:CLA:HBC2	20:K:1146:CLA:HMC1	1.35	1.08
17:N:51:ASP:C	17:N:52:LEU:HD23	1.74	1.08
18:R:39:UNK:C	18:R:41:UNK:CB	2.30	1.08
20:2:1212:CLA:HMC1	20:2:1212:CLA:CBC	1.83	1.07
3:3:198:PHE:HA	3:3:201:ALA:HB2	1.36	1.07
20:A:1780:CLA:H92	20:A:1780:CLA:OBD	1.51	1.07
21:A:7032:LMU:O2'	21:A:7032:LMU:H12	1.45	1.07
6:B:302:LYS:O	6:B:303:TYR:HB2	1.50	1.07
6:B:594:TRP:O	6:B:595:HIS:HB3	1.49	1.07
20:J:1043:CLA:HED3	20:J:1043:CLA:CHA	1.83	1.07
5:A:316:MET:HB3	5:A:317:TYR:HB2	1.18	1.07
20:A:1797:CLA:H71	20:A:1797:CLA:H121	1.34	1.07
21:A:7021:LMU:H1'	21:A:7021:LMU:C3	1.81	1.07
21:A:7023:LMU:C8	21:A:7023:LMU:H32	1.84	1.07
21:A:7036:LMU:C2	21:A:7036:LMU:C8	2.30	1.07
21:A:7043:LMU:C11	21:A:7043:LMU:C7	2.30	1.07
20:B:1753:CLA:O2D	20:B:1753:CLA:H2A	1.52	1.07
20:B:1755:CLA:HHD	20:B:1755:CLA:HBC2	1.15	1.07
9:E:52:VAL:HG12	9:E:53:VAL:H	1.18	1.07
11:G:46:ALA:HA	11:G:48:ASP:OD2	1.53	1.07
20:J:1044:CLA:O2D	20:J:1045:CLA:H92	1.50	1.07
20:J:1045:CLA:CBC	20:J:1045:CLA:CHD	2.30	1.07
21:R:1056:LMU:O6B	21:R:1056:LMU:H1B	1.50	1.07
20:1:1198:CLA:H102	20:1:1198:CLA:C5	1.81	1.07
20:1:1198:CLA:HHD	20:1:1198:CLA:CBC	1.82	1.07
20:3:3008:CLA:CBD	20:3:3008:CLA:CBA	2.30	1.07
20:3:3008:CLA:HMC1	20:3:3008:CLA:HBC2	1.09	1.07
4:4:95:PHE:HZ	20:4:1208:CLA:C3C	1.67	1.07
10:F:42:ILE:HG13	10:F:43:LYS:H	1.15	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:164:PRO:HA	16:L:165:TYR:CE2	1.90	1.07
19:Q:1:GLC:C1	19:Q:2:FRU:H5	1.84	1.07
20:A:1782:CLA:HMC1	20:A:1782:CLA:HBC2	1.33	1.07
21:A:7016:LMU:H22	21:A:7016:LMU:C6	1.57	1.07
21:A:7023:LMU:O3B	21:A:7023:LMU:H6'1	1.46	1.07
6:B:58:PHE:HB2	6:B:146:SER:CB	1.83	1.07
20:J:1044:CLA:CGD	20:J:1045:CLA:C9	2.32	1.07
16:L:164:PRO:C	16:L:165:TYR:CG	2.28	1.07
17:N:45:ASN:HD22	17:N:54:LYS:CB	1.64	1.07
20:2:1220:CLA:H42	3:3:140:LYS:HG2	1.35	1.07
3:3:93:PHE:CD2	3:3:93:PHE:N	2.22	1.07
21:A:7023:LMU:H82	21:A:7023:LMU:H32	1.13	1.07
21:A:7039:LMU:H3'	21:A:7039:LMU:H6'2	1.08	1.07
6:B:729:THR:O	6:B:729:THR:HG22	1.53	1.07
20:B:1737:CLA:H62	20:B:1737:CLA:O1A	1.54	1.07
12:H:25:GLY:HA3	12:H:27:ASP:H	1.02	1.07
20:J:1045:CLA:HHD	20:J:1045:CLA:HBC2	1.19	1.07
16:L:66:GLY:HA3	20:L:1168:CLA:CHC	1.85	1.07
20:R:1054:CLA:HED3	20:R:1054:CLA:CHA	1.85	1.07
5:A:21:LEU:HA	5:A:22:VAL:HB	1.14	1.06
21:A:7042:LMU:O2B	21:A:7042:LMU:H5'	1.54	1.06
6:B:202:SER:O	6:B:245:GLY:HA2	1.52	1.06
17:N:54:LYS:HB3	17:N:57:LYS:CE	1.85	1.06
5:A:249:ILE:HG12	5:A:250:LEU:N	1.67	1.06
20:A:1797:CLA:H121	20:A:1797:CLA:C7	1.85	1.06
21:A:7020:LMU:C5B	21:A:7020:LMU:C6'	2.29	1.06
21:A:7026:LMU:C5	21:A:7026:LMU:H12	1.82	1.06
6:B:25:ILE:HG23	22:L:1169:BCR:H282	1.37	1.06
12:H:58:ILE:HD11	16:L:97:MET:SD	1.94	1.06
20:J:1044:CLA:H41	20:J:1044:CLA:C8	1.84	1.06
3:3:87:GLU:C	22:3:1220:BCR:H381	1.75	1.06
5:A:23:ASP:OD2	5:A:24:ARG:HD3	1.54	1.06
5:A:605:MET:HA	5:A:608:SER:OG	1.55	1.06
20:A:1779:CLA:CAB	22:A:1805:BCR:H351	1.85	1.06
20:A:1781:CLA:HBC2	20:A:1781:CLA:HHD	1.07	1.06
20:A:1781:CLA:HHD	20:A:1781:CLA:CBC	1.86	1.06
22:A:1807:BCR:C31	20:A:1813:CLA:H142	1.84	1.06
20:B:1768:CLA:H152	22:B:1779:BCR:H312	1.09	1.06
11:G:28:ARG:HG2	11:G:28:ARG:HH21	1.20	1.06
22:I:1032:BCR:H322	22:I:1032:BCR:HC42	1.10	1.06
16:L:164:PRO:CA	16:L:165:TYR:CD2	2.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:164:PRO:C	16:L:165:TYR:CD2	2.28	1.06
20:L:1168:CLA:HHD	20:L:1168:CLA:CBC	1.83	1.06
3:3:98:ILE:O	17:N:63:ASP:O	1.72	1.06
20:3:3011:CLA:HMA2	20:3:3011:CLA:H12	1.27	1.06
5:A:197:GLN:HA	5:A:197:GLN:HE21	0.92	1.06
21:A:7030:LMU:H91	21:A:7030:LMU:H51	1.34	1.06
6:B:282:PHE:HZ	20:B:1746:CLA:C1	1.69	1.06
10:F:5:LEU:HG	10:F:6:THR:N	1.66	1.06
16:L:161:LEU:CD1	16:L:162:ASP:N	2.18	1.06
17:N:52:LEU:HD23	17:N:52:LEU:N	1.65	1.06
4:4:95:PHE:CZ	20:4:1208:CLA:C2C	2.38	1.06
4:4:107:GLN:HA	20:4:1196:CLA:HMA3	1.16	1.06
5:A:21:LEU:N	5:A:22:VAL:HB	1.69	1.06
20:A:1770:CLA:CHC	22:A:1803:BCR:C19	2.34	1.06
6:B:310:PRO:HG3	20:B:1753:CLA:HMA1	1.09	1.06
6:B:531:THR:HG22	20:B:1755:CLA:HMC2	1.11	1.06
6:B:663:PHE:O	6:B:664:LEU:HB2	1.49	1.06
20:B:1761:CLA:HBC2	20:B:1761:CLA:HHD	1.35	1.06
23:B:1773:PQN:C16	22:B:1780:BCR:H333	1.80	1.06
5:A:267:THR:O	5:A:269:PHE:HD2	1.39	1.05
9:E:87:VAL:O	9:E:87:VAL:HG12	1.56	1.05
11:G:42:SER:OG	11:G:45:GLU:HB2	1.56	1.05
11:G:45:GLU:HG3	11:G:49:THR:CG2	1.79	1.05
22:I:1032:BCR:HC22	20:I:1033:CLA:C4C	1.85	1.05
20:J:1044:CLA:C10	20:J:1044:CLA:C15	2.30	1.05
17:N:58:VAL:CB	17:N:59:PRO:CD	2.30	1.05
20:3:3008:CLA:HMC1	20:3:3008:CLA:CBC	1.87	1.05
20:4:1198:CLA:H151	20:4:1198:CLA:H202	1.27	1.05
20:4:1209:CLA:HBD	20:4:1209:CLA:HBA1	1.37	1.05
22:A:1803:BCR:H311	22:A:1803:BCR:HC8	1.07	1.05
6:B:560:ASP:OD1	6:B:561:GLY:N	1.90	1.05
20:B:1735:CLA:HMD3	22:B:1778:BCR:HC41	1.36	1.05
22:B:1780:BCR:H17C	20:B:1786:CLA:H101	1.39	1.05
11:G:46:ALA:H	11:G:48:ASP:CB	1.69	1.05
11:G:68:ILE:CG2	11:G:72:LEU:HD13	1.86	1.05
21:1:7004:LMU:O6B	21:1:7004:LMU:H1B	1.50	1.05
20:4:1198:CLA:H151	20:4:1198:CLA:H203	1.34	1.05
5:A:454:GLY:H	5:A:457:SER:HB3	1.15	1.05
20:A:1816:CLA:CBC	20:A:1816:CLA:CHD	2.33	1.05
6:B:474:PHE:HE2	6:B:476:ILE:HG13	1.19	1.05
20:B:1761:CLA:HHD	20:B:1761:CLA:CBC	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:46:PHE:O	17:N:47:THR:HG23	1.54	1.05
17:N:48:GLY:HA3	17:N:49:CYS:O	1.55	1.05
20:4:1198:CLA:H2A	20:4:1198:CLA:O1D	1.56	1.05
5:A:599:PHE:CE2	5:A:735:VAL:HG21	1.92	1.05
21:A:7037:LMU:C1	21:A:7037:LMU:H51	1.87	1.05
21:A:7043:LMU:H102	21:A:7043:LMU:H62	1.06	1.05
23:B:1773:PQN:H192	22:B:1780:BCR:H10C	1.35	1.05
11:G:12:THR:CG2	11:G:72:LEU:HG	1.85	1.05
12:H:25:GLY:HA3	12:H:27:ASP:CB	1.86	1.05
20:J:1045:CLA:HHD	20:J:1045:CLA:HBC3	1.39	1.05
17:N:65:LEU:HD23	17:N:65:LEU:O	1.54	1.05
20:A:1781:CLA:H72	20:A:1782:CLA:HED2	1.30	1.05
22:A:1807:BCR:C31	22:A:1807:BCR:HC8	1.86	1.05
21:A:7016:LMU:C2	21:A:7016:LMU:C6	2.30	1.05
21:A:7036:LMU:C3	21:A:7036:LMU:H71	1.82	1.05
6:B:174:ARG:HB2	20:B:1743:CLA:HBC2	1.39	1.05
9:E:72:VAL:O	9:E:73:ASN:HB3	1.56	1.05
14:J:2:ARG:HH12	14:J:8:LEU:HD13	1.21	1.05
16:L:64:LEU:HB3	16:L:68:PHE:HE1	1.18	1.05
16:L:163:LEU:CD2	16:L:164:PRO:CD	2.30	1.05
20:1:1197:CLA:HED2	20:1:1197:CLA:OBD	1.56	1.04
5:A:402:ILE:CG1	20:A:1784:CLA:HBB2	1.87	1.04
20:A:1782:CLA:HMC1	20:A:1782:CLA:CBC	1.86	1.04
22:A:1804:BCR:H23C	22:A:1804:BCR:H402	1.38	1.04
10:F:151:ASP:O	10:F:154:PHE:HB3	1.56	1.04
11:G:43:HIS:O	11:G:45:GLU:HB2	1.56	1.04
16:L:161:LEU:HD11	16:L:162:ASP:O	1.57	1.04
5:A:316:MET:CB	5:A:317:TYR:HD1	1.64	1.04
6:B:560:ASP:HB2	7:C:66:ARG:NE	1.71	1.04
16:L:163:LEU:CG	16:L:164:PRO:HD2	1.85	1.04
17:N:45:ASN:HD22	17:N:57:LYS:NZ	1.53	1.04
21:A:7016:LMU:H51	21:A:7016:LMU:H6'	1.19	1.04
20:B:1755:CLA:CED	20:B:1756:CLA:HMD1	1.88	1.04
8:D:78:ALA:HB3	8:D:82:GLN:HE22	1.16	1.04
9:E:85:ASP:O	9:E:86:GLU:HB3	1.52	1.04
3:3:64:TYR:HB3	20:3:1218:CLA:H42	1.33	1.04
3:3:110:SER:O	3:3:111:TYR:CD2	2.10	1.04
20:4:1198:CLA:C20	20:4:1198:CLA:C15	2.30	1.04
5:A:21:LEU:CA	5:A:22:VAL:CB	2.35	1.04
5:A:81:ALA:HB1	20:A:1760:CLA:HMA1	1.38	1.04
20:A:1772:CLA:H172	20:A:1772:CLA:C14	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7042:LMU:C7	21:A:7042:LMU:C2	2.30	1.04
7:C:1:MET:HG2	7:C:4:SER:HB3	1.37	1.04
22:I:1032:BCR:C3	20:I:1033:CLA:CAC	2.36	1.04
6:B:310:PRO:HG2	6:B:311:PRO:HD2	1.37	1.04
20:B:1739:CLA:H92	20:B:1739:CLA:CBB	1.86	1.04
10:F:23:LYS:O	10:F:26:GLN:HB2	1.57	1.04
10:F:24:LYS:CA	10:F:24:LYS:CE	2.36	1.04
10:F:130:LEU:HG	10:F:131:PHE:H	1.16	1.04
20:J:1045:CLA:HBD	20:J:1045:CLA:HBA2	1.04	1.04
19:O:2:FRU:H62	19:O:2:FRU:H11	1.07	1.04
5:A:370:ILE:HG22	5:A:400:MET:HA	1.40	1.03
20:A:1770:CLA:HMB2	22:A:1803:BCR:C38	1.87	1.03
21:A:7032:LMU:H31	21:A:7032:LMU:H2B	1.34	1.03
22:B:1779:BCR:C27	22:B:1779:BCR:C40	2.30	1.03
11:G:45:GLU:HG3	11:G:49:THR:HG23	1.08	1.03
17:N:61:LEU:HD11	17:N:63:ASP:N	1.73	1.03
20:3:1219:CLA:C10	20:3:1219:CLA:C14	2.34	1.03
20:A:1771:CLA:CBB	22:A:1803:BCR:H352	1.87	1.03
21:A:7021:LMU:H22	21:A:7021:LMU:H62	1.07	1.03
6:B:708:VAL:O	6:B:712:HIS:HB2	1.56	1.03
20:J:1045:CLA:O2A	20:J:1045:CLA:H2A	1.55	1.03
20:3:1219:CLA:C14	20:3:1219:CLA:H102	1.89	1.03
5:A:316:MET:CB	5:A:317:TYR:HB2	1.88	1.03
6:B:419:ILE:O	6:B:420:SER:OG	1.77	1.03
7:C:1:MET:HB3	7:C:4:SER:OG	1.54	1.03
7:C:54:CYS:CB	25:C:1082:SF4:S1	2.47	1.03
11:G:68:ILE:HG23	11:G:72:LEU:HD13	1.34	1.03
20:J:1044:CLA:C15	20:J:1044:CLA:H102	1.87	1.03
5:A:23:ASP:C	5:A:24:ARG:HD2	1.78	1.03
5:A:116:ILE:HG23	5:A:137:GLY:HA3	1.41	1.03
10:F:24:LYS:O	10:F:27:ALA:HB2	1.59	1.03
11:G:44:PHE:N	11:G:45:GLU:HB2	1.71	1.03
20:1:1198:CLA:H41	20:1:1198:CLA:C7	1.78	1.03
20:4:1199:CLA:HMC1	20:4:1199:CLA:CBC	1.88	1.03
5:A:365:LEU:HD23	20:A:1761:CLA:CED	1.87	1.03
5:A:545:HIS:ND1	20:A:1792:CLA:HBB2	1.74	1.03
20:A:1776:CLA:HMD3	20:A:1778:CLA:CBB	1.87	1.03
20:A:1796:CLA:C14	22:A:1807:BCR:C2	2.37	1.03
6:B:340:SER:HA	20:B:1756:CLA:H51	1.40	1.03
12:H:20:GLN:HB3	12:H:22:ASP:HB3	1.03	1.03
22:I:1032:BCR:C2	20:I:1033:CLA:C3C	2.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:71:GLY:O	15:K:72:VAL:O	1.76	1.03
20:2:1220:CLA:H41	3:3:140:LYS:HD3	1.40	1.02
5:A:707:ILE:HG22	5:A:711:HIS:NE2	1.74	1.02
6:B:65:LEU:HD22	6:B:124:TRP:HE3	1.21	1.02
20:B:1753:CLA:H43	20:B:1753:CLA:HAA1	1.41	1.02
23:B:1773:PQN:C16	22:B:1780:BCR:H331	1.87	1.02
9:E:51:SER:HB3	9:E:68:ARG:CZ	1.89	1.02
2:2:120:ASN:ND2	14:J:5:LYS:HE3	1.73	1.02
20:K:1085:CLA:CMB	20:K:1142:CLA:HED2	1.90	1.02
17:N:76:LYS:HG3	17:N:77:CYS:H	1.22	1.02
20:2:1213:CLA:HHD	20:2:1213:CLA:HBC2	1.41	1.02
20:A:1791:CLA:CGA	20:A:1797:CLA:CBB	2.36	1.02
22:B:1779:BCR:H403	22:B:1779:BCR:H271	1.03	1.02
10:F:24:LYS:HE2	10:F:24:LYS:HA	1.42	1.02
20:J:1044:CLA:C15	20:J:1044:CLA:H91	1.90	1.02
5:A:401:TRP:CD1	20:A:1783:CLA:HHC	1.95	1.02
20:A:1762:CLA:H43	20:A:1785:CLA:H11	1.40	1.02
22:A:1807:BCR:C31	20:A:1813:CLA:H143	1.87	1.02
6:B:247:THR:HA	6:B:250:ALA:HB2	1.05	1.02
6:B:558:PRO:HG2	6:B:703:VAL:HB	1.37	1.02
14:J:31:ARG:NH2	20:J:1043:CLA:C4B	2.21	1.02
15:K:1:ASP:HA	15:K:5:SER:HB3	1.40	1.02
20:A:1772:CLA:HBC3	20:A:1772:CLA:CMC	1.82	1.02
10:F:23:LYS:C	10:F:24:LYS:HE2	1.79	1.02
16:L:88:ALA:C	16:L:90:GLY:H	1.56	1.02
20:2:1212:CLA:H42	20:2:1212:CLA:CGA	1.89	1.01
20:3:1217:CLA:C2A	20:3:3011:CLA:HAC2	1.89	1.01
4:4:160:MET:HE3	20:4:1201:CLA:CBB	1.87	1.01
5:A:23:ASP:HB2	5:A:24:ARG:CZ	1.90	1.01
5:A:27:ILE:O	5:A:27:ILE:HG22	1.54	1.01
21:A:7042:LMU:H1B	21:A:7042:LMU:O3'	1.57	1.01
20:B:1768:CLA:HBC1	10:F:83:PHE:CZ	1.95	1.01
9:E:45:TRP:CH2	9:E:78:SER:OG	2.12	1.01
11:G:43:HIS:C	11:G:45:GLU:HB2	1.79	1.01
11:G:48:ASP:HB3	11:G:49:THR:CG2	1.89	1.01
20:3:1217:CLA:CHA	20:3:3011:CLA:HBC2	1.90	1.01
5:A:239:PRO:HA	5:A:242:ILE:CD1	1.90	1.01
5:A:355:HIS:ND1	5:A:416:ILE:HG21	1.76	1.01
5:A:511:THR:HG23	20:A:1773:CLA:O1A	1.58	1.01
6:B:382:ILE:HG22	6:B:383:MET:H	1.25	1.01
11:G:47:GLY:H	11:G:48:ASP:CB	1.73	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:CD1	17:N:63:ASP:CB	2.38	1.01
21:1:7004:LMU:O2'	21:1:7004:LMU:H11	1.56	1.01
20:3:1217:CLA:CHA	20:3:3011:CLA:HBC1	1.87	1.01
20:3:3008:CLA:CGD	20:3:3008:CLA:CGA	2.38	1.01
5:A:249:ILE:HG12	5:A:250:LEU:H	0.89	1.01
5:A:328:LYS:HE2	5:A:332:GLU:HG3	1.38	1.01
20:B:1735:CLA:H2A	20:B:1735:CLA:HED3	1.40	1.01
20:B:1753:CLA:C4A	20:B:1753:CLA:H42	1.90	1.01
20:B:1767:CLA:HMC1	20:B:1767:CLA:HBC3	1.42	1.01
22:B:1780:BCR:H19C	20:B:1786:CLA:H151	1.41	1.01
12:H:44:ALA:CB	16:L:145:PHE:HD1	1.73	1.01
16:L:108:LYS:O	16:L:132:SER:HB2	1.59	1.01
20:A:1769:CLA:HBA1	20:A:1780:CLA:H41	1.41	1.01
20:A:1812:CLA:HMB3	20:B:1785:CLA:H18	1.43	1.01
21:A:7033:LMU:H3'	21:A:7033:LMU:H6'2	1.05	1.01
20:B:1755:CLA:HED1	20:B:1756:CLA:HMD1	1.42	1.01
11:G:12:THR:HG22	11:G:72:LEU:CG	1.88	1.01
16:L:122:GLY:C	16:L:124:LYS:H	1.61	1.01
2:2:169:LEU:HD22	20:2:1215:CLA:CAB	1.90	1.01
3:3:194:ILE:HD11	20:3:1212:CLA:HMC2	1.39	1.01
21:A:7023:LMU:H6'2	21:A:7023:LMU:C2B	1.87	1.01
25:B:1784:SF4:S4	25:B:1784:SF4:S3	2.59	1.01
20:K:1085:CLA:NA	20:K:1142:CLA:HMD1	1.74	1.01
16:L:163:LEU:HD13	16:L:164:PRO:HB2	1.36	1.01
5:A:368:LEU:CD2	20:A:1774:CLA:C9	2.38	1.00
20:A:1781:CLA:C7	20:A:1782:CLA:CED	2.38	1.00
22:A:1807:BCR:HC8	22:A:1807:BCR:H311	1.01	1.00
22:A:1808:BCR:H23C	22:A:1808:BCR:H393	1.04	1.00
20:B:1768:CLA:H152	22:B:1779:BCR:H313	1.43	1.00
7:C:8:TYR:O	7:C:60:THR:HA	1.59	1.00
4:4:146:THR:OG1	20:4:1200:CLA:C5	2.09	1.00
20:A:1788:CLA:H161	22:L:1169:BCR:C36	1.91	1.00
20:B:1735:CLA:HBB2	20:B:1735:CLA:C10	1.91	1.00
3:3:48:PHE:HD2	3:3:49:ILE:HG22	0.85	1.00
5:A:390:ALA:HB2	5:A:754:ILE:HB	1.43	1.00
5:A:588:GLY:HA3	6:B:668:ARG:HD3	1.41	1.00
20:A:1797:CLA:C7	20:A:1797:CLA:C12	2.35	1.00
21:A:7013:LMU:O6B	21:A:7013:LMU:H1B	1.57	1.00
20:B:1740:CLA:H41	22:B:1781:BCR:C23	1.90	1.00
10:F:26:GLN:OE1	10:F:26:GLN:HA	1.61	1.00
20:J:1044:CLA:H152	20:J:1044:CLA:C8	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:72:LYS:HB3	17:N:73:ASP:C	1.81	1.00
20:A:1759:CLA:H42	20:A:1796:CLA:H61	1.03	1.00
20:A:1774:CLA:HBB2	20:A:1774:CLA:H121	1.42	1.00
21:A:7026:LMU:H41	21:A:7026:LMU:H82	1.41	1.00
20:B:1753:CLA:C4A	20:B:1753:CLA:C4	2.30	1.00
7:C:44:ARG:HH21	8:D:127:ARG:HB3	1.23	1.00
17:N:1:GLY:O	17:N:2:VAL:HG13	1.59	1.00
17:N:61:LEU:CD1	17:N:63:ASP:C	2.30	1.00
17:N:70:GLU:C	17:N:72:LYS:H	1.65	1.00
20:2:1220:CLA:C6	3:3:140:LYS:NZ	2.24	1.00
10:F:22:LEU:O	10:F:25:LEU:HB2	1.58	1.00
17:N:45:ASN:ND2	17:N:53:ALA:O	1.93	1.00
6:B:521:HIS:HE1	20:B:1768:CLA:NA	1.60	1.00
20:K:1085:CLA:HMB2	20:K:1142:CLA:HED2	1.40	1.00
17:N:42:PHE:CD1	17:N:43:PRO:N	2.30	1.00
7:C:39:ILE:HG12	7:C:40:ALA:H	1.26	1.00
9:E:39:LEU:H	9:E:40:ARG:NH1	1.58	1.00
10:F:23:LYS:C	10:F:24:LYS:CE	2.30	1.00
11:G:43:HIS:HA	11:G:44:PHE:CB	1.91	1.00
17:N:54:LYS:CG	17:N:57:LYS:HZ3	1.74	1.00
9:E:83:ALA:O	9:E:86:GLU:HG2	1.61	0.99
20:J:1043:CLA:CHA	20:J:1043:CLA:CED	2.39	0.99
3:3:74:ALA:HB3	3:3:75:PRO:HD3	1.45	0.99
20:A:1782:CLA:O1D	20:A:1782:CLA:HBA1	1.62	0.99
21:R:1057:LMU:H11	21:R:1057:LMU:C6	1.90	0.99
20:A:1801:CLA:CMA	16:L:27:VAL:HA	1.90	0.99
22:A:1807:BCR:H313	20:A:1813:CLA:H142	1.43	0.99
6:B:269:TRP:HB2	6:B:497:TRP:HH2	1.22	0.99
20:2:1224:CLA:H152	20:2:1224:CLA:H192	1.43	0.99
10:F:102:ARG:CG	10:F:106:ILE:HD11	1.92	0.99
17:N:18:ASP:CB	17:N:22:LEU:HG	1.92	0.99
5:A:328:LYS:HE3	5:A:332:GLU:CG	1.90	0.99
20:A:1781:CLA:HBC2	20:A:1781:CLA:CHD	1.92	0.99
11:G:48:ASP:HB3	11:G:49:THR:HG22	1.45	0.99
16:L:37:LEU:O	16:L:42:ALA:HB3	1.62	0.99
17:N:47:THR:OG1	17:N:54:LYS:HD3	1.61	0.99
21:A:7021:LMU:C6'	21:A:7021:LMU:H41	1.91	0.99
17:N:62:SER:CB	17:N:66:ASP:CG	2.29	0.99
3:3:205:GLY:N	5:A:252:ARG:NH2	1.99	0.99
6:B:361:ILE:HG23	6:B:368:GLN:OE1	1.63	0.99
16:L:82:ALA:CB	16:L:86:LEU:HD13	1.93	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:52:UNK:CA	18:R:53:UNK:CB	2.36	0.99
5:A:22:VAL:CG1	5:A:23:ASP:H	1.75	0.99
5:A:370:ILE:HG23	5:A:403:GLY:HA3	1.44	0.99
5:A:412:ALA:HB2	5:A:598:VAL:HG11	1.45	0.99
21:A:7037:LMU:O2B	21:A:7037:LMU:H5B	1.63	0.99
17:N:66:ASP:C	17:N:67:LEU:CD1	2.30	0.99
20:2:1220:CLA:HBD	20:2:1220:CLA:CBA	1.92	0.99
21:A:7021:LMU:H31	21:A:7021:LMU:H1'	0.99	0.99
11:G:42:SER:CB	11:G:45:GLU:CD	2.30	0.99
20:2:1215:CLA:O1A	20:2:1220:CLA:HBC2	1.61	0.99
5:A:453:LEU:HD21	20:A:1793:CLA:HBB2	1.41	0.99
5:A:672:LEU:O	5:A:674:ALA:N	1.95	0.99
20:A:1763:CLA:C2B	22:A:1808:BCR:H331	1.92	0.99
22:A:1807:BCR:H311	22:A:1807:BCR:C8	1.85	0.99
20:B:1786:CLA:H93	20:B:1787:CLA:C9	1.93	0.99
11:G:45:GLU:CA	11:G:49:THR:HG21	1.91	0.99
17:N:32:ALA:HB1	17:N:35:VAL:HG22	1.45	0.99
8:D:44:GLU:HB2	8:D:46:TYR:HE2	1.26	0.98
11:G:42:SER:HB2	11:G:45:GLU:OE1	1.63	0.98
17:N:72:LYS:HB3	17:N:74:LYS:N	1.78	0.98
4:4:193:ILE:HG21	14:J:42:PHE:HD1	1.25	0.98
20:A:1770:CLA:CHC	22:A:1803:BCR:H19C	1.92	0.98
21:A:7021:LMU:H22	21:A:7021:LMU:C6	1.93	0.98
20:B:1787:CLA:H43	20:B:1787:CLA:HHB	1.45	0.98
17:N:63:ASP:CA	17:N:64:ASP:C	2.29	0.98
20:1:1200:CLA:HMC1	20:1:1200:CLA:HBC2	1.00	0.98
20:B:1768:CLA:H93	20:B:1768:CLA:HBB2	0.99	0.98
10:F:5:LEU:HG	10:F:6:THR:H	0.84	0.98
5:A:355:HIS:CE1	5:A:416:ILE:HG21	1.98	0.98
5:A:451:ILE:CD1	20:A:1788:CLA:CED	2.40	0.98
21:A:7009:LMU:H3'	21:A:7009:LMU:O5B	1.61	0.98
20:B:1737:CLA:O1A	20:B:1737:CLA:H2	1.19	0.98
4:4:169:GLN:NE2	20:4:1199:CLA:HHD	1.77	0.98
5:A:281:LEU:CG	20:A:1772:CLA:CED	2.40	0.98
21:A:7042:LMU:H3'	21:A:7042:LMU:H2B	1.44	0.98
20:B:1746:CLA:HHD	20:B:1746:CLA:HBC2	1.44	0.98
17:N:18:ASP:HB2	17:N:22:LEU:HG	1.42	0.98
19:T:1:GLC:C2	19:T:2:FRU:H11	1.92	0.98
5:A:170:GLY:O	5:A:173:VAL:HG22	1.63	0.98
5:A:204:ASN:O	5:A:205:HIS:HB2	1.63	0.98
5:A:302:HIS:O	5:A:306:ILE:HG12	1.64	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1815:CLA:HMC1	20:A:1815:CLA:HBC3	1.43	0.98
20:B:1758:CLA:H142	22:B:1776:BCR:H10C	1.42	0.98
10:F:22:LEU:H	10:F:22:LEU:HD12	0.83	0.98
11:G:44:PHE:HD2	11:G:44:PHE:O	1.46	0.98
11:G:48:ASP:HB2	11:G:49:THR:CG2	1.91	0.98
22:I:1032:BCR:C31	22:I:1032:BCR:C8	2.29	0.98
15:K:64:GLY:O	15:K:68:HIS:ND1	1.96	0.98
3:3:74:ALA:CA	20:3:1215:CLA:C3D	2.41	0.98
5:A:210:LEU:CD1	20:A:1769:CLA:HMB2	1.94	0.98
9:E:68:ARG:HE	9:E:68:ARG:C	1.66	0.98
11:G:46:ALA:H	11:G:49:THR:CG2	1.75	0.98
17:N:62:SER:HB3	17:N:66:ASP:HB3	1.41	0.98
2:2:103:GLY:N	20:2:1222:CLA:HBB2	1.79	0.98
5:A:114:THR:OG1	5:A:525:ASN:HB2	1.63	0.98
5:A:281:LEU:CD1	20:A:1772:CLA:O2D	2.11	0.98
20:B:1737:CLA:O1A	20:B:1737:CLA:C2	2.11	0.98
20:J:1045:CLA:CHD	20:J:1045:CLA:HBC2	1.92	0.98
17:N:51:ASP:C	17:N:52:LEU:CD2	2.32	0.98
3:3:173:GLU:HG2	3:3:174:LYS:H	1.29	0.98
4:4:107:GLN:C	20:4:1196:CLA:HMA2	1.82	0.98
20:A:1794:CLA:HMC1	20:A:1794:CLA:HBC3	1.43	0.98
20:A:1796:CLA:C14	22:A:1807:BCR:HC22	1.93	0.98
11:G:43:HIS:HA	11:G:44:PHE:HB3	0.99	0.98
22:A:1803:BCR:HC8	22:A:1803:BCR:C31	1.91	0.97
22:A:1804:BCR:C40	22:A:1804:BCR:C23	2.36	0.97
6:B:608:GLN:HA	6:B:608:GLN:NE2	1.79	0.97
10:F:5:LEU:CG	10:F:6:THR:H	1.74	0.97
5:A:365:LEU:CD2	20:A:1761:CLA:HED3	1.94	0.97
21:A:7023:LMU:H2B	21:A:7023:LMU:H6'2	0.98	0.97
20:J:1043:CLA:C1A	20:J:1043:CLA:CED	2.42	0.97
16:L:160:VAL:O	16:L:160:VAL:HG22	1.64	0.97
20:4:1201:CLA:HAA2	20:4:1201:CLA:O1D	1.63	0.97
5:A:197:GLN:HA	5:A:197:GLN:NE2	1.72	0.97
6:B:11:GLY:HA3	7:C:71:HIS:HD2	1.26	0.97
6:B:269:TRP:HB2	6:B:497:TRP:CH2	2.00	0.97
17:N:61:LEU:CD1	17:N:63:ASP:CA	2.42	0.97
5:A:98:PHE:CZ	20:A:1763:CLA:HMD3	1.99	0.97
6:B:588:GLY:O	6:B:592:PHE:HB2	1.62	0.97
6:B:247:THR:HA	6:B:250:ALA:CB	1.94	0.97
22:B:1780:BCR:C19	20:B:1786:CLA:H151	1.94	0.97
17:N:63:ASP:HA	17:N:64:ASP:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:65:LEU:C	17:N:65:LEU:CD2	2.30	0.97
21:A:7037:LMU:H51	21:A:7037:LMU:H12	1.45	0.97
20:B:1768:CLA:C15	22:B:1779:BCR:H313	1.90	0.97
10:F:61:LEU:HD23	10:F:69:PRO:HB2	1.45	0.97
11:G:94:ASP:N	11:G:95:PRO:HD3	1.79	0.97
20:J:1043:CLA:HBC3	20:J:1043:CLA:HHD	1.43	0.97
17:N:45:ASN:ND2	17:N:57:LYS:HZ1	1.61	0.97
5:A:246:HIS:O	5:A:248:PHE:HD2	1.46	0.97
6:B:295:PHE:H	6:B:295:PHE:HD2	1.06	0.97
20:3:3008:CLA:O1A	20:3:3008:CLA:HED3	1.65	0.97
5:A:79:PHE:CZ	5:A:185:HIS:NE2	2.31	0.97
5:A:368:LEU:HD21	20:A:1774:CLA:H92	1.47	0.97
20:A:1800:CLA:HMD3	22:B:1780:BCR:HC31	1.43	0.97
21:A:7023:LMU:H82	21:A:7023:LMU:C4	1.74	0.97
20:A:1771:CLA:HBB1	22:A:1803:BCR:H352	0.99	0.97
20:A:1781:CLA:CED	20:A:1782:CLA:C3D	2.43	0.97
20:A:1796:CLA:H141	22:A:1807:BCR:HC22	0.98	0.97
21:A:7032:LMU:C2B	21:A:7032:LMU:C3	2.42	0.97
6:B:461:GLN:O	6:B:464:GLN:HG2	1.65	0.97
22:B:1777:BCR:H23C	22:B:1777:BCR:C38	1.92	0.97
17:N:70:GLU:O	17:N:72:LYS:CD	2.12	0.97
4:4:160:MET:CE	20:4:1201:CLA:HBB1	1.80	0.97
20:A:1759:CLA:H42	20:A:1796:CLA:C6	1.93	0.97
20:A:1796:CLA:H141	22:A:1807:BCR:HC21	1.45	0.97
6:B:292:ARG:NE	6:B:292:ARG:HA	1.80	0.97
22:A:1808:BCR:H23C	22:A:1808:BCR:C39	1.91	0.96
20:A:1812:CLA:H11	6:B:616:LEU:HG	1.47	0.96
6:B:586:THR:O	6:B:588:GLY:N	1.98	0.96
13:I:11:LEU:HD12	22:I:1032:BCR:C10	1.94	0.96
20:K:1146:CLA:HMA2	20:K:1146:CLA:O1A	1.64	0.96
16:L:82:ALA:HB2	16:L:86:LEU:CD1	1.94	0.96
16:L:163:LEU:HD22	16:L:164:PRO:HD2	1.00	0.96
20:1:1187:CLA:HMA2	20:1:1187:CLA:HBA1	1.46	0.96
6:B:22:TRP:HE1	20:B:1770:CLA:HBB1	0.80	0.96
6:B:530:THR:HG21	20:B:1755:CLA:HAC1	1.42	0.96
24:B:1783:LMG:O3	7:C:70:TRP:CZ2	2.16	0.96
13:I:26:LEU:HA	13:I:29:GLU:O	1.64	0.96
20:A:1797:CLA:C12	20:A:1797:CLA:H72	1.94	0.96
6:B:122:GLN:O	6:B:126:THR:OG1	1.83	0.96
17:N:72:LYS:HB3	17:N:73:ASP:HA	0.97	0.96
5:A:40:PHE:HE1	5:A:53:TRP:CD1	1.83	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:1784:SF4:S2	25:B:1784:SF4:S3	2.63	0.96
11:G:44:PHE:N	11:G:45:GLU:CB	2.29	0.96
17:N:61:LEU:CD1	17:N:62:SER:C	2.34	0.96
20:1:1187:CLA:CMC	20:1:1187:CLA:CBC	2.30	0.96
5:A:114:THR:HG22	5:A:115:HIS:CE1	1.98	0.96
5:A:345:GLY:O	5:A:347:TYR:N	1.96	0.96
5:A:361:ASN:HD21	20:A:1761:CLA:CED	1.76	0.96
17:N:79:SER:HA	17:N:80:ASN:C	1.84	0.96
1:1:37:GLU:HA	1:1:40:LYS:HB2	1.45	0.96
2:2:120:ASN:HB3	14:J:5:LYS:HD2	1.45	0.96
5:A:368:LEU:HD21	20:A:1774:CLA:H93	1.44	0.96
5:A:451:ILE:CD1	20:A:1788:CLA:HED3	1.95	0.96
5:A:545:HIS:HB3	20:A:1792:CLA:HBB1	1.46	0.96
6:B:732:LYS:CG	6:B:734:GLY:CA	2.43	0.96
20:B:1735:CLA:H191	10:F:104:TYR:HB3	1.43	0.96
22:B:1780:BCR:H19C	20:B:1786:CLA:H112	1.44	0.96
11:G:28:ARG:HG2	11:G:29:GLU:N	1.80	0.96
12:H:44:ALA:HB2	16:L:145:PHE:CD1	1.99	0.96
17:N:67:LEU:HD12	17:N:67:LEU:N	1.79	0.96
5:A:79:PHE:HE2	5:A:185:HIS:CD2	1.81	0.96
20:A:1783:CLA:C20	22:A:1808:BCR:C17	2.35	0.96
6:B:87:ILE:CA	6:B:115:ASN:HA	1.94	0.96
10:F:24:LYS:N	10:F:24:LYS:CE	2.27	0.96
3:3:84:ILE:H	20:A:1798:CLA:C3	1.78	0.96
21:A:7016:LMU:C2	21:A:7016:LMU:H61	1.92	0.96
7:C:62:PHE:HE2	9:E:42:GLU:OE1	1.49	0.96
12:H:20:GLN:CB	12:H:22:ASP:CB	2.34	0.96
5:A:714:LEU:HD13	22:B:1779:BCR:C39	1.96	0.96
17:N:57:LYS:N	17:N:60:PHE:O	1.88	0.96
2:2:127:ASN:ND2	14:J:2:ARG:NH1	2.14	0.96
3:3:83:LEU:CA	20:A:1798:CLA:H43	1.96	0.96
20:4:1209:CLA:HBC3	20:4:1209:CLA:HHD	1.46	0.96
5:A:368:LEU:CD2	20:A:1774:CLA:H92	1.93	0.96
20:B:1768:CLA:C16	22:B:1779:BCR:C31	2.41	0.96
11:G:94:ASP:N	11:G:95:PRO:CD	2.29	0.96
5:A:331:LEU:HD21	5:A:343:HIS:C	1.85	0.95
20:A:1816:CLA:HBC3	20:A:1816:CLA:CHD	1.92	0.95
21:A:7027:LMU:O2'	21:A:7027:LMU:H12	1.64	0.95
5:A:335:LYS:HG2	5:A:336:GLY:N	1.82	0.95
6:B:421:HIS:NE2	20:B:1761:CLA:ND	2.13	0.95
9:E:68:ARG:HH21	9:E:69:PHE:HA	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:62:SER:HB3	17:N:66:ASP:CA	1.96	0.95
20:1:1200:CLA:HBC2	20:1:1200:CLA:CMC	1.91	0.95
5:A:328:LYS:HE3	5:A:332:GLU:HG3	0.98	0.95
5:A:382:TYR:OH	20:A:1784:CLA:H42	1.64	0.95
5:A:547:PHE:O	5:A:551:VAL:HG13	1.64	0.95
20:A:1764:CLA:CHC	20:A:1765:CLA:HMD2	1.96	0.95
20:A:1797:CLA:H12	20:A:1797:CLA:CMA	1.94	0.95
6:B:608:GLN:HE21	6:B:608:GLN:CA	1.80	0.95
17:N:56:LYS:O	17:N:60:PHE:HD1	1.49	0.95
20:2:1220:CLA:C6	3:3:140:LYS:CE	2.44	0.95
5:A:246:HIS:O	5:A:248:PHE:N	1.99	0.95
7:C:63:LEU:HG	7:C:64:SER:N	1.78	0.95
5:A:87:SER:HB2	5:A:178:MET:O	1.65	0.95
5:A:328:LYS:HE2	5:A:332:GLU:CG	1.94	0.95
5:A:394:SER:HB2	20:A:1783:CLA:HMA1	1.44	0.95
5:A:472:ARG:NH1	16:L:74:LEU:HG	1.81	0.95
20:A:1783:CLA:HBA1	20:A:1783:CLA:H43	1.48	0.95
21:A:7009:LMU:H5B	21:A:7009:LMU:C3'	1.96	0.95
20:B:1743:CLA:H151	20:B:1758:CLA:HMD2	1.47	0.95
9:E:52:VAL:O	9:E:53:VAL:HG22	1.64	0.95
20:F:1157:CLA:OBD	20:F:1157:CLA:HED2	1.66	0.95
1:1:89:VAL:HB	1:1:90:PRO:HD3	1.46	0.95
20:B:1786:CLA:HBB2	20:B:1787:CLA:C1B	1.97	0.95
11:G:13:GLY:HA2	11:G:16:LEU:HG	1.47	0.95
5:A:23:ASP:CG	5:A:24:ARG:CD	2.35	0.95
5:A:51:THR:HG21	20:A:1795:CLA:HBB2	1.11	0.95
5:A:545:HIS:CG	20:A:1792:CLA:CBB	2.49	0.95
20:A:1781:CLA:HED3	20:A:1782:CLA:HMD1	1.45	0.95
6:B:167:TRP:HB2	11:G:41:MET:HE2	1.47	0.95
7:C:52:LYS:O	7:C:52:LYS:HG3	1.66	0.95
16:L:161:LEU:C	16:L:161:LEU:CD1	2.30	0.95
3:3:110:SER:C	3:3:111:TYR:CD2	2.40	0.95
5:A:21:LEU:N	5:A:22:VAL:CB	2.30	0.95
5:A:442:ILE:HG23	20:A:1786:CLA:HMC3	1.47	0.95
5:A:599:PHE:CE2	5:A:731:ARG:HB3	2.02	0.95
6:B:648:TRP:CZ3	22:B:1780:BCR:H392	2.01	0.95
7:C:1:MET:HG2	7:C:4:SER:CB	1.96	0.95
7:C:1:MET:HB3	7:C:4:SER:HG	1.29	0.95
11:G:46:ALA:H	11:G:48:ASP:HB3	1.16	0.95
11:G:60:SER:HA	11:G:63:PRO:HD2	1.49	0.95
20:1:1198:CLA:H71	20:1:1198:CLA:C4	1.93	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:87:GLU:CB	22:3:1220:BCR:H382	1.95	0.95
20:A:1759:CLA:C4	20:A:1796:CLA:H61	1.96	0.95
21:A:7032:LMU:C3	21:A:7032:LMU:H2B	1.96	0.95
9:E:56:ASP:HB2	9:E:64:PRO:HB3	1.46	0.95
20:J:1043:CLA:H143	20:J:1043:CLA:O1A	1.67	0.95
4:4:95:PHE:CZ	20:4:1208:CLA:C3C	2.50	0.95
5:A:23:ASP:OD1	5:A:33:GLN:OE1	1.83	0.95
5:A:567:ARG:HH11	8:D:35:GLY:HA2	1.31	0.95
20:B:1771:CLA:HBC2	20:B:1771:CLA:HMC1	1.47	0.95
10:F:23:LYS:CB	10:F:24:LYS:NZ	2.30	0.95
18:R:40:UNK:N	18:R:41:UNK:CB	2.30	0.95
1:1:161:PHE:H	20:1:1189:CLA:CBB	1.79	0.94
20:4:1198:CLA:H203	20:4:1198:CLA:C15	1.95	0.94
21:A:7026:LMU:O4'	19:Z:2:FRU:C3	1.98	0.94
21:A:7042:LMU:H32	21:A:7042:LMU:H6D	0.96	0.94
18:R:34:UNK:N	18:R:36:UNK:CB	2.30	0.94
21:R:1056:LMU:O6'	21:R:1056:LMU:H1'	1.65	0.94
20:2:1220:CLA:H42	3:3:140:LYS:CG	1.92	0.94
4:4:52:MET:HG3	4:4:160:MET:HG3	1.47	0.94
5:A:21:LEU:N	5:A:22:VAL:CG2	2.30	0.94
11:G:47:GLY:N	11:G:48:ASP:CB	2.30	0.94
17:N:54:LYS:CG	17:N:57:LYS:NZ	2.30	0.94
20:A:1781:CLA:CHC	22:A:1806:BCR:H373	1.97	0.94
6:B:266:GLN:O	6:B:267:SER:HB3	1.66	0.94
20:B:1755:CLA:CBB	20:B:1769:CLA:HMB3	1.96	0.94
7:C:73:THR:OG1	7:C:76:SER:HB3	1.67	0.94
22:I:1032:BCR:C3	20:I:1033:CLA:HAC1	1.98	0.94
5:A:340:GLY:O	5:A:343:HIS:HB2	1.68	0.94
6:B:422:LEU:HD13	6:B:535:VAL:HG11	1.46	0.94
10:F:100:VAL:HA	10:F:103:SER:OG	1.66	0.94
17:N:52:LEU:N	17:N:52:LEU:CD2	2.30	0.94
17:N:61:LEU:CD1	17:N:62:SER:N	2.29	0.94
3:3:74:ALA:CA	20:3:1215:CLA:C2D	2.45	0.94
5:A:22:VAL:CG1	5:A:23:ASP:N	2.30	0.94
13:I:12:VAL:O	13:I:17:PRO:HD3	1.65	0.94
20:2:1212:CLA:HMC1	20:2:1212:CLA:HBC3	1.49	0.94
5:A:114:THR:HG22	5:A:115:HIS:ND1	1.82	0.94
5:A:246:HIS:HE1	20:A:1798:CLA:HMA3	1.31	0.94
5:A:316:MET:CG	5:A:317:TYR:HD1	1.70	0.94
13:I:11:LEU:HD12	22:I:1032:BCR:H10C	0.97	0.94
17:N:54:LYS:CB	17:N:57:LYS:NZ	2.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:67:LEU:C	17:N:68:GLU:CG	2.33	0.94
20:2:1220:CLA:H93	3:3:137:SER:HB2	1.45	0.94
20:4:1201:CLA:HMA2	20:4:1201:CLA:HBA1	0.95	0.94
11:G:46:ALA:CA	11:G:48:ASP:CG	2.36	0.94
16:L:82:ALA:HB2	16:L:86:LEU:HD13	0.98	0.94
17:N:66:ASP:O	17:N:67:LEU:HG	1.68	0.94
19:Z:1:GLC:O2	19:Z:1:GLC:H5	1.66	0.94
5:A:23:ASP:HB2	5:A:24:ARG:CD	1.93	0.94
5:A:81:ALA:HB2	20:A:1760:CLA:HMA2	1.50	0.94
5:A:381:PRO:HB2	20:A:1774:CLA:HAA2	1.48	0.94
20:A:1816:CLA:HAA1	20:A:1816:CLA:O2D	1.66	0.94
21:A:7021:LMU:H41	21:A:7021:LMU:O6'	1.67	0.94
21:A:7023:LMU:C2	21:A:7023:LMU:C9	2.30	0.94
20:B:1747:CLA:H52	20:B:1756:CLA:HMB1	1.47	0.94
20:B:1751:CLA:HBC2	20:B:1751:CLA:CHD	1.96	0.94
20:B:1755:CLA:HBC2	20:B:1755:CLA:CHD	1.96	0.94
8:D:39:LYS:HD2	8:D:42:VAL:CG1	1.98	0.94
11:G:46:ALA:N	11:G:48:ASP:CB	2.30	0.94
20:3:1219:CLA:HMC1	20:3:1219:CLA:CBC	1.96	0.94
6:B:493:TRP:CH2	20:B:1765:CLA:HMA2	2.02	0.94
17:N:62:SER:CB	17:N:66:ASP:HB3	1.96	0.94
17:N:72:LYS:NZ	17:N:74:LYS:HG2	1.82	0.94
3:3:64:TYR:HB3	20:3:1218:CLA:H41	1.49	0.94
20:A:1764:CLA:H142	22:A:1808:BCR:C14	1.98	0.94
22:I:1032:BCR:C4	22:I:1032:BCR:C32	2.39	0.94
20:J:1044:CLA:H41	20:J:1044:CLA:H72	0.95	0.94
17:N:51:ASP:O	17:N:52:LEU:HD22	1.67	0.94
5:A:328:LYS:HG2	5:A:332:GLU:CB	1.98	0.93
5:A:331:LEU:CD1	5:A:346:LEU:HB3	1.96	0.93
6:B:50:HIS:HD2	20:B:1737:CLA:HAA2	1.31	0.93
6:B:127:ILE:HD13	6:B:198:ALA:HB2	1.51	0.93
20:B:1755:CLA:HED1	20:B:1756:CLA:CMD	1.97	0.93
7:C:1:MET:H1	7:C:4:SER:N	1.66	0.93
20:J:1044:CLA:HED3	20:J:1044:CLA:OBD	1.66	0.93
17:N:63:ASP:H	17:N:64:ASP:HB3	1.32	0.93
17:N:72:LYS:CB	17:N:73:ASP:CA	2.31	0.93
20:A:1816:CLA:HHD	20:A:1816:CLA:HBC2	1.47	0.93
6:B:390:GLY:O	22:B:1777:BCR:HC42	1.69	0.93
6:B:715:VAL:HG23	6:B:719:PHE:CD2	2.03	0.93
6:B:732:LYS:HG2	6:B:734:GLY:H	1.23	0.93
20:K:1085:CLA:NA	20:K:1142:CLA:CMD	2.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:61:LEU:CD1	17:N:63:ASP:N	2.30	0.93
2:2:99:LEU:CD2	20:2:1222:CLA:HMC3	1.99	0.93
5:A:162:LEU:O	5:A:165:TYR:HB3	1.66	0.93
20:B:1743:CLA:H42	22:B:1775:BCR:H10C	1.50	0.93
22:B:1779:BCR:C8	22:B:1779:BCR:C32	2.29	0.93
17:N:47:THR:HG21	17:N:54:LYS:HZ3	0.88	0.93
21:2:7006:LMU:H22	21:2:7006:LMU:O2'	1.69	0.93
22:A:1804:BCR:H402	22:A:1804:BCR:C23	1.96	0.93
6:B:517:PHE:O	6:B:517:PHE:HD2	1.36	0.93
20:3:3011:CLA:H122	20:3:3011:CLA:H172	1.51	0.93
20:4:4014:CLA:HMC1	20:4:4014:CLA:CBC	1.98	0.93
5:A:358:LEU:HD11	5:A:413:HIS:CG	2.03	0.93
20:A:1776:CLA:C9	22:A:1805:BCR:C37	2.12	0.93
20:A:1813:CLA:HMD3	6:B:578:LEU:CD2	1.99	0.93
21:A:7032:LMU:H1B	21:A:7032:LMU:O1'	1.68	0.93
7:C:5:VAL:C	7:C:65:VAL:HG22	1.88	0.93
17:N:72:LYS:CB	17:N:74:LYS:N	2.31	0.93
5:A:23:ASP:CB	5:A:24:ARG:NE	2.30	0.93
20:A:1783:CLA:C7	22:A:1807:BCR:C37	2.47	0.93
21:A:7041:LMU:O2'	21:A:7041:LMU:H5'	1.66	0.93
11:G:68:ILE:O	11:G:72:LEU:HB3	1.68	0.93
6:B:124:TRP:NE1	6:B:129:LEU:HD22	1.84	0.93
6:B:556:SER:C	6:B:558:PRO:HD2	1.88	0.93
15:K:69:ILE:CG2	15:K:70:MET:N	2.29	0.93
1:1:160:GLY:HA3	20:1:1189:CLA:HBB2	1.48	0.93
4:4:160:MET:HE3	20:4:1201:CLA:HBB2	1.51	0.93
22:A:1805:BCR:H23C	22:A:1805:BCR:C38	1.99	0.93
21:A:7016:LMU:H51	21:A:7016:LMU:O6'	1.67	0.93
22:B:1778:BCR:H371	10:F:93:ILE:HG21	1.51	0.93
5:A:73:GLU:O	5:A:76:ARG:N	2.02	0.93
5:A:81:ALA:HB1	20:A:1760:CLA:CMA	1.91	0.93
5:A:239:PRO:HA	5:A:242:ILE:HD11	1.49	0.93
20:A:1770:CLA:HHC	22:A:1803:BCR:C17	1.98	0.93
22:A:1803:BCR:H402	22:A:1803:BCR:C23	1.94	0.93
21:A:7033:LMU:H3'	21:A:7033:LMU:C5B	1.99	0.93
11:G:45:GLU:HG2	11:G:49:THR:CG2	1.87	0.93
2:2:90:ASP:HB3	2:2:94:LEU:HB2	1.49	0.92
5:A:103:PHE:HE1	20:A:1763:CLA:O1D	1.51	0.92
5:A:462:ILE:HD11	20:B:1786:CLA:H51	1.47	0.92
20:3:3008:CLA:HBA2	20:3:3008:CLA:HBD	0.93	0.92
5:A:626:GLY:HA3	5:A:636:HIS:HA	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1781:CLA:H2	20:A:1781:CLA:O1A	1.67	0.92
20:A:1781:CLA:H2	20:A:1782:CLA:HED3	1.52	0.92
22:A:1808:BCR:H393	22:A:1808:BCR:C23	1.94	0.92
11:G:93:TYR:CA	11:G:94:ASP:CB	2.30	0.92
7:C:79:LEU:HD22	7:C:81:TYR:O	1.70	0.92
9:E:61:THR:HG22	9:E:62:ARG:H	1.34	0.92
16:L:118:LEU:HD12	16:L:119:THR:H	1.31	0.92
5:A:331:LEU:HD11	5:A:346:LEU:HB2	1.50	0.92
22:B:1779:BCR:C40	22:B:1779:BCR:H271	1.95	0.92
11:G:7:VAL:CG2	11:G:8:ILE:H	1.83	0.92
15:K:67:GLY:O	15:K:70:MET:HB2	1.69	0.92
19:W:2:FRU:H11	19:W:2:FRU:C6	2.00	0.92
1:1:25:ASP:H	6:B:314:ARG:HH22	1.17	0.92
4:4:107:GLN:CA	20:4:1196:CLA:HMA2	1.99	0.92
4:4:124:TYR:HB2	4:4:143:PHE:CD1	2.05	0.92
5:A:100:GLY:HA3	5:A:153:TRP:CH2	2.05	0.92
5:A:715:LYS:HD2	10:F:153:ASN:OD1	1.70	0.92
19:O:2:FRU:C1	19:O:2:FRU:C6	2.39	0.92
8:D:111:TYR:HD2	8:D:114:PRO:HB3	1.33	0.92
3:3:64:TYR:CB	20:3:1218:CLA:H42	1.91	0.92
10:F:40:LEU:HA	10:F:42:ILE:HG12	1.50	0.92
20:2:1220:CLA:CHA	20:2:1220:CLA:CBA	2.44	0.92
4:4:122:LYS:HG2	4:4:150:LYS:HD2	1.48	0.92
5:A:259:TYR:HB3	5:A:260:PRO:HD2	1.51	0.92
20:A:1788:CLA:H52	22:B:1780:BCR:C34	1.99	0.92
20:A:1788:CLA:C16	22:L:1169:BCR:C36	2.47	0.92
21:A:7009:LMU:C3'	21:A:7009:LMU:C5B	2.47	0.92
22:B:1780:BCR:H23C	22:B:1780:BCR:C38	1.99	0.92
5:A:195:TRP:CZ2	20:A:1766:CLA:HMA1	2.05	0.92
22:A:1807:BCR:H313	20:A:1813:CLA:H143	1.48	0.92
21:A:7016:LMU:H81	21:A:7016:LMU:H21	0.94	0.92
6:B:612:SER:HA	6:B:615:TYR:HE1	1.32	0.92
6:B:697:PRO:O	7:C:79:LEU:CD1	2.17	0.92
7:C:1:MET:CG	7:C:4:SER:OG	2.17	0.92
11:G:46:ALA:N	11:G:49:THR:CG2	2.31	0.92
11:G:47:GLY:H	11:G:48:ASP:CA	1.82	0.92
20:K:1085:CLA:H3A	20:K:1085:CLA:CGA	2.00	0.92
17:N:47:THR:CG2	17:N:54:LYS:HZ3	1.81	0.92
17:N:72:LYS:NZ	17:N:74:LYS:CG	2.32	0.92
4:4:169:GLN:CG	20:4:1199:CLA:HAC2	1.99	0.91
5:A:103:PHE:CE1	20:A:1763:CLA:O1D	2.23	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:478:SER:HB3	5:A:644:GLN:OE1	1.70	0.91
5:A:648:THR:HG23	5:A:651:GLY:H	1.33	0.91
17:N:72:LYS:CG	17:N:74:LYS:HB2	1.99	0.91
20:A:1763:CLA:C3B	22:A:1808:BCR:H333	1.99	0.91
20:A:1779:CLA:C1D	22:A:1805:BCR:H19C	2.00	0.91
20:A:1816:CLA:HAA1	20:A:1816:CLA:O1D	1.71	0.91
7:C:5:VAL:HB	7:C:65:VAL:HA	1.52	0.91
12:H:25:GLY:HA2	12:H:27:ASP:OD2	1.68	0.91
16:L:30:SER:OG	16:L:32:LEU:HB2	1.67	0.91
3:3:93:PHE:H	3:3:95:THR:H	1.10	0.91
4:4:154:ILE:HG13	4:4:155:ALA:H	1.36	0.91
5:A:304:LEU:CD2	20:A:1772:CLA:HBB2	2.00	0.91
20:A:1779:CLA:NC	22:A:1805:BCR:H19C	1.84	0.91
20:A:1783:CLA:H203	22:A:1808:BCR:H17C	0.92	0.91
6:B:492:ILE:H	6:B:492:ILE:HD13	1.36	0.91
23:B:1773:PQN:H191	22:B:1780:BCR:H10C	0.92	0.91
5:A:25:ASP:CG	5:A:26:PRO:HG3	1.89	0.91
21:A:7022:LMU:C2	21:A:7022:LMU:C2'	2.32	0.91
6:B:596:TRP:HH2	6:B:612:SER:O	1.48	0.91
6:B:602:TRP:O	6:B:604:GLY:N	2.02	0.91
11:G:46:ALA:C	11:G:48:ASP:CG	2.29	0.91
11:G:93:TYR:HA	11:G:94:ASP:CG	1.90	0.91
17:N:61:LEU:HD11	17:N:63:ASP:CB	1.98	0.91
21:A:7036:LMU:H31	21:A:7036:LMU:H71	0.93	0.91
6:B:189:ALA:HB2	20:B:1758:CLA:H203	1.49	0.91
2:2:120:ASN:ND2	14:J:5:LYS:CE	2.33	0.91
5:A:281:LEU:CD1	20:A:1772:CLA:CED	0.92	0.91
21:A:7009:LMU:H3'	21:A:7009:LMU:C5B	2.00	0.91
21:A:7020:LMU:H6E	21:A:7020:LMU:H5B	1.29	0.91
20:B:1786:CLA:C9	20:B:1787:CLA:C9	2.48	0.91
10:F:42:ILE:HG13	10:F:43:LYS:N	1.82	0.91
6:B:525:LEU:O	6:B:525:LEU:HD22	1.70	0.91
11:G:45:GLU:CB	11:G:49:THR:HG21	1.99	0.91
11:G:48:ASP:HB2	11:G:49:THR:HG22	0.94	0.91
20:4:1196:CLA:CBC	20:4:1196:CLA:CHD	2.44	0.91
5:A:453:LEU:HB3	5:A:547:PHE:HB2	1.52	0.91
6:B:661:PHE:HB2	20:B:1787:CLA:CMC	2.00	0.91
8:D:124:ASN:HB3	8:D:125:PRO:HD3	1.52	0.91
20:2:1220:CLA:H71	3:3:140:LYS:HZ2	1.33	0.91
5:A:217:SER:HA	22:A:1803:BCR:H351	1.51	0.91
20:A:1811:CLA:HAA1	20:B:1785:CLA:HBB2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:5:ILE:HB	6:B:6:PRO:HD2	1.51	0.91
6:B:353:TYR:CG	6:B:594:TRP:HZ3	1.88	0.91
11:G:40:GLY:O	11:G:41:MET:SD	2.29	0.91
19:T:1:GLC:O2	19:T:2:FRU:H11	1.71	0.91
4:4:169:GLN:CD	20:4:1199:CLA:HHD	1.91	0.91
21:A:7042:LMU:H22	21:A:7042:LMU:H71	0.92	0.91
11:G:42:SER:HB2	11:G:45:GLU:OE2	1.70	0.91
8:D:102:ARG:NH1	8:D:104:PHE:CE1	2.39	0.90
13:I:11:LEU:HG	22:I:1032:BCR:C7	2.00	0.90
16:L:123:ARG:CZ	16:L:123:ARG:HA	2.00	0.90
20:3:1219:CLA:O1A	20:3:1219:CLA:HMA2	1.71	0.90
22:3:1220:BCR:C8	22:3:1220:BCR:H311	1.99	0.90
5:A:248:PHE:HD2	5:A:248:PHE:H	1.11	0.90
5:A:328:LYS:HG3	5:A:332:GLU:HB2	1.50	0.90
20:A:1813:CLA:CMD	6:B:578:LEU:HD23	2.00	0.90
21:A:7021:LMU:H62	21:A:7021:LMU:C2	1.98	0.90
6:B:369:ALA:O	6:B:725:LEU:HD11	1.71	0.90
20:B:1740:CLA:HBB2	20:B:1786:CLA:H13	1.53	0.90
20:H:1079:CLA:HMA2	20:H:1079:CLA:O2A	1.71	0.90
16:L:95:LEU:HD13	22:L:1169:BCR:C31	2.01	0.90
20:L:1168:CLA:HAA1	20:L:1168:CLA:CGD	1.99	0.90
17:N:47:THR:CG2	17:N:54:LYS:NZ	2.32	0.90
18:R:33:UNK:C	18:R:36:UNK:CB	2.50	0.90
2:2:120:ASN:HD22	14:J:5:LYS:HE3	1.35	0.90
7:C:78:GLY:O	7:C:81:TYR:HE1	1.54	0.90
1:1:160:GLY:CA	20:1:1189:CLA:HBB2	2.01	0.90
6:B:120:VAL:HA	6:B:123:TRP:NE1	1.85	0.90
7:C:44:ARG:NH2	8:D:127:ARG:HB3	1.85	0.90
10:F:23:LYS:C	10:F:24:LYS:HZ3	1.74	0.90
20:A:1791:CLA:O1A	20:A:1797:CLA:HBB1	1.72	0.90
6:B:382:ILE:CG2	6:B:383:MET:H	1.85	0.90
16:L:161:LEU:CD1	16:L:162:ASP:O	2.19	0.90
20:R:1054:CLA:CHA	20:R:1054:CLA:CED	2.49	0.90
20:1:1192:CLA:HHD	20:1:1192:CLA:CBC	2.01	0.90
6:B:504:ASN:HD22	6:B:504:ASN:H	1.14	0.90
11:G:46:ALA:H	11:G:49:THR:HG21	1.33	0.90
17:N:54:LYS:CB	17:N:57:LYS:HZ1	1.84	0.90
17:N:63:ASP:HA	17:N:64:ASP:C	1.91	0.90
20:2:1220:CLA:H91	3:3:137:SER:HB2	1.52	0.90
20:A:1780:CLA:HMD2	20:A:1780:CLA:H142	1.51	0.90
6:B:382:ILE:O	6:B:384:THR:N	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:732:LYS:CB	6:B:733:PHE:C	2.39	0.90
20:B:1786:CLA:HBB2	20:B:1787:CLA:CHB	2.00	0.90
8:D:48:ILE:HB	8:D:100:PHE:HB3	1.52	0.90
20:3:1218:CLA:H2A	20:3:1218:CLA:O1D	1.70	0.90
5:A:361:ASN:HD21	20:A:1761:CLA:HED3	1.37	0.90
5:A:472:ARG:HE	5:A:474:GLN:HG3	1.33	0.90
20:A:1781:CLA:C6	20:A:1782:CLA:CED	2.50	0.90
20:A:1781:CLA:C6	20:A:1782:CLA:HED1	2.02	0.90
6:B:5:ILE:HB	6:B:6:PRO:CD	2.01	0.90
6:B:65:LEU:HD22	6:B:124:TRP:CE3	2.06	0.90
20:4:1196:CLA:HBC2	20:4:1196:CLA:CHD	2.01	0.90
6:B:666:SER:HB3	6:B:671:TRP:HE1	1.36	0.90
6:B:672:GLN:HE21	6:B:672:GLN:CA	1.85	0.90
6:B:370:ALA:O	20:B:1757:CLA:HMA1	1.71	0.90
17:N:45:ASN:HB2	17:N:57:LYS:HZ2	1.35	0.90
19:O:1:GLC:H5	19:O:2:FRU:O5	1.72	0.90
2:2:76:THR:HG23	17:N:7:LEU:HB2	1.54	0.89
5:A:452:PHE:HE1	20:A:1793:CLA:HBB1	1.07	0.89
6:B:172:GLU:O	6:B:176:ASN:HB2	1.72	0.89
17:N:40:CYS:O	17:N:40:CYS:SG	2.30	0.89
20:1:1188:CLA:HMC1	20:1:1188:CLA:HBC3	1.54	0.89
5:A:210:LEU:HD13	20:A:1769:CLA:HMB2	1.53	0.89
5:A:368:LEU:HD11	20:A:1782:CLA:H61	1.52	0.89
5:A:452:PHE:HE1	20:A:1793:CLA:CBB	1.84	0.89
5:A:659:ALA:O	5:A:662:SER:OG	1.88	0.89
20:B:1752:CLA:HBC2	20:B:1753:CLA:HBA1	1.54	0.89
20:A:1772:CLA:HMC1	20:A:1772:CLA:HBC3	0.91	0.89
22:A:1807:BCR:H23C	22:A:1807:BCR:H393	1.52	0.89
21:A:7038:LMU:H101	21:A:7038:LMU:C6	2.00	0.89
6:B:11:GLY:HA3	7:C:71:HIS:CD2	2.07	0.89
20:2:1212:CLA:CGA	20:2:1212:CLA:C4	2.50	0.89
5:A:131:ILE:O	5:A:671:SER:HA	1.72	0.89
21:A:7026:LMU:H4O1	19:Z:2:FRU:H3	1.32	0.89
6:B:351:HIS:HB3	20:B:1747:CLA:HED1	1.52	0.89
4:4:158:ARG:HB2	20:4:1202:CLA:C3A	2.02	0.89
20:A:1781:CLA:C7	20:A:1782:CLA:HED1	2.02	0.89
20:B:1755:CLA:HBB1	20:B:1769:CLA:HMB2	1.54	0.89
12:H:44:ALA:CB	16:L:145:PHE:CD1	2.56	0.89
21:A:7040:LMU:O3'	21:A:7040:LMU:H1B	1.65	0.89
20:B:1755:CLA:CBC	20:B:1755:CLA:CHD	2.46	0.89
20:B:1768:CLA:H161	22:B:1779:BCR:C31	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1220:CLA:H41	3:3:140:LYS:CE	2.02	0.89
3:3:84:ILE:N	20:A:1798:CLA:C4	2.34	0.89
20:4:1204:CLA:C10	20:4:1204:CLA:H41	2.02	0.89
5:A:402:ILE:CD1	20:A:1784:CLA:HBB2	2.02	0.89
20:A:1779:CLA:CBB	22:A:1805:BCR:H353	2.02	0.89
20:A:1779:CLA:C1D	22:A:1805:BCR:C19	2.49	0.89
6:B:292:ARG:O	6:B:293:THR:OG1	1.91	0.89
6:B:362:ALA:HB2	6:B:368:GLN:HG2	1.55	0.89
6:B:635:ILE:O	6:B:636:THR:O	1.91	0.89
20:B:1753:CLA:C2	20:B:1753:CLA:H71	2.00	0.89
7:C:62:PHE:CZ	9:E:42:GLU:OE1	2.26	0.89
20:A:1781:CLA:C7	20:A:1782:CLA:HED2	2.01	0.89
21:A:7039:LMU:H4'	21:A:7039:LMU:O6B	1.73	0.89
6:B:174:ARG:HB2	20:B:1743:CLA:CBC	2.02	0.89
8:D:102:ARG:HE	8:D:110:GLN:HB2	1.38	0.89
16:L:64:LEU:HB3	16:L:68:PHE:CE1	2.08	0.89
19:W:1:GLC:H3	19:W:2:FRU:O5	1.72	0.89
20:1:1198:CLA:HBC3	20:1:1198:CLA:HHD	0.91	0.89
20:3:1219:CLA:H142	20:3:1219:CLA:H102	1.50	0.89
5:A:269:PHE:HE1	15:K:14:THR:HG21	1.06	0.89
6:B:393:PHE:HD2	6:B:397:ASP:OD1	1.55	0.89
6:B:442:VAL:HG21	20:B:1763:CLA:HAC2	1.55	0.89
17:N:72:LYS:CG	17:N:74:LYS:N	2.35	0.89
4:4:147:LEU:HD22	4:4:148:GLU:H	1.38	0.89
4:4:154:ILE:HG13	4:4:155:ALA:N	1.88	0.89
20:4:1198:CLA:C2A	20:4:1198:CLA:CGD	2.50	0.89
5:A:24:ARG:N	5:A:24:ARG:CD	2.34	0.89
6:B:282:PHE:CZ	20:B:1746:CLA:C1	2.55	0.89
6:B:574:ASP:HA	6:B:577:TYR:HB3	1.52	0.89
10:F:93:ILE:O	10:F:96:TRP:HD1	1.56	0.89
20:3:1218:CLA:HHD	20:3:1218:CLA:HBC2	1.54	0.88
20:A:1779:CLA:CAB	22:A:1805:BCR:C35	2.48	0.88
20:A:1796:CLA:C14	22:A:1807:BCR:HC21	2.00	0.88
21:A:7030:LMU:C9	21:A:7030:LMU:H52	2.01	0.88
22:B:1777:BCR:H321	22:B:1777:BCR:HC8	1.55	0.88
19:W:1:GLC:O2	19:W:2:FRU:H12	1.71	0.88
20:1:1198:CLA:H52	20:1:1198:CLA:H102	0.92	0.88
21:A:7032:LMU:H3'	21:A:7032:LMU:C5B	2.03	0.88
6:B:91:ILE:HD12	6:B:104:PHE:HE2	1.38	0.88
6:B:621:ARG:O	6:B:625:TRP:HB3	1.72	0.88
20:B:1738:CLA:H2A	20:B:1738:CLA:O1D	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1795:CLA:C1C	20:B:1735:CLA:HBC2	2.03	0.88
21:A:7036:LMU:H82	21:A:7036:LMU:H22	0.90	0.88
6:B:87:ILE:HA	6:B:115:ASN:CA	2.04	0.88
20:B:1746:CLA:HHD	20:B:1746:CLA:CBC	2.02	0.88
25:B:1784:SF4:S1	25:B:1784:SF4:FE3	1.65	0.88
18:R:39:UNK:HA	18:R:42:UNK:CB	2.04	0.88
2:2:81:THR:HG23	2:2:82:ALA:H	1.36	0.88
5:A:470:LEU:CD1	6:B:95:HIS:HB3	2.03	0.88
5:A:578:ARG:HB2	5:A:578:ARG:CZ	2.02	0.88
20:A:1765:CLA:CBB	20:B:1763:CLA:HMD2	2.03	0.88
6:B:137:THR:HA	6:B:140:ILE:HG13	1.54	0.88
6:B:167:TRP:HB2	11:G:41:MET:CE	2.04	0.88
25:B:1784:SF4:S2	25:B:1784:SF4:FE1	1.64	0.88
20:J:1044:CLA:HED2	20:J:1045:CLA:CMA	2.03	0.88
20:J:1044:CLA:HED2	20:J:1045:CLA:HMA3	1.53	0.88
20:2:1218:CLA:HMD2	20:2:1220:CLA:HMD3	1.55	0.88
5:A:355:HIS:ND1	5:A:416:ILE:CG2	2.36	0.88
20:A:1771:CLA:HMC1	20:A:1771:CLA:HBC3	1.55	0.88
24:B:1783:LMG:O3	7:C:70:TRP:CE2	2.24	0.88
20:K:1085:CLA:CMB	20:K:1142:CLA:HED1	1.96	0.88
3:3:205:GLY:CA	5:A:252:ARG:HH22	1.85	0.88
4:4:193:ILE:HG21	14:J:42:PHE:CD1	2.07	0.88
20:B:1735:CLA:H101	20:B:1735:CLA:CBB	2.03	0.88
5:A:309:LEU:HD21	20:A:1776:CLA:CMC	2.03	0.88
5:A:267:THR:O	5:A:269:PHE:CD2	2.26	0.88
6:B:732:LYS:HG2	6:B:734:GLY:CA	2.04	0.88
15:K:74:ILE:HG22	15:K:75:VAL:HG22	1.56	0.88
6:B:50:HIS:CD2	20:B:1737:CLA:HAA2	2.09	0.88
6:B:119:GLY:CA	20:B:1758:CLA:HED1	2.01	0.88
20:B:1739:CLA:HBB2	20:B:1739:CLA:H92	0.90	0.88
7:C:14:CYS:HA	7:C:17:CYS:HG	1.01	0.88
16:L:115:ALA:H	16:L:116:PRO:HD2	1.36	0.88
3:3:112:THR:OG1	3:3:113:LEU:N	2.04	0.87
5:A:246:HIS:CE1	20:A:1798:CLA:HMA3	2.08	0.87
5:A:356:ALA:HB2	5:A:417:PHE:HD2	1.39	0.87
5:A:358:LEU:HD11	5:A:413:HIS:CB	2.03	0.87
5:A:581:CYS:CB	5:A:590:CYS:HA	2.04	0.87
20:A:1781:CLA:C5	20:A:1782:CLA:HED1	2.03	0.87
6:B:275:HIS:O	6:B:279:ALA:N	2.05	0.87
6:B:531:THR:O	6:B:535:VAL:HG12	1.74	0.87
6:B:561:GLY:HA3	7:C:52:LYS:HG2	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:30:ALA:O	16:L:18:PRO:HB2	1.74	0.87
17:N:67:LEU:HB2	17:N:68:GLU:HG2	0.90	0.87
20:2:1220:CLA:C6	3:3:140:LYS:HD3	2.03	0.87
4:4:160:MET:HE1	20:4:1201:CLA:CBB	2.02	0.87
5:A:22:VAL:HG12	5:A:23:ASP:N	1.82	0.87
5:A:151:GLN:NE2	5:A:384:TYR:O	2.06	0.87
5:A:249:ILE:CG1	5:A:250:LEU:H	1.83	0.87
6:B:91:ILE:HG21	20:B:1740:CLA:HMD1	1.57	0.87
16:L:163:LEU:HD13	16:L:164:PRO:CA	2.04	0.87
17:N:48:GLY:HA2	17:N:49:CYS:HG	1.05	0.87
5:A:425:THR:HG1	5:A:428:TYR:HE1	0.93	0.87
21:A:7023:LMU:C3	21:A:7023:LMU:C9	2.50	0.87
9:E:42:GLU:HG2	9:E:43:SER:N	1.90	0.87
10:F:23:LYS:HB2	10:F:24:LYS:NZ	1.88	0.87
16:L:56:VAL:HA	20:L:1167:CLA:HED2	1.55	0.87
5:A:349:ILE:HG23	5:A:352:THR:O	1.72	0.87
20:A:1760:CLA:HBB2	20:A:1762:CLA:C3D	2.04	0.87
21:A:7032:LMU:H31	21:A:7032:LMU:O5B	1.73	0.87
6:B:310:PRO:CG	6:B:311:PRO:HD2	2.04	0.87
8:D:113:HIS:H	8:D:114:PRO:HD2	1.39	0.87
5:A:567:ARG:HH12	8:D:35:GLY:HA2	1.34	0.87
20:A:1761:CLA:H42	22:A:1804:BCR:H313	1.56	0.87
6:B:279:ALA:O	20:B:1746:CLA:HMB3	1.73	0.87
8:D:113:HIS:NE2	8:D:118:VAL:CG1	2.37	0.87
17:N:32:ALA:CB	17:N:35:VAL:HG22	2.05	0.87
20:A:1781:CLA:HMB3	22:A:1806:BCR:C18	2.04	0.87
6:B:427:LEU:HD23	6:B:431:PHE:CZ	2.09	0.87
9:E:68:ARG:NE	9:E:68:ARG:O	2.06	0.87
3:3:84:ILE:CA	20:A:1798:CLA:H51	2.04	0.87
21:A:7043:LMU:H71	21:A:7043:LMU:H111	1.57	0.87
6:B:70:TRP:CD1	6:B:71:GLN:OE1	2.27	0.87
6:B:230:TRP:HB3	20:B:1746:CLA:HED3	1.55	0.87
6:B:661:PHE:HB2	20:B:1787:CLA:HMC3	1.56	0.87
6:B:732:LYS:CG	6:B:733:PHE:CA	2.49	0.87
20:B:1765:CLA:HMB1	22:B:1777:BCR:H292	1.56	0.87
20:2:1220:CLA:C4	3:3:140:LYS:CD	2.42	0.87
20:4:1198:CLA:H202	20:4:1198:CLA:C15	2.00	0.87
5:A:661:ALA:O	5:A:664:VAL:HG22	1.75	0.87
6:B:469:LYS:HG2	6:B:471:THR:OG1	1.75	0.87
5:A:194:ALA:O	5:A:198:ASP:N	2.07	0.87
21:A:7041:LMU:O6'	21:A:7041:LMU:H1B	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:317:ARG:NH1	6:B:405:ASP:O	2.08	0.87
11:G:68:ILE:O	11:G:72:LEU:CB	2.22	0.87
12:H:21:TRP:H	12:H:22:ASP:HA	1.38	0.87
13:I:24:LEU:C	13:I:26:LEU:H	1.77	0.87
17:N:48:GLY:CA	17:N:49:CYS:CB	2.50	0.87
20:A:1792:CLA:O1D	20:A:1792:CLA:HBA2	1.74	0.86
6:B:110:LEU:HD12	6:B:111:GLY:H	1.40	0.86
6:B:203:ARG:HG2	6:B:204:GLY:N	1.88	0.86
6:B:732:LYS:HG2	6:B:733:PHE:CA	2.04	0.86
16:L:95:LEU:HD13	22:L:1169:BCR:H312	1.57	0.86
5:A:393:LEU:HG	5:A:394:SER:H	1.40	0.86
20:A:1795:CLA:CGA	20:A:1795:CLA:H42	2.03	0.86
6:B:474:PHE:CE2	6:B:476:ILE:HG13	2.10	0.86
20:B:1755:CLA:H52	20:B:1769:CLA:CAD	2.05	0.86
20:1:1193:CLA:HMC1	20:1:1193:CLA:HBC3	1.54	0.86
20:1:1198:CLA:CHD	20:1:1198:CLA:CBC	2.45	0.86
20:3:1218:CLA:H91	20:3:1218:CLA:H121	1.54	0.86
4:4:104:ARG:HH11	4:4:105:ARG:HB2	1.38	0.86
5:A:370:ILE:HD11	20:A:1781:CLA:C3D	2.05	0.86
20:A:1790:CLA:OBD	20:A:1791:CLA:HAC1	1.75	0.86
20:B:1753:CLA:C2	20:B:1753:CLA:C7	2.51	0.86
20:B:1755:CLA:CBB	20:B:1769:CLA:HHB	2.05	0.86
23:B:1773:PQN:H162	22:B:1780:BCR:H333	0.88	0.86
20:J:1043:CLA:H2	20:J:1043:CLA:C16	2.05	0.86
4:4:75:TRP:HA	20:4:1204:CLA:HMD3	1.58	0.86
6:B:25:ILE:CG2	22:L:1169:BCR:H291	2.04	0.86
6:B:86:PRO:O	6:B:87:ILE:HG13	1.74	0.86
15:K:69:ILE:HG22	15:K:70:MET:N	1.84	0.86
19:Q:1:GLC:C1	19:Q:2:FRU:C4	2.52	0.86
5:A:356:ALA:HB2	5:A:417:PHE:CD2	2.09	0.86
5:A:411:ALA:HB2	22:A:1806:BCR:H392	1.57	0.86
20:A:1816:CLA:H2	20:A:1816:CLA:HED3	1.58	0.86
10:F:20:GLN:NE2	10:F:20:GLN:C	2.29	0.86
20:J:1044:CLA:H91	20:J:1044:CLA:C16	2.05	0.86
17:N:32:ALA:HB1	17:N:35:VAL:CG2	2.06	0.86
1:1:57:ILE:HG23	1:1:58:LEU:H	1.41	0.86
20:2:1220:CLA:H91	3:3:137:SER:CB	2.06	0.86
20:A:1783:CLA:H171	22:A:1808:BCR:H15C	1.55	0.86
20:A:1788:CLA:C16	22:L:1169:BCR:H361	2.06	0.86
22:A:1806:BCR:HC8	22:A:1806:BCR:C33	2.06	0.86
20:B:1735:CLA:C19	10:F:104:TYR:HB3	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:281:LEU:HD12	20:A:1772:CLA:O2D	1.73	0.86
20:A:1761:CLA:H151	22:A:1803:BCR:H393	1.57	0.86
20:A:1788:CLA:C5	22:B:1780:BCR:H343	2.05	0.86
20:A:1790:CLA:CBC	20:A:1790:CLA:HMC1	2.06	0.86
6:B:693:TRP:HD1	20:B:1770:CLA:C2D	1.89	0.86
10:F:153:ASN:C	10:F:153:ASN:HD22	1.78	0.86
16:L:161:LEU:HD12	16:L:162:ASP:CA	2.04	0.86
3:3:132:TRP:HZ3	3:3:155:GLU:HG2	1.07	0.86
5:A:370:ILE:CG2	5:A:400:MET:HA	2.06	0.86
5:A:599:PHE:CE2	5:A:735:VAL:CG2	2.59	0.86
5:A:723:ARG:CG	5:A:723:ARG:HH11	1.87	0.86
7:C:1:MET:CG	7:C:4:SER:CB	2.54	0.86
7:C:14:CYS:SG	7:C:18:VAL:O	2.32	0.86
17:N:61:LEU:HD11	17:N:63:ASP:O	1.76	0.86
20:2:1212:CLA:HMC1	20:2:1212:CLA:HBC2	1.55	0.86
3:3:63:ARG:HH22	3:3:189:LEU:HD23	1.40	0.86
5:A:606:TYR:O	5:A:610:SER:HB2	1.76	0.86
20:A:1800:CLA:CMD	22:B:1780:BCR:HC31	2.05	0.86
21:A:7042:LMU:C2	21:A:7042:LMU:H61	2.01	0.86
6:B:142:LEU:CD2	22:B:1776:BCR:H333	2.06	0.86
6:B:216:LEU:HD21	6:B:221:GLY:HA2	1.57	0.86
6:B:310:PRO:CG	20:B:1753:CLA:HMA1	2.02	0.86
6:B:527:LEU:HD12	20:B:1755:CLA:C1D	2.05	0.86
10:F:24:LYS:CA	10:F:26:GLN:H	1.89	0.86
2:2:120:ASN:CG	14:J:5:LYS:HD2	1.95	0.86
5:A:581:CYS:SG	25:B:1784:SF4:S2	2.73	0.86
20:A:1763:CLA:CBA	20:A:1765:CLA:H12	2.06	0.86
6:B:551:LYS:NZ	8:D:140:ASN:O	2.09	0.86
7:C:1:MET:N	7:C:3:HIS:C	2.29	0.86
16:L:164:PRO:O	16:L:165:TYR:CD1	2.29	0.86
17:N:58:VAL:HG23	17:N:60:PHE:CE1	2.11	0.86
5:A:21:LEU:HD12	5:A:21:LEU:O	1.75	0.85
5:A:331:LEU:HD23	5:A:331:LEU:C	1.95	0.85
20:A:1815:CLA:H61	20:A:1815:CLA:HMA1	1.56	0.85
6:B:432:HIS:HE1	20:B:1762:CLA:NB	1.74	0.85
20:B:1761:CLA:H12	20:B:1761:CLA:HMA2	1.56	0.85
7:C:74:THR:OG1	7:C:80:ALA:HB2	1.75	0.85
16:L:56:VAL:HA	20:L:1167:CLA:CED	2.04	0.85
17:N:63:ASP:H	17:N:64:ASP:CA	1.89	0.85
2:2:70:LYS:HG3	2:2:73:ILE:HG13	1.56	0.85
20:4:1201:CLA:CGD	20:4:1201:CLA:CAA	2.52	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1807:BCR:C31	22:A:1807:BCR:C8	2.47	0.85
6:B:310:PRO:HG3	20:B:1753:CLA:CMA	2.03	0.85
6:B:374:HIS:HB2	20:B:1757:CLA:C1B	2.06	0.85
20:B:1743:CLA:H141	20:B:1748:CLA:H2	1.59	0.85
10:F:23:LYS:CB	10:F:24:LYS:HZ1	1.89	0.85
12:H:25:GLY:HA3	12:H:27:ASP:CA	2.04	0.85
12:H:45:ALA:O	12:H:48:THR:N	2.08	0.85
12:H:69:SER:CB	20:H:1079:CLA:H61	2.04	0.85
13:I:1:MET:O	13:I:2:ILE:HG22	1.75	0.85
17:N:72:LYS:HG3	17:N:74:LYS:N	1.89	0.85
20:A:1783:CLA:H72	22:A:1807:BCR:H371	1.57	0.85
12:H:21:TRP:H	12:H:22:ASP:CA	1.88	0.85
16:L:66:GLY:HA3	20:L:1168:CLA:HHC	1.57	0.85
16:L:164:PRO:O	16:L:165:TYR:CG	2.30	0.85
17:N:70:GLU:HB3	17:N:72:LYS:N	1.89	0.85
3:3:132:TRP:CH2	3:3:155:GLU:HG3	2.08	0.85
5:A:453:LEU:CD2	20:A:1793:CLA:CBB	2.50	0.85
20:A:1776:CLA:H92	22:A:1805:BCR:H371	1.51	0.85
6:B:142:LEU:HD22	22:B:1776:BCR:H333	1.58	0.85
6:B:594:TRP:O	6:B:595:HIS:CB	2.24	0.85
10:F:20:GLN:CD	10:F:21:ALA:H	1.78	0.85
20:L:1168:CLA:HBC3	20:L:1168:CLA:CHD	2.04	0.85
17:N:5:GLU:OE1	17:N:6:TYR:CD2	2.30	0.85
17:N:5:GLU:OE1	17:N:6:TYR:CG	2.30	0.85
17:N:42:PHE:H	17:N:43:PRO:CD	1.88	0.85
1:1:185:TRP:O	1:1:186:HIS:HB2	1.75	0.85
5:A:197:GLN:HE21	5:A:197:GLN:CA	1.84	0.85
5:A:349:ILE:O	5:A:349:ILE:HG22	1.74	0.85
20:A:1767:CLA:HMC1	20:A:1767:CLA:HBC3	1.58	0.85
20:A:1796:CLA:NC	20:A:1796:CLA:C4	2.40	0.85
6:B:388:ALA:C	6:B:391:PRO:HD2	1.95	0.85
6:B:571:SER:OG	6:B:574:ASP:OD1	1.95	0.85
9:E:39:LEU:N	9:E:40:ARG:NH1	2.24	0.85
17:N:63:ASP:N	17:N:64:ASP:CB	2.38	0.85
20:1:1191:CLA:HMC1	20:1:1194:CLA:CHD	2.03	0.85
9:E:35:LYS:NZ	9:E:89:GLU:OE2	2.09	0.85
12:H:25:GLY:HA3	12:H:27:ASP:HB2	1.56	0.85
17:N:61:LEU:HD21	17:N:63:ASP:O	1.74	0.85
2:2:169:LEU:HD22	20:2:1215:CLA:CBB	2.05	0.85
3:3:98:ILE:C	17:N:63:ASP:O	2.15	0.85
21:A:7020:LMU:H5B	21:A:7020:LMU:O6'	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:374:HIS:HB2	20:B:1757:CLA:NB	1.91	0.85
20:B:1768:CLA:H121	22:B:1779:BCR:H312	1.58	0.85
17:N:4:GLU:HG3	17:N:4:GLU:O	1.74	0.85
3:3:80:LYS:HD3	3:3:105:ASN:HB2	1.59	0.85
5:A:62:HIS:HB2	20:A:1785:CLA:HBA1	1.58	0.85
20:A:1781:CLA:H52	20:A:1782:CLA:HED1	1.57	0.85
20:A:1816:CLA:HED1	20:A:1816:CLA:CGA	2.00	0.85
21:A:7023:LMU:O6'	21:A:7023:LMU:H1'	1.75	0.85
6:B:304:ILE:HD11	20:B:1749:CLA:CED	2.07	0.85
6:B:656:VAL:HG22	20:B:1771:CLA:HMB3	1.59	0.85
20:B:1753:CLA:CBC	20:B:1753:CLA:CMC	2.31	0.85
20:B:1757:CLA:O1D	20:B:1758:CLA:HMA1	1.77	0.85
20:4:1199:CLA:HAA1	20:F:1157:CLA:C4	2.05	0.85
20:A:1797:CLA:HBC3	20:A:1797:CLA:CHD	2.05	0.85
7:C:59:PRO:O	25:C:1083:SF4:S3	2.35	0.85
10:F:20:GLN:CD	10:F:21:ALA:N	2.29	0.85
16:L:163:LEU:HD11	16:L:164:PRO:HG2	1.57	0.85
5:A:58:HIS:HE1	20:A:1759:CLA:ND	1.73	0.85
5:A:207:LEU:HA	5:A:211:LEU:HG	1.57	0.85
20:A:1817:CLA:O1D	20:A:1817:CLA:HBA2	1.76	0.85
20:B:1753:CLA:HMD2	20:B:1754:CLA:CBB	2.06	0.85
10:F:96:TRP:HZ3	10:F:134:PHE:HB2	1.42	0.85
5:A:685:VAL:CG2	20:A:1796:CLA:CBB	2.55	0.84
22:B:1774:BCR:H343	11:G:21:PHE:CD1	2.11	0.84
20:1:1197:CLA:HAA2	20:1:1197:CLA:CGD	2.05	0.84
2:2:99:LEU:HD22	20:2:1222:CLA:HMC3	1.58	0.84
3:3:158:TYR:HB3	3:3:159:PRO:CD	2.06	0.84
5:A:370:ILE:CD1	20:A:1781:CLA:CAD	2.54	0.84
20:A:1776:CLA:C3C	20:A:1782:CLA:H172	2.06	0.84
22:A:1803:BCR:H311	22:A:1803:BCR:C8	1.98	0.84
6:B:230:TRP:CH2	11:G:11:SER:HB2	2.12	0.84
9:E:58:ASP:OD2	9:E:60:LYS:HG2	1.76	0.84
16:L:48:ASN:HB3	16:L:49:PRO:HD2	1.56	0.84
4:4:58:MET:SD	4:4:59:LEU:N	2.50	0.84
6:B:464:GLN:CD	6:B:469:LYS:HD3	1.96	0.84
24:B:1783:LMG:HC61	7:C:70:TRP:CH2	2.12	0.84
20:H:1079:CLA:HBB2	13:I:13:GLY:O	1.77	0.84
17:N:45:ASN:ND2	17:N:57:LYS:NZ	2.22	0.84
5:A:208:ALA:HB2	5:A:314:GLY:HA3	1.57	0.84
21:A:7033:LMU:H6'2	21:A:7033:LMU:O2'	1.77	0.84
21:A:7037:LMU:H6E	21:A:7037:LMU:O3'	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:174:ARG:CB	20:B:1743:CLA:HBC2	2.06	0.84
20:A:1763:CLA:HAA2	20:A:1765:CLA:CED	2.07	0.84
6:B:391:PRO:HB3	6:B:538:ALA:HA	1.58	0.84
10:F:24:LYS:C	10:F:26:GLN:N	2.30	0.84
21:K:1086:LMU:H81	21:K:1086:LMU:H42	0.85	0.84
21:1:7004:LMU:H3'	21:1:7004:LMU:C1	2.06	0.84
10:F:23:LYS:C	10:F:24:LYS:NZ	2.29	0.84
12:H:20:GLN:CA	12:H:22:ASP:HB3	2.07	0.84
5:A:581:CYS:HB2	5:A:590:CYS:CA	2.05	0.84
6:B:427:LEU:HD23	6:B:431:PHE:HZ	1.41	0.84
25:B:1784:SF4:S1	25:B:1784:SF4:FE2	1.69	0.84
7:C:63:LEU:HG	7:C:64:SER:H	1.39	0.84
12:H:28:ALA:N	12:H:29:PRO:HD3	1.89	0.84
3:3:88:THR:N	22:3:1220:BCR:H383	1.93	0.84
3:3:199:VAL:HG22	20:3:1214:CLA:C3C	2.07	0.84
20:A:1797:CLA:H72	20:A:1797:CLA:H122	1.59	0.84
11:G:44:PHE:O	11:G:44:PHE:CD2	2.30	0.84
20:J:1044:CLA:C7	20:J:1044:CLA:C4	2.30	0.84
17:N:5:GLU:OE1	17:N:6:TYR:CD1	2.31	0.84
20:2:1220:CLA:CBD	20:2:1220:CLA:CBA	2.55	0.84
21:A:7042:LMU:C2	21:A:7042:LMU:C6	2.30	0.84
20:A:1783:CLA:H71	22:A:1807:BCR:H372	1.58	0.84
21:A:7038:LMU:H101	21:A:7038:LMU:H61	1.59	0.84
20:B:1739:CLA:H141	20:B:1757:CLA:H91	1.60	0.84
16:L:14:LEU:HA	16:L:24:GLU:HG3	1.59	0.84
4:4:106:TRP:CD1	20:4:1196:CLA:CED	2.60	0.83
5:A:53:TRP:HA	5:A:56:ASN:HB2	1.60	0.83
5:A:269:PHE:CD1	15:K:14:THR:HG21	2.12	0.83
6:B:202:SER:HB3	6:B:270:LEU:HD11	1.60	0.83
20:B:1739:CLA:H102	20:B:1739:CLA:H142	1.60	0.83
20:B:1768:CLA:C20	22:B:1779:BCR:HC41	2.07	0.83
10:F:61:LEU:HD23	10:F:69:PRO:CB	2.06	0.83
12:H:65:LEU:HD23	20:H:1079:CLA:H52	1.60	0.83
3:3:74:ALA:N	20:3:1215:CLA:C2D	2.41	0.83
21:A:7037:LMU:C5	21:A:7037:LMU:H11	2.05	0.83
6:B:560:ASP:HB2	7:C:66:ARG:HE	1.39	0.83
25:B:1784:SF4:S2	25:B:1784:SF4:FE4	1.68	0.83
22:L:1169:BCR:H271	22:L:1169:BCR:H403	1.60	0.83
17:N:5:GLU:OE2	17:N:5:GLU:HA	1.75	0.83
17:N:61:LEU:CG	17:N:62:SER:N	2.35	0.83
2:2:181:HIS:CD2	20:2:1214:CLA:C1D	2.62	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:133:ASN:ND2	5:A:142:GLY:HA2	1.92	0.83
5:A:393:LEU:HG	5:A:394:SER:N	1.92	0.83
6:B:516:ASP:O	6:B:520:HIS:HB2	1.78	0.83
22:B:1776:BCR:H331	22:B:1776:BCR:C8	2.06	0.83
20:1:1198:CLA:C10	20:1:1198:CLA:C5	2.41	0.83
3:3:74:ALA:HA	20:3:1215:CLA:C1D	2.09	0.83
3:3:132:TRP:HZ3	3:3:155:GLU:CG	1.60	0.83
5:A:110:LEU:HD11	5:A:239:PRO:HG2	1.58	0.83
5:A:207:LEU:CB	20:A:1776:CLA:HBB2	2.07	0.83
20:A:1800:CLA:C20	16:L:64:LEU:HD21	2.08	0.83
22:A:1807:BCR:C39	22:A:1807:BCR:H23C	2.09	0.83
6:B:294:ASN:HB3	11:G:36:PRO:HD2	1.58	0.83
11:G:26:PHE:HB2	11:G:27:GLN:HE21	1.41	0.83
15:K:69:ILE:HA	15:K:72:VAL:HG12	1.60	0.83
3:3:80:LYS:HD3	3:3:105:ASN:CB	2.07	0.83
20:A:1800:CLA:H201	16:L:64:LEU:HD21	1.61	0.83
21:A:7038:LMU:C6	21:A:7038:LMU:C10	2.49	0.83
20:B:1753:CLA:C1A	20:B:1753:CLA:C4	2.41	0.83
9:E:60:LYS:HG3	9:E:61:THR:H	1.41	0.83
5:A:711:HIS:NE2	20:A:1795:CLA:HAC1	1.94	0.83
6:B:353:TYR:CG	6:B:594:TRP:CZ3	2.66	0.83
6:B:711:VAL:O	6:B:711:VAL:HG12	1.76	0.83
8:D:78:ALA:HB3	8:D:82:GLN:NE2	1.92	0.83
20:3:1218:CLA:HBC2	20:3:1218:CLA:CHD	2.09	0.83
5:A:28:LYS:O	5:A:29:THR:HG22	1.78	0.83
5:A:207:LEU:HD12	5:A:310:PHE:HD1	1.42	0.83
5:A:269:PHE:HE1	15:K:14:THR:CG2	1.88	0.83
5:A:567:ARG:NH1	8:D:35:GLY:CA	2.35	0.83
20:A:1788:CLA:O1A	20:A:1800:CLA:H11	1.78	0.83
21:A:7042:LMU:H32	21:A:7042:LMU:C5'	2.09	0.83
22:I:1032:BCR:HC22	20:I:1033:CLA:C3C	2.03	0.83
16:L:124:LYS:HB2	16:L:124:LYS:NZ	1.93	0.83
20:L:1168:CLA:CBC	20:L:1168:CLA:CHD	2.55	0.83
19:T:1:GLC:H2	19:T:2:FRU:H11	1.61	0.83
20:2:1220:CLA:C7	3:3:140:LYS:NZ	2.41	0.83
5:A:451:ILE:CD1	20:A:1788:CLA:HED1	2.07	0.83
5:A:497:ALA:HB2	5:A:515:TRP:HB2	1.59	0.83
6:B:732:LYS:HG3	6:B:733:PHE:C	1.98	0.83
20:B:1735:CLA:CMD	22:B:1778:BCR:HC41	2.08	0.83
10:F:62:LEU:HG	10:F:72:ILE:HD13	1.59	0.83
12:H:25:GLY:C	12:H:27:ASP:H	1.74	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:397:THR:HB	5:A:613:ILE:CG1	2.09	0.83
5:A:586:ARG:HG3	7:C:49:VAL:HG21	1.61	0.83
21:A:7037:LMU:H51	21:A:7037:LMU:H11	1.57	0.83
20:B:1768:CLA:C15	22:B:1779:BCR:H312	1.94	0.83
17:N:56:LYS:O	17:N:60:PHE:CD1	2.30	0.83
17:N:67:LEU:O	17:N:68:GLU:HG3	1.78	0.83
20:1:1200:CLA:HBC2	20:4:1198:CLA:HMB3	1.60	0.83
3:3:83:LEU:HD12	20:A:1798:CLA:HED2	1.61	0.83
3:3:89:ALA:HB1	3:3:90:LEU:HG	1.61	0.83
5:A:207:LEU:HD21	5:A:314:GLY:HA2	1.61	0.83
6:B:131:THR:HB	6:B:134:ASP:CB	2.06	0.83
7:C:2:SER:O	7:C:69:LEU:HB2	1.79	0.83
8:D:39:LYS:HD2	8:D:42:VAL:HG13	1.59	0.83
16:L:63:LEU:HD22	16:L:64:LEU:H	1.41	0.83
17:N:58:VAL:HB	17:N:59:PRO:HD2	0.83	0.83
17:N:59:PRO:HB3	17:N:75:TYR:HE1	1.43	0.83
17:N:63:ASP:N	17:N:64:ASP:C	2.33	0.83
20:A:1760:CLA:O2D	20:A:1760:CLA:H2A	1.79	0.82
22:B:1778:BCR:C37	10:F:93:ILE:HG21	2.08	0.82
17:N:48:GLY:HA3	17:N:49:CYS:CB	2.08	0.82
18:R:41:UNK:CB	18:R:42:UNK:CB	2.56	0.82
1:1:24:PHE:HB3	6:B:314:ARG:HH21	1.43	0.82
3:3:87:GLU:C	22:3:1220:BCR:H383	1.96	0.82
5:A:668:TYR:OH	6:B:441:ASP:OD1	1.96	0.82
21:A:7020:LMU:H6E	21:A:7020:LMU:O6B	1.78	0.82
20:B:1744:CLA:HMB2	22:B:1776:BCR:C8	2.09	0.82
20:B:1755:CLA:HMB3	22:B:1777:BCR:C35	2.10	0.82
11:G:16:LEU:HD23	11:G:68:ILE:CG2	2.09	0.82
3:3:157:ALA:C	3:3:158:TYR:HD2	1.83	0.82
5:A:373:ALA:HB1	5:A:396:PHE:HD1	1.44	0.82
6:B:664:LEU:C	6:B:667:TRP:HZ3	1.81	0.82
20:B:1771:CLA:H102	13:I:21:MET:SD	2.19	0.82
22:B:1780:BCR:H19C	20:B:1786:CLA:C11	2.09	0.82
25:B:1784:SF4:S1	25:B:1784:SF4:FE4	1.69	0.82
20:B:1787:CLA:H3A	20:B:1787:CLA:O2A	1.79	0.82
22:I:1032:BCR:HC21	20:I:1033:CLA:C3C	2.08	0.82
14:J:9:SER:O	14:J:10:VAL:HB	1.79	0.82
21:R:1056:LMU:O5B	21:R:1056:LMU:H6D	1.80	0.82
5:A:100:GLY:HA3	5:A:153:TRP:HH2	1.42	0.82
20:A:1817:CLA:HBC2	20:A:1817:CLA:CMC	2.09	0.82
21:A:7041:LMU:H1B	21:A:7041:LMU:O6B	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1768:CLA:H121	22:B:1779:BCR:C31	2.09	0.82
10:F:130:LEU:HG	10:F:131:PHE:N	1.94	0.82
11:G:47:GLY:N	11:G:48:ASP:CA	2.41	0.82
20:1:1190:CLA:HBC3	20:1:1190:CLA:HMC1	1.61	0.82
2:2:120:ASN:CA	14:J:5:LYS:HD2	2.10	0.82
21:2:7006:LMU:H5'	21:2:7006:LMU:O5B	1.74	0.82
5:A:349:ILE:O	5:A:349:ILE:CG2	2.27	0.82
15:K:6:SER:O	15:K:10:ILE:HD13	1.80	0.82
20:R:1055:CLA:HBA2	20:R:1055:CLA:CBD	2.08	0.82
5:A:693:LEU:HD21	5:A:735:VAL:H	1.44	0.82
5:A:711:HIS:NE2	20:A:1795:CLA:CAC	2.43	0.82
21:A:7016:LMU:H32	21:A:7016:LMU:H91	1.60	0.82
5:A:90:PHE:CE1	20:A:1761:CLA:H91	2.15	0.82
5:A:239:PRO:HA	5:A:242:ILE:HD13	1.62	0.82
20:A:1812:CLA:C3B	6:B:589:TRP:HH2	1.93	0.82
6:B:53:GLN:C	6:B:55:ALA:H	1.83	0.82
1:1:97:ILE:HG22	20:1:1197:CLA:HBB2	1.59	0.82
20:1:1187:CLA:HMA2	20:1:1187:CLA:CBA	2.08	0.82
2:2:102:ILE:C	20:2:1222:CLA:HBB2	1.97	0.82
5:A:141:ARG:HG3	5:A:141:ARG:HH21	1.42	0.82
5:A:286:GLY:C	5:A:287:LEU:HD22	2.00	0.82
22:A:1807:BCR:H312	20:A:1813:CLA:H143	1.61	0.82
6:B:414:HIS:CD2	20:B:1760:CLA:HMA3	2.15	0.82
23:B:1773:PQN:H161	22:B:1780:BCR:H331	1.61	0.82
7:C:7:ILE:HG22	7:C:65:VAL:CG2	2.09	0.82
7:C:74:THR:C	7:C:76:SER:N	2.30	0.82
5:A:368:LEU:CD1	20:A:1782:CLA:H61	2.09	0.82
5:A:393:LEU:CD1	5:A:750:PHE:CE1	2.62	0.82
20:A:1770:CLA:HMC2	22:A:1803:BCR:C16	2.10	0.82
21:A:7026:LMU:H41	21:A:7026:LMU:H81	1.62	0.82
10:F:81:GLY:O	14:J:38:THR:HG23	1.79	0.82
16:L:88:ALA:C	16:L:90:GLY:N	2.31	0.82
16:L:163:LEU:CD1	16:L:164:PRO:HD2	2.00	0.82
20:2:1223:CLA:HMC1	20:2:1223:CLA:HBC3	1.62	0.82
5:A:555:ILE:HG21	20:B:1787:CLA:HMD1	1.62	0.82
20:A:1770:CLA:C3B	22:A:1803:BCR:C19	2.54	0.82
21:A:7022:LMU:H2'	21:A:7022:LMU:H21	0.83	0.82
6:B:323:TYR:CE1	20:B:1754:CLA:HBC1	2.15	0.82
20:B:1742:CLA:HAC2	20:B:1743:CLA:HBB2	0.86	0.82
9:E:45:TRP:HH2	9:E:78:SER:OG	1.63	0.82
17:N:61:LEU:C	17:N:61:LEU:CD1	2.37	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1220:CLA:C9	3:3:137:SER:CB	2.58	0.81
4:4:154:ILE:HD12	20:4:1202:CLA:CHA	2.10	0.81
5:A:470:LEU:HD11	6:B:95:HIS:HB3	1.61	0.81
17:N:45:ASN:HD22	17:N:57:LYS:HZ1	1.17	0.81
20:A:1787:CLA:H52	20:A:1801:CLA:HHB	1.61	0.81
21:A:7017:LMU:O3'	21:A:7017:LMU:H1B	1.78	0.81
20:B:1753:CLA:HAA1	20:B:1753:CLA:H12	1.60	0.81
17:N:72:LYS:HZ3	17:N:74:LYS:HG2	1.43	0.81
20:4:1199:CLA:CAA	20:F:1157:CLA:H42	2.09	0.81
5:A:187:HIS:CD2	20:A:1767:CLA:NC	2.29	0.81
5:A:621:GLN:HG2	5:A:637:ILE:HD12	1.60	0.81
20:A:1781:CLA:CHC	22:A:1806:BCR:C37	2.57	0.81
6:B:464:GLN:OE1	6:B:469:LYS:HD3	1.79	0.81
20:B:1751:CLA:HHD	20:B:1751:CLA:CBC	2.00	0.81
12:H:53:LEU:HG	12:H:54:LEU:H	1.44	0.81
16:L:122:GLY:C	16:L:124:LYS:N	2.31	0.81
19:W:1:GLC:C3	19:W:2:FRU:O5	2.28	0.81
19:Z:2:FRU:H12	19:Z:2:FRU:O6	1.80	0.81
2:2:189:ILE:HD13	2:2:189:ILE:H	1.45	0.81
5:A:373:ALA:HB1	5:A:396:PHE:CD1	2.16	0.81
5:A:599:PHE:HD1	5:A:600:LEU:HD23	1.43	0.81
6:B:697:PRO:O	7:C:79:LEU:HD13	1.78	0.81
8:D:44:GLU:HB2	8:D:46:TYR:CE2	2.15	0.81
8:D:124:ASN:CB	8:D:125:PRO:HD3	2.10	0.81
10:F:26:GLN:O	10:F:27:ALA:HB3	1.80	0.81
2:2:181:HIS:NE2	20:2:1214:CLA:C4D	2.44	0.81
5:A:746:THR:HA	5:A:749:PHE:HB3	1.62	0.81
20:A:1781:CLA:HBA2	20:A:1794:CLA:CED	2.05	0.81
21:A:7032:LMU:O5B	21:A:7032:LMU:C1	2.29	0.81
20:B:1740:CLA:H41	22:B:1781:BCR:H23C	1.62	0.81
7:C:74:THR:OG1	7:C:80:ALA:CB	2.29	0.81
17:N:47:THR:HB	17:N:52:LEU:O	1.79	0.81
17:N:72:LYS:CD	17:N:72:LYS:N	2.42	0.81
20:A:1774:CLA:H202	20:A:1782:CLA:H3A	1.62	0.81
21:A:7039:LMU:C6B	21:A:7039:LMU:C4'	2.58	0.81
8:D:94:TYR:O	8:D:95:LYS:HG2	1.78	0.81
11:G:8:ILE:O	11:G:8:ILE:HG13	1.79	0.81
16:L:118:LEU:CD1	16:L:119:THR:H	1.93	0.81
17:N:34:THR:OG1	17:N:36:GLU:HB3	1.79	0.81
5:A:23:ASP:CG	5:A:24:ARG:HD2	2.00	0.81
5:A:362:LEU:HB3	5:A:410:ALA:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1812:CLA:HED2	20:A:1812:CLA:CAD	2.09	0.81
9:E:88:GLU:O	9:E:90:VAL:CB	2.29	0.81
17:N:47:THR:HG21	17:N:54:LYS:HZ2	1.41	0.81
20:2:1220:CLA:C7	3:3:140:LYS:HZ2	1.94	0.81
5:A:108:ALA:HB1	5:A:138:GLY:HA3	1.61	0.81
5:A:466:THR:HG21	20:B:1740:CLA:CBB	2.11	0.81
5:A:711:HIS:CE1	20:A:1795:CLA:HAC1	2.15	0.81
20:A:1800:CLA:HBB2	20:B:1770:CLA:HMD1	1.63	0.81
21:A:7016:LMU:O6'	21:A:7016:LMU:C1	2.29	0.81
6:B:131:THR:O	6:B:135:LEU:N	2.14	0.81
6:B:293:THR:O	6:B:294:ASN:ND2	2.14	0.81
8:D:104:PHE:HB3	8:D:106:SER:H	1.46	0.81
5:A:244:LEU:HD22	5:A:247:GLU:OE2	1.81	0.81
6:B:128:GLY:HA2	6:B:130:ARG:HE	1.44	0.81
6:B:212:PHE:HE1	20:B:1744:CLA:HHD	1.44	0.81
6:B:334:LEU:HG	6:B:334:LEU:O	1.79	0.81
25:B:1784:SF4:S4	25:B:1784:SF4:FE2	1.72	0.81
20:B:1787:CLA:H3A	20:B:1787:CLA:CGA	2.11	0.81
8:D:102:ARG:NH1	8:D:104:PHE:CD1	2.47	0.81
10:F:20:GLN:NE2	10:F:21:ALA:N	2.29	0.81
15:K:67:GLY:O	15:K:70:MET:CB	2.29	0.81
17:N:18:ASP:HB2	17:N:22:LEU:CG	2.11	0.81
20:A:1783:CLA:C7	22:A:1807:BCR:H371	2.10	0.81
20:A:1816:CLA:CED	20:A:1816:CLA:C1	2.54	0.81
21:A:7013:LMU:O6B	21:A:7013:LMU:C1B	2.29	0.81
21:A:7038:LMU:O6'	21:A:7038:LMU:H1B	1.81	0.81
11:G:17:PHE:O	11:G:20:ARG:HB2	1.81	0.81
16:L:160:VAL:O	16:L:160:VAL:CG2	2.29	0.81
20:A:1791:CLA:H3A	20:A:1797:CLA:CBB	2.11	0.80
21:A:7016:LMU:C3	21:A:7016:LMU:O6'	2.30	0.80
21:A:7032:LMU:C1B	21:A:7032:LMU:O1'	2.29	0.80
6:B:189:ALA:HB1	20:B:1758:CLA:H203	1.61	0.80
6:B:586:THR:C	6:B:588:GLY:H	1.84	0.80
8:D:93:LYS:NZ	8:D:93:LYS:HB3	1.95	0.80
11:G:16:LEU:HD12	11:G:17:PHE:CE2	2.15	0.80
17:N:50:GLN:CA	17:N:51:ASP:O	2.28	0.80
1:1:45:ILE:HD12	20:1:1195:CLA:HMD2	1.63	0.80
3:3:86:GLN:HB2	3:3:88:THR:HB	1.60	0.80
5:A:21:LEU:O	5:A:21:LEU:CD1	2.30	0.80
5:A:588:GLY:N	6:B:668:ARG:HD3	1.96	0.80
5:A:596:ASP:HA	5:A:599:PHE:HB3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7020:LMU:O6'	21:A:7020:LMU:C1B	2.30	0.80
21:A:7038:LMU:O6'	21:A:7038:LMU:C1B	2.29	0.80
6:B:373:THR:HA	6:B:376:GLN:HB2	1.62	0.80
18:R:33:UNK:O	18:R:36:UNK:CB	2.30	0.80
19:X:1:GLC:C5	19:X:2:FRU:O1	2.29	0.80
5:A:269:PHE:CE1	15:K:14:THR:CG2	2.57	0.80
5:A:284:ARG:HA	5:A:284:ARG:CZ	2.09	0.80
21:A:7033:LMU:C6B	21:A:7033:LMU:O2'	2.30	0.80
21:A:7037:LMU:O3'	21:A:7037:LMU:C6'	2.29	0.80
6:B:85:ARG:O	6:B:86:PRO:O	1.98	0.80
6:B:542:ARG:NH2	8:D:143:PRO:HG3	1.96	0.80
9:E:43:SER:HB2	9:E:82:TYR:HE1	1.45	0.80
11:G:46:ALA:CA	11:G:48:ASP:OD2	2.30	0.80
14:J:23:ALA:O	14:J:26:LEU:HB3	1.82	0.80
20:J:1044:CLA:OBD	20:J:1044:CLA:CED	2.30	0.80
20:J:1045:CLA:O1D	20:J:1045:CLA:C1	2.30	0.80
17:N:48:GLY:CA	17:N:49:CYS:O	2.30	0.80
3:3:104:TYR:HB2	3:3:106:TYR:N	1.96	0.80
20:3:3008:CLA:HBC2	20:3:3008:CLA:CMC	2.00	0.80
20:3:3008:CLA:O1A	20:3:3008:CLA:CED	2.30	0.80
5:A:21:LEU:HA	5:A:22:VAL:CB	2.05	0.80
5:A:27:ILE:O	5:A:27:ILE:CG2	2.28	0.80
5:A:423:ASP:CB	5:A:424:PRO:HD3	2.09	0.80
5:A:545:HIS:O	5:A:549:ILE:HG13	1.81	0.80
6:B:395:ILE:HD12	6:B:396:ARG:HG2	1.63	0.80
6:B:404:ALA:C	6:B:406:ASN:H	1.84	0.80
7:C:7:ILE:O	7:C:8:TYR:C	2.18	0.80
9:E:85:ASP:O	9:E:86:GLU:CB	2.30	0.80
12:H:25:GLY:CA	12:H:27:ASP:OD2	2.30	0.80
19:U:1:GLC:O2	19:U:2:FRU:C1	2.30	0.80
5:A:393:LEU:O	5:A:397:THR:HG23	1.82	0.80
5:A:545:HIS:CG	20:A:1792:CLA:HBB2	2.14	0.80
5:A:684:PHE:C	5:A:684:PHE:CD2	2.55	0.80
21:A:7021:LMU:O6'	21:A:7021:LMU:C2	2.30	0.80
21:A:7026:LMU:O3'	21:A:7026:LMU:H2B	1.80	0.80
7:C:73:THR:OG1	7:C:76:SER:CB	2.30	0.80
9:E:88:GLU:O	9:E:90:VAL:CA	2.29	0.80
11:G:43:HIS:C	11:G:45:GLU:N	2.30	0.80
19:T:1:GLC:O2	19:T:2:FRU:C1	2.30	0.80
22:3:1220:BCR:H311	22:3:1220:BCR:HC8	1.62	0.80
20:4:1198:CLA:O1D	20:4:1198:CLA:C2A	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1800:CLA:C9	22:L:1169:BCR:H321	2.12	0.80
21:A:7028:LMU:O6'	21:A:7028:LMU:C1'	2.30	0.80
21:A:7043:LMU:C11	21:A:7043:LMU:H62	2.12	0.80
10:F:22:LEU:O	10:F:25:LEU:CB	2.30	0.80
10:F:26:GLN:OE1	10:F:26:GLN:CA	2.29	0.80
11:G:16:LEU:HD23	11:G:68:ILE:HG23	1.64	0.80
13:I:12:VAL:HG21	20:I:1031:CLA:O1A	1.81	0.80
20:J:1044:CLA:C15	20:J:1044:CLA:C9	2.59	0.80
17:N:72:LYS:HZ2	17:N:74:LYS:CG	1.91	0.80
19:O:2:FRU:C6	19:O:2:FRU:O1	2.29	0.80
5:A:21:LEU:N	5:A:22:VAL:HG23	1.95	0.80
5:A:107:GLU:OE1	5:A:161:GLU:HG3	1.82	0.80
20:A:1789:CLA:H41	16:L:64:LEU:HD23	1.62	0.80
21:A:7032:LMU:C3	21:A:7032:LMU:H1B	2.08	0.80
6:B:557:PHE:N	6:B:558:PRO:CD	2.44	0.80
20:B:1756:CLA:C8	22:B:1777:BCR:H14C	2.11	0.80
10:F:24:LYS:O	10:F:27:ALA:CB	2.30	0.80
11:G:60:SER:OG	11:G:63:PRO:HB2	1.81	0.80
12:H:20:GLN:HB3	12:H:22:ASP:HB2	1.60	0.80
16:L:165:TYR:CD2	16:L:165:TYR:N	2.50	0.80
17:N:45:ASN:HD21	17:N:54:LYS:CB	1.93	0.80
17:N:67:LEU:HB2	17:N:68:GLU:CB	2.11	0.80
17:N:72:LYS:HG2	17:N:74:LYS:CG	2.04	0.80
5:A:207:LEU:O	5:A:310:PHE:HB3	1.80	0.80
5:A:615:HIS:CE1	20:A:1792:CLA:HBC3	2.16	0.80
20:A:1816:CLA:CGA	20:A:1816:CLA:O2D	2.30	0.80
21:A:7020:LMU:O6'	21:A:7020:LMU:H3B	1.81	0.80
21:A:7021:LMU:H1'	21:A:7021:LMU:O6'	1.82	0.80
21:A:7028:LMU:C1	21:A:7028:LMU:O2'	2.30	0.80
21:A:7032:LMU:C3	21:A:7032:LMU:O5B	2.29	0.80
21:A:7039:LMU:C3'	21:A:7039:LMU:O6B	2.30	0.80
8:D:46:TYR:HE1	8:D:80:LYS:HE2	1.44	0.80
11:G:7:VAL:HG22	11:G:8:ILE:H	1.46	0.80
11:G:73:ALA:O	11:G:75:GLY:N	2.15	0.80
16:L:56:VAL:HG13	20:L:1167:CLA:CED	2.12	0.80
18:R:34:UNK:O	18:R:38:UNK:CB	2.30	0.80
5:A:496:HIS:HB3	5:A:515:TRP:CE3	2.17	0.80
5:A:726:SER:O	5:A:728:VAL:N	2.15	0.80
20:A:1781:CLA:CHB	22:A:1806:BCR:H363	2.11	0.80
21:A:7016:LMU:C7	21:A:7016:LMU:H112	2.12	0.80
21:A:7020:LMU:C6'	21:A:7020:LMU:O5B	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:317:ARG:NE	6:B:317:ARG:HA	1.95	0.80
12:H:50:ARG:HH12	12:H:53:LEU:C	1.86	0.80
20:J:1045:CLA:O1D	20:J:1045:CLA:CGA	2.29	0.80
20:K:1146:CLA:O1A	20:K:1146:CLA:C2A	2.30	0.80
16:L:8:TYR:HE1	16:L:11:ILE:HG23	1.47	0.80
17:N:5:GLU:OE2	17:N:6:TYR:CB	2.29	0.80
17:N:63:ASP:N	17:N:65:LEU:N	2.29	0.80
17:N:66:ASP:O	17:N:67:LEU:CD1	2.29	0.80
18:R:35:UNK:O	18:R:38:UNK:CB	2.29	0.80
19:O:1:GLC:C5	19:O:2:FRU:O5	2.29	0.80
20:1:1192:CLA:HAA1	21:1:1202:LMU:O3'	1.82	0.80
20:2:1215:CLA:H43	20:2:1220:CLA:HBC3	1.61	0.80
4:4:107:GLN:HA	20:4:1196:CLA:HMA2	1.57	0.80
5:A:248:PHE:N	5:A:248:PHE:CD2	2.49	0.80
5:A:680:LEU:HB3	20:A:1812:CLA:O2A	1.81	0.80
21:A:7016:LMU:O6'	21:A:7016:LMU:C1'	2.30	0.80
21:A:7021:LMU:C1'	21:A:7021:LMU:O6'	2.30	0.80
21:A:7021:LMU:C3	21:A:7021:LMU:O6'	2.30	0.80
21:A:7042:LMU:O2B	21:A:7042:LMU:C5'	2.30	0.80
20:B:1759:CLA:H62	24:B:1783:LMG:H182	1.64	0.80
22:B:1778:BCR:C37	10:F:93:ILE:CG2	2.60	0.80
11:G:47:GLY:H	11:G:48:ASP:HB3	1.45	0.80
22:I:1032:BCR:HC8	22:I:1032:BCR:H313	0.84	0.80
17:N:65:LEU:O	17:N:65:LEU:CD2	2.30	0.80
19:Z:2:FRU:O6	19:Z:2:FRU:C1	2.30	0.80
20:3:3008:CLA:CGA	20:3:3008:CLA:O1D	2.30	0.79
5:A:308:ILE:O	5:A:312:ILE:N	2.15	0.79
20:A:1781:CLA:CMA	20:A:1782:CLA:O1A	2.30	0.79
20:A:1787:CLA:H42	16:L:33:ILE:HG12	1.64	0.79
21:A:7036:LMU:C6'	21:A:7036:LMU:O5B	2.30	0.79
21:A:7039:LMU:H6'2	21:A:7039:LMU:C4'	2.11	0.79
21:A:7039:LMU:O6B	21:A:7039:LMU:C4'	2.29	0.79
6:B:655:LEU:HD21	20:B:1771:CLA:CBB	2.11	0.79
20:B:1753:CLA:HAA2	20:B:1753:CLA:HBD	1.64	0.79
9:E:60:LYS:HG3	9:E:61:THR:N	1.97	0.79
10:F:102:ARG:HG2	10:F:106:ILE:CD1	2.05	0.79
10:F:103:SER:C	10:F:105:LEU:H	1.86	0.79
11:G:19:GLY:C	11:G:21:PHE:N	2.30	0.79
12:H:21:TRP:N	12:H:22:ASP:HB3	1.96	0.79
20:K:1146:CLA:O1A	20:K:1146:CLA:C3A	2.30	0.79
17:N:61:LEU:CD1	17:N:63:ASP:O	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:36:UNK:O	18:R:38:UNK:CB	2.30	0.79
19:M:1:GLC:O2	19:M:2:FRU:C5	2.29	0.79
19:W:1:GLC:O2	19:W:2:FRU:C2	2.30	0.79
2:2:181:HIS:NE2	20:2:1214:CLA:C3D	2.46	0.79
3:3:107:TRP:CG	3:3:108:ALA:N	2.38	0.79
20:4:1201:CLA:O1D	20:4:1201:CLA:CAA	2.30	0.79
20:A:1791:CLA:CGA	20:A:1797:CLA:HBB2	2.12	0.79
21:A:7020:LMU:C5B	21:A:7020:LMU:O6'	2.30	0.79
21:A:7020:LMU:O6'	21:A:7020:LMU:C3B	2.29	0.79
21:A:7041:LMU:O6'	21:A:7041:LMU:C1B	2.30	0.79
21:A:7042:LMU:O6'	21:A:7042:LMU:C4	2.29	0.79
6:B:398:TYR:HD1	6:B:542:ARG:HH21	1.28	0.79
20:B:1737:CLA:H43	22:B:1775:BCR:H313	1.63	0.79
20:B:1742:CLA:CAC	20:B:1743:CLA:CBB	2.48	0.79
20:J:1043:CLA:O1A	20:J:1043:CLA:C14	2.30	0.79
20:K:1146:CLA:O1A	20:K:1146:CLA:CMA	2.29	0.79
17:N:48:GLY:C	17:N:49:CYS:SG	2.58	0.79
17:N:66:ASP:O	17:N:67:LEU:CG	2.30	0.79
18:R:38:UNK:O	18:R:42:UNK:CA	2.29	0.79
19:W:1:GLC:C1	19:W:1:GLC:O6	2.30	0.79
2:2:196:HIS:CE1	19:M:1:GLC:O3	2.34	0.79
20:2:1220:CLA:H71	3:3:140:LYS:NZ	1.95	0.79
5:A:78:VAL:O	5:A:82:HIS:HB2	1.82	0.79
20:A:1783:CLA:H71	22:A:1807:BCR:C37	2.10	0.79
21:A:7040:LMU:O3'	21:A:7040:LMU:C1B	2.29	0.79
21:A:7042:LMU:C3	21:A:7042:LMU:O6'	2.30	0.79
6:B:119:GLY:HA3	20:B:1758:CLA:CED	2.04	0.79
6:B:546:LEU:HD11	6:B:567:THR:HG22	1.62	0.79
20:B:1755:CLA:CED	20:B:1756:CLA:OBD	2.30	0.79
10:F:22:LEU:O	10:F:25:LEU:CD1	2.29	0.79
11:G:45:GLU:CG	11:G:49:THR:HG21	2.12	0.79
11:G:45:GLU:CB	11:G:49:THR:CG2	2.59	0.79
16:L:152:THR:O	16:L:156:PHE:N	2.11	0.79
20:L:1167:CLA:HBC3	20:L:1167:CLA:HMC1	1.63	0.79
17:N:4:GLU:O	17:N:4:GLU:CG	2.29	0.79
17:N:45:ASN:CB	17:N:57:LYS:NZ	2.45	0.79
2:2:68:LEU:HD11	20:2:1217:CLA:H192	1.64	0.79
5:A:401:TRP:CD1	20:A:1783:CLA:CHC	2.65	0.79
6:B:331:HIS:CE1	6:B:392:ILE:HG21	2.17	0.79
11:G:30:ASN:O	11:G:33:LYS:NZ	2.16	0.79
12:H:23:VAL:O	12:H:23:VAL:CG1	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:51:ASP:O	17:N:52:LEU:CD2	2.30	0.79
17:N:60:PHE:CA	17:N:61:LEU:O	2.30	0.79
1:1:185:TRP:O	1:1:186:HIS:CB	2.30	0.79
2:2:124:ILE:HB	2:2:129:LYS:HB3	1.63	0.79
20:4:1198:CLA:CAA	20:4:1198:CLA:O2D	2.30	0.79
21:A:7020:LMU:O6'	21:A:7020:LMU:C2B	2.30	0.79
6:B:672:GLN:HA	6:B:672:GLN:NE2	1.94	0.79
22:B:1779:BCR:H321	22:B:1779:BCR:HC8	0.83	0.79
17:N:61:LEU:CD2	17:N:63:ASP:O	2.29	0.79
3:3:158:TYR:O	3:3:160:GLY:N	2.16	0.79
5:A:281:LEU:HD12	20:A:1772:CLA:CED	1.28	0.79
21:A:7026:LMU:H12	21:A:7026:LMU:H51	1.64	0.79
6:B:278:LEU:HD12	20:B:1746:CLA:CMA	2.12	0.79
6:B:415:LYS:HE3	6:B:539:LEU:O	1.82	0.79
6:B:531:THR:HG22	20:B:1755:CLA:CMC	2.05	0.79
20:B:1753:CLA:O2D	20:B:1753:CLA:C2A	2.31	0.79
20:B:1762:CLA:HBB2	22:B:1778:BCR:H272	1.65	0.79
25:B:1784:SF4:S3	25:B:1784:SF4:FE1	1.73	0.79
9:E:90:VAL:O	9:E:90:VAL:CG1	2.30	0.79
10:F:30:LYS:O	10:F:31:LEU:HB2	1.80	0.79
20:F:1157:CLA:OBD	20:F:1157:CLA:CED	2.31	0.79
11:G:28:ARG:HG2	11:G:28:ARG:NH2	1.94	0.79
11:G:46:ALA:HA	11:G:48:ASP:CG	2.01	0.79
20:J:1043:CLA:HBC3	20:J:1043:CLA:CHD	2.13	0.79
16:L:148:VAL:O	16:L:149:SER:HB3	1.80	0.79
16:L:163:LEU:HD11	16:L:164:PRO:CG	2.11	0.79
17:N:45:ASN:HB2	17:N:57:LYS:NZ	1.98	0.79
1:1:160:GLY:HA3	20:1:1189:CLA:CBB	2.11	0.79
21:A:7010:LMU:O2B	21:A:7010:LMU:C3'	2.30	0.79
21:A:7023:LMU:C6B	21:A:7023:LMU:O3B	2.30	0.79
21:A:7026:LMU:H3O1	19:Z:2:FRU:H5	1.48	0.79
25:B:1784:SF4:S2	25:B:1784:SF4:FE3	1.70	0.79
7:C:39:ILE:CG1	7:C:40:ALA:H	1.92	0.79
20:F:1156:CLA:HBC2	20:F:1156:CLA:HHD	1.64	0.79
11:G:42:SER:OG	11:G:45:GLU:CB	2.30	0.79
11:G:67:ASN:HA	11:G:70:ASP:OD2	1.83	0.79
17:N:62:SER:CB	17:N:66:ASP:OD1	2.30	0.79
20:A:1770:CLA:HMC2	22:A:1803:BCR:C17	2.13	0.79
21:A:7016:LMU:O6'	21:A:7016:LMU:C4	2.30	0.79
21:A:7032:LMU:O5B	21:A:7032:LMU:C2	2.29	0.79
6:B:255:LEU:HD13	6:B:275:HIS:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1781:BCR:H392	20:I:1031:CLA:H142	1.63	0.79
11:G:43:HIS:O	11:G:45:GLU:CB	2.29	0.79
1:1:39:TYR:CB	20:1:1196:CLA:OBD	2.31	0.79
3:3:92:TRP:HA	3:3:93:PHE:CG	2.18	0.79
20:4:1196:CLA:HHD	20:4:1196:CLA:HBC3	1.62	0.79
22:A:1803:BCR:C23	22:A:1803:BCR:C40	2.61	0.79
21:A:7016:LMU:C2	21:A:7016:LMU:O6'	2.30	0.79
6:B:120:VAL:HA	6:B:123:TRP:HD1	1.46	0.79
20:B:1744:CLA:HMA1	22:B:1776:BCR:H313	1.64	0.79
20:B:1756:CLA:H122	22:B:1777:BCR:C14	2.13	0.79
20:B:1759:CLA:H72	24:B:1783:LMG:H311	1.64	0.79
7:C:1:MET:N	7:C:4:SER:N	2.31	0.79
10:F:147:GLY:CA	10:F:150:VAL:HB	2.13	0.79
20:F:1157:CLA:HED2	20:F:1157:CLA:CAD	2.12	0.79
14:J:11:ALA:CB	14:J:12:PRO:HD2	2.13	0.79
17:N:1:GLY:O	17:N:2:VAL:CG1	2.30	0.79
17:N:29:PHE:CD1	17:N:32:ALA:HB3	2.18	0.79
19:W:1:GLC:O2	19:W:2:FRU:C1	2.30	0.79
5:A:58:HIS:CE1	20:A:1759:CLA:ND	2.50	0.79
5:A:555:ILE:HG22	6:B:670:TYR:CE2	2.18	0.79
20:A:1772:CLA:C17	20:A:1772:CLA:C14	2.45	0.79
20:A:1781:CLA:O1A	20:A:1782:CLA:HED3	1.83	0.79
21:A:7016:LMU:O6'	21:A:7016:LMU:C5	2.30	0.79
21:A:7023:LMU:O6'	21:A:7023:LMU:C1'	2.29	0.79
21:A:7030:LMU:H52	21:A:7030:LMU:H92	1.64	0.79
6:B:438:VAL:HG22	20:B:1763:CLA:CMC	2.12	0.79
6:B:558:PRO:CG	6:B:703:VAL:HB	2.13	0.79
7:C:26:LEU:H	7:C:43:PRO:HG3	1.48	0.79
7:C:63:LEU:CG	7:C:64:SER:H	1.96	0.79
12:H:65:LEU:HD23	20:H:1079:CLA:C5	2.12	0.79
19:Q:1:GLC:C1	19:Q:2:FRU:O4	2.30	0.79
1:1:25:ASP:H	6:B:314:ARG:NH2	1.81	0.78
21:1:7004:LMU:O2'	21:1:7004:LMU:C1	2.30	0.78
21:A:7021:LMU:H41	21:A:7021:LMU:H6D	1.65	0.78
21:A:7021:LMU:O6'	21:A:7021:LMU:C4	2.30	0.78
22:B:1778:BCR:H371	10:F:93:ILE:CG2	2.13	0.78
25:B:1784:SF4:S3	25:B:1784:SF4:FE4	1.74	0.78
9:E:51:SER:HB3	9:E:68:ARG:NH1	1.97	0.78
22:I:1032:BCR:HC32	20:I:1033:CLA:HAC1	1.65	0.78
17:N:61:LEU:HD13	17:N:63:ASP:HB2	1.64	0.78
19:X:1:GLC:H5	19:X:2:FRU:HO1	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:2:FRU:C6	19:Z:2:FRU:C1	2.48	0.78
2:2:70:LYS:HG3	2:2:73:ILE:CG1	2.13	0.78
20:3:1218:CLA:O1D	20:3:1218:CLA:C2A	2.31	0.78
4:4:119:PRO:CG	20:4:1206:CLA:C2D	2.51	0.78
5:A:27:ILE:O	5:A:28:LYS:CG	2.29	0.78
5:A:157:GLY:HA2	5:A:229:ILE:HG21	1.66	0.78
5:A:242:ILE:HG12	5:A:243:PRO:HD3	1.64	0.78
5:A:669:GLY:H	6:B:445:ALA:HA	1.47	0.78
17:N:45:ASN:HD22	17:N:54:LYS:HG2	0.79	0.78
20:4:1201:CLA:CBA	20:4:1201:CLA:CMA	2.30	0.78
5:A:700:TRP:O	5:A:704:ILE:HB	1.83	0.78
20:A:1760:CLA:HMC3	20:A:1762:CLA:O2D	1.82	0.78
20:A:1776:CLA:C1C	20:A:1782:CLA:H171	2.13	0.78
7:C:17:CYS:CB	7:C:58:CYS:SG	2.68	0.78
17:N:5:GLU:OE2	17:N:5:GLU:CA	2.30	0.78
17:N:54:LYS:CB	17:N:57:LYS:CE	2.61	0.78
5:A:197:GLN:HE22	5:A:351:THR:HB	1.49	0.78
5:A:217:SER:CA	22:A:1803:BCR:H351	2.12	0.78
5:A:308:ILE:HG22	5:A:309:LEU:N	1.99	0.78
21:A:7041:LMU:O2'	21:A:7041:LMU:C5'	2.29	0.78
6:B:172:GLU:O	6:B:176:ASN:CB	2.32	0.78
6:B:353:TYR:O	6:B:354:SER:OG	2.01	0.78
20:B:1739:CLA:HMC2	22:B:1780:BCR:H281	1.64	0.78
11:G:88:THR:OG1	11:G:92:GLY:HA3	1.83	0.78
16:L:124:LYS:C	16:L:126:GLN:H	1.86	0.78
17:N:62:SER:O	17:N:63:ASP:CB	2.30	0.78
20:A:1776:CLA:C2C	20:A:1782:CLA:C17	2.61	0.78
21:A:7033:LMU:C3'	21:A:7033:LMU:O5B	2.29	0.78
6:B:120:VAL:CA	6:B:123:TRP:CD1	2.64	0.78
20:B:1749:CLA:OBD	20:B:1752:CLA:HBC3	1.83	0.78
11:G:21:PHE:O	11:G:23:PHE:HB2	1.82	0.78
12:H:25:GLY:CA	12:H:27:ASP:N	2.29	0.78
16:L:99:LEU:CD1	22:L:1169:BCR:HC7	2.13	0.78
16:L:123:ARG:HA	16:L:123:ARG:NE	1.97	0.78
17:N:45:ASN:CB	17:N:57:LYS:HZ2	1.96	0.78
2:2:54:TRP:CG	20:2:1222:CLA:O1D	2.37	0.78
20:A:1794:CLA:HBA2	20:A:1794:CLA:CHA	2.12	0.78
20:A:1813:CLA:H11	6:B:431:PHE:CE1	2.18	0.78
20:A:1816:CLA:O2D	20:A:1816:CLA:CBA	2.31	0.78
6:B:382:ILE:HG22	6:B:383:MET:N	1.98	0.78
7:C:79:LEU:CD2	7:C:81:TYR:O	2.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:68:HIS:O	15:K:70:MET:CB	2.29	0.78
15:K:69:ILE:CG2	15:K:70:MET:H	1.90	0.78
17:N:62:SER:O	17:N:63:ASP:HB2	1.80	0.78
2:2:59:ALA:O	2:2:62:ILE:HG22	1.83	0.78
20:2:1220:CLA:H43	3:3:140:LYS:HG2	1.62	0.78
5:A:23:ASP:OD2	5:A:24:ARG:CD	2.29	0.78
5:A:146:THR:O	20:A:1783:CLA:HMA2	1.83	0.78
21:A:7009:LMU:O3'	21:A:7009:LMU:C5B	2.30	0.78
21:A:7026:LMU:H12	21:A:7026:LMU:H52	1.63	0.78
21:A:7037:LMU:H11	21:A:7037:LMU:H61	1.65	0.78
6:B:280:ILE:HA	6:B:283:LEU:HD12	1.64	0.78
6:B:348:VAL:HA	20:B:1748:CLA:H42	1.66	0.78
6:B:438:VAL:CG2	20:B:1763:CLA:HMC1	2.12	0.78
13:I:8:PHE:HB2	20:I:1031:CLA:OBD	1.84	0.78
20:A:1816:CLA:CED	20:A:1816:CLA:O1A	2.31	0.78
10:F:12:LYS:HG2	10:F:13:GLN:N	1.99	0.78
4:4:149:ALA:HB1	4:4:150:LYS:HE3	1.66	0.78
6:B:58:PHE:HB3	6:B:146:SER:HB3	1.65	0.78
6:B:521:HIS:CE1	20:B:1768:CLA:NA	2.49	0.78
7:C:1:MET:H2	7:C:3:HIS:CA	1.96	0.78
11:G:47:GLY:N	11:G:48:ASP:CG	2.37	0.78
20:J:1044:CLA:H102	20:J:1044:CLA:H151	1.65	0.78
17:N:70:GLU:HB3	17:N:72:LYS:H	1.47	0.78
3:3:112:THR:O	3:3:114:PHE:N	2.17	0.78
3:3:205:GLY:H	5:A:252:ARG:HH22	0.78	0.78
5:A:443:ILE:HG21	5:A:558:LYS:HB2	1.66	0.78
5:A:545:HIS:CB	20:A:1792:CLA:HBB1	2.14	0.78
20:A:1781:CLA:O2A	20:A:1794:CLA:O2D	2.02	0.78
20:A:1800:CLA:H92	22:L:1169:BCR:H321	1.64	0.78
21:A:7013:LMU:H1B	21:A:7013:LMU:H6B	1.49	0.78
21:A:7025:LMU:O2'	21:A:7025:LMU:H21	1.84	0.78
6:B:188:LEU:O	6:B:191:ALA:N	2.17	0.78
20:B:1761:CLA:CBC	20:B:1761:CLA:CHD	2.62	0.78
8:D:48:ILE:HG22	8:D:83:CYS:HB2	1.65	0.78
11:G:42:SER:CB	11:G:45:GLU:OE1	2.29	0.78
15:K:27:ALA:CB	15:K:28:PRO:HD3	2.14	0.78
16:L:163:LEU:HD21	16:L:164:PRO:HD2	1.57	0.78
22:L:1170:BCR:H23C	22:L:1170:BCR:H383	1.64	0.78
19:X:1:GLC:O5	19:X:2:FRU:C1	2.30	0.78
4:4:33:ASP:HB3	4:4:34:PRO:CD	2.10	0.77
20:A:1764:CLA:H111	22:A:1808:BCR:C11	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1787:CLA:HBB1	20:A:1793:CLA:H192	1.64	0.77
20:A:1791:CLA:HBC1	22:A:1806:BCR:HC31	1.66	0.77
21:A:7033:LMU:H6'2	21:A:7033:LMU:C2'	2.13	0.77
21:A:7037:LMU:O2B	21:A:7037:LMU:C5B	2.31	0.77
6:B:160:LYS:HG3	6:B:161:TRP:H	1.48	0.77
11:G:42:SER:CB	11:G:45:GLU:OE2	2.30	0.77
20:J:1045:CLA:CHD	20:J:1045:CLA:HBC3	2.05	0.77
15:K:51:ASP:HB3	15:K:52:PRO:CD	2.13	0.77
17:N:5:GLU:OE1	17:N:6:TYR:CE1	2.37	0.77
17:N:54:LYS:HB2	17:N:57:LYS:HZ1	1.48	0.77
2:2:128:ASN:ND2	14:J:4:PHE:H	1.83	0.77
2:2:197:LEU:HD21	5:A:162:LEU:HD21	1.66	0.77
20:2:1220:CLA:O1A	20:2:1220:CLA:CBD	2.30	0.77
5:A:168:ALA:O	5:A:171:ALA:HB3	1.82	0.77
5:A:454:GLY:H	5:A:457:SER:CB	1.96	0.77
5:A:723:ARG:HH11	5:A:723:ARG:HG2	1.50	0.77
6:B:137:THR:HA	6:B:140:ILE:CG1	2.14	0.77
6:B:190:TRP:HA	20:B:1744:CLA:HBB2	1.66	0.77
6:B:527:LEU:HD12	20:B:1755:CLA:CHD	2.13	0.77
11:G:93:TYR:HA	11:G:94:ASP:HB2	0.78	0.77
17:N:46:PHE:O	17:N:47:THR:CG2	2.29	0.77
1:1:28:GLY:HA2	20:1:1199:CLA:C3C	2.15	0.77
21:1:7004:LMU:O6B	21:1:7004:LMU:C1B	2.30	0.77
5:A:80:SER:O	5:A:83:PHE:HB2	1.84	0.77
5:A:375:HIS:CE1	20:A:1782:CLA:NC	2.53	0.77
20:A:1781:CLA:CBC	20:A:1781:CLA:CHD	2.53	0.77
22:A:1807:BCR:H393	22:A:1807:BCR:C23	2.12	0.77
20:A:1816:CLA:C2	20:A:1816:CLA:O1A	2.32	0.77
20:A:1816:CLA:CAA	20:A:1816:CLA:O2D	2.31	0.77
21:A:7022:LMU:O2'	21:A:7022:LMU:H5'	1.83	0.77
21:A:7037:LMU:H32	21:A:7037:LMU:H72	0.78	0.77
6:B:76:ALA:O	6:B:78:VAL:N	2.18	0.77
6:B:655:LEU:CD2	20:B:1771:CLA:CBB	2.61	0.77
20:B:1746:CLA:CBA	20:B:1746:CLA:HED2	2.13	0.77
17:N:79:SER:CA	17:N:80:ASN:O	2.29	0.77
18:R:27:UNK:O	18:R:29:UNK:O	2.03	0.77
20:R:1054:CLA:C1A	20:R:1054:CLA:CED	2.58	0.77
20:1:1197:CLA:O1D	20:1:1197:CLA:CAA	2.31	0.77
5:A:214:GLY:HA3	22:A:1804:BCR:H15C	1.66	0.77
5:A:331:LEU:CD2	5:A:331:LEU:C	2.53	0.77
20:A:1787:CLA:O2A	16:L:27:VAL:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:124:TRP:O	6:B:129:LEU:HB3	1.85	0.77
6:B:409:ALA:O	6:B:411:MET:N	2.17	0.77
6:B:664:LEU:O	6:B:667:TRP:CZ3	2.37	0.77
20:B:1764:CLA:HMD2	20:B:1765:CLA:C2C	2.14	0.77
9:E:52:VAL:HG12	9:E:53:VAL:N	1.99	0.77
10:F:62:LEU:HG	10:F:72:ILE:CD1	2.13	0.77
20:J:1045:CLA:CBA	20:J:1045:CLA:CB D	2.51	0.77
5:A:28:LYS:C	5:A:29:THR:HG22	2.04	0.77
5:A:737:HIS:HA	5:A:740:LEU:CD2	2.14	0.77
20:A:1783:CLA:C10	22:A:1807:BCR:H372	2.14	0.77
21:A:7021:LMU:C6B	21:A:7021:LMU:O3B	2.29	0.77
13:I:11:LEU:CD1	22:I:1032:BCR:C10	2.56	0.77
18:R:3:UNK:O	18:R:4:UNK:CB	2.33	0.77
5:A:40:PHE:HE1	5:A:53:TRP:HD1	1.29	0.77
5:A:422:TYR:N	5:A:422:TYR:CD1	2.51	0.77
20:A:1776:CLA:HAA2	20:A:1780:CLA:HBB2	1.67	0.77
20:A:1781:CLA:CBA	20:A:1794:CLA:HED1	2.10	0.77
21:A:7042:LMU:O3'	21:A:7042:LMU:C1B	2.29	0.77
6:B:278:LEU:HD12	20:B:1746:CLA:HMA2	1.66	0.77
8:D:78:ALA:CB	8:D:82:GLN:HE22	1.97	0.77
17:N:5:GLU:OE1	17:N:6:TYR:CE2	2.37	0.77
5:A:392:GLN:HA	5:A:395:LEU:HD23	1.67	0.77
5:A:624:VAL:O	5:A:636:HIS:CD2	2.38	0.77
6:B:75:GLU:HB2	6:B:132:ASN:HB3	1.67	0.77
6:B:317:ARG:HA	6:B:317:ARG:HE	1.48	0.77
20:B:1755:CLA:HMB3	22:B:1777:BCR:H352	1.67	0.77
10:F:23:LYS:CB	10:F:24:LYS:HZ3	1.98	0.77
17:N:45:ASN:HD21	17:N:54:LYS:CG	1.93	0.77
5:A:423:ASP:HB3	5:A:424:PRO:CD	2.07	0.77
6:B:353:TYR:CD2	6:B:594:TRP:CZ3	2.72	0.77
6:B:507:SER:O	6:B:508:LEU:HB2	1.82	0.77
20:B:1739:CLA:HBA1	20:B:1757:CLA:OBD	1.85	0.77
7:C:14:CYS:C	7:C:17:CYS:SG	2.62	0.77
9:E:44:TYR:CE1	9:E:73:ASN:HA	2.20	0.77
17:N:57:LYS:O	17:N:60:PHE:CD1	2.37	0.77
19:Q:1:GLC:O3	19:Q:1:GLC:H62	1.85	0.77
20:4:1209:CLA:HBC3	20:4:1209:CLA:CHD	2.14	0.77
5:A:107:GLU:CD	5:A:161:GLU:HG3	2.05	0.77
6:B:437:TYR:HB3	6:B:616:LEU:CD2	2.14	0.77
6:B:732:LYS:HB3	6:B:733:PHE:HA	0.79	0.77
20:B:1760:CLA:HED2	20:B:1760:CLA:CAA	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1760:CLA:HED2	20:B:1760:CLA:HAA1	1.67	0.77
20:B:1768:CLA:HBC1	10:F:83:PHE:HZ	1.44	0.77
10:F:25:LEU:HD22	10:F:46:MET:HB3	1.65	0.77
20:K:1085:CLA:HBC2	20:K:1085:CLA:HMC1	1.67	0.77
17:N:65:LEU:CD2	17:N:66:ASP:O	2.33	0.77
19:U:1:GLC:O2	19:U:2:FRU:C2	2.33	0.77
5:A:132:LEU:HD11	5:A:674:ALA:HB2	1.65	0.77
20:A:1815:CLA:HMC1	20:A:1815:CLA:CBC	2.13	0.77
6:B:354:SER:O	6:B:355:LEU:HD13	1.85	0.77
11:G:44:PHE:H	11:G:45:GLU:HB2	1.49	0.77
20:2:1212:CLA:O1A	20:2:1212:CLA:C1A	2.33	0.76
20:2:1220:CLA:CBD	20:2:1220:CLA:HBA2	2.15	0.76
3:3:48:PHE:HD2	3:3:49:ILE:CG2	1.82	0.76
5:A:121:GLN:NE2	20:A:1765:CLA:HMD1	2.00	0.76
21:A:7023:LMU:H91	21:A:7023:LMU:C3	2.08	0.76
6:B:189:ALA:HB2	20:B:1758:CLA:C20	2.14	0.76
7:C:1:MET:N	7:C:4:SER:OG	2.18	0.76
13:I:23:SER:O	13:I:26:LEU:HD23	1.85	0.76
1:1:161:PHE:H	20:1:1189:CLA:HBB2	1.51	0.76
20:1:1192:CLA:HHD	20:1:1192:CLA:HBC2	1.66	0.76
2:2:103:GLY:CA	20:2:1222:CLA:HBB2	2.16	0.76
20:4:1199:CLA:O2A	20:4:1199:CLA:H2A	1.85	0.76
5:A:491:TRP:CD1	5:A:492:ILE:HG23	2.20	0.76
5:A:711:HIS:HB3	5:A:717:ALA:HB2	1.66	0.76
6:B:475:ASP:HA	6:B:480:SER:O	1.85	0.76
20:B:1759:CLA:HMC1	20:B:1759:CLA:HBC3	1.67	0.76
10:F:33:ALA:HA	10:F:36:SER:HB2	1.65	0.76
1:1:161:PHE:N	20:1:1189:CLA:HBB2	2.00	0.76
3:3:74:ALA:CA	20:3:1215:CLA:C4D	2.59	0.76
4:4:33:ASP:CB	4:4:34:PRO:HD2	2.11	0.76
5:A:28:LYS:O	5:A:29:THR:CB	2.30	0.76
5:A:747:TRP:CD2	22:A:1807:BCR:C40	2.67	0.76
6:B:127:ILE:CD1	6:B:198:ALA:HB2	2.14	0.76
20:B:1755:CLA:CMB	22:B:1777:BCR:H352	2.15	0.76
19:O:2:FRU:O1	19:O:2:FRU:C4	2.30	0.76
20:2:1220:CLA:H61	3:3:140:LYS:NZ	1.94	0.76
4:4:154:ILE:HB	20:4:1202:CLA:CHA	2.16	0.76
20:A:1791:CLA:CGA	20:A:1797:CLA:HBB1	2.14	0.76
6:B:374:HIS:CG	6:B:374:HIS:O	2.38	0.76
11:G:45:GLU:O	11:G:46:ALA:HB3	1.84	0.76
20:J:1044:CLA:H41	20:J:1044:CLA:C9	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:259:TYR:CB	5:A:260:PRO:HD2	2.14	0.76
20:A:1760:CLA:C1	20:A:1767:CLA:H61	2.12	0.76
20:A:1793:CLA:CGA	20:A:1793:CLA:C1A	2.63	0.76
21:A:7032:LMU:O2'	21:A:7032:LMU:C1	2.30	0.76
21:A:7038:LMU:H4'	21:A:7038:LMU:O2B	1.84	0.76
6:B:454:LEU:HD11	10:F:69:PRO:O	1.84	0.76
9:E:90:VAL:O	9:E:90:VAL:HG12	1.85	0.76
17:N:5:GLU:OE2	17:N:6:TYR:CG	2.38	0.76
17:N:70:GLU:CD	17:N:72:LYS:O	2.24	0.76
18:R:34:UNK:H	18:R:36:UNK:CB	1.99	0.76
4:4:106:TRP:CG	20:4:1196:CLA:CED	2.69	0.76
5:A:233:LEU:O	5:A:235:ALA:N	2.19	0.76
5:A:464:ASN:HD22	5:A:464:ASN:N	1.82	0.76
6:B:323:TYR:CD1	20:B:1754:CLA:HBC1	2.21	0.76
9:E:48:ASN:ND2	9:E:71:LYS:NZ	2.34	0.76
20:J:1043:CLA:O1A	20:J:1043:CLA:C16	2.34	0.76
18:R:37:UNK:O	18:R:42:UNK:C	2.34	0.76
3:3:173:GLU:CG	3:3:174:LYS:H	1.98	0.76
5:A:714:LEU:HD13	22:B:1779:BCR:H392	1.66	0.76
6:B:325:THR:O	6:B:329:SER:HB2	1.86	0.76
6:B:596:TRP:CD1	6:B:623:TYR:HB2	2.19	0.76
7:C:20:ALA:O	7:C:21:CYS:HB2	1.84	0.76
17:N:42:PHE:H	17:N:43:PRO:HD3	1.50	0.76
20:A:1783:CLA:C7	22:A:1807:BCR:H372	2.15	0.76
20:A:1783:CLA:C17	22:A:1808:BCR:H15C	2.14	0.76
21:A:7037:LMU:H11	21:A:7037:LMU:C6	2.16	0.76
6:B:414:HIS:HD2	20:B:1760:CLA:HMA3	1.48	0.76
6:B:693:TRP:CD1	20:B:1770:CLA:C2D	2.69	0.76
11:G:41:MET:O	11:G:42:SER:O	2.04	0.76
20:R:1055:CLA:H92	21:R:1056:LMU:O4'	1.85	0.76
21:R:1057:LMU:H62	21:R:1057:LMU:C1	2.08	0.76
2:2:68:LEU:CG	20:2:1217:CLA:H192	2.15	0.76
5:A:259:TYR:CE2	5:A:280:PHE:HA	2.21	0.76
6:B:195:VAL:HA	6:B:199:ILE:HG13	1.66	0.76
6:B:503:GLU:HB3	6:B:507:SER:CB	2.16	0.76
7:C:70:TRP:O	7:C:72:GLU:HB2	1.85	0.76
11:G:44:PHE:H	11:G:45:GLU:CB	1.96	0.76
20:2:1223:CLA:HMC1	20:2:1223:CLA:CBC	2.15	0.76
5:A:23:ASP:CG	5:A:24:ARG:HD3	2.02	0.76
5:A:353:SER:O	5:A:354:TRP:HB2	1.85	0.76
7:C:29:ILE:HG23	8:D:126:GLY:HA2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:59:PRO:HB3	17:N:75:TYR:CE1	2.20	0.76
19:M:1:GLC:C2	19:M:2:FRU:O5	2.32	0.76
3:3:87:GLU:CB	22:3:1220:BCR:C38	2.64	0.75
20:A:1781:CLA:HMA2	20:A:1782:CLA:O1A	1.86	0.75
6:B:295:PHE:CD2	6:B:295:PHE:N	2.54	0.75
10:F:94:ALA:HA	10:F:97:ILE:HG12	1.68	0.75
10:F:96:TRP:CZ3	10:F:134:PHE:HB2	2.20	0.75
20:J:1043:CLA:O1A	20:J:1043:CLA:C15	2.33	0.75
15:K:24:PHE:HB3	15:K:52:PRO:HG2	1.68	0.75
16:L:164:PRO:HA	16:L:165:TYR:CZ	2.21	0.75
17:N:11:LYS:HG2	17:N:12:THR:H	1.51	0.75
5:A:402:ILE:HG13	20:A:1784:CLA:CBB	2.14	0.75
5:A:626:GLY:CA	5:A:636:HIS:HA	2.17	0.75
20:A:1769:CLA:HMA2	20:A:1769:CLA:C2	2.16	0.75
6:B:130:ARG:O	6:B:135:LEU:HD23	1.85	0.75
6:B:337:ALA:HA	20:B:1754:CLA:HAA1	1.68	0.75
6:B:493:TRP:HE1	20:B:1746:CLA:HAC2	1.51	0.75
8:D:32:SER:O	16:L:21:GLY:HA2	1.85	0.75
9:E:44:TYR:CD1	9:E:73:ASN:HB2	2.20	0.75
10:F:83:PHE:O	10:F:87:GLY:HA3	1.87	0.75
16:L:164:PRO:HB3	16:L:165:TYR:HD2	1.48	0.75
21:R:1056:LMU:O6B	21:R:1056:LMU:C1B	2.31	0.75
4:4:106:TRP:CG	20:4:1196:CLA:HED3	2.20	0.75
5:A:735:VAL:O	5:A:739:LEU:HG	1.86	0.75
20:A:1782:CLA:HBA1	20:A:1782:CLA:CGD	2.17	0.75
20:B:1756:CLA:HED1	20:B:1764:CLA:CBB	2.15	0.75
7:C:12:ILE:N	7:C:12:ILE:HD12	2.01	0.75
11:G:7:VAL:CG2	11:G:8:ILE:N	2.48	0.75
16:L:64:LEU:HA	16:L:67:PRO:CG	2.16	0.75
17:N:50:GLN:HA	17:N:51:ASP:O	1.86	0.75
17:N:65:LEU:HD23	17:N:66:ASP:C	2.07	0.75
5:A:558:LYS:NZ	6:B:674:LEU:HB3	2.01	0.75
5:A:661:ALA:HA	5:A:664:VAL:HG13	1.68	0.75
21:A:7020:LMU:H6E	21:A:7020:LMU:C6B	2.16	0.75
6:B:596:TRP:NE1	6:B:623:TYR:HB2	2.01	0.75
6:B:630:GLN:HE21	6:B:731:GLY:HA3	1.50	0.75
20:B:1758:CLA:O1D	20:B:1758:CLA:OBD	1.93	0.75
7:C:7:ILE:HG22	7:C:65:VAL:HG23	1.69	0.75
19:X:1:GLC:O5	19:X:2:FRU:H12	1.86	0.75
5:A:56:ASN:O	5:A:57:LEU:HB3	1.86	0.75
20:A:1788:CLA:C16	22:L:1169:BCR:H362	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1796:CLA:H62	20:A:1813:CLA:H193	1.68	0.75
21:A:7022:LMU:C6B	21:A:7022:LMU:O3B	2.30	0.75
6:B:123:TRP:CZ3	20:B:1743:CLA:H191	2.22	0.75
6:B:315:LEU:O	6:B:315:LEU:HD13	1.87	0.75
20:B:1739:CLA:H42	20:B:1739:CLA:C4C	2.17	0.75
8:D:93:LYS:HB3	8:D:93:LYS:HZ3	1.49	0.75
10:F:20:GLN:O	10:F:21:ALA:CB	2.31	0.75
22:I:1032:BCR:H391	22:L:1169:BCR:H401	1.66	0.75
16:L:115:ALA:N	16:L:116:PRO:HD2	2.01	0.75
16:L:164:PRO:HB3	16:L:165:TYR:HE2	1.44	0.75
4:4:193:ILE:CG2	14:J:42:PHE:HD1	1.99	0.75
5:A:281:LEU:CD1	20:A:1772:CLA:H2A	2.13	0.75
5:A:342:GLY:HA3	5:A:430:ASP:HB2	0.82	0.75
5:A:370:ILE:HD11	20:A:1781:CLA:CAD	2.14	0.75
5:A:648:THR:CG2	5:A:651:GLY:H	2.00	0.75
20:A:1783:CLA:H43	20:A:1783:CLA:CBA	2.16	0.75
6:B:292:ARG:NH1	6:B:296:GLY:H	1.85	0.75
20:B:1753:CLA:H151	20:B:1753:CLA:H102	0.81	0.75
8:D:28:ILE:HG12	8:D:67:ILE:HG13	1.69	0.75
14:J:26:LEU:C	14:J:26:LEU:HD23	2.07	0.75
2:2:68:LEU:HD21	20:2:1217:CLA:H172	1.68	0.75
5:A:246:HIS:O	5:A:248:PHE:CD2	2.37	0.75
5:A:361:ASN:ND2	20:A:1761:CLA:CED	2.50	0.75
5:A:591:GLN:HA	5:A:591:GLN:HE21	1.50	0.75
5:A:636:HIS:C	5:A:638:THR:N	2.39	0.75
20:A:1777:CLA:CAD	20:A:1778:CLA:HMA1	2.17	0.75
20:A:1817:CLA:HMC1	20:A:1817:CLA:CBC	2.10	0.75
15:K:27:ALA:HB3	15:K:28:PRO:HD3	1.67	0.75
16:L:124:LYS:HB2	16:L:124:LYS:HZ2	1.48	0.75
1:1:97:ILE:HG22	20:1:1197:CLA:CBB	2.16	0.75
20:2:1220:CLA:H42	3:3:140:LYS:CB	2.16	0.75
4:4:38:ARG:HG3	4:4:39:TRP:H	1.52	0.75
5:A:284:ARG:HA	5:A:284:ARG:NH1	2.01	0.75
5:A:567:ARG:HH11	8:D:35:GLY:CA	1.97	0.75
20:A:1789:CLA:C4	16:L:64:LEU:HD23	2.16	0.75
21:A:7032:LMU:H6'2	21:A:7032:LMU:H22	1.66	0.75
21:A:7043:LMU:C6	21:A:7043:LMU:C11	2.63	0.75
6:B:196:HIS:CE1	20:B:1745:CLA:HED2	2.21	0.75
22:B:1777:BCR:H382	22:B:1777:BCR:C23	2.09	0.75
7:C:52:LYS:O	7:C:52:LYS:CG	2.35	0.75
11:G:13:GLY:CA	11:G:16:LEU:HG	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1215:CLA:O1A	20:2:1220:CLA:CBC	2.34	0.75
3:3:112:THR:OG1	3:3:113:LEU:HG	1.87	0.75
6:B:347:LEU:HD22	6:B:351:HIS:CE1	2.22	0.75
20:B:1739:CLA:HMC2	22:B:1780:BCR:C28	2.17	0.75
7:C:31:TRP:O	7:C:33:GLY:N	2.19	0.75
8:D:78:ALA:O	8:D:79:ARG:HD3	1.85	0.75
20:J:1045:CLA:HBD	20:J:1045:CLA:CGA	2.16	0.75
17:N:4:GLU:OE2	17:N:5:GLU:HB2	1.87	0.75
19:U:1:GLC:O2	19:U:2:FRU:H11	1.87	0.75
2:2:169:LEU:CD2	20:2:1215:CLA:CBB	2.65	0.74
20:2:1212:CLA:C4	20:2:1212:CLA:O2A	2.30	0.74
5:A:29:THR:HG23	5:A:29:THR:O	1.85	0.74
5:A:54:ILE:O	5:A:58:HIS:CD2	2.40	0.74
5:A:91:LEU:O	20:A:1763:CLA:HMC3	1.87	0.74
5:A:491:TRP:HE1	20:A:1792:CLA:H12	1.51	0.74
5:A:690:LEU:HD23	5:A:693:LEU:HD12	1.69	0.74
5:A:747:TRP:CE3	22:A:1807:BCR:H401	2.22	0.74
20:A:1761:CLA:C4	22:A:1804:BCR:H313	2.17	0.74
6:B:180:SER:HB2	6:B:288:GLY:HA3	1.68	0.74
20:B:1764:CLA:HBB2	22:B:1777:BCR:H381	1.67	0.74
7:C:54:CYS:SG	25:C:1082:SF4:S1	2.85	0.74
8:D:111:TYR:CD2	8:D:114:PRO:HB3	2.21	0.74
11:G:28:ARG:HA	20:G:1099:CLA:HMA3	1.68	0.74
17:N:54:LYS:HG2	17:N:57:LYS:HZ3	1.50	0.74
5:A:462:ILE:CD1	20:B:1786:CLA:H72	2.17	0.74
5:A:488:PHE:CE2	5:A:533:PRO:HB3	2.22	0.74
5:A:684:PHE:HD2	5:A:685:VAL:N	1.85	0.74
20:A:1815:CLA:HMA2	20:A:1815:CLA:H2	1.69	0.74
6:B:709:GLY:O	6:B:710:LEU:HB2	1.86	0.74
9:E:58:ASP:OD2	9:E:60:LYS:NZ	2.18	0.74
14:J:31:ARG:NH2	20:J:1043:CLA:C3B	2.50	0.74
5:A:32:GLU:OE2	20:A:1767:CLA:HMA2	1.87	0.74
5:A:711:HIS:CD2	20:A:1795:CLA:CBC	2.68	0.74
6:B:58:PHE:HB2	6:B:146:SER:HB2	1.69	0.74
6:B:122:GLN:HG3	6:B:361:ILE:HG12	1.69	0.74
11:G:40:GLY:C	11:G:41:MET:SD	2.65	0.74
11:G:94:ASP:H	11:G:95:PRO:CD	1.99	0.74
18:R:44:UNK:O	18:R:45:UNK:C	2.35	0.74
1:1:39:TYR:HB3	20:1:1196:CLA:OBD	1.87	0.74
2:2:36:SER:O	2:2:37:ASP:HB2	1.87	0.74
2:2:99:LEU:HD21	20:2:1222:CLA:HMC3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:84:ILE:CB	20:A:1798:CLA:O1A	2.29	0.74
3:3:87:GLU:CA	22:3:1220:BCR:C38	2.65	0.74
20:4:1199:CLA:HBC3	20:4:1199:CLA:CMC	2.03	0.74
5:A:214:GLY:O	5:A:215:SER:HB3	1.86	0.74
5:A:411:ALA:HB2	22:A:1806:BCR:C39	2.17	0.74
5:A:472:ARG:HH22	16:L:74:LEU:HD21	1.52	0.74
20:A:1776:CLA:C2C	20:A:1782:CLA:H171	2.18	0.74
20:A:1787:CLA:H3A	6:B:685:THR:OG1	1.87	0.74
6:B:269:TRP:CB	6:B:497:TRP:HH2	2.00	0.74
20:B:1746:CLA:HED2	20:B:1746:CLA:HBA2	1.67	0.74
12:H:23:VAL:O	12:H:23:VAL:HG12	1.87	0.74
14:J:11:ALA:HB1	14:J:12:PRO:CD	2.16	0.74
18:R:24:UNK:O	18:R:27:UNK:CB	2.35	0.74
20:2:1224:CLA:H151	20:2:1224:CLA:H8	1.69	0.74
20:A:1772:CLA:CBC	20:A:1772:CLA:CMC	2.46	0.74
6:B:471:THR:HG23	6:B:502:ASN:ND2	2.02	0.74
20:J:1043:CLA:HED3	20:J:1043:CLA:C2A	2.17	0.74
16:L:36:TYR:CG	16:L:36:TYR:O	2.40	0.74
17:N:45:ASN:HD22	17:N:57:LYS:HZ3	1.33	0.74
17:N:61:LEU:CG	17:N:62:SER:H	1.98	0.74
5:A:103:PHE:CD2	5:A:103:PHE:N	2.55	0.74
5:A:588:GLY:H	6:B:668:ARG:NH1	1.85	0.74
5:A:692:PHE:CZ	20:A:1796:CLA:HBC3	2.22	0.74
7:C:12:ILE:HB	7:C:39:ILE:HA	1.68	0.74
10:F:7:PRO:HA	10:F:61:LEU:O	1.88	0.74
12:H:44:ALA:HB3	16:L:145:PHE:HD1	1.51	0.74
18:R:7:UNK:O	18:R:11:UNK:N	2.20	0.74
20:1:1190:CLA:HMC1	20:1:1190:CLA:CBC	2.16	0.74
5:A:78:VAL:HG11	20:A:1761:CLA:HBC3	1.69	0.74
5:A:187:HIS:CE1	20:A:1767:CLA:C4D	2.67	0.74
5:A:224:HIS:O	5:A:225:VAL:HG22	1.88	0.74
5:A:475:ASP:OD2	16:L:74:LEU:HA	1.87	0.74
6:B:292:ARG:HA	6:B:292:ARG:CZ	2.16	0.74
6:B:347:LEU:CD2	6:B:351:HIS:CE1	2.71	0.74
20:B:1753:CLA:H43	20:B:1753:CLA:CAA	2.16	0.74
11:G:46:ALA:H	11:G:49:THR:HG22	1.53	0.74
11:G:47:GLY:H	11:G:48:ASP:HA	1.52	0.74
21:1:7004:LMU:C1	21:1:7004:LMU:C3'	2.66	0.74
4:4:126:LEU:N	4:4:127:PRO:HD3	2.03	0.74
5:A:76:ARG:NH1	5:A:192:LYS:CG	2.45	0.74
5:A:270:PHE:CE1	20:A:1797:CLA:H2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1788:CLA:CBC	20:A:1793:CLA:HBC2	2.17	0.74
20:A:1792:CLA:HBA2	20:A:1792:CLA:CGD	2.17	0.74
20:A:1801:CLA:HED1	16:L:32:LEU:HD13	1.69	0.74
6:B:292:ARG:C	6:B:293:THR:HG1	1.91	0.74
20:B:1755:CLA:H72	20:B:1769:CLA:C2D	2.18	0.74
14:J:10:VAL:HG13	14:J:14:LEU:HG	1.69	0.74
5:A:216:LEU:HD12	22:A:1803:BCR:H353	1.70	0.74
5:A:457:SER:O	5:A:544:ILE:HD13	1.87	0.74
9:E:88:GLU:O	9:E:90:VAL:HB	1.88	0.74
21:1:7004:LMU:H12	21:1:7004:LMU:C3'	2.01	0.74
3:3:80:LYS:HB2	20:3:1214:CLA:C3D	2.17	0.74
6:B:233:TYR:CD2	20:B:1746:CLA:HED1	2.23	0.74
20:B:1748:CLA:CGA	20:B:1748:CLA:H3A	2.18	0.74
3:3:194:ILE:CG1	20:3:1212:CLA:HMC2	2.18	0.73
5:A:459:GLY:O	5:A:462:ILE:HG22	1.88	0.73
5:A:553:VAL:H	5:A:556:LEU:HD12	1.53	0.73
20:A:1760:CLA:H2A	20:A:1760:CLA:CED	2.18	0.73
20:A:1779:CLA:HBB2	22:A:1805:BCR:H351	1.70	0.73
20:A:1787:CLA:H52	20:A:1801:CLA:CHB	2.18	0.73
21:A:7010:LMU:O3'	21:A:7010:LMU:H1B	1.88	0.73
6:B:732:LYS:HG3	6:B:734:GLY:CA	2.18	0.73
9:E:55:VAL:HG23	9:E:65:VAL:HB	1.70	0.73
16:L:8:TYR:CE1	16:L:11:ILE:HG23	2.23	0.73
20:2:1215:CLA:C3	20:2:1220:CLA:CBC	2.66	0.73
5:A:452:PHE:CE1	20:A:1793:CLA:CBB	2.57	0.73
20:A:1796:CLA:NC	20:A:1796:CLA:H43	2.03	0.73
6:B:98:GLN:C	6:B:100:ALA:H	1.92	0.73
6:B:700:LEU:N	6:B:700:LEU:HD23	2.02	0.73
16:L:49:PRO:HB2	16:L:139:PHE:HB2	1.70	0.73
17:N:63:ASP:H	17:N:64:ASP:C	1.90	0.73
18:R:35:UNK:O	18:R:36:UNK:C	2.35	0.73
1:1:45:ILE:HA	1:1:48:ARG:HB2	1.68	0.73
2:2:68:LEU:CD1	20:2:1217:CLA:H192	2.18	0.73
20:4:1199:CLA:HED1	20:4:1199:CLA:H2	1.69	0.73
5:A:227:LEU:HD23	5:A:231:GLN:HE22	1.53	0.73
20:A:1763:CLA:CMB	22:A:1808:BCR:HC7	2.17	0.73
20:A:1790:CLA:HMC1	20:A:1790:CLA:HBC2	1.70	0.73
6:B:91:ILE:HD12	6:B:104:PHE:CE2	2.23	0.73
6:B:664:LEU:O	6:B:667:TRP:HZ3	1.71	0.73
16:L:63:LEU:HD22	16:L:64:LEU:N	2.02	0.73
20:L:1168:CLA:HAA1	20:L:1168:CLA:O1D	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:72:LYS:HZ2	17:N:74:LYS:HG3	1.53	0.73
2:2:127:ASN:CG	14:J:2:ARG:NH1	2.41	0.73
20:3:1217:CLA:C2A	20:3:3011:CLA:CAC	2.64	0.73
5:A:364:MET:O	5:A:368:LEU:N	2.20	0.73
17:N:5:GLU:OE1	17:N:6:TYR:CZ	2.41	0.73
18:R:38:UNK:O	18:R:41:UNK:CB	2.36	0.73
2:2:64:ILE:O	2:2:68:LEU:CB	2.35	0.73
3:3:98:ILE:HB	17:N:61:LEU:HB2	1.70	0.73
5:A:28:LYS:O	5:A:29:THR:CG2	2.36	0.73
5:A:684:PHE:C	5:A:684:PHE:HD2	1.91	0.73
22:A:1807:BCR:H312	20:A:1813:CLA:C14	2.17	0.73
21:A:7020:LMU:H6E	21:A:7020:LMU:O5B	1.86	0.73
6:B:489:GLY:O	6:B:490:ARG:HG2	1.89	0.73
5:A:328:LYS:HE2	5:A:332:GLU:CD	2.09	0.73
20:A:1776:CLA:C8	22:A:1805:BCR:H373	2.18	0.73
20:A:1783:CLA:H172	22:A:1808:BCR:H17C	1.70	0.73
6:B:124:TRP:CG	6:B:129:LEU:HD13	2.23	0.73
10:F:30:LYS:O	10:F:31:LEU:CB	2.37	0.73
17:N:60:PHE:HA	17:N:61:LEU:O	1.87	0.73
20:1:1190:CLA:HMC3	20:1:1196:CLA:CAC	2.18	0.73
3:3:50:GLU:N	3:3:51:PRO:CD	2.52	0.73
20:4:1209:CLA:HBA1	20:4:1209:CLA:CBF	2.17	0.73
5:A:387:THR:CG2	5:A:523:VAL:HG11	2.18	0.73
5:A:447:ASN:ND2	6:B:678:LEU:HD21	2.04	0.73
5:A:542:HIS:HA	5:A:545:HIS:HD2	1.54	0.73
5:A:628:ILE:HG13	5:A:632:GLY:HA2	1.69	0.73
22:A:1806:BCR:HC8	22:A:1806:BCR:H331	1.70	0.73
6:B:8:PHE:O	6:B:35:ASP:HB2	1.87	0.73
6:B:394:PHE:O	6:B:542:ARG:NE	2.18	0.73
20:B:1771:CLA:C19	13:I:21:MET:HB3	2.18	0.73
9:E:39:LEU:O	9:E:40:ARG:HD3	1.88	0.73
9:E:86:GLU:HG3	9:E:87:VAL:H	0.71	0.73
20:K:1085:CLA:C1A	20:K:1142:CLA:CMD	2.67	0.73
17:N:67:LEU:CB	17:N:68:GLU:CG	2.45	0.73
5:A:309:LEU:HD21	20:A:1776:CLA:HMC3	1.71	0.73
5:A:316:MET:CB	5:A:317:TYR:CB	2.56	0.73
5:A:472:ARG:HH12	16:L:74:LEU:CG	1.91	0.73
5:A:692:PHE:CE2	20:A:1796:CLA:HBC3	2.24	0.73
20:A:1779:CLA:CHD	22:A:1805:BCR:C20	2.66	0.73
20:A:1800:CLA:HMB2	20:L:1167:CLA:HBC1	1.69	0.73
6:B:329:SER:O	6:B:330:ILE:HG22	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:438:VAL:HG23	20:B:1763:CLA:HAC1	1.71	0.73
9:E:39:LEU:C	9:E:40:ARG:HD3	2.08	0.73
17:N:67:LEU:CA	17:N:68:GLU:HG2	2.18	0.73
3:3:194:ILE:HG13	20:3:1212:CLA:CMC	2.19	0.73
4:4:38:ARG:HG3	4:4:38:ARG:NH1	1.94	0.73
20:4:1201:CLA:C2	20:4:1201:CLA:O1A	2.29	0.73
5:A:393:LEU:HD11	5:A:750:PHE:CE1	2.23	0.73
20:A:1783:CLA:H102	22:A:1807:BCR:H372	1.70	0.73
20:A:1787:CLA:HAC2	20:A:1801:CLA:HMC3	1.71	0.73
21:A:7016:LMU:C7	21:A:7016:LMU:C11	2.67	0.73
21:A:7032:LMU:H1B	21:A:7032:LMU:H32	1.70	0.73
6:B:533:ILE:HD11	6:B:575:ASP:O	1.88	0.73
7:C:1:MET:H1	7:C:4:SER:CB	2.00	0.73
17:N:72:LYS:CG	17:N:74:LYS:H	1.98	0.73
21:R:1056:LMU:O5B	21:R:1056:LMU:C5'	2.33	0.73
3:3:208:PRO:HB3	3:3:210:GLN:OE1	1.89	0.73
5:A:54:ILE:O	5:A:58:HIS:HD2	1.71	0.73
5:A:270:PHE:CZ	20:A:1797:CLA:H2	2.24	0.73
5:A:289:PRO:O	5:A:290:LEU:HB2	1.89	0.73
5:A:442:ILE:CG2	20:A:1786:CLA:HMC3	2.18	0.73
20:A:1816:CLA:CHD	20:A:1816:CLA:HBC2	2.10	0.73
6:B:304:ILE:HG22	20:B:1752:CLA:CGD	2.19	0.73
10:F:125:LEU:O	10:F:126:ALA:CB	2.36	0.73
11:G:13:GLY:O	11:G:16:LEU:HG	1.89	0.73
12:H:42:THR:HG22	12:H:45:ALA:HB2	1.70	0.73
20:4:1198:CLA:O1A	20:4:1198:CLA:C2	2.29	0.72
5:A:220:ARG:O	5:A:221:HIS:HB2	1.88	0.72
20:A:1770:CLA:CHC	22:A:1803:BCR:C17	2.66	0.72
20:A:1781:CLA:H61	20:A:1782:CLA:CED	2.19	0.72
22:A:1807:BCR:C32	22:A:1808:BCR:H391	2.19	0.72
21:A:1810:LMU:O6B	21:A:1810:LMU:O1'	2.06	0.72
21:A:7021:LMU:O6'	21:A:7021:LMU:C1	2.37	0.72
20:B:1756:CLA:H122	22:B:1777:BCR:C13	2.18	0.72
20:J:1045:CLA:CBD	20:J:1045:CLA:CGA	2.67	0.72
16:L:36:TYR:O	16:L:36:TYR:CD1	2.41	0.72
17:N:75:TYR:C	17:N:76:LYS:O	2.26	0.72
2:2:99:LEU:HB3	20:2:1222:CLA:HBB1	1.71	0.72
21:2:7006:LMU:H22	21:2:7006:LMU:C2'	2.19	0.72
4:4:169:GLN:HG2	20:4:1199:CLA:HAC2	1.71	0.72
5:A:281:LEU:HD11	20:A:1772:CLA:CED	0.95	0.72
5:A:707:ILE:O	5:A:711:HIS:CD2	2.42	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1763:CLA:HBA2	20:A:1765:CLA:H12	1.71	0.72
20:A:1769:CLA:HBA1	20:A:1780:CLA:C4	2.18	0.72
20:A:1781:CLA:HED3	20:A:1782:CLA:CMD	2.09	0.72
6:B:378:ILE:O	6:B:380:GLY:N	2.21	0.72
20:B:1738:CLA:H91	20:B:1738:CLA:H193	1.71	0.72
20:B:1753:CLA:HMC1	20:B:1753:CLA:HBC3	0.78	0.72
20:B:1755:CLA:HMB2	20:B:1769:CLA:O1A	1.89	0.72
7:C:6:LYS:HB3	7:C:63:LEU:HD21	1.71	0.72
13:I:12:VAL:O	13:I:17:PRO:CD	2.36	0.72
17:N:72:LYS:CB	17:N:74:LYS:HB2	2.19	0.72
5:A:131:ILE:HD13	6:B:446:PHE:C	2.10	0.72
5:A:210:LEU:HD12	20:A:1769:CLA:HMB2	1.72	0.72
11:G:68:ILE:HG23	11:G:72:LEU:CD1	2.14	0.72
17:N:41:LYS:HB2	17:N:42:PHE:HB3	0.80	0.72
5:A:51:THR:CB	20:A:1795:CLA:CBB	2.53	0.72
5:A:98:PHE:HZ	20:A:1763:CLA:HMD3	1.54	0.72
5:A:755:ILE:O	5:A:756:ALA:HB3	1.87	0.72
20:A:1776:CLA:HMD2	20:A:1778:CLA:HBB2	1.67	0.72
6:B:38:THR:OG1	6:B:41:ARG:HB2	1.89	0.72
3:3:52:LYS:HA	3:3:55:ALA:HB3	1.70	0.72
5:A:426:THR:HA	5:A:428:TYR:CE2	2.25	0.72
5:A:514:THR:O	5:A:531:PRO:O	2.07	0.72
5:A:685:VAL:CG2	20:A:1796:CLA:HBB1	2.12	0.72
12:H:49:LYS:O	12:H:51:GLY:N	2.22	0.72
17:N:47:THR:CB	17:N:52:LEU:O	2.37	0.72
17:N:61:LEU:HD12	17:N:62:SER:CA	2.19	0.72
17:N:62:SER:CB	17:N:66:ASP:CA	2.65	0.72
17:N:72:LYS:NZ	17:N:74:LYS:HG3	2.03	0.72
20:2:1212:CLA:O2A	20:2:1212:CLA:H43	1.89	0.72
3:3:106:TYR:CD2	3:3:107:TRP:CD1	2.78	0.72
20:4:1201:CLA:CMA	20:4:1201:CLA:CGA	2.66	0.72
5:A:23:ASP:OD1	5:A:33:GLN:CD	2.26	0.72
21:A:7016:LMU:H81	21:A:7016:LMU:H32	1.46	0.72
17:N:48:GLY:HA3	17:N:49:CYS:HB2	1.71	0.72
19:T:1:GLC:C2	19:T:2:FRU:C1	2.64	0.72
5:A:76:ARG:O	5:A:186:TYR:HD2	1.71	0.72
5:A:79:PHE:HE2	5:A:185:HIS:CE1	2.06	0.72
5:A:85:GLN:O	5:A:89:ILE:HG13	1.90	0.72
5:A:187:HIS:CD2	20:A:1767:CLA:C4C	2.73	0.72
5:A:218:TRP:O	5:A:222:GLN:HB2	1.89	0.72
5:A:479:ASP:HA	5:A:536:THR:HG23	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1800:CLA:HMD3	22:B:1780:BCR:C3	2.20	0.72
20:A:1815:CLA:CMA	20:A:1815:CLA:C6	2.64	0.72
6:B:707:LEU:CD1	6:B:711:VAL:HG21	2.20	0.72
20:B:1768:CLA:H61	22:B:1779:BCR:H323	1.70	0.72
8:D:69:ARG:O	8:D:70:GLU:HB2	1.90	0.72
22:I:1032:BCR:H382	22:I:1032:BCR:H402	1.71	0.72
16:L:48:ASN:HD22	16:L:115:ALA:HB2	1.54	0.72
19:Q:1:GLC:O3	19:Q:1:GLC:C6	2.30	0.72
3:3:52:LYS:O	3:3:56:TYR:HD2	1.63	0.72
5:A:340:GLY:O	5:A:343:HIS:N	2.22	0.72
20:A:1815:CLA:CMA	20:A:1815:CLA:H2	2.20	0.72
10:F:28:SER:O	10:F:29:LEU:C	2.27	0.72
10:F:53:PHE:C	10:F:55:ASN:H	1.93	0.72
22:L:1169:BCR:H403	22:L:1169:BCR:C27	2.18	0.72
6:B:492:ILE:H	6:B:492:ILE:CD1	2.01	0.72
11:G:92:GLY:C	11:G:94:ASP:OD1	2.28	0.72
20:K:1085:CLA:C1A	20:K:1142:CLA:HMD1	2.20	0.72
16:L:40:LEU:HB3	16:L:41:PRO:HD3	1.71	0.72
16:L:107:PHE:HB2	16:L:109:GLU:OE1	1.89	0.72
16:L:124:LYS:O	16:L:126:GLN:N	2.23	0.72
19:W:1:GLC:HO2	19:W:2:FRU:H12	1.53	0.72
2:2:120:ASN:HA	14:J:5:LYS:HB2	1.71	0.72
20:2:1224:CLA:H18	20:2:1224:CLA:ND	2.04	0.72
5:A:103:PHE:N	5:A:103:PHE:HD2	1.87	0.72
5:A:174:PHE:CE2	20:A:1761:CLA:H152	2.24	0.72
20:A:1765:CLA:CBB	20:B:1763:CLA:CMD	2.66	0.72
21:A:7027:LMU:H2B	21:A:7027:LMU:C6B	2.18	0.72
7:C:11:CYS:SG	7:C:12:ILE:N	2.63	0.72
8:D:60:MET:SD	8:D:61:PRO:HD2	2.30	0.72
11:G:13:GLY:O	11:G:16:LEU:CG	2.38	0.72
12:H:37:SER:HB3	16:L:51:LEU:HG	1.72	0.72
16:L:66:GLY:N	16:L:67:PRO:HD2	2.05	0.72
17:N:5:GLU:CD	17:N:6:TYR:CG	2.63	0.72
4:4:39:TRP:CG	4:4:40:PHE:N	2.58	0.71
5:A:41:SER:O	5:A:44:ILE:HA	1.89	0.71
5:A:668:TYR:CE2	6:B:617:MET:SD	2.83	0.71
5:A:747:TRP:CD2	22:A:1807:BCR:H401	2.25	0.71
20:A:1763:CLA:HAA2	20:A:1765:CLA:HED1	1.72	0.71
20:A:1789:CLA:HMC1	20:A:1789:CLA:HBC3	1.71	0.71
22:A:1803:BCR:C12	22:A:1803:BCR:H341	2.17	0.71
22:A:1807:BCR:HC31	22:B:1778:BCR:H17C	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7028:LMU:O6'	21:A:7028:LMU:H1'	1.86	0.71
6:B:427:LEU:HD13	20:B:1735:CLA:OBD	1.90	0.71
6:B:504:ASN:H	6:B:504:ASN:ND2	1.87	0.71
6:B:615:TYR:HD1	6:B:615:TYR:H	1.38	0.71
7:C:1:MET:N	7:C:3:HIS:N	2.30	0.71
11:G:21:PHE:O	11:G:23:PHE:CB	2.37	0.71
11:G:42:SER:OG	11:G:45:GLU:CD	2.29	0.71
12:H:21:TRP:H	12:H:22:ASP:HB3	1.55	0.71
16:L:95:LEU:HA	16:L:98:CYS:HB2	1.71	0.71
20:L:1167:CLA:HHC	22:L:1170:BCR:HC8	1.71	0.71
17:N:50:GLN:HA	17:N:51:ASP:C	2.10	0.71
19:M:1:GLC:O2	19:M:2:FRU:H5	1.87	0.71
20:1:1187:CLA:CBA	20:1:1187:CLA:CMA	2.59	0.71
3:3:92:TRP:CZ2	5:A:250:LEU:HD12	2.25	0.71
3:3:93:PHE:H	3:3:93:PHE:HD2	1.38	0.71
20:4:4014:CLA:O1A	20:4:4014:CLA:HED3	1.90	0.71
5:A:119:SER:HB2	5:A:136:VAL:HG21	1.71	0.71
5:A:475:ASP:HB3	20:A:1789:CLA:HED3	1.72	0.71
6:B:188:LEU:HD11	20:B:1745:CLA:CBB	2.19	0.71
20:B:1752:CLA:CBB	20:B:1752:CLA:H72	2.19	0.71
10:F:93:ILE:O	10:F:96:TRP:CD1	2.40	0.71
5:A:79:PHE:CE2	5:A:185:HIS:CE1	2.79	0.71
5:A:381:PRO:CB	20:A:1774:CLA:HAA2	2.18	0.71
5:A:708:VAL:HA	5:A:711:HIS:HD2	1.54	0.71
5:A:747:TRP:CE3	22:A:1807:BCR:C40	2.73	0.71
21:A:7027:LMU:H2B	21:A:7027:LMU:H6'1	1.72	0.71
6:B:145:LEU:HA	6:B:148:ILE:HD12	1.71	0.71
6:B:437:TYR:HB3	6:B:616:LEU:HD23	1.72	0.71
20:B:1745:CLA:O2D	20:B:1745:CLA:OBD	2.06	0.71
23:B:1773:PQN:H291	24:B:1783:LMG:H201	1.71	0.71
8:D:94:TYR:O	8:D:95:LYS:CG	2.38	0.71
8:D:113:HIS:N	8:D:114:PRO:HD2	2.05	0.71
10:F:17:ARG:HA	10:F:17:ARG:HE	1.54	0.71
10:F:42:ILE:CG1	10:F:43:LYS:H	1.99	0.71
10:F:80:TRP:HE3	20:F:1157:CLA:HMC2	1.54	0.71
16:L:10:VAL:HG22	16:L:10:VAL:O	1.89	0.71
17:N:49:CYS:O	17:N:50:GLN:C	2.29	0.71
5:A:397:THR:HB	5:A:613:ILE:HD11	1.73	0.71
20:A:1759:CLA:C4	20:A:1796:CLA:H8	2.20	0.71
22:A:1806:BCR:H331	22:A:1806:BCR:C8	2.20	0.71
21:A:7042:LMU:H1B	21:A:7042:LMU:H3O2	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:91:ILE:CD1	6:B:104:PHE:HE2	2.04	0.71
6:B:444:LEU:O	6:B:445:ALA:HB3	1.90	0.71
7:C:74:THR:CB	7:C:80:ALA:HB2	2.20	0.71
20:J:1044:CLA:H91	20:J:1044:CLA:H151	1.71	0.71
16:L:118:LEU:HD12	16:L:119:THR:N	2.04	0.71
17:N:45:ASN:CG	17:N:45:ASN:O	2.29	0.71
20:3:1219:CLA:H102	20:3:1219:CLA:H143	1.70	0.71
5:A:370:ILE:HG22	5:A:400:MET:CA	2.19	0.71
5:A:443:ILE:HD11	5:A:557:LEU:HG	1.73	0.71
20:A:1796:CLA:H161	22:A:1807:BCR:HC22	1.70	0.71
6:B:299:HIS:CE1	20:B:1752:CLA:HMD1	2.26	0.71
6:B:654:HIS:CE1	20:B:1785:CLA:NB	2.58	0.71
9:E:53:VAL:HG12	9:E:54:ALA:H	1.55	0.71
14:J:31:ARG:HA	14:J:34:PRO:HA	1.72	0.71
15:K:51:ASP:HB3	15:K:52:PRO:HD3	1.70	0.71
17:N:35:VAL:HG12	17:N:37:PHE:CZ	2.26	0.71
17:N:54:LYS:O	17:N:56:LYS:N	2.22	0.71
2:2:98:GLU:HG2	2:2:99:LEU:HG	1.71	0.71
5:A:387:THR:HG23	5:A:523:VAL:HG11	1.71	0.71
5:A:550:HIS:O	5:A:552:THR:O	2.07	0.71
5:A:555:ILE:HG22	6:B:670:TYR:HE2	1.53	0.71
20:A:1788:CLA:H152	22:L:1169:BCR:C36	2.20	0.71
20:A:1796:CLA:H102	20:A:1813:CLA:H152	1.73	0.71
6:B:44:GLN:OE1	6:B:163:PRO:HB2	1.90	0.71
6:B:496:GLY:O	6:B:499:ASN:HB2	1.91	0.71
6:B:545:LYS:HG2	6:B:546:LEU:N	2.03	0.71
9:E:39:LEU:H	9:E:40:ARG:HH11	1.37	0.71
9:E:44:TYR:CG	9:E:73:ASN:HB2	2.25	0.71
16:L:99:LEU:HD11	22:L:1169:BCR:HC7	1.72	0.71
3:3:52:LYS:O	3:3:56:TYR:N	2.21	0.71
5:A:281:LEU:HA	5:A:297:THR:O	1.91	0.71
6:B:25:ILE:HG22	22:L:1169:BCR:C29	2.14	0.71
6:B:46:ILE:HD11	20:B:1737:CLA:H192	1.72	0.71
6:B:144:PHE:CD2	6:B:144:PHE:O	2.42	0.71
6:B:334:LEU:HB2	20:B:1737:CLA:HMD3	1.72	0.71
6:B:362:ALA:O	6:B:363:GLN:HG3	1.90	0.71
22:B:1775:BCR:HC8	22:B:1775:BCR:C33	2.20	0.71
7:C:26:LEU:N	7:C:43:PRO:HG3	2.05	0.71
9:E:68:ARG:NH2	9:E:69:PHE:HA	2.05	0.71
17:N:74:LYS:O	17:N:76:LYS:N	2.24	0.71
1:1:163:VAL:HA	1:1:166:SER:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:1200:CLA:HMC1	20:4:1198:CLA:HMB3	1.73	0.71
20:A:1781:CLA:H2	20:A:1782:CLA:CED	2.20	0.71
6:B:375:HIS:HE1	20:B:1758:CLA:NC	1.89	0.71
20:B:1749:CLA:C3	20:B:1754:CLA:H92	2.20	0.71
20:B:1753:CLA:HAA2	20:B:1753:CLA:CBD	2.20	0.71
20:B:1756:CLA:H8	22:B:1777:BCR:H12C	1.71	0.71
23:B:1773:PQN:H192	22:B:1780:BCR:C8	2.21	0.71
15:K:47:ILE:HG23	15:K:48:GLN:H	1.54	0.71
20:2:1220:CLA:C6	3:3:140:LYS:HZ2	2.04	0.71
5:A:249:ILE:O	5:A:251:ASN:N	2.23	0.71
20:A:1782:CLA:O2A	20:A:1782:CLA:C4	2.39	0.71
21:A:7009:LMU:H12	21:A:7009:LMU:O2'	1.90	0.71
6:B:152:ALA:O	6:B:153:GLY:C	2.28	0.71
6:B:454:LEU:CD1	10:F:69:PRO:O	2.38	0.71
10:F:24:LYS:C	10:F:26:GLN:H	1.93	0.71
11:G:28:ARG:CG	11:G:29:GLU:N	2.53	0.71
17:N:61:LEU:HG	17:N:62:SER:H	1.55	0.71
17:N:65:LEU:O	17:N:66:ASP:C	2.29	0.71
5:A:166:CYS:HB3	20:A:1798:CLA:HBB1	1.73	0.71
5:A:223:VAL:HG23	5:A:227:LEU:HD13	1.73	0.71
5:A:479:ASP:OD2	5:A:536:THR:HG23	1.90	0.71
20:A:1783:CLA:H111	22:A:1808:BCR:H353	1.73	0.71
6:B:25:ILE:HG21	22:L:1169:BCR:H292	0.72	0.71
11:G:46:ALA:C	11:G:48:ASP:OD1	2.28	0.71
16:L:52:ARG:O	16:L:56:VAL:HG23	1.90	0.71
16:L:126:GLN:N	16:L:127:PRO:HD2	2.05	0.71
17:N:11:LYS:HD2	17:N:12:THR:O	1.91	0.71
20:4:1199:CLA:CBC	20:4:1199:CLA:CMC	2.65	0.70
5:A:211:LEU:O	5:A:214:GLY:O	2.09	0.70
20:A:1774:CLA:O1A	20:A:1784:CLA:H71	1.91	0.70
20:A:1776:CLA:C4C	20:A:1782:CLA:H172	2.20	0.70
20:A:1800:CLA:H112	20:A:1800:CLA:C6	2.18	0.70
6:B:295:PHE:HD2	6:B:295:PHE:N	1.85	0.70
6:B:400:PRO:HD2	8:D:143:PRO:HD3	1.74	0.70
17:N:42:PHE:O	17:N:43:PRO:C	2.30	0.70
3:3:106:TYR:O	3:3:108:ALA:HB2	1.91	0.70
20:3:3011:CLA:HMA2	20:3:3011:CLA:C1	2.14	0.70
5:A:331:LEU:CD2	5:A:331:LEU:O	2.30	0.70
5:A:445:HIS:O	5:A:446:LEU:CB	2.39	0.70
5:A:454:GLY:N	5:A:457:SER:HB3	1.99	0.70
6:B:130:ARG:HG2	6:B:130:ARG:HH11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:463:ILE:O	6:B:464:GLN:HB3	1.91	0.70
8:D:28:ILE:HG12	8:D:67:ILE:CG1	2.21	0.70
17:N:42:PHE:HD1	17:N:43:PRO:N	1.84	0.70
3:3:74:ALA:CA	20:3:1215:CLA:C1D	2.69	0.70
4:4:126:LEU:O	4:4:126:LEU:HG	1.89	0.70
5:A:645:SER:HB3	6:B:637:PRO:HG3	1.72	0.70
6:B:199:ILE:HG23	6:B:270:LEU:HD22	1.71	0.70
20:B:1755:CLA:HED2	20:B:1756:CLA:OBD	1.91	0.70
24:B:1783:LMG:O3	7:C:70:TRP:NE1	2.24	0.70
9:E:42:GLU:HG2	9:E:43:SER:H	1.54	0.70
11:G:68:ILE:HG22	11:G:72:LEU:HD13	1.70	0.70
20:J:1044:CLA:H72	20:J:1044:CLA:H42	1.71	0.70
17:N:79:SER:CA	17:N:80:ASN:C	2.57	0.70
18:R:37:UNK:O	18:R:43:UNK:N	2.24	0.70
1:1:24:PHE:HB3	6:B:314:ARG:NH2	2.06	0.70
2:2:120:ASN:CG	14:J:5:LYS:CD	2.59	0.70
20:2:1218:CLA:O1D	20:2:1218:CLA:H2A	1.91	0.70
3:3:157:ALA:C	3:3:158:TYR:CD2	2.64	0.70
20:4:1198:CLA:CAA	20:4:1198:CLA:CGD	2.69	0.70
5:A:51:THR:OG1	20:A:1795:CLA:CBB	2.40	0.70
5:A:485:GLN:O	5:A:487:VAL:N	2.24	0.70
5:A:497:ALA:HB2	5:A:515:TRP:CB	2.20	0.70
20:A:1763:CLA:C4B	22:A:1808:BCR:C33	2.67	0.70
20:A:1795:CLA:H42	20:A:1795:CLA:O1A	1.91	0.70
21:A:7016:LMU:O6'	21:A:7016:LMU:H12	1.89	0.70
6:B:172:GLU:HG3	6:B:301:ILE:HG13	1.72	0.70
7:C:17:CYS:C	7:C:58:CYS:HB2	2.11	0.70
10:F:116:GLN:C	10:F:118:GLU:H	1.93	0.70
13:I:20:ALA:O	13:I:24:LEU:HB3	1.91	0.70
20:J:1043:CLA:H152	20:J:1044:CLA:HMB1	1.73	0.70
17:N:4:GLU:OE2	17:N:4:GLU:C	2.30	0.70
17:N:54:LYS:HG2	17:N:57:LYS:NZ	2.06	0.70
20:2:1213:CLA:H93	20:2:1213:CLA:H51	1.71	0.70
4:4:159:LEU:O	4:4:163:PHE:HB2	1.91	0.70
20:4:4014:CLA:CED	20:4:4014:CLA:O1A	2.39	0.70
6:B:438:VAL:HG22	20:B:1763:CLA:HMC3	1.72	0.70
7:C:5:VAL:HB	7:C:65:VAL:CA	2.13	0.70
9:E:52:VAL:C	9:E:53:VAL:HG23	2.10	0.70
17:N:70:GLU:C	17:N:72:LYS:N	2.34	0.70
2:2:169:LEU:CD2	20:2:1215:CLA:HBB2	2.21	0.70
5:A:242:ILE:HG12	5:A:243:PRO:CD	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:467:MET:HA	5:A:470:LEU:HB2	1.72	0.70
5:A:690:LEU:HD21	5:A:738:TYR:HE1	1.56	0.70
20:A:1782:CLA:O2A	20:A:1782:CLA:H42	1.91	0.70
6:B:607:SER:HA	6:B:610:ASN:HD22	1.57	0.70
6:B:730:SER:C	6:B:731:GLY:O	2.29	0.70
23:B:1773:PQN:H2M1	23:B:1773:PQN:H142	1.74	0.70
7:C:1:MET:H2	7:C:3:HIS:C	1.91	0.70
10:F:83:PHE:O	10:F:87:GLY:CA	2.39	0.70
12:H:21:TRP:H	12:H:22:ASP:CB	2.03	0.70
20:K:3009:CLA:HBA1	20:K:3009:CLA:O2D	1.92	0.70
22:L:1170:BCR:HC8	22:L:1170:BCR:C33	2.22	0.70
17:N:63:ASP:H	17:N:65:LEU:N	1.88	0.70
19:W:1:GLC:C2	19:W:2:FRU:O5	2.35	0.70
2:2:120:ASN:HA	14:J:5:LYS:CB	2.21	0.70
3:3:163:PHE:O	3:3:164:PHE:HB2	1.91	0.70
5:A:438:HIS:CE1	5:A:442:ILE:HD11	2.26	0.70
5:A:458:PHE:CD2	20:B:1786:CLA:HMB2	2.26	0.70
5:A:723:ARG:HG2	5:A:723:ARG:NH1	2.06	0.70
20:A:1781:CLA:HBB2	20:A:1794:CLA:H3A	1.73	0.70
6:B:293:THR:HG22	6:B:294:ASN:ND2	2.07	0.70
6:B:294:ASN:OD1	11:G:38:GLN:N	2.20	0.70
8:D:28:ILE:HG21	8:D:67:ILE:HG13	1.74	0.70
10:F:63:CYS:HA	10:F:69:PRO:HA	1.74	0.70
12:H:45:ALA:HB3	12:H:46:PRO:CD	2.21	0.70
20:2:1215:CLA:C5	20:2:1220:CLA:HBC1	2.21	0.70
5:A:545:HIS:CE1	5:A:612:VAL:HG22	2.27	0.70
5:A:680:LEU:HD21	6:B:617:MET:CE	2.22	0.70
5:A:685:VAL:HG12	5:A:741:GLY:HA2	1.74	0.70
6:B:29:HIS:CG	20:B:1737:CLA:HBB2	2.27	0.70
6:B:91:ILE:CD1	6:B:104:PHE:CE2	2.75	0.70
6:B:174:ARG:NH1	20:B:1754:CLA:CMD	2.54	0.70
6:B:174:ARG:NH1	20:B:1754:CLA:HMD1	2.07	0.70
6:B:293:THR:O	11:G:38:GLN:CD	2.29	0.70
6:B:561:GLY:HA3	7:C:52:LYS:CG	2.22	0.70
20:B:1787:CLA:CBC	20:B:1787:CLA:HMC1	2.21	0.70
7:C:1:MET:CA	7:C:4:SER:OG	2.40	0.70
7:C:5:VAL:CB	7:C:65:VAL:HG22	2.22	0.70
20:2:1220:CLA:C4	3:3:140:LYS:HD3	2.18	0.70
5:A:396:PHE:CE2	5:A:616:PHE:CG	2.80	0.70
21:A:7022:LMU:O2'	21:A:7022:LMU:C5'	2.30	0.70
21:A:7042:LMU:H32	21:A:7042:LMU:O5'	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1780:BCR:H17C	20:B:1786:CLA:C10	2.18	0.70
13:I:9:VAL:HG12	13:I:10:PRO:HD3	1.73	0.70
16:L:5:LYS:HA	16:L:5:LYS:HE2	1.73	0.70
17:N:76:LYS:HG3	17:N:77:CYS:N	2.00	0.70
4:4:95:PHE:CE2	20:4:1208:CLA:C2C	2.75	0.70
6:B:230:TRP:HH2	11:G:11:SER:HB2	1.54	0.70
8:D:47:VAL:HB	8:D:76:LYS:HA	1.74	0.70
12:H:45:ALA:O	12:H:47:PHE:N	2.25	0.70
5:A:558:LYS:HZ2	6:B:674:LEU:HB3	1.56	0.69
5:A:697:ARG:NH2	6:B:566:GLY:O	2.18	0.69
6:B:141:PHE:O	6:B:143:LEU:N	2.25	0.69
6:B:421:HIS:NE2	20:B:1761:CLA:C4D	2.55	0.69
7:C:44:ARG:HH22	8:D:127:ARG:NE	1.90	0.69
11:G:37:GLU:OE2	11:G:42:SER:HA	1.92	0.69
17:N:74:LYS:O	17:N:75:TYR:C	2.30	0.69
4:4:38:ARG:CG	4:4:39:TRP:H	2.04	0.69
5:A:207:LEU:HD12	5:A:310:PHE:CD1	2.26	0.69
5:A:453:LEU:HD13	5:A:547:PHE:HA	1.74	0.69
5:A:691:MET:HE2	23:A:1802:PQN:H2M2	1.75	0.69
21:A:7042:LMU:O6'	21:A:7042:LMU:H41	1.91	0.69
6:B:15:ASP:O	6:B:20:ARG:HG2	1.90	0.69
6:B:594:TRP:CD1	6:B:594:TRP:C	2.66	0.69
6:B:696:LYS:HG2	7:C:80:ALA:HA	1.72	0.69
9:E:90:VAL:O	9:E:91:ALA:C	2.30	0.69
12:H:53:LEU:CG	12:H:54:LEU:H	2.03	0.69
20:J:1045:CLA:O1D	20:J:1045:CLA:H12	1.91	0.69
20:L:1166:CLA:HED2	20:L:1166:CLA:HAA2	1.74	0.69
5:A:25:ASP:OD1	5:A:26:PRO:CG	2.32	0.69
20:A:1764:CLA:HMB1	20:A:1765:CLA:H11	1.74	0.69
20:A:1782:CLA:CBC	20:A:1782:CLA:CMC	2.65	0.69
6:B:269:TRP:HE3	6:B:270:LEU:H	1.38	0.69
7:C:44:ARG:HH21	8:D:127:ARG:CB	2.04	0.69
8:D:111:TYR:HD2	8:D:114:PRO:CB	2.05	0.69
10:F:47:GLU:CG	10:F:51:LYS:HE3	2.09	0.69
11:G:62:ASP:HB2	11:G:63:PRO:HD3	1.73	0.69
20:A:1790:CLA:CAD	20:A:1791:CLA:HAC1	2.21	0.69
6:B:188:LEU:HD11	20:B:1745:CLA:HBB2	1.74	0.69
6:B:242:HIS:O	6:B:243:LEU:HG	1.92	0.69
6:B:645:VAL:HG11	20:B:1739:CLA:HAC1	1.74	0.69
20:B:1747:CLA:H52	20:B:1756:CLA:CMB	2.22	0.69
20:B:1764:CLA:HMD2	20:B:1765:CLA:C1C	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1773:PQN:H192	22:B:1780:BCR:C10	2.09	0.69
16:L:64:LEU:HA	16:L:67:PRO:HG2	1.73	0.69
21:R:1056:LMU:O5B	21:R:1056:LMU:C6'	2.39	0.69
5:A:390:ALA:HA	5:A:393:LEU:HD23	1.74	0.69
5:A:472:ARG:O	5:A:474:GLN:HG3	1.92	0.69
6:B:655:LEU:HD21	20:B:1771:CLA:HBB1	1.74	0.69
7:C:31:TRP:HB2	7:C:39:ILE:HG21	1.75	0.69
11:G:13:GLY:HA2	11:G:16:LEU:CG	2.22	0.69
16:L:43:TYR:O	16:L:44:ARG:HB2	1.90	0.69
17:N:54:LYS:HG3	17:N:57:LYS:HZ3	1.55	0.69
18:R:51:UNK:O	18:R:52:UNK:CB	2.41	0.69
6:B:369:ALA:O	6:B:725:LEU:CD1	2.39	0.69
20:B:1771:CLA:H192	13:I:21:MET:HB3	1.73	0.69
7:C:75:ARG:HH22	8:D:110:GLN:CD	1.95	0.69
9:E:72:VAL:O	9:E:73:ASN:CB	2.39	0.69
10:F:22:LEU:C	10:F:24:LYS:H	1.93	0.69
10:F:47:GLU:HG3	10:F:51:LYS:CE	2.10	0.69
20:J:1045:CLA:CGA	20:J:1045:CLA:CGD	2.69	0.69
16:L:96:SER:OG	16:L:143:PHE:HD2	1.76	0.69
16:L:158:MET:CG	16:L:159:TYR:H	2.04	0.69
17:N:18:ASP:HB3	17:N:22:LEU:HG	1.74	0.69
20:2:1215:CLA:C4	20:2:1220:CLA:CBC	2.71	0.69
22:3:1220:BCR:H23C	22:3:1220:BCR:H393	0.77	0.69
4:4:165:GLY:O	4:4:169:GLN:HG2	1.93	0.69
5:A:259:TYR:CD2	5:A:280:PHE:HA	2.28	0.69
5:A:402:ILE:HD11	20:A:1784:CLA:HBB2	1.74	0.69
20:A:1764:CLA:C4	22:A:1807:BCR:H383	2.23	0.69
21:A:7037:LMU:C1	21:A:7037:LMU:C6	2.71	0.69
6:B:124:TRP:O	6:B:124:TRP:HD1	1.76	0.69
6:B:409:ALA:C	6:B:411:MET:H	1.96	0.69
6:B:693:TRP:HD1	20:B:1770:CLA:C1D	2.06	0.69
22:I:1032:BCR:HC21	20:I:1033:CLA:C2C	2.23	0.69
20:K:1085:CLA:C4A	20:K:1142:CLA:HMD1	2.22	0.69
5:A:157:GLY:HA2	5:A:229:ILE:CG2	2.23	0.69
5:A:225:VAL:O	5:A:229:ILE:HB	1.91	0.69
5:A:281:LEU:HD13	20:A:1772:CLA:H2A	1.71	0.69
20:A:1774:CLA:OBD	20:A:1784:CLA:H43	1.92	0.69
20:A:1800:CLA:HMC2	20:B:1770:CLA:H11	1.75	0.69
22:A:1807:BCR:H311	20:A:1813:CLA:H142	1.73	0.69
6:B:503:GLU:HB3	6:B:507:SER:HB2	1.73	0.69
6:B:595:HIS:HD2	6:B:623:TYR:OH	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1750:CLA:NB	20:B:1750:CLA:H2	2.07	0.69
20:B:1755:CLA:H72	20:B:1769:CLA:C3D	2.23	0.69
20:B:1756:CLA:H41	20:B:1756:CLA:H72	1.73	0.69
20:B:1768:CLA:H202	22:B:1779:BCR:HC41	1.75	0.69
20:J:1045:CLA:O2A	20:J:1045:CLA:C2A	2.30	0.69
19:V:1:GLC:O2	19:V:2:FRU:C3	2.30	0.69
3:3:83:LEU:HA	20:A:1798:CLA:C4	2.15	0.69
5:A:396:PHE:HE2	5:A:616:PHE:CB	2.06	0.69
5:A:453:LEU:HD21	20:A:1793:CLA:CBB	2.17	0.69
5:A:618:TRP:CZ2	5:A:655:ASP:HB2	2.27	0.69
23:A:1802:PQN:C13	22:B:1778:BCR:H322	2.23	0.69
21:A:7016:LMU:C2	21:A:7016:LMU:C7	2.71	0.69
6:B:347:LEU:HD13	6:B:351:HIS:HD1	1.58	0.69
6:B:404:ALA:C	6:B:406:ASN:N	2.45	0.69
20:B:1759:CLA:HBC2	20:B:1759:CLA:CMC	2.11	0.69
9:E:52:VAL:CG1	9:E:53:VAL:H	1.95	0.69
10:F:21:ALA:O	10:F:22:LEU:C	2.29	0.69
12:H:44:ALA:HB2	16:L:145:PHE:CE1	2.27	0.69
16:L:77:THR:HG21	16:L:82:ALA:HB1	1.74	0.69
16:L:99:LEU:HD11	22:L:1169:BCR:H313	1.74	0.69
18:R:34:UNK:C	18:R:38:UNK:CB	2.71	0.69
3:3:97:PHE:CD2	3:3:97:PHE:N	2.59	0.69
20:3:3007:CLA:HAC2	20:K:3009:CLA:H91	1.75	0.69
5:A:466:THR:O	5:A:470:LEU:HG	1.92	0.69
20:A:1782:CLA:H143	20:A:1782:CLA:H101	1.73	0.69
21:A:7026:LMU:H11	21:A:7026:LMU:H3'	1.72	0.69
21:A:7027:LMU:O2'	21:A:7027:LMU:C1	2.39	0.69
6:B:124:TRP:CD1	6:B:129:LEU:HD13	2.27	0.69
6:B:124:TRP:HE1	6:B:129:LEU:HD22	1.58	0.69
6:B:693:TRP:CD1	20:B:1770:CLA:C1D	2.76	0.69
20:B:1747:CLA:CAD	20:B:1756:CLA:CBB	2.71	0.69
20:B:1762:CLA:H51	22:B:1779:BCR:H401	1.75	0.69
8:D:102:ARG:NE	8:D:110:GLN:HB2	2.07	0.69
13:I:8:PHE:CB	20:I:1031:CLA:OBD	2.40	0.69
16:L:163:LEU:CG	16:L:164:PRO:CD	2.60	0.69
5:A:193:LEU:HA	5:A:196:PHE:CE2	2.28	0.68
5:A:385:LEU:O	5:A:386:ALA:CB	2.39	0.68
5:A:545:HIS:CE1	20:A:1792:CLA:HBB2	2.26	0.68
5:A:620:MET:HG3	5:A:625:TRP:CE2	2.28	0.68
20:A:1760:CLA:H12	20:A:1767:CLA:C6	2.16	0.68
6:B:46:ILE:HG21	20:B:1737:CLA:HBC3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:65:VAL:HG12	7:C:66:ARG:H	1.57	0.68
12:H:14:ILE:HG13	12:H:17:THR:OG1	1.93	0.68
2:2:81:THR:HG23	2:2:82:ALA:N	2.06	0.68
5:A:207:LEU:HB2	20:A:1776:CLA:HBB2	1.73	0.68
5:A:582:ASP:OD1	5:A:586:ARG:NH1	2.18	0.68
6:B:697:PRO:HB3	20:B:1770:CLA:HBC3	1.75	0.68
7:C:78:GLY:O	7:C:81:TYR:CE1	2.42	0.68
20:1:1198:CLA:C9	20:1:1198:CLA:C12	2.72	0.68
3:3:52:LYS:C	3:3:56:TYR:CD2	2.65	0.68
3:3:74:ALA:HA	20:3:1215:CLA:ND	2.09	0.68
20:4:1198:CLA:HAA2	20:4:1198:CLA:HED3	0.73	0.68
5:A:28:LYS:O	5:A:29:THR:HB	1.93	0.68
5:A:59:ALA:O	5:A:61:ALA:N	2.25	0.68
20:A:1811:CLA:HBC3	20:A:1811:CLA:HHD	1.75	0.68
6:B:438:VAL:CG2	20:B:1763:CLA:CMC	2.69	0.68
6:B:711:VAL:O	6:B:711:VAL:CG1	2.42	0.68
20:B:1749:CLA:HBB2	20:B:1754:CLA:H41	1.76	0.68
22:B:1779:BCR:HC32	20:F:1156:CLA:CMA	2.23	0.68
8:D:48:ILE:CG2	8:D:83:CYS:HB2	2.22	0.68
20:J:1045:CLA:H2A	20:J:1045:CLA:C2	2.24	0.68
5:A:51:THR:OG1	20:A:1795:CLA:HBB2	1.93	0.68
5:A:370:ILE:HG23	5:A:403:GLY:CA	2.22	0.68
20:A:1763:CLA:HMB3	20:A:1764:CLA:HBB	1.74	0.68
20:A:1782:CLA:HBA1	20:A:1782:CLA:HBD	1.74	0.68
6:B:438:VAL:HG21	20:B:1763:CLA:HMC1	1.75	0.68
13:I:14:LEU:C	13:I:17:PRO:HD2	2.14	0.68
15:K:16:THR:O	15:K:20:PHE:HB3	1.94	0.68
16:L:161:LEU:CD1	16:L:162:ASP:C	2.60	0.68
20:3:3008:CLA:CBC	20:3:3008:CLA:CMC	2.63	0.68
4:4:169:GLN:NE2	20:4:1199:CLA:CHD	2.55	0.68
5:A:309:LEU:O	5:A:310:PHE:HB2	1.93	0.68
5:A:464:ASN:HD22	5:A:464:ASN:H	1.40	0.68
6:B:576:PHE:CE2	20:B:1759:CLA:HAC1	2.28	0.68
20:B:1744:CLA:HMB3	22:B:1776:BCR:H311	1.73	0.68
7:C:1:MET:SD	7:C:4:SER:CB	2.82	0.68
10:F:95:GLY:O	10:F:99:TRP:HB2	1.93	0.68
21:R:1056:LMU:O6'	21:R:1056:LMU:C1'	2.41	0.68
1:1:97:ILE:CG2	20:1:1197:CLA:CBB	2.71	0.68
3:3:63:ARG:CZ	3:3:185:LYS:HG2	2.24	0.68
5:A:431:LEU:O	5:A:435:VAL:HG12	1.93	0.68
20:A:1776:CLA:H111	20:A:1776:CLA:H162	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:290:MET:HA	20:B:1751:CLA:HAC2	1.74	0.68
6:B:388:ALA:C	6:B:391:PRO:CD	2.61	0.68
6:B:468:GLY:O	6:B:470:THR:N	2.26	0.68
6:B:568:CYS:O	6:B:570:ILE:N	2.26	0.68
20:B:1758:CLA:H101	22:B:1776:BCR:H343	1.75	0.68
7:C:20:ALA:O	7:C:21:CYS:CB	2.42	0.68
9:E:34:SER:O	9:E:35:LYS:HB3	1.92	0.68
16:L:163:LEU:O	16:L:164:PRO:C	2.29	0.68
4:4:39:TRP:HE1	4:4:41:VAL:HG23	1.59	0.68
4:4:171:ASN:O	4:4:172:VAL:HB	1.92	0.68
5:A:370:ILE:HD13	20:A:1781:CLA:CAD	2.24	0.68
5:A:625:TRP:CB	5:A:637:ILE:HD11	2.23	0.68
20:A:1771:CLA:CED	20:A:1771:CLA:HAA1	2.23	0.68
20:A:1816:CLA:H2	20:A:1816:CLA:H72	1.75	0.68
6:B:140:ILE:HD13	6:B:140:ILE:H	1.59	0.68
6:B:711:VAL:HG22	24:B:1783:LMG:H391	1.75	0.68
22:B:1780:BCR:C20	20:B:1786:CLA:H151	2.23	0.68
9:E:44:TYR:CZ	9:E:73:ASN:HA	2.29	0.68
9:E:53:VAL:O	9:E:55:VAL:N	2.25	0.68
10:F:25:LEU:HD23	10:F:46:MET:HB3	1.72	0.68
11:G:12:THR:HG22	11:G:72:LEU:CD1	2.24	0.68
20:J:1045:CLA:HBA2	20:J:1045:CLA:CHA	2.24	0.68
3:3:93:PHE:H	3:3:95:THR:N	1.89	0.68
5:A:585:GLY:O	5:A:589:THR:OG1	2.12	0.68
6:B:438:VAL:O	6:B:441:ASP:N	2.27	0.68
20:B:1753:CLA:HAA1	20:B:1753:CLA:C4	2.20	0.68
20:B:1755:CLA:HHD	20:B:1755:CLA:HBC3	1.76	0.68
8:D:49:THR:HG22	8:D:99:GLN:HB3	1.76	0.68
11:G:28:ARG:HD2	11:G:33:LYS:HE2	1.76	0.68
15:K:67:GLY:O	15:K:68:HIS:O	2.12	0.68
16:L:69:VAL:HG11	16:L:84:GLY:H	1.58	0.68
1:1:161:PHE:N	20:1:1189:CLA:CBB	2.54	0.68
3:3:92:TRP:CA	3:3:93:PHE:CG	2.74	0.68
20:3:1219:CLA:H2A	20:3:1219:CLA:O2D	1.94	0.68
5:A:618:TRP:O	5:A:622:SER:HB3	1.94	0.68
5:A:663:GLN:HB3	5:A:752:ALA:O	1.93	0.68
20:A:1779:CLA:HBB2	22:A:1805:BCR:C35	2.19	0.68
20:A:1781:CLA:H172	22:A:1805:BCR:H332	1.75	0.68
14:J:22:LEU:O	14:J:25:LEU:N	2.27	0.68
14:J:31:ARG:NH2	20:J:1043:CLA:CHC	2.56	0.68
17:N:65:LEU:HD23	17:N:66:ASP:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:1188:CLA:HED2	20:1:1188:CLA:OBD	1.93	0.68
3:3:50:GLU:O	3:3:53:TRP:N	2.27	0.68
3:3:84:ILE:HA	20:A:1798:CLA:C5	2.15	0.68
5:A:141:ARG:HD3	10:F:39:ALA:HA	1.75	0.68
21:A:7016:LMU:C11	21:A:7016:LMU:H71	2.24	0.68
6:B:450:GLU:O	6:B:452:GLN:N	2.25	0.68
22:B:1781:BCR:C4	20:B:1787:CLA:H142	2.24	0.68
20:J:1044:CLA:H152	20:J:1044:CLA:C9	2.24	0.68
3:3:93:PHE:N	3:3:95:THR:H	1.89	0.67
5:A:203:LEU:H	5:A:203:LEU:HD12	1.59	0.67
5:A:204:ASN:O	5:A:205:HIS:CB	2.36	0.67
5:A:396:PHE:HE2	5:A:616:PHE:CG	2.11	0.67
5:A:400:MET:O	5:A:609:ILE:HD12	1.94	0.67
5:A:470:LEU:HD13	6:B:95:HIS:HB3	1.74	0.67
20:A:1785:CLA:H152	20:A:1785:CLA:H101	1.76	0.67
6:B:30:ASP:OD2	6:B:396:ARG:NH1	2.25	0.67
6:B:174:ARG:O	6:B:175:LEU:HB3	1.95	0.67
20:B:1753:CLA:H42	20:B:1753:CLA:CHB	2.23	0.67
5:A:390:ALA:HA	5:A:393:LEU:CD2	2.24	0.67
20:A:1759:CLA:H42	20:A:1796:CLA:H8	1.75	0.67
21:A:7041:LMU:O6B	21:A:7041:LMU:C1B	2.42	0.67
6:B:141:PHE:HD2	6:B:144:PHE:CE1	2.12	0.67
6:B:160:LYS:HZ3	6:B:160:LYS:HB2	1.58	0.67
6:B:160:LYS:HE3	6:B:161:TRP:CD2	2.29	0.67
6:B:269:TRP:CD1	6:B:497:TRP:CH2	2.82	0.67
6:B:646:TRP:CH2	6:B:726:ILE:HD13	2.28	0.67
20:B:1755:CLA:CAD	20:B:1767:CLA:HBB1	2.24	0.67
20:B:1762:CLA:HBB2	22:B:1778:BCR:C27	2.25	0.67
22:B:1780:BCR:C33	22:B:1780:BCR:HC8	2.24	0.67
7:C:55:GLU:C	7:C:57:ALA:H	1.98	0.67
14:J:10:VAL:CG1	14:J:11:ALA:N	2.57	0.67
20:J:1044:CLA:H41	20:J:1044:CLA:H93	1.76	0.67
15:K:4:GLY:HA2	15:K:7:THR:HB	1.75	0.67
20:K:1085:CLA:H43	20:K:1085:CLA:O2A	1.93	0.67
17:N:67:LEU:CA	17:N:68:GLU:CG	2.71	0.67
18:R:26:UNK:O	18:R:27:UNK:C	2.42	0.67
5:A:263:ALA:O	5:A:264:GLU:HG3	1.95	0.67
21:A:7020:LMU:O2'	21:A:7020:LMU:H5'	1.92	0.67
6:B:290:MET:HA	20:B:1751:CLA:CAC	2.23	0.67
20:B:1735:CLA:H191	10:F:104:TYR:CB	2.20	0.67
7:C:66:ARG:HG2	7:C:66:ARG:NH2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:91:ARG:HH12	8:D:119:TYR:HE1	1.39	0.67
10:F:15:ALA:O	10:F:18:GLU:HB2	1.94	0.67
10:F:52:ARG:NH1	10:F:55:ASN:OD1	2.28	0.67
16:L:113:SER:O	16:L:116:PRO:HD2	1.93	0.67
5:A:88:ILE:HG22	5:A:89:ILE:N	2.09	0.67
5:A:382:TYR:CE2	20:A:1784:CLA:HED3	2.29	0.67
5:A:603:PHE:HZ	5:A:693:LEU:HD21	1.60	0.67
5:A:720:THR:O	5:A:720:THR:HG22	1.94	0.67
6:B:178:HIS:O	6:B:180:SER:N	2.27	0.67
20:B:1787:CLA:HHB	20:B:1787:CLA:C4	2.23	0.67
7:C:12:ILE:HB	7:C:38:GLN:O	1.95	0.67
8:D:39:LYS:CD	8:D:42:VAL:CG1	2.72	0.67
12:H:67:TYR:O	12:H:70:ALA:O	2.13	0.67
15:K:69:ILE:HA	15:K:72:VAL:CG1	2.23	0.67
17:N:61:LEU:HD12	17:N:63:ASP:HB2	1.74	0.67
2:2:126:PRO:CD	2:2:129:LYS:HB2	2.25	0.67
5:A:408:VAL:HG11	5:A:602:LEU:HD23	1.76	0.67
5:A:436:LEU:O	5:A:439:ARG:HB3	1.95	0.67
20:A:1790:CLA:C3D	20:A:1791:CLA:HAC1	2.24	0.67
20:A:1815:CLA:HAA2	20:A:1815:CLA:O1D	1.94	0.67
6:B:127:ILE:CD1	6:B:193:HIS:CE1	2.78	0.67
6:B:273:VAL:O	6:B:277:HIS:HD2	1.76	0.67
6:B:426:SER:O	6:B:430:GLY:N	2.26	0.67
20:B:1764:CLA:HMB3	20:B:1767:CLA:HED3	1.77	0.67
22:B:1779:BCR:H333	20:F:1156:CLA:HHB	1.76	0.67
20:B:1786:CLA:H91	20:B:1787:CLA:C9	2.24	0.67
11:G:28:ARG:NH2	11:G:29:GLU:O	2.28	0.67
22:L:1170:BCR:H23C	22:L:1170:BCR:C38	2.25	0.67
18:R:26:UNK:O	18:R:28:UNK:N	2.27	0.67
4:4:38:ARG:HH11	4:4:38:ARG:CG	2.01	0.67
4:4:192:THR:HG22	4:4:193:ILE:H	1.58	0.67
5:A:107:GLU:OE1	5:A:161:GLU:CG	2.43	0.67
20:A:1790:CLA:O1A	20:A:1791:CLA:HBC3	1.94	0.67
20:A:1812:CLA:CAD	20:A:1812:CLA:CED	2.72	0.67
20:A:1817:CLA:O1D	20:A:1817:CLA:CBA	2.43	0.67
6:B:98:GLN:O	6:B:100:ALA:N	2.28	0.67
6:B:347:LEU:HD21	6:B:351:HIS:HE1	1.60	0.67
6:B:612:SER:HA	6:B:615:TYR:CE1	2.23	0.67
20:F:1157:CLA:CED	20:F:1157:CLA:CAD	2.73	0.67
12:H:10:ASP:HB3	12:H:13:ASP:HB2	1.75	0.67
20:I:1192:CLA:H61	20:I:1192:CLA:H122	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1220:CLA:C6	3:3:140:LYS:HZ3	2.07	0.67
3:3:107:TRP:CD1	3:3:108:ALA:CA	2.77	0.67
5:A:170:GLY:O	5:A:173:VAL:CG2	2.40	0.67
5:A:491:TRP:NE1	20:A:1792:CLA:H12	2.10	0.67
20:A:1800:CLA:H152	22:L:1170:BCR:H352	1.76	0.67
6:B:469:LYS:HE2	6:B:471:THR:OG1	1.94	0.67
6:B:633:ASN:ND2	6:B:636:THR:HB	2.09	0.67
6:B:694:ARG:HE	16:L:105:ALA:HA	1.60	0.67
7:C:2:SER:O	7:C:3:HIS:ND1	2.28	0.67
15:K:31:ASN:H	15:K:32:ARG:HH11	1.39	0.67
17:N:62:SER:HB2	17:N:66:ASP:OD1	1.95	0.67
2:2:114:LEU:O	2:2:116:PRO:HD3	1.94	0.67
5:A:397:THR:HB	5:A:613:ILE:CD1	2.25	0.67
20:A:1776:CLA:H61	22:A:1806:BCR:H19C	1.76	0.67
20:A:1781:CLA:O1A	20:A:1781:CLA:C2	2.41	0.67
20:A:1812:CLA:C1	6:B:616:LEU:HG	2.22	0.67
6:B:154:TRP:HD1	6:B:158:GLN:HG2	1.58	0.67
6:B:178:HIS:C	6:B:180:SER:H	1.96	0.67
6:B:598:HIS:HB3	6:B:602:TRP:CZ3	2.30	0.67
6:B:689:ASN:O	6:B:691:ILE:N	2.27	0.67
8:D:28:ILE:CG2	8:D:67:ILE:HG13	2.25	0.67
12:H:74:GLN:OE1	12:H:74:GLN:O	2.13	0.67
22:I:1032:BCR:C2	20:I:1033:CLA:CAC	2.72	0.67
20:K:1085:CLA:O2A	20:K:1085:CLA:C4	2.42	0.67
16:L:25:THR:O	16:L:28:THR:HB	1.94	0.67
3:3:47:GLY:O	3:3:49:ILE:N	2.27	0.67
5:A:164:LEU:HA	5:A:167:THR:HG23	1.75	0.67
20:A:1764:CLA:H43	22:A:1807:BCR:H383	1.77	0.67
20:A:1788:CLA:O1A	20:A:1800:CLA:C1	2.43	0.67
6:B:390:GLY:HA3	22:B:1777:BCR:HC22	1.76	0.67
20:B:1755:CLA:HED2	20:B:1756:CLA:HMD1	1.76	0.67
8:D:31:GLY:HA3	16:L:23:LEU:HD21	1.77	0.67
16:L:13:PRO:O	16:L:14:LEU:HB2	1.95	0.67
17:N:40:CYS:N	17:N:41:LYS:HA	2.10	0.67
17:N:80:ASN:OD1	17:N:82:PHE:HA	1.95	0.67
20:2:1220:CLA:H62	3:3:140:LYS:CE	2.24	0.67
3:3:63:ARG:NH1	3:3:185:LYS:O	2.28	0.67
3:3:173:GLU:CG	3:3:174:LYS:N	2.57	0.67
5:A:368:LEU:HD21	20:A:1774:CLA:H91	1.69	0.67
20:A:1787:CLA:C4	16:L:33:ILE:HG12	2.24	0.67
20:A:1812:CLA:H122	20:A:1812:CLA:H92	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7043:LMU:H62	21:A:7043:LMU:H111	1.76	0.67
6:B:81:PRO:HG2	6:B:360:PHE:CD1	2.30	0.67
6:B:576:PHE:HE2	20:B:1759:CLA:HAC1	1.59	0.67
7:C:66:ARG:HH21	7:C:66:ARG:CG	2.03	0.67
2:2:108:ARG:NH2	20:2:1224:CLA:O1D	2.28	0.66
3:3:97:PHE:O	3:3:98:ILE:HG23	1.95	0.66
4:4:52:MET:HG3	4:4:160:MET:CG	2.22	0.66
5:A:708:VAL:HA	5:A:711:HIS:CD2	2.30	0.66
6:B:418:ILE:O	6:B:422:LEU:HD12	1.94	0.66
10:F:140:ALA:O	10:F:144:LEU:HB3	1.96	0.66
16:L:65:VAL:C	16:L:67:PRO:HD2	2.14	0.66
2:2:49:LEU:HB3	20:2:1215:CLA:HAC2	1.76	0.66
3:3:106:TYR:CG	3:3:107:TRP:CD1	2.84	0.66
4:4:108:ASP:N	20:4:1196:CLA:HMA2	2.08	0.66
5:A:114:THR:CG2	5:A:115:HIS:CE1	2.75	0.66
5:A:425:THR:O	5:A:427:ARG:NE	2.28	0.66
5:A:555:ILE:HG23	20:B:1787:CLA:OBD	1.95	0.66
6:B:190:TRP:HE3	20:B:1744:CLA:CBB	2.08	0.66
6:B:267:SER:HA	6:B:356:PRO:O	1.95	0.66
6:B:692:ARG:HH22	6:B:694:ARG:HG2	1.60	0.66
20:B:1739:CLA:CMC	22:B:1780:BCR:H282	2.25	0.66
20:B:1740:CLA:HAA1	20:B:1740:CLA:H12	1.76	0.66
7:C:70:TRP:O	7:C:72:GLU:CB	2.43	0.66
5:A:129:GLN:O	5:A:130:GLU:HB2	1.95	0.66
5:A:216:LEU:HD12	22:A:1803:BCR:C35	2.25	0.66
5:A:370:ILE:HD12	20:A:1781:CLA:O1D	1.94	0.66
5:A:539:PHE:HD2	5:A:539:PHE:O	1.78	0.66
5:A:629:ASN:HD21	5:A:633:VAL:HG23	1.59	0.66
5:A:660:GLN:O	5:A:661:ALA:CB	2.42	0.66
20:A:1785:CLA:H152	20:A:1785:CLA:C10	2.26	0.66
20:A:1811:CLA:HBC3	20:A:1811:CLA:CHD	2.25	0.66
20:A:1815:CLA:HMA1	20:A:1815:CLA:C6	2.24	0.66
21:A:7026:LMU:C8	21:A:7026:LMU:C4	2.65	0.66
6:B:127:ILE:CD1	6:B:193:HIS:HE1	2.08	0.66
20:B:1746:CLA:CBC	20:B:1746:CLA:CHD	2.74	0.66
20:B:1748:CLA:CGA	20:B:1748:CLA:C3A	2.73	0.66
17:N:33:TYR:O	17:N:34:THR:HG22	1.96	0.66
17:N:40:CYS:H	17:N:41:LYS:HA	1.59	0.66
19:Q:1:GLC:H2	19:Q:2:FRU:O4	1.96	0.66
20:1:1192:CLA:HHD	20:1:1192:CLA:HBC3	1.76	0.66
5:A:173:VAL:HG23	5:A:174:PHE:HD1	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:578:ARG:O	5:A:579:PHE:CD1	2.49	0.66
21:A:1810:LMU:H5'	21:A:1810:LMU:O5B	1.94	0.66
6:B:349:ALA:HB2	6:B:375:HIS:HB3	1.78	0.66
20:B:1736:CLA:HBC3	20:B:1759:CLA:H51	1.77	0.66
7:C:55:GLU:O	7:C:57:ALA:N	2.21	0.66
12:H:63:SER:O	12:H:67:TYR:HB2	1.95	0.66
3:3:84:ILE:N	20:A:1798:CLA:H43	2.10	0.66
3:3:114:PHE:CD1	20:3:1216:CLA:CHA	2.79	0.66
4:4:118:ASP:O	4:4:122:LYS:HA	1.96	0.66
5:A:154:ARG:HH21	5:A:233:LEU:HD13	1.60	0.66
5:A:229:ILE:CG1	5:A:243:PRO:HB3	2.25	0.66
5:A:255:LEU:CD1	5:A:280:PHE:HZ	2.09	0.66
6:B:187:SER:O	6:B:189:ALA:N	2.28	0.66
6:B:203:ARG:H	6:B:270:LEU:HD11	1.60	0.66
6:B:292:ARG:NH2	6:B:297:ILE:HG13	2.10	0.66
6:B:649:MET:O	6:B:653:GLY:N	2.27	0.66
22:B:1780:BCR:H19C	20:B:1786:CLA:C15	2.23	0.66
7:C:73:THR:N	7:C:76:SER:OG	2.29	0.66
9:E:87:VAL:O	9:E:89:GLU:N	2.27	0.66
20:H:1079:CLA:HBB2	13:I:13:GLY:C	2.15	0.66
15:K:71:GLY:O	15:K:72:VAL:C	2.31	0.66
16:L:161:LEU:HD11	16:L:162:ASP:C	2.15	0.66
17:N:45:ASN:HD21	17:N:54:LYS:HB2	1.51	0.66
17:N:70:GLU:HB3	17:N:72:LYS:CA	2.25	0.66
5:A:68:THR:C	5:A:70:ASP:H	1.99	0.66
5:A:636:HIS:O	5:A:638:THR:N	2.29	0.66
20:A:1788:CLA:C15	22:L:1169:BCR:C36	2.74	0.66
21:A:7026:LMU:H52	21:A:7026:LMU:C1	2.22	0.66
6:B:141:PHE:HA	6:B:144:PHE:CD1	2.31	0.66
7:C:74:THR:O	7:C:76:SER:N	2.28	0.66
8:D:39:LYS:NZ	8:D:43:GLU:OE2	2.28	0.66
16:L:69:VAL:HG11	16:L:84:GLY:N	2.10	0.66
17:N:18:ASP:HB2	17:N:22:LEU:CD1	2.24	0.66
20:R:1054:CLA:H2A	20:R:1054:CLA:O1A	1.94	0.66
5:A:123:VAL:HG22	5:A:133:ASN:OD1	1.94	0.66
20:A:1812:CLA:HMB3	20:B:1785:CLA:C18	2.24	0.66
21:A:7016:LMU:H112	21:A:7016:LMU:H71	1.78	0.66
6:B:247:THR:CG2	6:B:250:ALA:HB3	2.25	0.66
6:B:292:ARG:NH2	6:B:297:ILE:H	1.94	0.66
7:C:1:MET:CB	7:C:4:SER:HG	1.92	0.66
8:D:126:GLY:C	8:D:127:ARG:HG2	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:147:GLY:HA2	10:F:150:VAL:HB	1.78	0.66
20:K:1085:CLA:O1A	20:K:1085:CLA:C3A	2.32	0.66
16:L:10:VAL:O	16:L:10:VAL:CG2	2.44	0.66
17:N:61:LEU:O	17:N:62:SER:HB2	1.93	0.66
20:3:1219:CLA:O1A	20:3:1219:CLA:CMA	2.43	0.66
4:4:91:PHE:CD1	20:4:1205:CLA:C3C	2.79	0.66
5:A:160:SER:HB2	5:A:163:GLN:OE1	1.96	0.66
5:A:206:HIS:C	5:A:211:LEU:HD23	2.16	0.66
5:A:302:HIS:HB2	20:A:1773:CLA:C1B	2.25	0.66
5:A:624:VAL:O	5:A:636:HIS:HD2	1.77	0.66
20:A:1777:CLA:H2A	20:A:1777:CLA:O1D	1.95	0.66
20:A:1781:CLA:C3B	22:A:1806:BCR:H373	2.26	0.66
20:A:1816:CLA:HED3	20:A:1816:CLA:O1A	1.96	0.66
6:B:55:ALA:HB1	6:B:150:LEU:CD1	2.26	0.66
6:B:595:HIS:CD2	6:B:623:TYR:OH	2.49	0.66
10:F:22:LEU:O	10:F:24:LYS:N	2.28	0.66
11:G:49:THR:OG1	11:G:50:ARG:N	2.29	0.66
20:K:1146:CLA:O1A	20:K:1146:CLA:H2A	1.95	0.66
17:N:62:SER:HB3	17:N:66:ASP:OD1	1.89	0.66
19:W:1:GLC:HO2	19:W:2:FRU:C1	2.07	0.66
3:3:93:PHE:HD2	3:3:95:THR:H	1.41	0.66
5:A:118:PRO:HB3	5:A:150:PHE:CE2	2.31	0.66
5:A:207:LEU:HA	5:A:211:LEU:CG	2.25	0.66
5:A:244:LEU:HB2	5:A:247:GLU:HB2	1.77	0.66
5:A:631:GLN:HG3	5:A:631:GLN:O	1.96	0.66
5:A:691:MET:CE	23:A:1802:PQN:H2M2	2.26	0.66
21:A:7038:LMU:H1B	21:A:7038:LMU:C6'	2.26	0.66
6:B:124:TRP:O	6:B:124:TRP:CD1	2.48	0.66
6:B:247:THR:C	6:B:250:ALA:HB2	2.15	0.66
26:B:8057:UNL:C2	26:B:8057:UNL:C6	2.65	0.66
9:E:65:VAL:HG13	9:E:82:TYR:O	1.95	0.66
11:G:24:PHE:CE1	11:G:27:GLN:O	2.49	0.66
20:K:1085:CLA:CGA	20:K:1085:CLA:C3A	2.73	0.66
17:N:44:GLU:O	17:N:46:PHE:N	2.29	0.66
17:N:49:CYS:C	17:N:51:ASP:O	2.34	0.66
17:N:65:LEU:O	17:N:67:LEU:N	2.29	0.66
2:2:131:THR:HG23	2:2:132:GLY:H	1.60	0.66
20:2:1215:CLA:C4	20:2:1220:CLA:HBC3	2.24	0.66
5:A:206:HIS:O	5:A:211:LEU:HD23	1.96	0.66
5:A:374:GLN:O	5:A:377:TYR:HD2	1.79	0.66
5:A:615:HIS:ND1	20:A:1792:CLA:HBC3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1764:CLA:HMC3	20:A:1765:CLA:HHD	1.76	0.66
20:A:1776:CLA:H8	22:A:1806:BCR:H19C	1.76	0.66
21:A:7037:LMU:C1	21:A:7037:LMU:H61	2.25	0.66
21:A:7042:LMU:H32	21:A:7042:LMU:O6'	1.92	0.66
7:C:79:LEU:CD2	7:C:81:TYR:C	2.64	0.66
8:D:44:GLU:CB	8:D:46:TYR:HE2	2.05	0.66
8:D:101:TYR:CD1	8:D:114:PRO:HD3	2.30	0.66
9:E:89:GLU:HG2	9:E:92:ALA:H	1.61	0.66
22:I:1032:BCR:H403	22:I:1032:BCR:C27	2.19	0.66
16:L:36:TYR:O	16:L:37:LEU:HB3	1.95	0.66
17:N:69:CYS:O	17:N:72:LYS:CE	2.44	0.66
19:Q:1:GLC:C2	19:Q:2:FRU:O4	2.43	0.66
5:A:606:TYR:O	5:A:610:SER:CB	2.43	0.65
21:A:7022:LMU:O2'	21:A:7022:LMU:H1B	1.96	0.65
21:A:7031:LMU:H4'	21:A:7031:LMU:O2B	1.94	0.65
6:B:336:LEU:HD13	20:B:1754:CLA:HBB1	1.78	0.65
10:F:21:ALA:O	10:F:23:LYS:N	2.29	0.65
10:F:151:ASP:C	10:F:154:PHE:HB3	2.15	0.65
11:G:13:GLY:O	11:G:16:LEU:CB	2.44	0.65
17:N:58:VAL:O	17:N:60:PHE:N	2.29	0.65
20:2:1213:CLA:HBC2	20:2:1213:CLA:CHD	2.21	0.65
5:A:328:LYS:O	5:A:330:ILE:N	2.30	0.65
20:A:1777:CLA:HBC3	20:A:1779:CLA:HED1	1.77	0.65
20:A:1781:CLA:C4B	22:A:1806:BCR:C37	2.67	0.65
20:A:1781:CLA:C6	20:A:1782:CLA:HED2	2.24	0.65
6:B:366:THR:HG23	6:B:729:THR:HG22	1.78	0.65
6:B:388:ALA:O	6:B:391:PRO:HD2	1.94	0.65
11:G:23:PHE:CD2	11:G:24:PHE:HB2	2.31	0.65
11:G:28:ARG:HG2	11:G:29:GLU:H	1.57	0.65
11:G:33:LYS:HE3	11:G:33:LYS:CA	2.16	0.65
22:I:1032:BCR:C8	22:I:1032:BCR:H311	2.24	0.65
16:L:60:HIS:HD2	20:L:1167:CLA:HED1	1.61	0.65
16:L:64:LEU:HD22	16:L:91:LEU:HD22	1.79	0.65
16:L:128:ASP:OD2	16:L:129:GLN:N	2.27	0.65
17:N:80:ASN:OD1	17:N:82:PHE:N	2.30	0.65
17:N:82:PHE:O	17:N:84:LYS:N	2.30	0.65
1:1:45:ILE:HD12	20:1:1195:CLA:CMD	2.25	0.65
1:1:97:ILE:CG2	20:1:1197:CLA:HBB2	2.27	0.65
20:2:1215:CLA:C3	20:2:1220:CLA:HBC1	2.25	0.65
3:3:52:LYS:O	3:3:56:TYR:CG	2.49	0.65
5:A:42:ARG:C	5:A:44:ILE:H	1.99	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:95:GLY:H	20:A:1763:CLA:HMC3	1.60	0.65
20:A:1792:CLA:H2	20:A:1792:CLA:O1A	1.96	0.65
6:B:119:GLY:O	6:B:121:TYR:N	2.29	0.65
20:J:1044:CLA:HBA2	20:J:1044:CLA:C4A	2.25	0.65
3:3:107:TRP:CD1	3:3:108:ALA:HA	2.32	0.65
4:4:103:ILE:HG13	20:4:1197:CLA:HMD1	1.78	0.65
5:A:679:PHE:CE2	5:A:683:HIS:HD2	2.14	0.65
20:A:1776:CLA:HMC1	20:A:1776:CLA:CBC	2.25	0.65
20:A:1782:CLA:HBC2	20:A:1782:CLA:CMC	2.18	0.65
20:A:1782:CLA:HBA1	20:A:1782:CLA:CBD	2.26	0.65
6:B:20:ARG:HB3	6:B:20:ARG:HH11	1.60	0.65
6:B:247:THR:HG23	6:B:250:ALA:HB3	1.77	0.65
6:B:293:THR:C	6:B:294:ASN:ND2	2.50	0.65
20:B:1756:CLA:HED1	20:B:1764:CLA:HBB1	1.77	0.65
20:B:1762:CLA:HBB2	22:B:1778:BCR:C26	2.26	0.65
7:C:1:MET:N	7:C:4:SER:CB	2.60	0.65
7:C:7:ILE:C	7:C:8:TYR:O	2.34	0.65
7:C:74:THR:O	7:C:75:ARG:C	2.30	0.65
8:D:32:SER:H	16:L:23:LEU:HG	1.59	0.65
11:G:47:GLY:N	11:G:48:ASP:OD1	2.30	0.65
11:G:83:TYR:O	11:G:83:TYR:CG	2.48	0.65
14:J:4:PHE:O	14:J:5:LYS:HB2	1.95	0.65
20:2:1220:CLA:H91	3:3:137:SER:OG	1.97	0.65
3:3:163:PHE:HD1	3:3:163:PHE:C	1.99	0.65
5:A:23:ASP:OD2	5:A:24:ARG:NH1	2.29	0.65
5:A:432:LEU:HA	5:A:435:VAL:HG13	1.78	0.65
20:A:1783:CLA:H202	22:A:1808:BCR:C15	2.26	0.65
20:A:1791:CLA:O1A	20:A:1797:CLA:CBB	2.38	0.65
6:B:62:SER:OG	6:B:63:GLY:N	2.29	0.65
6:B:174:ARG:HH11	20:B:1754:CLA:HMD1	1.60	0.65
6:B:324:ASP:O	6:B:328:ASN:HB2	1.96	0.65
6:B:349:ALA:CB	6:B:375:HIS:HB3	2.26	0.65
6:B:646:TRP:CH2	6:B:726:ILE:HG21	2.32	0.65
6:B:663:PHE:O	6:B:664:LEU:CB	2.33	0.65
10:F:22:LEU:O	10:F:25:LEU:N	2.30	0.65
12:H:50:ARG:HG2	16:L:137:ALA:HB1	1.77	0.65
12:H:69:SER:OG	20:H:1079:CLA:H2	1.96	0.65
14:J:2:ARG:NH1	14:J:8:LEU:HD13	2.04	0.65
20:J:1044:CLA:CED	20:J:1045:CLA:HMA3	2.24	0.65
20:J:1045:CLA:H2A	20:J:1045:CLA:H2	1.77	0.65
15:K:27:ALA:HB3	15:K:28:PRO:CD	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:68:HIS:O	15:K:70:MET:N	2.29	0.65
17:N:61:LEU:HD21	17:N:63:ASP:C	2.16	0.65
17:N:65:LEU:HD23	17:N:66:ASP:N	2.10	0.65
21:2:7006:LMU:O5B	21:2:7006:LMU:C5'	2.42	0.65
5:A:81:ALA:CB	20:A:1760:CLA:HMA3	2.22	0.65
20:A:1776:CLA:HMD1	20:A:1777:CLA:HHD	1.79	0.65
20:A:1812:CLA:H11	6:B:616:LEU:CG	2.23	0.65
21:A:7033:LMU:C3'	21:A:7033:LMU:O6B	2.44	0.65
6:B:398:TYR:HD1	6:B:542:ARG:NH2	1.94	0.65
7:C:60:THR:CG2	7:C:63:LEU:O	2.44	0.65
8:D:31:GLY:HA2	16:L:13:PRO:HB3	1.79	0.65
10:F:62:LEU:CG	10:F:72:ILE:HD13	2.25	0.65
12:H:30:SER:O	12:H:31:PRO:O	2.13	0.65
13:I:10:PRO:HA	13:I:14:LEU:HB2	1.78	0.65
13:I:14:LEU:O	13:I:17:PRO:HD2	1.97	0.65
17:N:54:LYS:O	17:N:57:LYS:N	2.29	0.65
17:N:81:VAL:O	17:N:83:TRP:N	2.30	0.65
5:A:197:GLN:NE2	5:A:351:THR:HB	2.11	0.65
5:A:362:LEU:CB	5:A:410:ALA:HB2	2.26	0.65
20:A:1786:CLA:HMB2	20:A:1787:CLA:C1D	2.26	0.65
6:B:414:HIS:O	6:B:414:HIS:CG	2.50	0.65
6:B:551:LYS:CE	8:D:143:PRO:HA	2.26	0.65
20:B:1740:CLA:H91	22:B:1781:BCR:H361	1.77	0.65
22:B:1778:BCR:C39	10:F:90:PHE:HA	2.27	0.65
7:C:14:CYS:SG	7:C:14:CYS:O	2.54	0.65
11:G:16:LEU:HA	11:G:68:ILE:HG13	1.77	0.65
18:R:36:UNK:O	18:R:38:UNK:N	2.30	0.65
5:A:217:SER:CB	22:A:1803:BCR:H351	2.26	0.65
5:A:353:SER:HB2	5:A:356:ALA:HB3	1.79	0.65
23:A:1802:PQN:H142	22:B:1778:BCR:HC22	1.78	0.65
21:A:7021:LMU:O6'	21:A:7021:LMU:H12	1.96	0.65
6:B:131:THR:CB	6:B:134:ASP:HB2	2.11	0.65
6:B:175:LEU:O	6:B:179:LEU:HG	1.96	0.65
6:B:392:ILE:HD13	20:B:1759:CLA:CED	2.27	0.65
6:B:607:SER:HA	6:B:610:ASN:ND2	2.12	0.65
20:B:1747:CLA:HBD	20:B:1756:CLA:HBB2	1.77	0.65
8:D:93:LYS:NZ	8:D:93:LYS:CB	2.60	0.65
8:D:102:ARG:HE	8:D:110:GLN:CB	2.08	0.65
10:F:42:ILE:C	10:F:43:LYS:HE3	2.17	0.65
10:F:123:VAL:HB	10:F:126:ALA:C	2.17	0.65
12:H:54:LEU:HD13	12:H:55:LYS:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:13:PRO:HG2	16:L:18:PRO:HB3	1.77	0.65
20:2:1220:CLA:H41	3:3:140:LYS:HE2	1.77	0.65
5:A:368:LEU:HD22	20:A:1774:CLA:H92	1.79	0.65
5:A:618:TRP:CZ2	5:A:655:ASP:CB	2.79	0.65
10:F:104:TYR:O	10:F:104:TYR:CD2	2.49	0.65
10:F:130:LEU:HD12	10:F:131:PHE:CD1	2.32	0.65
14:J:2:ARG:HH12	14:J:8:LEU:CD1	2.04	0.65
17:N:2:VAL:HG23	17:N:2:VAL:O	1.97	0.65
17:N:61:LEU:HD12	17:N:62:SER:O	1.95	0.65
20:1:1198:CLA:C12	20:1:1198:CLA:H91	2.26	0.65
3:3:84:ILE:H	20:A:1798:CLA:H43	1.56	0.65
5:A:98:PHE:O	5:A:99:HIS:HB2	1.96	0.65
5:A:158:ILE:HG22	20:A:1770:CLA:HED3	1.79	0.65
5:A:361:ASN:HD22	5:A:362:LEU:N	1.95	0.65
5:A:455:PHE:HD1	20:A:1788:CLA:CMA	2.10	0.65
5:A:705:GLU:HA	5:A:708:VAL:HB	1.79	0.65
6:B:224:PRO:HA	6:B:227:THR:OG1	1.97	0.65
6:B:387:PHE:O	6:B:391:PRO:HD3	1.97	0.65
6:B:493:TRP:HB3	20:B:1765:CLA:HED2	1.78	0.65
6:B:538:ALA:O	6:B:540:ASP:N	2.30	0.65
6:B:558:PRO:HG2	6:B:703:VAL:CB	2.21	0.65
20:B:1759:CLA:CBC	20:B:1759:CLA:CMC	2.57	0.65
7:C:7:ILE:HG22	7:C:65:VAL:HG21	1.76	0.65
9:E:40:ARG:HB2	9:E:42:GLU:OE2	1.97	0.65
19:Y:1:GLC:O5	19:Y:2:FRU:H12	1.96	0.65
2:2:120:ASN:HA	14:J:5:LYS:CG	2.27	0.64
2:2:128:ASN:HD21	14:J:4:PHE:H	1.44	0.64
20:4:1198:CLA:O2D	20:4:1198:CLA:HAA1	1.96	0.64
5:A:281:LEU:O	5:A:283:PHE:N	2.29	0.64
5:A:334:HIS:HB3	20:A:1777:CLA:CMA	2.26	0.64
20:A:1796:CLA:H192	14:J:19:PHE:CD2	2.32	0.64
21:A:7042:LMU:H3'	21:A:7042:LMU:C2B	2.11	0.64
6:B:551:LYS:HE2	8:D:143:PRO:HA	1.79	0.64
6:B:661:PHE:CB	20:B:1787:CLA:CMC	2.75	0.64
6:B:666:SER:O	6:B:667:TRP:HB2	1.96	0.64
20:B:1742:CLA:H61	20:B:1742:CLA:H11	1.79	0.64
8:D:60:MET:HG3	8:D:61:PRO:O	1.97	0.64
10:F:130:LEU:HD12	10:F:131:PHE:HD1	1.62	0.64
11:G:28:ARG:HH21	11:G:29:GLU:H	1.46	0.64
11:G:48:ASP:OD1	11:G:48:ASP:N	2.29	0.64
20:K:1085:CLA:CHB	20:K:1142:CLA:OBD	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:126:LEU:H	4:4:127:PRO:HD3	1.61	0.64
5:A:544:ILE:O	5:A:548:THR:OG1	2.09	0.64
20:A:1763:CLA:HMB2	22:A:1808:BCR:HC7	1.79	0.64
20:A:1812:CLA:H91	20:A:1812:CLA:H152	1.78	0.64
21:A:7033:LMU:H3'	21:A:7033:LMU:O5B	1.78	0.64
6:B:527:LEU:HD13	6:B:586:THR:HG21	1.78	0.64
6:B:625:TRP:HE3	6:B:626:LEU:N	1.95	0.64
6:B:708:VAL:O	6:B:710:LEU:O	2.16	0.64
8:D:113:HIS:CD2	8:D:118:VAL:HG21	2.32	0.64
8:D:118:VAL:CG1	8:D:119:TYR:N	2.59	0.64
10:F:151:ASP:O	10:F:154:PHE:CB	2.40	0.64
11:G:93:TYR:N	11:G:94:ASP:OD1	2.29	0.64
16:L:40:LEU:HB3	16:L:41:PRO:CD	2.28	0.64
16:L:163:LEU:HD12	16:L:164:PRO:HB2	1.72	0.64
17:N:41:LYS:HB2	17:N:42:PHE:CA	2.25	0.64
19:O:2:FRU:O1	19:O:2:FRU:H4	1.96	0.64
20:1:1200:CLA:CBC	20:1:1200:CLA:CMC	2.57	0.64
20:2:1212:CLA:O1A	20:2:1212:CLA:NA	2.30	0.64
4:4:118:ASP:C	4:4:122:LYS:HA	2.18	0.64
5:A:390:ALA:HB1	5:A:754:ILE:HD13	1.80	0.64
21:A:7036:LMU:O5B	21:A:7036:LMU:H6E	1.95	0.64
21:A:7042:LMU:H71	21:A:7042:LMU:C1	2.26	0.64
6:B:424:TRP:CZ2	20:B:1761:CLA:HAC1	2.33	0.64
6:B:527:LEU:HB3	20:B:1755:CLA:C4C	2.27	0.64
6:B:661:PHE:CB	20:B:1787:CLA:HMC1	2.27	0.64
22:B:1780:BCR:C35	20:B:1787:CLA:H111	2.27	0.64
16:L:48:ASN:HB3	16:L:49:PRO:CD	2.27	0.64
18:R:38:UNK:C	18:R:39:UNK:O	2.45	0.64
20:1:1197:CLA:OBD	20:1:1197:CLA:HMD1	1.96	0.64
2:2:68:LEU:HG	20:2:1217:CLA:H192	1.80	0.64
20:3:1217:CLA:C2A	20:3:3011:CLA:CBC	2.76	0.64
5:A:453:LEU:HD23	20:A:1793:CLA:CBB	2.13	0.64
20:A:1759:CLA:O1D	20:A:1759:CLA:HBA2	1.96	0.64
20:B:1735:CLA:CBC	22:B:1778:BCR:H332	2.28	0.64
20:B:1751:CLA:CHD	20:B:1751:CLA:CBC	2.65	0.64
8:D:90:LEU:O	8:D:90:LEU:HD13	1.97	0.64
9:E:35:LYS:CE	9:E:89:GLU:OE2	2.46	0.64
9:E:36:VAL:C	9:E:49:VAL:HG13	2.18	0.64
12:H:75:ASP:CG	12:H:77:LEU:HG	2.18	0.64
16:L:30:SER:HG	16:L:32:LEU:HB2	1.62	0.64
16:L:158:MET:SD	16:L:159:TYR:N	2.67	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:39:SER:OG	17:N:40:CYS:N	2.29	0.64
17:N:83:TRP:O	17:N:83:TRP:HE3	1.79	0.64
3:3:73:ILE:C	20:3:1215:CLA:C2D	2.65	0.64
3:3:198:PHE:HA	3:3:201:ALA:CB	2.18	0.64
3:3:205:GLY:CA	5:A:252:ARG:HH12	2.09	0.64
5:A:401:TRP:O	5:A:405:PHE:HB2	1.97	0.64
20:A:1770:CLA:CHC	22:A:1803:BCR:C18	2.75	0.64
6:B:17:THR:HA	6:B:696:LYS:H	1.62	0.64
6:B:37:ILE:HD12	6:B:37:ILE:O	1.97	0.64
6:B:171:ALA:O	6:B:172:GLU:HB2	1.98	0.64
6:B:334:LEU:O	6:B:334:LEU:CG	2.46	0.64
20:B:1755:CLA:HMB3	22:B:1777:BCR:H351	1.79	0.64
20:B:1787:CLA:CBA	20:B:1787:CLA:HED3	2.28	0.64
9:E:89:GLU:O	9:E:90:VAL:HB	1.97	0.64
14:J:10:VAL:HG13	14:J:11:ALA:H	1.61	0.64
15:K:69:ILE:O	15:K:70:MET:C	2.35	0.64
17:N:63:ASP:CA	17:N:64:ASP:O	2.40	0.64
5:A:207:LEU:CD2	5:A:314:GLY:HA2	2.28	0.64
5:A:302:HIS:HE1	20:A:1774:CLA:CHB	2.11	0.64
5:A:340:GLY:O	5:A:343:HIS:CB	2.43	0.64
20:A:1760:CLA:HBC3	20:A:1760:CLA:HHD	1.78	0.64
20:A:1770:CLA:HED2	20:A:1770:CLA:H2A	1.80	0.64
20:A:1790:CLA:HMC1	20:A:1790:CLA:HBC3	1.79	0.64
20:A:1817:CLA:O1D	20:A:1817:CLA:CAA	2.46	0.64
20:B:1768:CLA:HHB	20:B:1769:CLA:OBD	1.97	0.64
20:B:1786:CLA:CBB	20:B:1787:CLA:CHB	2.73	0.64
20:J:1043:CLA:C16	20:J:1043:CLA:O2A	2.45	0.64
1:1:185:TRP:O	1:1:186:HIS:ND1	2.30	0.64
20:1:1197:CLA:H41	20:1:1198:CLA:O1D	1.96	0.64
3:3:64:TYR:CB	20:3:1218:CLA:H41	2.15	0.64
20:3:3007:CLA:HAC2	20:K:3009:CLA:C9	2.28	0.64
4:4:75:TRP:HA	20:4:1204:CLA:CMD	2.27	0.64
5:A:187:HIS:CE1	20:A:1767:CLA:C1A	2.67	0.64
20:A:1788:CLA:H101	20:A:1788:CLA:C14	2.28	0.64
20:A:1793:CLA:ND	20:A:1793:CLA:H11	2.12	0.64
6:B:545:LYS:HD3	6:B:546:LEU:H	1.61	0.64
12:H:45:ALA:HB3	12:H:46:PRO:HD3	1.78	0.64
12:H:63:SER:O	12:H:67:TYR:CB	2.46	0.64
3:3:87:GLU:CA	22:3:1220:BCR:H382	2.27	0.64
20:3:3008:CLA:H2A	20:3:3008:CLA:O2A	1.96	0.64
4:4:91:PHE:CG	20:4:1205:CLA:C3C	2.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:434:ARG:O	5:A:437:ARG:HB2	1.98	0.64
5:A:631:GLN:O	21:A:1809:LMU:H6E	1.98	0.64
5:A:668:TYR:CD1	6:B:445:ALA:HB2	2.33	0.64
20:A:1784:CLA:CHD	22:A:1804:BCR:H333	2.28	0.64
20:A:1795:CLA:O1A	20:A:1795:CLA:C3	2.46	0.64
6:B:577:TYR:HE2	6:B:578:LEU:HD12	1.63	0.64
20:B:1771:CLA:HED1	24:B:1783:LMG:C21	2.28	0.64
22:B:1779:BCR:H333	20:F:1156:CLA:HMA1	1.79	0.64
10:F:153:ASN:C	10:F:153:ASN:ND2	2.48	0.64
11:G:7:VAL:HG23	11:G:8:ILE:N	2.12	0.64
11:G:28:ARG:NH2	11:G:29:GLU:H	1.95	0.64
15:K:69:ILE:HG23	15:K:70:MET:N	2.13	0.64
17:N:77:CYS:O	17:N:79:SER:N	2.29	0.64
20:4:4014:CLA:CBC	20:4:4014:CLA:CMC	2.74	0.64
5:A:40:PHE:CE1	5:A:53:TRP:CD1	2.76	0.64
5:A:132:LEU:HD11	5:A:674:ALA:CB	2.27	0.64
6:B:366:THR:HG23	6:B:729:THR:CG2	2.28	0.64
6:B:535:VAL:HG13	6:B:536:LYS:N	2.13	0.64
6:B:556:SER:C	6:B:558:PRO:CD	2.62	0.64
10:F:125:LEU:O	10:F:126:ALA:HB2	1.98	0.64
11:G:68:ILE:O	11:G:72:LEU:HB2	1.96	0.64
17:N:11:LYS:HG2	17:N:12:THR:N	2.13	0.64
17:N:24:THR:O	17:N:26:GLY:N	2.31	0.64
17:N:59:PRO:C	17:N:66:ASP:OD1	2.37	0.64
18:R:27:UNK:O	18:R:29:UNK:N	2.31	0.64
4:4:169:GLN:CD	20:4:1199:CLA:HAC2	2.19	0.64
5:A:101:ALA:O	5:A:104:SER:HA	1.98	0.64
5:A:131:ILE:HD13	6:B:447:GLY:N	2.13	0.64
5:A:202:MET:HG3	20:A:1769:CLA:HBC2	1.79	0.64
5:A:207:LEU:O	5:A:310:PHE:CB	2.46	0.64
5:A:362:LEU:HD11	20:A:1785:CLA:HBB2	1.78	0.64
5:A:492:ILE:HA	5:A:495:THR:HG23	1.78	0.64
20:A:1760:CLA:HBB2	20:A:1762:CLA:C4D	2.27	0.64
20:A:1779:CLA:NC	22:A:1805:BCR:H17C	2.12	0.64
20:A:1796:CLA:H142	20:A:1813:CLA:H143	1.80	0.64
20:A:1812:CLA:HED1	20:B:1785:CLA:H61	1.80	0.64
21:A:7016:LMU:C3	21:A:7016:LMU:C7	2.76	0.64
6:B:73:ASN:HB3	6:B:76:ALA:HB3	1.78	0.64
6:B:103:ALA:O	6:B:104:PHE:CB	2.34	0.64
11:G:16:LEU:HD23	11:G:68:ILE:HG21	1.81	0.64
11:G:28:ARG:HG3	11:G:29:GLU:CG	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:10:VAL:HG13	14:J:11:ALA:N	2.13	0.64
16:L:99:LEU:O	16:L:102:TYR:N	2.29	0.64
19:X:1:GLC:C5	19:X:2:FRU:C1	2.75	0.64
3:3:163:PHE:C	3:3:163:PHE:CD1	2.72	0.63
5:A:126:ILE:HG12	20:A:1765:CLA:HMA3	1.80	0.63
5:A:360:ILE:HD13	22:A:1805:BCR:H371	1.79	0.63
5:A:418:MET:O	5:A:564:ARG:HD2	1.98	0.63
5:A:700:TRP:CZ2	23:A:1802:PQN:H2M3	2.33	0.63
20:A:1796:CLA:C6	20:A:1813:CLA:H193	2.27	0.63
20:A:1815:CLA:H61	20:A:1815:CLA:HMA2	1.74	0.63
6:B:216:LEU:O	6:B:218:TYR:N	2.31	0.63
6:B:292:ARG:HH22	6:B:297:ILE:HG13	1.62	0.63
20:B:1756:CLA:H8	22:B:1777:BCR:H14C	1.79	0.63
7:C:28:MET:HG2	7:C:38:GLN:HE21	1.63	0.63
7:C:55:GLU:C	7:C:57:ALA:N	2.51	0.63
8:D:46:TYR:HE1	8:D:80:LYS:CE	2.11	0.63
10:F:11:SER:OG	10:F:14:PHE:HB3	1.98	0.63
11:G:42:SER:OG	11:G:43:HIS:C	2.37	0.63
3:3:106:TYR:HB3	3:3:107:TRP:CD1	2.32	0.63
5:A:53:TRP:HA	5:A:56:ASN:CB	2.28	0.63
5:A:281:LEU:HD13	20:A:1772:CLA:CED	1.04	0.63
5:A:360:ILE:O	5:A:361:ASN:CB	2.45	0.63
5:A:625:TRP:HB2	5:A:637:ILE:HD11	1.79	0.63
20:A:1763:CLA:CGA	20:A:1765:CLA:H12	2.28	0.63
21:A:7042:LMU:C3	21:A:7042:LMU:O5'	2.46	0.63
6:B:67:HIS:O	6:B:68:VAL:HG23	1.98	0.63
20:B:1742:CLA:CMC	22:B:1775:BCR:H373	2.27	0.63
20:B:1756:CLA:H71	22:B:1777:BCR:H14C	1.79	0.63
22:B:1780:BCR:C17	20:B:1786:CLA:H101	2.22	0.63
10:F:12:LYS:HG2	10:F:13:GLN:H	1.60	0.63
10:F:62:LEU:CD2	10:F:72:ILE:HD13	2.28	0.63
10:F:100:VAL:CA	10:F:103:SER:OG	2.45	0.63
10:F:123:VAL:HB	10:F:126:ALA:O	1.99	0.63
10:F:147:GLY:C	10:F:150:VAL:HB	2.19	0.63
20:J:1043:CLA:O1A	20:J:1043:CLA:H152	1.98	0.63
16:L:63:LEU:CD2	16:L:64:LEU:H	2.10	0.63
16:L:128:ASP:CG	16:L:129:GLN:H	2.01	0.63
17:N:41:LYS:CB	17:N:42:PHE:CB	2.55	0.63
4:4:91:PHE:O	4:4:95:PHE:HD1	1.82	0.63
5:A:114:THR:CG2	5:A:115:HIS:ND1	2.59	0.63
5:A:205:HIS:CE1	20:A:1769:CLA:HMC2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:229:ILE:HG12	5:A:243:PRO:HB3	1.80	0.63
6:B:79:GLN:O	6:B:80:ASP:HB3	1.96	0.63
6:B:203:ARG:HG2	6:B:204:GLY:H	1.63	0.63
6:B:317:ARG:NE	6:B:317:ARG:CA	2.56	0.63
8:D:36:LEU:HD12	8:D:78:ALA:H	1.63	0.63
9:E:44:TYR:HB3	9:E:45:TRP:CE3	2.33	0.63
20:J:1043:CLA:C16	20:J:1043:CLA:CGA	2.77	0.63
17:N:29:PHE:CE1	17:N:32:ALA:HB3	2.33	0.63
3:3:180:LYS:O	3:3:182:LYS:N	2.31	0.63
5:A:24:ARG:HG2	5:A:29:THR:HG21	1.81	0.63
5:A:249:ILE:C	5:A:251:ASN:H	2.00	0.63
5:A:308:ILE:CG2	5:A:309:LEU:N	2.61	0.63
5:A:520:LEU:O	5:A:522:ALA:N	2.27	0.63
5:A:547:PHE:HE2	20:B:1787:CLA:O1A	1.82	0.63
5:A:558:LYS:NZ	6:B:674:LEU:HD23	2.14	0.63
20:A:1783:CLA:H102	22:A:1807:BCR:C37	2.29	0.63
20:A:1793:CLA:CHA	20:A:1793:CLA:O1A	2.47	0.63
21:A:7043:LMU:C6B	21:A:7043:LMU:O3B	2.45	0.63
6:B:282:PHE:O	6:B:286:ILE:HG13	1.98	0.63
6:B:510:LEU:HD21	20:B:1767:CLA:HHD	1.80	0.63
20:B:1758:CLA:H142	22:B:1776:BCR:C10	2.24	0.63
8:D:79:ARG:O	8:D:82:GLN:HB2	1.98	0.63
21:2:7006:LMU:C2'	21:2:7006:LMU:C2	2.77	0.63
5:A:284:ARG:HH12	5:A:507:ALA:HB1	1.63	0.63
5:A:426:THR:HA	5:A:428:TYR:CZ	2.33	0.63
5:A:455:PHE:HD1	20:A:1788:CLA:HMA2	1.63	0.63
5:A:530:LEU:HB2	5:A:531:PRO:HD2	1.81	0.63
5:A:612:VAL:O	5:A:615:HIS:HB3	1.98	0.63
5:A:618:TRP:CH2	5:A:655:ASP:HB2	2.34	0.63
21:A:7010:LMU:O3'	21:A:7010:LMU:C1B	2.47	0.63
6:B:193:HIS:HB2	20:B:1744:CLA:CHC	2.28	0.63
10:F:20:GLN:C	10:F:20:GLN:CD	2.54	0.63
10:F:22:LEU:O	10:F:25:LEU:HD12	1.97	0.63
11:G:60:SER:CA	11:G:63:PRO:HD2	2.27	0.63
16:L:36:TYR:OH	20:L:1167:CLA:HBA2	1.97	0.63
16:L:99:LEU:HD11	22:L:1169:BCR:C31	2.28	0.63
17:N:72:LYS:N	17:N:72:LYS:HD2	2.07	0.63
18:R:7:UNK:O	18:R:10:UNK:CB	2.47	0.63
3:3:205:GLY:HA3	5:A:252:ARG:HH12	1.62	0.63
5:A:370:ILE:CD1	20:A:1781:CLA:C3D	2.75	0.63
6:B:178:HIS:HE1	20:B:1743:CLA:NC	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:224:PRO:CB	6:B:227:THR:HB	2.28	0.63
20:B:1760:CLA:HMB2	20:B:1761:CLA:CHB	2.28	0.63
17:N:66:ASP:N	17:N:66:ASP:OD2	2.29	0.63
20:R:1054:CLA:HED3	20:R:1054:CLA:NA	2.11	0.63
5:A:398:HIS:CD2	20:A:1783:CLA:ND	2.67	0.63
5:A:439:ARG:NH1	5:A:565:SER:O	2.32	0.63
5:A:472:ARG:N	5:A:473:PRO:HD2	2.13	0.63
20:A:1774:CLA:H93	20:A:1774:CLA:H193	1.78	0.63
7:C:12:ILE:CB	7:C:39:ILE:HA	2.28	0.63
11:G:93:TYR:CA	11:G:94:ASP:CG	2.59	0.63
12:H:14:ILE:O	12:H:16:ASN:N	2.31	0.63
16:L:122:GLY:O	16:L:124:LYS:N	2.32	0.63
2:2:196:HIS:NE2	19:M:1:GLC:O3	2.28	0.63
20:2:1220:CLA:HBC3	20:2:1220:CLA:HHD	1.80	0.63
3:3:50:GLU:N	3:3:51:PRO:HD3	2.13	0.63
4:4:107:GLN:HB3	20:4:1196:CLA:HMA3	1.75	0.63
5:A:281:LEU:O	5:A:282:THR:C	2.36	0.63
5:A:451:ILE:HD11	20:A:1788:CLA:HED1	1.79	0.63
5:A:520:LEU:HD22	21:A:1809:LMU:O2'	1.98	0.63
5:A:701:GLN:O	5:A:704:ILE:N	2.32	0.63
20:A:1765:CLA:HBA2	20:A:1765:CLA:HBD	1.80	0.63
20:A:1781:CLA:HMA3	20:A:1782:CLA:O1A	1.98	0.63
6:B:429:LEU:HB3	6:B:525:LEU:HB2	1.80	0.63
6:B:670:TYR:C	6:B:670:TYR:CD1	2.72	0.63
7:C:77:MET:O	7:C:79:LEU:N	2.29	0.63
11:G:92:GLY:O	11:G:93:TYR:C	2.36	0.63
17:N:57:LYS:HG3	17:N:58:VAL:H	0.61	0.63
2:2:54:TRP:CD1	20:2:1222:CLA:O1D	2.52	0.63
4:4:124:TYR:CB	4:4:143:PHE:CD1	2.80	0.63
5:A:330:ILE:HG22	5:A:330:ILE:O	1.99	0.63
5:A:346:LEU:HD11	20:A:1779:CLA:CHD	2.29	0.63
20:A:1764:CLA:H142	22:A:1808:BCR:H14C	1.79	0.63
20:A:1816:CLA:HED1	20:A:1816:CLA:O2A	1.99	0.63
6:B:25:ILE:CB	22:L:1169:BCR:H292	2.28	0.63
6:B:92:TRP:O	6:B:92:TRP:CD1	2.52	0.63
6:B:438:VAL:CG2	20:B:1763:CLA:HAC1	2.29	0.63
6:B:458:ILE:HG23	20:B:1768:CLA:CMD	2.29	0.63
6:B:545:LYS:CG	6:B:546:LEU:N	2.61	0.63
6:B:704:GLN:O	6:B:708:VAL:HG23	1.99	0.63
20:L:1167:CLA:CHC	22:L:1170:BCR:HC8	2.28	0.63
17:N:80:ASN:O	17:N:82:PHE:N	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:80:ASN:C	17:N:82:PHE:H	2.02	0.63
18:R:31:UNK:C	18:R:32:UNK:O	2.47	0.63
1:1:160:GLY:O	1:1:162:CYS:N	2.32	0.62
20:4:1198:CLA:H2A	20:4:1198:CLA:CGD	2.18	0.62
5:A:665:ILE:C	5:A:665:ILE:HD12	2.19	0.62
6:B:49:SER:O	6:B:52:GLY:N	2.33	0.62
6:B:378:ILE:HG22	6:B:379:ALA:H	1.63	0.62
6:B:687:LEU:HD12	22:L:1170:BCR:HC31	1.81	0.62
20:B:1747:CLA:CBD	20:B:1756:CLA:CBB	2.77	0.62
20:B:1771:CLA:C19	13:I:21:MET:CB	2.76	0.62
7:C:62:PHE:CE1	9:E:42:GLU:HB2	2.34	0.62
15:K:7:THR:HA	15:K:10:ILE:HB	1.81	0.62
1:1:57:ILE:O	1:1:59:VAL:N	2.32	0.62
5:A:24:ARG:C	5:A:25:ASP:O	2.33	0.62
5:A:195:TRP:CZ2	20:A:1766:CLA:CMA	2.80	0.62
5:A:599:PHE:CD2	5:A:735:VAL:HG21	2.35	0.62
5:A:664:VAL:CG2	5:A:665:ILE:HG23	2.29	0.62
6:B:269:TRP:HD1	6:B:497:TRP:CH2	2.17	0.62
6:B:371:LEU:HD21	20:B:1758:CLA:HED3	1.80	0.62
20:B:1742:CLA:HMC1	22:B:1775:BCR:H373	1.80	0.62
23:B:1773:PQN:H162	22:B:1780:BCR:H332	1.64	0.62
2:2:174:VAL:O	2:2:178:TRP:HD1	1.82	0.62
4:4:70:ILE:O	4:4:73:PRO:HD3	1.99	0.62
4:4:147:LEU:CD2	4:4:148:GLU:H	2.12	0.62
5:A:79:PHE:HE2	5:A:185:HIS:CG	2.17	0.62
5:A:109:TRP:HA	5:A:116:ILE:HG13	1.81	0.62
5:A:174:PHE:O	5:A:175:ALA:HB2	1.98	0.62
20:A:1796:CLA:H62	20:A:1813:CLA:H171	1.80	0.62
20:A:1812:CLA:HED1	20:B:1785:CLA:H2	1.80	0.62
6:B:77:TRP:CZ2	6:B:122:GLN:NE2	2.68	0.62
6:B:661:PHE:HB3	20:B:1787:CLA:HBC3	1.81	0.62
20:B:1771:CLA:HMC1	20:B:1771:CLA:CBC	2.27	0.62
20:F:1156:CLA:HBC2	20:F:1156:CLA:CHD	2.27	0.62
11:G:28:ARG:HA	20:G:1099:CLA:CMA	2.28	0.62
11:G:37:GLU:OE2	11:G:42:SER:N	2.32	0.62
13:I:24:LEU:C	13:I:26:LEU:N	2.51	0.62
16:L:64:LEU:HA	16:L:67:PRO:HG3	1.80	0.62
3:3:59:ILE:O	3:3:63:ARG:HG3	1.99	0.62
5:A:23:ASP:CA	5:A:24:ARG:CD	2.63	0.62
5:A:201:SER:O	5:A:204:ASN:HB2	1.99	0.62
5:A:254:LEU:C	5:A:256:ALA:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:302:HIS:HB2	20:A:1773:CLA:CHB	2.28	0.62
5:A:393:LEU:HD11	5:A:750:PHE:CD1	2.33	0.62
20:A:1781:CLA:C3B	22:A:1806:BCR:C22	2.78	0.62
6:B:221:GLY:C	6:B:223:GLY:H	2.03	0.62
6:B:284:PHE:O	6:B:288:GLY:N	2.27	0.62
20:B:1768:CLA:C12	22:B:1779:BCR:C31	2.76	0.62
22:B:1776:BCR:H331	22:B:1776:BCR:HC8	1.80	0.62
7:C:28:MET:HB3	8:D:122:LYS:O	1.98	0.62
7:C:59:PRO:HB3	7:C:61:ASP:OD1	2.00	0.62
8:D:94:TYR:O	8:D:95:LYS:CB	2.48	0.62
12:H:21:TRP:N	12:H:22:ASP:CB	2.61	0.62
5:A:377:TYR:CD1	5:A:616:PHE:HE1	2.18	0.62
20:A:1783:CLA:C18	22:A:1808:BCR:H17C	2.28	0.62
20:A:1791:CLA:HAA2	20:A:1797:CLA:HBB2	1.81	0.62
20:A:1797:CLA:CHD	20:A:1797:CLA:CBC	2.77	0.62
20:A:1812:CLA:C3B	6:B:589:TRP:CH2	2.78	0.62
6:B:53:GLN:C	6:B:55:ALA:N	2.53	0.62
6:B:530:THR:HG22	20:B:1755:CLA:HMC1	1.80	0.62
20:B:1738:CLA:HBB2	20:B:1758:CLA:HHC	1.79	0.62
20:B:1756:CLA:H41	20:B:1756:CLA:C7	2.29	0.62
7:C:73:THR:C	7:C:76:SER:OG	2.37	0.62
11:G:33:LYS:HA	11:G:33:LYS:NZ	2.14	0.62
22:L:1170:BCR:C38	22:L:1170:BCR:C23	2.76	0.62
1:1:61:GLU:HG2	1:1:61:GLU:O	1.98	0.62
20:1:1187:CLA:HBC3	20:1:1187:CLA:HMC1	0.70	0.62
3:3:104:TYR:HB2	3:3:106:TYR:H	1.64	0.62
5:A:281:LEU:HG	5:A:282:THR:H	1.63	0.62
5:A:466:THR:HG22	20:B:1740:CLA:HHC	1.80	0.62
5:A:514:THR:HB	5:A:532:ILE:HG23	1.82	0.62
5:A:604:TRP:O	5:A:607:ASN:N	2.28	0.62
20:A:1787:CLA:CBB	20:A:1793:CLA:H192	2.30	0.62
21:A:7010:LMU:C3'	21:A:7010:LMU:C2B	2.77	0.62
21:A:7032:LMU:C1B	21:A:7032:LMU:H32	2.25	0.62
6:B:42:LEU:O	6:B:43:TYR:C	2.36	0.62
6:B:374:HIS:HB2	20:B:1757:CLA:C4B	2.29	0.62
20:B:1743:CLA:C4	22:B:1775:BCR:H10C	2.27	0.62
22:B:1780:BCR:H382	22:B:1780:BCR:C23	2.11	0.62
8:D:118:VAL:HG12	8:D:119:TYR:N	2.14	0.62
9:E:61:THR:HG22	9:E:62:ARG:N	2.11	0.62
12:H:25:GLY:CA	12:H:27:ASP:HB2	2.28	0.62
13:I:22:ALA:O	13:I:23:SER:C	2.36	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:27:ALA:CB	15:K:28:PRO:CD	2.78	0.62
17:N:34:THR:C	17:N:36:GLU:H	2.02	0.62
17:N:62:SER:CA	17:N:66:ASP:H	2.13	0.62
17:N:72:LYS:HZ3	17:N:74:LYS:CG	2.01	0.62
4:4:106:TRP:CE3	20:4:1207:CLA:HMA2	2.35	0.62
5:A:308:ILE:HG22	5:A:309:LEU:H	1.64	0.62
5:A:553:VAL:O	5:A:557:LEU:N	2.29	0.62
5:A:705:GLU:CB	6:B:545:LYS:HZ2	2.12	0.62
20:A:1783:CLA:H72	22:A:1807:BCR:C37	2.20	0.62
20:A:1788:CLA:HAA1	22:L:1170:BCR:C13	2.29	0.62
20:A:1816:CLA:HAA1	20:A:1816:CLA:CED	2.28	0.62
21:A:7016:LMU:H1'	21:A:7016:LMU:H31	1.81	0.62
21:A:7043:LMU:C6	21:A:7043:LMU:H111	2.28	0.62
6:B:247:THR:HG23	6:B:250:ALA:CB	2.29	0.62
6:B:456:GLU:HG2	10:F:70:HIS:HB3	1.80	0.62
10:F:103:SER:C	10:F:105:LEU:N	2.53	0.62
17:N:5:GLU:OE2	17:N:6:TYR:HB2	1.99	0.62
20:1:1193:CLA:CGA	20:1:1193:CLA:H43	2.29	0.62
2:2:41:LEU:O	2:2:43:TRP:N	2.30	0.62
5:A:66:SER:O	5:A:67:HIS:HB2	2.00	0.62
5:A:210:LEU:CD1	20:A:1769:CLA:CMB	2.75	0.62
5:A:445:HIS:O	5:A:446:LEU:HB2	1.99	0.62
5:A:555:ILE:CG2	20:B:1787:CLA:OBD	2.47	0.62
5:A:578:ARG:HA	5:A:595:TRP:HB2	1.80	0.62
5:A:690:LEU:CD2	6:B:661:PHE:HE1	2.13	0.62
5:A:707:ILE:C	5:A:711:HIS:CD2	2.73	0.62
6:B:334:LEU:CA	20:B:1737:CLA:HMD3	2.30	0.62
6:B:664:LEU:C	6:B:667:TRP:CZ3	2.69	0.62
6:B:697:PRO:CB	20:B:1770:CLA:HBC3	2.30	0.62
9:E:45:TRP:CZ3	9:E:78:SER:OG	2.53	0.62
10:F:40:LEU:HA	10:F:42:ILE:CG1	2.26	0.62
17:N:81:VAL:O	17:N:82:PHE:C	2.38	0.62
4:4:151:GLU:HA	4:4:154:ILE:HG23	1.81	0.62
5:A:425:THR:OG1	5:A:428:TYR:HE1	1.74	0.62
5:A:709:TRP:CH2	6:B:417:ALA:HB2	2.35	0.62
20:B:1746:CLA:HED2	20:B:1746:CLA:HBA1	1.81	0.62
7:C:62:PHE:CE2	8:D:137:ILE:HB	2.34	0.62
12:H:26:SER:C	12:H:27:ASP:O	2.33	0.62
16:L:163:LEU:CD1	16:L:164:PRO:N	2.51	0.62
20:2:1213:CLA:H42	20:2:1213:CLA:C4C	2.29	0.62
5:A:207:LEU:HB3	20:A:1776:CLA:HBB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:270:PHE:CZ	20:A:1797:CLA:C2	2.83	0.62
5:A:448:TRP:CD1	20:A:1788:CLA:HED2	2.35	0.62
20:A:1774:CLA:C20	20:A:1782:CLA:H3A	2.30	0.62
6:B:456:GLU:OE1	10:F:70:HIS:ND1	2.32	0.62
10:F:84:ILE:O	10:F:87:GLY:N	2.26	0.62
10:F:151:ASP:HA	10:F:154:PHE:HB3	1.80	0.62
12:H:16:ASN:HD22	12:H:19:GLY:HA2	1.65	0.62
16:L:30:SER:C	16:L:32:LEU:H	2.03	0.62
3:3:62:GLY:HA2	3:3:65:ALA:HB3	1.82	0.61
4:4:169:GLN:HE22	20:4:1199:CLA:HHD	1.62	0.61
22:A:1807:BCR:H353	20:A:1812:CLA:H41	1.82	0.61
6:B:633:ASN:ND2	6:B:636:THR:CB	2.62	0.61
6:B:658:ALA:O	6:B:661:PHE:HD2	1.83	0.61
8:D:48:ILE:CB	8:D:100:PHE:HB3	2.29	0.61
20:1:1191:CLA:HMC3	20:1:1194:CLA:HHD	1.77	0.61
20:1:1198:CLA:C9	20:1:1198:CLA:H121	2.30	0.61
2:2:52:SER:OG	2:2:169:LEU:HG	1.99	0.61
5:A:401:TRP:HD1	20:A:1783:CLA:CHC	2.13	0.61
5:A:449:VAL:HG22	20:A:1794:CLA:HMC3	1.82	0.61
5:A:472:ARG:O	5:A:474:GLN:CG	2.47	0.61
5:A:697:ARG:HD3	6:B:566:GLY:O	2.00	0.61
20:A:1765:CLA:H51	22:A:1808:BCR:H10C	1.83	0.61
21:A:7020:LMU:H92	21:A:7020:LMU:C5	2.19	0.61
6:B:31:PHE:HB2	6:B:42:LEU:CD1	2.29	0.61
6:B:475:ASP:HA	6:B:480:SER:HA	1.80	0.61
6:B:555:TYR:CD2	6:B:573:TRP:HB2	2.34	0.61
6:B:732:LYS:CD	6:B:734:GLY:N	2.61	0.61
10:F:130:LEU:CD1	10:F:131:PHE:HD1	2.13	0.61
16:L:30:SER:O	16:L:32:LEU:N	2.33	0.61
20:L:1167:CLA:HBC3	20:L:1167:CLA:CMC	2.30	0.61
4:4:106:TRP:HE3	20:4:1207:CLA:CMA	2.13	0.61
4:4:118:ASP:HB3	20:4:1200:CLA:HMB3	1.83	0.61
5:A:25:ASP:CB	5:A:26:PRO:HG3	2.30	0.61
5:A:58:HIS:HB3	20:A:1760:CLA:HBC1	1.80	0.61
5:A:307:ALA:O	5:A:308:ILE:C	2.39	0.61
21:A:7030:LMU:C2'	21:A:7030:LMU:C6'	2.64	0.61
6:B:447:GLY:O	6:B:449:PRO:HD3	2.00	0.61
6:B:622:ASP:HA	6:B:626:LEU:HB3	1.82	0.61
6:B:732:LYS:CG	6:B:733:PHE:O	2.43	0.61
20:B:1747:CLA:HBD	20:B:1756:CLA:CBB	2.30	0.61
20:B:1753:CLA:CMC	20:B:1753:CLA:HBC2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1771:CLA:HMC3	20:B:1787:CLA:HMB3	1.83	0.61
7:C:29:ILE:CG2	8:D:126:GLY:HA2	2.29	0.61
14:J:20:GLY:O	14:J:21:SER:HB2	2.01	0.61
1:1:140:LEU:HG	1:1:142:GLU:H	1.65	0.61
3:3:52:LYS:CA	3:3:55:ALA:HB3	2.30	0.61
5:A:87:SER:OG	5:A:179:LEU:HB2	1.99	0.61
5:A:224:HIS:CE1	20:A:1771:CLA:C4C	2.84	0.61
5:A:514:THR:HB	5:A:532:ILE:CG2	2.31	0.61
21:A:7036:LMU:H92	21:A:7036:LMU:H11	1.81	0.61
6:B:213:LEU:HD12	6:B:214:ASP:N	2.15	0.61
6:B:592:PHE:HA	6:B:721:TYR:OH	2.01	0.61
6:B:608:GLN:O	6:B:612:SER:HB3	1.99	0.61
6:B:689:ASN:OD1	6:B:689:ASN:N	2.32	0.61
20:B:1753:CLA:HAA1	20:B:1753:CLA:C1	2.30	0.61
20:B:1756:CLA:C10	22:B:1777:BCR:H14C	2.31	0.61
20:B:1761:CLA:HBC2	20:B:1761:CLA:CHD	2.20	0.61
9:E:32:ARG:HH22	9:E:53:VAL:HA	1.65	0.61
16:L:46:ALA:HB2	16:L:52:ARG:NH2	2.16	0.61
17:N:57:LYS:O	17:N:60:PHE:N	2.33	0.61
4:4:124:TYR:HD2	4:4:144:ALA:H	1.49	0.61
5:A:113:PRO:C	5:A:115:HIS:H	2.03	0.61
5:A:249:ILE:CG1	5:A:250:LEU:N	2.48	0.61
20:A:1768:CLA:C3D	20:A:1769:CLA:HMC3	2.31	0.61
20:A:1783:CLA:C17	22:A:1808:BCR:H17C	2.30	0.61
20:A:1787:CLA:H92	20:A:1801:CLA:H2	1.81	0.61
6:B:98:GLN:C	6:B:100:ALA:N	2.53	0.61
6:B:124:TRP:CD1	6:B:124:TRP:C	2.73	0.61
6:B:275:HIS:HD1	20:B:1747:CLA:HMB1	1.64	0.61
6:B:382:ILE:CG2	6:B:383:MET:N	2.53	0.61
6:B:433:THR:O	6:B:436:LEU:O	2.17	0.61
6:B:451:LYS:HD2	20:B:1763:CLA:O2D	2.00	0.61
6:B:475:ASP:CA	6:B:480:SER:HA	2.29	0.61
9:E:73:ASN:ND2	9:E:75:ALA:H	1.99	0.61
12:H:14:ILE:O	12:H:14:ILE:HD13	2.00	0.61
20:J:1045:CLA:CGD	20:J:1045:CLA:O1A	2.48	0.61
17:N:65:LEU:HD21	17:N:66:ASP:O	2.00	0.61
20:A:1779:CLA:C1B	22:A:1805:BCR:C15	2.79	0.61
6:B:560:ASP:CG	6:B:561:GLY:N	2.54	0.61
20:B:1768:CLA:CBC	10:F:83:PHE:HZ	2.13	0.61
8:D:84:LEU:HD12	8:D:100:PHE:HZ	1.64	0.61
20:G:1099:CLA:H3A	20:G:1099:CLA:O2A	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:58:VAL:C	17:N:60:PHE:H	2.04	0.61
17:N:73:ASP:OD1	17:N:73:ASP:N	2.32	0.61
3:3:158:TYR:OH	20:3:1213:CLA:C3B	2.49	0.61
4:4:193:ILE:HG22	4:4:194:VAL:H	1.66	0.61
5:A:210:LEU:HD13	20:A:1769:CLA:HBB	1.83	0.61
5:A:508:THR:O	5:A:509:ALA:CB	2.49	0.61
20:A:1781:CLA:H61	20:A:1782:CLA:HED2	1.82	0.61
6:B:130:ARG:HH11	6:B:130:ARG:CG	2.13	0.61
6:B:211:ASN:HB2	6:B:214:ASP:HB3	1.82	0.61
6:B:216:LEU:HD21	6:B:221:GLY:CA	2.31	0.61
6:B:697:PRO:O	7:C:79:LEU:HD11	2.00	0.61
20:B:1755:CLA:H52	20:B:1769:CLA:CBD	2.30	0.61
7:C:74:THR:C	7:C:76:SER:H	2.01	0.61
8:D:78:ALA:O	8:D:79:ARG:NH1	2.34	0.61
12:H:41:GLU:OE2	12:H:42:THR:OG1	2.16	0.61
20:2:1215:CLA:H2	20:2:1218:CLA:HMD3	1.82	0.61
5:A:360:ILE:O	5:A:361:ASN:HB3	2.01	0.61
20:A:1791:CLA:C3A	20:A:1797:CLA:CBB	2.79	0.61
6:B:91:ILE:HD11	6:B:104:PHE:CD2	2.35	0.61
6:B:462:TRP:HZ3	20:B:1764:CLA:CBC	2.13	0.61
20:B:1758:CLA:C14	22:B:1776:BCR:H10C	2.25	0.61
20:B:1768:CLA:C1A	20:B:1768:CLA:CGA	2.79	0.61
8:D:117:GLY:O	8:D:118:VAL:CG2	2.39	0.61
9:E:73:ASN:HD22	9:E:73:ASN:C	2.04	0.61
17:N:5:GLU:CD	17:N:6:TYR:CD2	2.74	0.61
17:N:66:ASP:C	17:N:67:LEU:CG	2.69	0.61
3:3:106:TYR:CD1	3:3:107:TRP:N	2.68	0.61
5:A:39:HIS:O	5:A:40:PHE:HB3	2.01	0.61
5:A:399:HIS:O	5:A:400:MET:HB2	1.98	0.61
5:A:458:PHE:CD2	20:B:1786:CLA:CMB	2.83	0.61
5:A:462:ILE:HD11	20:B:1786:CLA:H72	1.80	0.61
5:A:581:CYS:CB	5:A:590:CYS:O	2.49	0.61
20:A:1781:CLA:HED2	20:A:1781:CLA:CAA	2.30	0.61
20:A:1796:CLA:C10	20:A:1813:CLA:H152	2.31	0.61
6:B:493:TRP:HH2	20:B:1765:CLA:HMA2	1.65	0.61
6:B:552:ASP:HA	8:D:144:ILE:HG22	1.81	0.61
6:B:715:VAL:HG23	6:B:719:PHE:HD2	1.64	0.61
7:C:60:THR:HG23	7:C:63:LEU:O	2.01	0.61
9:E:41:ARG:HG3	9:E:46:PHE:CZ	2.36	0.61
2:2:196:HIS:CE1	19:M:1:GLC:HO3	2.17	0.61
5:A:105:ASN:HB2	5:A:140:PHE:HZ	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:368:LEU:CD1	20:A:1782:CLA:C6	2.79	0.61
5:A:389:TYR:HE1	5:A:625:TRP:CD1	2.19	0.61
5:A:604:TRP:HE1	20:B:1787:CLA:C1D	2.13	0.61
20:A:1781:CLA:HAA2	20:A:1782:CLA:CAD	2.31	0.61
20:A:1782:CLA:HMC1	20:A:1782:CLA:HBC3	1.77	0.61
21:A:7038:LMU:C10	21:A:7038:LMU:H62	2.30	0.61
6:B:120:VAL:CA	6:B:123:TRP:HD1	2.09	0.61
6:B:143:LEU:C	6:B:145:LEU:H	2.03	0.61
6:B:347:LEU:CD2	6:B:351:HIS:HE1	2.13	0.61
6:B:348:VAL:HG12	6:B:349:ALA:N	2.16	0.61
6:B:559:CYS:HB2	6:B:702:ILE:HD12	1.82	0.61
6:B:655:LEU:HD22	20:B:1771:CLA:CBB	2.29	0.61
6:B:707:LEU:HD12	6:B:711:VAL:HG21	1.80	0.61
20:B:1755:CLA:CMB	22:B:1777:BCR:C35	2.77	0.61
20:B:1755:CLA:H11	20:B:1769:CLA:CBD	2.31	0.61
8:D:102:ARG:NH2	8:D:109:VAL:O	2.34	0.61
12:H:39:PHE:O	12:H:40:PHE:CD1	2.53	0.61
20:J:1045:CLA:H2A	20:J:1045:CLA:C1	2.30	0.61
17:N:72:LYS:CB	17:N:73:ASP:C	2.59	0.61
1:1:44:LEU:HD22	1:1:154:ALA:HB3	1.82	0.60
2:2:148:TRP:O	2:2:150:SER:N	2.34	0.60
20:2:1220:CLA:H62	3:3:140:LYS:NZ	2.16	0.60
3:3:173:GLU:HG2	3:3:174:LYS:N	2.08	0.60
5:A:123:VAL:O	5:A:124:TRP:HB2	2.01	0.60
5:A:446:LEU:CD1	5:A:554:LEU:HA	2.30	0.60
5:A:662:SER:HA	5:A:665:ILE:HD11	1.82	0.60
20:A:1783:CLA:H172	22:A:1808:BCR:C17	2.30	0.60
20:A:1787:CLA:H93	16:L:36:TYR:CE1	2.35	0.60
20:A:1795:CLA:H42	20:A:1795:CLA:O2A	2.00	0.60
6:B:467:HIS:NE2	20:B:1764:CLA:C1A	2.64	0.60
6:B:494:LEU:HD12	20:B:1765:CLA:HED1	1.83	0.60
20:B:1739:CLA:HMC1	22:B:1780:BCR:H282	1.82	0.60
20:B:1756:CLA:C7	22:B:1777:BCR:H14C	2.31	0.60
10:F:17:ARG:HA	10:F:17:ARG:NE	2.15	0.60
20:J:1043:CLA:C16	20:J:1043:CLA:C2	2.76	0.60
18:R:41:UNK:CA	18:R:42:UNK:CB	2.77	0.60
4:4:150:LYS:HE3	4:4:150:LYS:H	1.66	0.60
5:A:84:GLY:O	5:A:87:SER:O	2.19	0.60
20:A:1800:CLA:H141	16:L:95:LEU:HD22	1.83	0.60
21:A:7028:LMU:O2'	21:A:7028:LMU:H11	2.00	0.60
21:A:7040:LMU:C1B	21:A:7040:LMU:H3O2	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:51:PHE:CD1	20:B:1743:CLA:HED1	2.36	0.60
6:B:500:ALA:HB2	6:B:508:LEU:HD22	1.83	0.60
8:D:37:LEU:O	8:D:39:LYS:N	2.34	0.60
13:I:26:LEU:HD13	13:I:30:LYS:HB3	1.82	0.60
20:J:1044:CLA:O1D	20:J:1045:CLA:H93	1.95	0.60
20:K:1146:CLA:HMC1	20:K:1146:CLA:CBC	2.20	0.60
18:R:35:UNK:C	18:R:38:UNK:CB	2.79	0.60
4:4:38:ARG:O	4:4:39:TRP:HD1	1.85	0.60
4:4:133:TYR:CD1	4:4:134:PRO:HD2	2.36	0.60
5:A:158:ILE:CG2	20:A:1770:CLA:HED3	2.32	0.60
5:A:406:LEU:HD11	20:A:1762:CLA:HMB3	1.83	0.60
20:A:1779:CLA:HBC1	22:A:1805:BCR:C39	2.31	0.60
20:A:1811:CLA:CAA	20:B:1785:CLA:HBB2	2.29	0.60
21:A:7016:LMU:H32	21:A:7016:LMU:H92	1.77	0.60
6:B:127:ILE:HG12	6:B:193:HIS:HE1	1.66	0.60
6:B:560:ASP:OD1	7:C:66:ARG:HB3	2.00	0.60
7:C:1:MET:H2	7:C:3:HIS:H	1.43	0.60
22:I:1032:BCR:C39	22:L:1169:BCR:H401	2.30	0.60
16:L:164:PRO:CB	16:L:165:TYR:HD2	2.01	0.60
22:L:1170:BCR:C33	22:L:1170:BCR:C8	2.73	0.60
17:N:54:LYS:CB	17:N:57:LYS:HE2	2.14	0.60
22:3:1220:BCR:C39	22:3:1220:BCR:C23	2.37	0.60
5:A:91:LEU:O	20:A:1763:CLA:CMC	2.49	0.60
5:A:346:LEU:O	5:A:347:TYR:HB2	2.01	0.60
5:A:389:TYR:CE1	5:A:625:TRP:CD1	2.89	0.60
21:A:7023:LMU:H91	21:A:7023:LMU:H21	0.65	0.60
6:B:154:TRP:CD1	6:B:158:GLN:CG	2.85	0.60
6:B:646:TRP:O	6:B:649:MET:HB2	2.00	0.60
20:B:1762:CLA:H71	22:B:1779:BCR:H402	1.84	0.60
16:L:9:GLN:C	16:L:11:ILE:H	2.03	0.60
5:A:22:VAL:HG13	5:A:23:ASP:N	2.15	0.60
5:A:40:PHE:CZ	5:A:56:ASN:HB3	2.37	0.60
5:A:257:GLN:O	5:A:258:LEU:HB2	2.02	0.60
5:A:261:SER:O	5:A:262:PHE:CD2	2.55	0.60
5:A:348:GLU:O	5:A:350:LEU:N	2.35	0.60
5:A:370:ILE:CD1	20:A:1781:CLA:O1D	2.48	0.60
5:A:693:LEU:HD11	5:A:738:TYR:CD1	2.37	0.60
5:A:700:TRP:CZ3	20:A:1813:CLA:O1D	2.54	0.60
20:A:1780:CLA:OBD	20:A:1780:CLA:H112	2.01	0.60
20:A:1786:CLA:HMB2	20:A:1787:CLA:C2D	2.30	0.60
6:B:91:ILE:HG22	20:B:1740:CLA:CAD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:393:PHE:CD2	6:B:397:ASP:OD1	2.47	0.60
6:B:534:LEU:HD21	6:B:579:ALA:CB	2.32	0.60
6:B:551:LYS:CG	6:B:552:ASP:H	2.14	0.60
6:B:651:LEU:HB3	20:B:1786:CLA:O2A	2.02	0.60
20:B:1739:CLA:CMC	22:B:1780:BCR:C28	2.79	0.60
22:3:1220:BCR:HC8	22:3:1220:BCR:H321	1.84	0.60
5:A:664:VAL:HG23	5:A:665:ILE:HG23	1.82	0.60
6:B:8:PHE:O	6:B:35:ASP:CB	2.49	0.60
6:B:166:SER:O	6:B:168:PHE:N	2.33	0.60
6:B:190:TRP:HE3	20:B:1744:CLA:HBB2	1.65	0.60
10:F:20:GLN:O	10:F:21:ALA:HB2	2.01	0.60
21:R:1056:LMU:H1'	21:R:1056:LMU:H6'	1.67	0.60
2:2:110:TRP:CE3	20:2:1222:CLA:HED1	2.37	0.60
20:2:1220:CLA:C7	3:3:140:LYS:HZ3	2.15	0.60
5:A:81:ALA:HB1	20:A:1760:CLA:HMA3	1.78	0.60
5:A:714:LEU:HA	10:F:149:LEU:HD11	1.82	0.60
20:A:1779:CLA:NC	22:A:1805:BCR:C19	2.56	0.60
20:A:1790:CLA:H2A	20:A:1790:CLA:O1D	2.00	0.60
20:A:1812:CLA:CED	20:B:1785:CLA:H2	2.31	0.60
21:A:7033:LMU:C1B	21:A:7033:LMU:C6'	2.72	0.60
6:B:464:GLN:HA	6:B:467:HIS:HB2	1.82	0.60
6:B:666:SER:HB3	6:B:671:TRP:NE1	2.12	0.60
20:B:1739:CLA:H142	20:B:1739:CLA:C10	2.31	0.60
7:C:28:MET:SD	8:D:122:LYS:C	2.80	0.60
9:E:37:LYS:HB2	9:E:49:VAL:HG22	1.82	0.60
18:R:35:UNK:N	18:R:38:UNK:CB	2.65	0.60
20:1:1192:CLA:CBC	20:1:1192:CLA:CHD	2.76	0.60
20:2:1220:CLA:H62	3:3:140:LYS:HE2	1.83	0.60
5:A:229:ILE:CG2	5:A:229:ILE:O	2.49	0.60
20:A:1783:CLA:HBA1	20:A:1783:CLA:C4	2.29	0.60
21:A:7039:LMU:H5'	21:A:7039:LMU:O2'	2.02	0.60
6:B:412:LEU:O	6:B:415:LYS:HB3	2.02	0.60
6:B:482:ASN:OD1	6:B:485:ALA:HB2	2.01	0.60
6:B:593:TYR:O	6:B:596:TRP:O	2.19	0.60
6:B:652:PHE:O	6:B:656:VAL:HG23	2.00	0.60
10:F:151:ASP:OD2	10:F:154:PHE:CD1	2.54	0.60
4:4:122:LYS:HB2	4:4:143:PHE:HD2	1.66	0.60
4:4:122:LYS:CG	4:4:150:LYS:HD2	2.27	0.60
5:A:412:ALA:HA	5:A:598:VAL:HG21	1.83	0.60
5:A:697:ARG:C	5:A:699:TYR:H	2.04	0.60
5:A:708:VAL:CA	5:A:711:HIS:HD2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1770:CLA:CMB	22:A:1803:BCR:H382	2.19	0.60
22:A:1807:BCR:H322	22:A:1808:BCR:H391	1.84	0.60
6:B:282:PHE:HE2	20:B:1746:CLA:H3A	1.66	0.60
6:B:661:PHE:HB2	20:B:1787:CLA:HMC1	1.81	0.60
10:F:10:GLU:OE1	10:F:11:SER:N	2.35	0.60
10:F:23:LYS:HB3	10:F:24:LYS:HZ3	1.67	0.60
11:G:26:PHE:HB2	11:G:27:GLN:NE2	2.16	0.60
12:H:57:LEU:O	12:H:57:LEU:HD13	2.01	0.60
16:L:135:GLY:O	16:L:138:LYS:HG2	2.01	0.60
20:1:1193:CLA:CGD	20:1:1193:CLA:HAA2	2.32	0.60
3:3:181:LEU:HD13	3:3:184:VAL:HG21	1.82	0.60
4:4:193:ILE:HG22	4:4:194:VAL:N	2.17	0.60
5:A:109:TRP:CH2	5:A:154:ARG:HD3	2.36	0.60
5:A:122:VAL:HA	5:A:133:ASN:HD21	1.67	0.60
5:A:711:HIS:HB3	5:A:717:ALA:CB	2.32	0.60
20:A:1760:CLA:HBA2	20:A:1767:CLA:H62	1.84	0.60
6:B:40:GLY:HA2	6:B:165:VAL:HG23	1.82	0.60
6:B:53:GLN:OE1	6:B:53:GLN:HA	1.91	0.60
6:B:439:HIS:CD2	6:B:453:ILE:HG22	2.37	0.60
6:B:632:ILE:C	6:B:634:GLY:H	2.05	0.60
20:B:1749:CLA:OBD	20:B:1752:CLA:CBC	2.48	0.60
22:B:1778:BCR:C37	10:F:93:ILE:HG22	2.31	0.60
7:C:49:VAL:HG22	7:C:50:GLY:H	1.67	0.60
7:C:74:THR:O	7:C:77:MET:N	2.30	0.60
8:D:79:ARG:H	8:D:82:GLN:NE2	2.00	0.60
10:F:46:MET:O	10:F:48:LYS:N	2.35	0.60
18:R:4:UNK:O	18:R:5:UNK:CB	2.50	0.60
20:2:1224:CLA:H152	20:2:1224:CLA:C19	2.22	0.59
3:3:74:ALA:HB2	20:3:1215:CLA:C1D	2.32	0.59
5:A:51:THR:HB	20:A:1795:CLA:HBB2	1.76	0.59
5:A:128:GLY:HA3	6:B:446:PHE:CD2	2.37	0.59
5:A:174:PHE:O	5:A:175:ALA:CB	2.49	0.59
5:A:218:TRP:CA	20:A:1770:CLA:HBB2	2.31	0.59
5:A:535:GLY:O	5:A:539:PHE:HB2	2.01	0.59
5:A:605:MET:HA	5:A:608:SER:HG	1.64	0.59
5:A:736:THR:HG21	20:A:1785:CLA:H91	1.84	0.59
20:A:1765:CLA:HMC1	20:A:1765:CLA:HBC3	1.82	0.59
20:A:1800:CLA:H201	16:L:64:LEU:CD2	2.32	0.59
6:B:277:HIS:HE1	20:B:1748:CLA:NC	2.00	0.59
6:B:357:ALA:O	6:B:358:TYR:CD1	2.54	0.59
6:B:493:TRP:NE1	20:B:1746:CLA:HAC2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:498:LEU:HD12	6:B:498:LEU:O	2.02	0.59
6:B:623:TYR:O	6:B:624:LEU:HB2	2.00	0.59
20:B:1738:CLA:C19	20:B:1757:CLA:H141	2.32	0.59
8:D:87:GLY:N	8:D:90:LEU:HB3	2.17	0.59
9:E:39:LEU:H	9:E:40:ARG:CZ	2.15	0.59
11:G:94:ASP:H	11:G:95:PRO:HD2	1.66	0.59
15:K:1:ASP:CA	15:K:5:SER:HB3	2.25	0.59
19:W:1:GLC:HO2	19:W:2:FRU:C2	2.13	0.59
20:2:1213:CLA:H2A	20:2:1213:CLA:O1D	2.02	0.59
20:A:1765:CLA:HBA2	20:A:1765:CLA:CHA	2.31	0.59
20:A:1793:CLA:CGA	20:A:1793:CLA:CHA	2.80	0.59
21:A:7021:LMU:C6'	21:A:7021:LMU:C4	2.75	0.59
6:B:305:LEU:HD22	20:B:1753:CLA:O1D	2.02	0.59
20:B:1741:CLA:HBD	20:B:1741:CLA:O2A	2.01	0.59
20:B:1757:CLA:HMC1	20:B:1757:CLA:HBC3	1.84	0.59
9:E:56:ASP:HB2	9:E:64:PRO:CB	2.29	0.59
10:F:22:LEU:CA	10:F:25:LEU:HD13	2.32	0.59
10:F:103:SER:O	10:F:105:LEU:N	2.34	0.59
11:G:71:VAL:O	11:G:73:ALA:O	2.20	0.59
13:I:2:ILE:HG12	13:I:3:ASN:ND2	2.17	0.59
17:N:39:SER:O	17:N:40:CYS:CB	2.49	0.59
3:3:141:GLN:HG2	3:3:142:TYR:N	2.16	0.59
4:4:117:GLN:O	4:4:123:GLN:HA	2.01	0.59
20:A:1772:CLA:H2A	20:A:1772:CLA:O2D	1.97	0.59
20:A:1795:CLA:ND	20:B:1735:CLA:HMC3	2.17	0.59
6:B:154:TRP:CD1	6:B:158:GLN:HG2	2.37	0.59
6:B:352:MET:SD	20:B:1758:CLA:OBD	2.60	0.59
6:B:707:LEU:O	6:B:710:LEU:HB3	2.02	0.59
8:D:75:LEU:HD21	16:L:19:PHE:CZ	2.36	0.59
20:G:1099:CLA:HAA2	20:G:1099:CLA:HBD	1.84	0.59
13:I:11:LEU:HG	22:I:1032:BCR:HC7	1.80	0.59
17:N:4:GLU:CD	17:N:5:GLU:HB2	2.22	0.59
2:2:169:LEU:CD2	20:2:1215:CLA:CAB	2.75	0.59
20:2:1220:CLA:H42	3:3:140:LYS:HB2	1.84	0.59
5:A:527:VAL:CG1	5:A:528:ALA:N	2.66	0.59
5:A:636:HIS:C	5:A:638:THR:H	2.05	0.59
5:A:684:PHE:CD2	5:A:685:VAL:N	2.70	0.59
5:A:737:HIS:HA	5:A:740:LEU:HD23	1.83	0.59
20:A:1771:CLA:HAA1	20:A:1771:CLA:HED2	1.84	0.59
20:A:1773:CLA:H52	20:A:1790:CLA:HBA1	1.84	0.59
6:B:82:PHE:O	6:B:84:VAL:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:194:LEU:O	6:B:198:ALA:HB3	2.02	0.59
6:B:330:ILE:HD11	20:B:1737:CLA:C19	2.33	0.59
6:B:436:LEU:O	6:B:437:TYR:HB2	2.02	0.59
11:G:34:GLN:O	11:G:35:VAL:C	2.40	0.59
20:J:1045:CLA:HMA3	20:J:1045:CLA:H2	1.85	0.59
1:1:25:ASP:HB3	1:1:26:PRO:CD	2.32	0.59
20:2:1220:CLA:C6	3:3:140:LYS:CD	2.62	0.59
3:3:90:LEU:H	3:3:90:LEU:HD12	1.67	0.59
4:4:169:GLN:OE1	20:4:1199:CLA:HHD	2.01	0.59
5:A:451:ILE:HD11	20:A:1788:CLA:CED	2.32	0.59
5:A:478:SER:HB3	5:A:644:GLN:CD	2.21	0.59
5:A:502:THR:H	5:A:504:ALA:HB3	1.68	0.59
5:A:586:ARG:CG	7:C:49:VAL:HG21	2.31	0.59
5:A:681:GLY:HA2	5:A:684:PHE:HB3	1.84	0.59
6:B:289:LEU:HD22	22:B:1774:BCR:H352	1.83	0.59
6:B:409:ALA:C	6:B:411:MET:N	2.55	0.59
6:B:555:TYR:O	6:B:571:SER:HB2	2.02	0.59
20:B:1743:CLA:C15	20:B:1758:CLA:HMD2	2.29	0.59
20:B:1761:CLA:HHD	20:B:1761:CLA:HBC3	1.80	0.59
8:D:58:PHE:HD2	8:D:59:GLU:H	1.47	0.59
8:D:111:TYR:CD2	8:D:114:PRO:CB	2.83	0.59
11:G:45:GLU:O	11:G:46:ALA:CB	2.49	0.59
11:G:64:VAL:O	11:G:64:VAL:HG12	2.02	0.59
11:G:93:TYR:C	11:G:95:PRO:HD3	2.22	0.59
20:G:1099:CLA:HBC3	20:G:1099:CLA:HHD	1.83	0.59
14:J:26:LEU:HD23	14:J:26:LEU:O	2.02	0.59
1:1:185:TRP:O	1:1:186:HIS:CG	2.55	0.59
5:A:165:TYR:CD2	5:A:165:TYR:O	2.55	0.59
5:A:358:LEU:HD21	5:A:413:HIS:ND1	2.17	0.59
5:A:472:ARG:N	5:A:473:PRO:CD	2.64	0.59
20:A:1763:CLA:C4B	22:A:1808:BCR:H333	2.32	0.59
20:A:1815:CLA:HMA1	20:A:1815:CLA:C2	2.32	0.59
6:B:625:TRP:CE3	6:B:626:LEU:N	2.70	0.59
6:B:732:LYS:CG	6:B:733:PHE:HA	2.22	0.59
15:K:69:ILE:O	15:K:72:VAL:N	2.36	0.59
16:L:58:LEU:HD21	16:L:153:TRP:CZ2	2.37	0.59
16:L:124:LYS:C	16:L:126:GLN:N	2.56	0.59
17:N:58:VAL:C	17:N:60:PHE:N	2.52	0.59
17:N:67:LEU:HB2	17:N:68:GLU:HB3	1.85	0.59
18:R:26:UNK:C	18:R:28:UNK:N	2.66	0.59
20:2:1215:CLA:HBC2	20:2:1215:CLA:HMC1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:143:ILE:HD12	5:A:144:GLN:H	1.68	0.59
5:A:396:PHE:CG	5:A:396:PHE:O	2.54	0.59
5:A:582:ASP:HB3	5:A:589:THR:HG22	1.83	0.59
20:A:1760:CLA:H12	20:A:1767:CLA:H92	1.83	0.59
20:A:1800:CLA:H112	20:A:1800:CLA:H61	1.83	0.59
21:A:7037:LMU:H61	21:A:7037:LMU:C2	2.33	0.59
6:B:289:LEU:HD21	20:B:1750:CLA:NA	2.18	0.59
6:B:310:PRO:HB2	6:B:311:PRO:CD	2.33	0.59
6:B:454:LEU:HD12	6:B:454:LEU:N	2.18	0.59
6:B:657:TRP:O	6:B:660:GLY:N	2.26	0.59
6:B:707:LEU:HD11	6:B:711:VAL:HG21	1.84	0.59
7:C:1:MET:CG	7:C:4:SER:HG	2.09	0.59
8:D:61:PRO:HD3	8:D:86:LEU:HD21	1.85	0.59
11:G:42:SER:OG	11:G:44:PHE:N	2.36	0.59
12:H:21:TRP:N	12:H:22:ASP:CA	2.60	0.59
13:I:10:PRO:O	13:I:15:LEU:N	2.35	0.59
16:L:33:ILE:CD1	16:L:36:TYR:HD1	2.16	0.59
18:R:39:UNK:CB	18:R:40:UNK:HA	2.33	0.59
21:R:1056:LMU:H1B	21:R:1056:LMU:H6B	1.63	0.59
20:1:1200:CLA:HBC2	20:4:1198:CLA:CMB	2.32	0.59
3:3:83:LEU:CD1	20:A:1798:CLA:HED2	2.32	0.59
5:A:295:TRP:HB2	5:A:298:ASP:OD2	2.02	0.59
5:A:680:LEU:HD21	6:B:617:MET:HE3	1.85	0.59
6:B:212:PHE:CZ	20:B:1744:CLA:HAC1	2.37	0.59
6:B:459:PHE:O	6:B:463:ILE:HD13	2.03	0.59
6:B:557:PHE:CD1	6:B:571:SER:HB3	2.37	0.59
6:B:727:ALA:C	6:B:728:SER:OG	2.40	0.59
20:B:1739:CLA:H42	20:B:1739:CLA:CHD	2.33	0.59
20:B:1768:CLA:C6	22:B:1779:BCR:H323	2.31	0.59
22:B:1781:BCR:H392	20:I:1031:CLA:C14	2.32	0.59
8:D:46:TYR:N	8:D:46:TYR:CD2	2.70	0.59
11:G:37:GLU:OE2	11:G:42:SER:CA	2.51	0.59
16:L:50:LEU:HG	16:L:51:LEU:HD23	1.85	0.59
20:L:1505:CLA:C10	20:L:1505:CLA:H41	2.33	0.59
21:2:7006:LMU:C5B	21:2:7006:LMU:H3'	2.33	0.59
20:4:1196:CLA:H2A	20:4:1196:CLA:O1D	2.03	0.59
5:A:432:LEU:C	5:A:434:ARG:N	2.55	0.59
20:A:1791:CLA:CAA	20:A:1797:CLA:HBB2	2.33	0.59
22:A:1804:BCR:H403	22:A:1804:BCR:C23	2.14	0.59
6:B:50:HIS:HA	6:B:53:GLN:HB2	1.85	0.59
6:B:55:ALA:HB1	6:B:150:LEU:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:156:HIS:O	6:B:163:PRO:HB3	2.03	0.59
12:H:25:GLY:C	12:H:27:ASP:N	2.38	0.59
19:Z:1:GLC:O6	19:Z:2:FRU:C2	2.50	0.59
3:3:86:GLN:HB2	3:3:88:THR:CB	2.30	0.59
20:4:1196:CLA:CHD	20:4:1196:CLA:HBC3	2.25	0.59
5:A:44:ILE:O	5:A:46:LYS:HA	2.03	0.59
5:A:163:GLN:O	5:A:166:CYS:N	2.36	0.59
5:A:497:ALA:O	5:A:498:LEU:HB2	2.02	0.59
5:A:657:LEU:HD23	20:A:1811:CLA:C1D	2.32	0.59
5:A:733:VAL:HG11	20:A:1796:CLA:C2D	2.33	0.59
20:A:1783:CLA:H18	20:A:1812:CLA:H18	1.85	0.59
21:A:7037:LMU:C7	21:A:7037:LMU:C3	2.30	0.59
6:B:70:TRP:NE1	6:B:71:GLN:OE1	2.35	0.59
6:B:190:TRP:CA	20:B:1744:CLA:HBB2	2.33	0.59
6:B:551:LYS:O	6:B:553:PHE:CD2	2.56	0.59
6:B:692:ARG:NH2	6:B:694:ARG:HG2	2.17	0.59
20:B:1755:CLA:CHB	20:B:1769:CLA:HAA2	2.33	0.59
9:E:40:ARG:HH22	9:E:87:VAL:HG22	1.68	0.59
9:E:48:ASN:ND2	9:E:71:LYS:HZ2	2.00	0.59
10:F:151:ASP:CA	10:F:154:PHE:HB3	2.33	0.59
22:I:1032:BCR:H382	22:I:1032:BCR:C40	2.33	0.59
14:J:2:ARG:HB3	14:J:7:TYR:CZ	2.38	0.59
16:L:111:GLU:OE1	21:L:1171:LMU:O6B	2.21	0.59
17:N:53:ALA:O	17:N:54:LYS:CD	2.51	0.59
3:3:194:ILE:HG23	3:3:197:TYR:OH	2.02	0.58
5:A:284:ARG:HH22	5:A:507:ALA:C	2.06	0.58
5:A:351:THR:HA	20:A:1780:CLA:H191	1.85	0.58
5:A:401:TRP:HB3	20:A:1783:CLA:HMC3	1.85	0.58
20:A:1773:CLA:HMC1	20:A:1773:CLA:HBC3	1.83	0.58
21:A:7032:LMU:H31	21:A:7032:LMU:C4B	2.33	0.58
6:B:142:LEU:HD21	22:B:1776:BCR:H333	1.82	0.58
6:B:196:HIS:CE1	20:B:1745:CLA:ND	2.71	0.58
6:B:376:GLN:OE1	6:B:376:GLN:HA	2.03	0.58
6:B:668:ARG:HG3	6:B:700:LEU:O	2.02	0.58
20:B:1737:CLA:H151	20:B:1737:CLA:OBD	2.03	0.58
20:B:1738:CLA:H191	20:B:1757:CLA:H141	1.85	0.58
20:B:1739:CLA:H102	20:B:1739:CLA:C14	2.32	0.58
20:B:1739:CLA:CGA	20:B:1739:CLA:C1A	2.81	0.58
20:B:1747:CLA:CBD	20:B:1756:CLA:HBB2	2.32	0.58
22:B:1778:BCR:H23C	10:F:90:PHE:CD1	2.38	0.58
11:G:30:ASN:C	11:G:30:ASN:HD22	2.05	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:27:ASP:C	12:H:29:PRO:HD3	2.23	0.58
2:2:181:HIS:CD2	20:2:1214:CLA:C2D	2.86	0.58
3:3:157:ALA:O	3:3:158:TYR:HB2	2.02	0.58
5:A:79:PHE:HE2	5:A:185:HIS:NE2	1.73	0.58
5:A:473:PRO:O	5:A:475:ASP:N	2.36	0.58
5:A:691:MET:HB2	20:A:1813:CLA:C1C	2.32	0.58
5:A:733:VAL:HG21	20:A:1796:CLA:HMD3	1.84	0.58
20:A:1781:CLA:HMA1	22:A:1806:BCR:H16C	1.83	0.58
20:A:1816:CLA:HED1	20:A:1816:CLA:H12	1.78	0.58
6:B:615:TYR:HD1	6:B:615:TYR:N	2.01	0.58
6:B:662:MET:HG2	23:B:1773:PQN:O1	2.03	0.58
10:F:80:TRP:HZ3	20:F:1156:CLA:CMC	2.16	0.58
17:N:72:LYS:HD3	17:N:72:LYS:N	2.18	0.58
5:A:112:ASP:O	5:A:116:ILE:HG12	2.02	0.58
5:A:131:ILE:CG2	5:A:132:LEU:N	2.66	0.58
5:A:154:ARG:NH2	5:A:233:LEU:HD13	2.18	0.58
5:A:230:ASN:HA	5:A:233:LEU:HB2	1.85	0.58
5:A:309:LEU:HA	5:A:312:ILE:O	2.02	0.58
5:A:691:MET:CE	23:A:1802:PQN:C2M	2.80	0.58
5:A:755:ILE:O	5:A:756:ALA:CB	2.52	0.58
20:A:1765:CLA:HBA2	20:A:1765:CLA:CBD	2.33	0.58
7:C:7:ILE:O	7:C:60:THR:HA	2.03	0.58
10:F:78:ARG:O	10:F:80:TRP:HD1	1.86	0.58
11:G:93:TYR:CA	11:G:94:ASP:OD1	2.50	0.58
16:L:108:LYS:O	16:L:132:SER:CB	2.41	0.58
20:4:1198:CLA:O1A	20:4:1198:CLA:H2	2.01	0.58
5:A:154:ARG:HG3	5:A:383:PRO:HB2	1.85	0.58
5:A:373:ALA:O	5:A:396:PHE:CD1	2.56	0.58
5:A:452:PHE:CD1	20:A:1793:CLA:HBB1	2.32	0.58
23:A:1802:PQN:H241	23:A:1802:PQN:H272	1.86	0.58
6:B:530:THR:CG2	20:B:1755:CLA:HMC1	2.33	0.58
6:B:710:LEU:C	6:B:712:HIS:N	2.55	0.58
9:E:69:PHE:CD2	9:E:71:LYS:HG2	2.38	0.58
10:F:123:VAL:HG13	14:J:7:TYR:H	1.68	0.58
22:I:1032:BCR:HC22	20:I:1033:CLA:CHD	2.33	0.58
16:L:45:THR:HA	16:L:52:ARG:HH12	1.67	0.58
18:R:35:UNK:C	18:R:36:UNK:O	2.51	0.58
20:2:1213:CLA:HHD	20:2:1213:CLA:CBC	2.25	0.58
3:3:92:TRP:HZ2	5:A:250:LEU:HB2	1.68	0.58
5:A:23:ASP:C	5:A:23:ASP:OD1	2.41	0.58
5:A:207:LEU:HD13	20:A:1776:CLA:HBB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:458:ILE:HG13	6:B:459:PHE:N	2.16	0.58
9:E:51:SER:O	9:E:68:ARG:N	2.27	0.58
13:I:28:VAL:O	13:I:29:GLU:CD	2.42	0.58
15:K:71:GLY:C	15:K:72:VAL:O	2.42	0.58
5:A:98:PHE:HD1	5:A:99:HIS:HD2	1.51	0.58
5:A:239:PRO:CA	5:A:242:ILE:HD11	2.30	0.58
5:A:243:PRO:O	5:A:244:LEU:O	2.20	0.58
5:A:592:VAL:HG23	5:A:593:SER:H	1.67	0.58
20:A:1763:CLA:HBA2	20:A:1765:CLA:C1	2.32	0.58
20:A:1763:CLA:HBB	20:A:1764:CLA:HMB3	1.85	0.58
20:A:1782:CLA:HBA2	22:A:1806:BCR:H12C	1.85	0.58
6:B:36:ASP:O	6:B:41:ARG:NE	2.37	0.58
6:B:646:TRP:CZ2	6:B:726:ILE:HG21	2.38	0.58
20:B:1759:CLA:H93	24:B:1783:LMG:H311	1.84	0.58
20:B:1787:CLA:HMC1	20:B:1787:CLA:HBC3	1.86	0.58
20:K:1085:CLA:ND	20:K:1142:CLA:HMD3	2.18	0.58
16:L:40:LEU:CB	16:L:41:PRO:CD	2.82	0.58
18:R:52:UNK:CB	18:R:53:UNK:CB	2.82	0.58
20:1:1191:CLA:HHC	20:1:1197:CLA:HBC1	1.86	0.58
2:2:79:TRP:CG	2:2:79:TRP:O	2.57	0.58
3:3:52:LYS:N	3:3:55:ALA:HB3	2.19	0.58
5:A:42:ARG:C	5:A:44:ILE:N	2.56	0.58
5:A:98:PHE:O	5:A:99:HIS:CB	2.51	0.58
5:A:157:GLY:O	5:A:158:ILE:HB	2.04	0.58
5:A:225:VAL:HG12	5:A:248:PHE:CD1	2.39	0.58
5:A:413:HIS:ND1	5:A:416:ILE:HD12	2.18	0.58
5:A:678:PHE:O	5:A:680:LEU:N	2.36	0.58
21:A:7030:LMU:H2'	21:A:7030:LMU:H6E	1.84	0.58
6:B:415:LYS:CE	6:B:539:LEU:O	2.51	0.58
6:B:569:ASP:HB3	6:B:574:ASP:HB3	1.86	0.58
6:B:628:SER:O	6:B:631:LEU:HD23	2.03	0.58
20:B:1754:CLA:H61	20:B:1754:CLA:HMA2	1.84	0.58
22:B:1778:BCR:H392	10:F:90:PHE:HA	1.86	0.58
22:B:1781:BCR:H342	20:H:1079:CLA:HAC2	1.85	0.58
20:B:1787:CLA:HED3	20:B:1787:CLA:HBA2	1.85	0.58
10:F:40:LEU:CA	10:F:42:ILE:HG12	2.30	0.58
19:O:2:FRU:H11	19:O:2:FRU:C6	1.99	0.58
2:2:103:GLY:HA2	20:2:1222:CLA:HBB2	1.84	0.58
5:A:122:VAL:HG22	5:A:142:GLY:HA2	1.85	0.58
5:A:455:PHE:O	20:A:1789:CLA:CBB	2.52	0.58
20:A:1783:CLA:H171	22:A:1808:BCR:H351	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1813:CLA:H3A	20:A:1813:CLA:CGA	2.34	0.58
6:B:5:ILE:CB	6:B:6:PRO:HD2	2.30	0.58
6:B:22:TRP:CE2	20:B:1770:CLA:HMB1	2.39	0.58
6:B:187:SER:O	6:B:188:LEU:C	2.41	0.58
6:B:278:LEU:O	6:B:281:ALA:N	2.37	0.58
6:B:304:ILE:HD11	20:B:1749:CLA:HED2	1.82	0.58
6:B:460:ALA:O	6:B:461:GLN:C	2.42	0.58
6:B:561:GLY:CA	7:C:52:LYS:HG2	2.32	0.58
7:C:79:LEU:HD22	7:C:81:TYR:C	2.23	0.58
16:L:97:MET:HA	16:L:100:THR:HG23	1.86	0.58
18:R:37:UNK:C	18:R:42:UNK:O	2.52	0.58
20:2:1220:CLA:HBC3	20:2:1220:CLA:CHD	2.33	0.58
5:A:158:ILE:O	5:A:243:PRO:HG2	2.03	0.58
5:A:170:GLY:C	5:A:173:VAL:HG22	2.22	0.58
5:A:185:HIS:O	5:A:188:LYS:N	2.37	0.58
6:B:392:ILE:HG12	6:B:555:TYR:CD1	2.38	0.58
6:B:594:TRP:C	6:B:594:TRP:HD1	2.07	0.58
20:B:1735:CLA:NC	20:B:1735:CLA:H52	2.18	0.58
20:B:1758:CLA:C17	22:B:1775:BCR:H363	2.34	0.58
10:F:2:ILE:HG22	10:F:3:ALA:N	2.19	0.58
20:K:1085:CLA:NA	20:K:1142:CLA:HMD3	2.18	0.58
16:L:56:VAL:HA	20:L:1167:CLA:HED1	1.86	0.58
17:N:33:TYR:O	17:N:34:THR:CG2	2.51	0.58
17:N:62:SER:O	17:N:66:ASP:CG	2.42	0.58
2:2:77:PRO:O	17:N:3:ILE:CD1	2.52	0.58
2:2:208:PHE:CG	2:2:209:THR:N	2.71	0.58
20:4:1199:CLA:H2	20:4:1199:CLA:CED	2.34	0.58
5:A:328:LYS:CG	5:A:332:GLU:CB	2.59	0.58
5:A:390:ALA:CB	5:A:754:ILE:HD13	2.33	0.58
5:A:651:GLY:O	5:A:655:ASP:N	2.37	0.58
5:A:705:GLU:HB3	6:B:545:LYS:NZ	2.18	0.58
6:B:261:PHE:CZ	6:B:500:ALA:HB2	2.39	0.58
6:B:715:VAL:O	6:B:716:GLY:C	2.42	0.58
8:D:31:GLY:HA2	16:L:13:PRO:CB	2.34	0.58
14:J:9:SER:O	14:J:10:VAL:CB	2.51	0.58
20:J:1044:CLA:C4	20:J:1044:CLA:H93	2.33	0.58
1:1:109:GLU:HB3	20:1:1196:CLA:HMA3	1.84	0.57
3:3:84:ILE:N	20:A:1798:CLA:H41	2.14	0.57
4:4:58:MET:O	4:4:60:LEU:N	2.37	0.57
5:A:40:PHE:CE1	5:A:53:TRP:HD1	2.17	0.57
5:A:214:GLY:HA3	22:A:1804:BCR:C15	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:592:VAL:HG23	5:A:593:SER:N	2.19	0.57
20:A:1788:CLA:HAA1	22:L:1170:BCR:C14	2.34	0.57
6:B:391:PRO:HB3	6:B:538:ALA:CA	2.33	0.57
6:B:422:LEU:CD1	6:B:535:VAL:HG11	2.27	0.57
6:B:594:TRP:CD2	6:B:598:HIS:CE1	2.92	0.57
8:D:29:PHE:O	8:D:30:ALA:HB3	2.04	0.57
16:L:161:LEU:HD12	16:L:162:ASP:C	2.22	0.57
17:N:61:LEU:HD13	17:N:63:ASP:CB	2.29	0.57
1:1:25:ASP:HB3	1:1:26:PRO:HD3	1.85	0.57
5:A:146:THR:HG21	5:A:751:LEU:HD22	1.86	0.57
5:A:309:LEU:HD23	5:A:309:LEU:C	2.24	0.57
5:A:708:VAL:O	5:A:711:HIS:HB2	2.04	0.57
20:A:1770:CLA:HMC2	22:A:1803:BCR:C15	2.33	0.57
20:A:1779:CLA:C1B	22:A:1805:BCR:H15C	2.34	0.57
20:A:1792:CLA:HBD	20:A:1792:CLA:CBA	2.34	0.57
20:A:1793:CLA:O1D	20:A:1793:CLA:H2A	2.04	0.57
20:A:1795:CLA:O1A	20:A:1795:CLA:C4	2.52	0.57
20:A:1800:CLA:H202	16:L:64:LEU:HD21	1.84	0.57
21:A:7038:LMU:H61	21:A:7038:LMU:C10	2.22	0.57
6:B:53:GLN:O	6:B:55:ALA:N	2.33	0.57
6:B:175:LEU:HA	6:B:178:HIS:HB2	1.86	0.57
6:B:353:TYR:C	6:B:355:LEU:H	2.07	0.57
6:B:553:PHE:O	6:B:554:GLY:C	2.41	0.57
6:B:665:ILE:HD12	20:B:1787:CLA:HBC1	1.86	0.57
22:B:1781:BCR:HC41	20:B:1787:CLA:H142	1.86	0.57
18:R:38:UNK:C	18:R:42:UNK:O	2.52	0.57
20:R:1055:CLA:H111	21:R:1056:LMU:O4'	2.04	0.57
2:2:64:ILE:HD13	20:2:1213:CLA:HMB1	1.86	0.57
3:3:162:PRO:HG2	3:3:164:PHE:CD1	2.40	0.57
20:4:1201:CLA:O1D	20:4:1201:CLA:C2A	2.52	0.57
5:A:56:ASN:O	5:A:57:LEU:CB	2.52	0.57
5:A:110:LEU:O	5:A:113:PRO:HD3	2.04	0.57
5:A:513:LEU:HB3	5:A:529:LEU:HD13	1.85	0.57
5:A:653:LEU:HD23	20:B:1785:CLA:HBC2	1.86	0.57
5:A:669:GLY:N	6:B:445:ALA:HA	2.15	0.57
6:B:310:PRO:CB	6:B:311:PRO:CD	2.82	0.57
6:B:557:PHE:HE2	7:C:66:ARG:HE	1.51	0.57
20:B:1740:CLA:HBB2	20:B:1786:CLA:C13	2.30	0.57
20:B:1771:CLA:H191	13:I:21:MET:HB2	1.86	0.57
17:N:63:ASP:N	17:N:64:ASP:CA	2.55	0.57
20:3:3011:CLA:H3A	20:3:3011:CLA:CGA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:131:ILE:HD13	6:B:447:GLY:CA	2.34	0.57
5:A:595:TRP:HE3	5:A:596:ASP:OD2	1.87	0.57
5:A:691:MET:HE3	23:A:1802:PQN:C2M	2.34	0.57
5:A:691:MET:O	23:A:1802:PQN:O1	2.23	0.57
20:A:1771:CLA:HBA2	20:A:1771:CLA:H42	1.86	0.57
20:A:1789:CLA:O1D	16:L:73:PRO:HA	2.05	0.57
8:D:86:LEU:C	8:D:90:LEU:HB3	2.25	0.57
10:F:83:PHE:O	10:F:87:GLY:N	2.38	0.57
11:G:46:ALA:CA	11:G:48:ASP:HB3	2.34	0.57
14:J:32:PHE:HE2	14:J:33:PHE:CZ	2.23	0.57
20:J:1045:CLA:CMA	20:J:1045:CLA:H2	2.34	0.57
16:L:125:LYS:C	16:L:127:PRO:HD2	2.24	0.57
2:2:73:ILE:HD12	2:2:73:ILE:N	2.20	0.57
3:3:92:TRP:HZ2	5:A:250:LEU:HD12	1.69	0.57
5:A:462:ILE:HD11	20:B:1786:CLA:C5	2.28	0.57
21:A:7021:LMU:C4	21:A:7021:LMU:H6D	2.35	0.57
21:A:7021:LMU:C6B	21:A:7021:LMU:H3O1	2.14	0.57
6:B:674:LEU:C	6:B:674:LEU:HD12	2.25	0.57
20:B:1747:CLA:C1A	20:B:1747:CLA:H12	2.35	0.57
10:F:22:LEU:O	10:F:25:LEU:HD13	2.02	0.57
14:J:13:VAL:HG12	14:J:15:SER:HB2	1.86	0.57
20:J:1043:CLA:H141	20:J:1044:CLA:HMB3	1.86	0.57
17:N:28:ASN:HA	17:N:30:ALA:H	1.69	0.57
17:N:39:SER:OG	17:N:41:LYS:HA	2.04	0.57
17:N:50:GLN:N	17:N:51:ASP:O	2.37	0.57
21:2:1225:LMU:H6D	21:2:1225:LMU:H41	1.87	0.57
3:3:121:MET:O	20:3:1218:CLA:HED1	2.05	0.57
5:A:105:ASN:HB2	5:A:140:PHE:CZ	2.40	0.57
5:A:193:LEU:O	5:A:194:ALA:C	2.42	0.57
5:A:499:ALA:HB3	20:A:1790:CLA:O2D	2.04	0.57
22:A:1807:BCR:C3	22:B:1778:BCR:H17C	2.34	0.57
6:B:299:HIS:HE1	20:B:1752:CLA:HMD1	1.69	0.57
6:B:334:LEU:CB	20:B:1737:CLA:HMD3	2.34	0.57
6:B:649:MET:CE	6:B:723:ALA:HB2	2.35	0.57
8:D:118:VAL:CG1	8:D:119:TYR:H	2.17	0.57
9:E:40:ARG:CB	9:E:42:GLU:OE2	2.52	0.57
16:L:95:LEU:HD11	16:L:143:PHE:CZ	2.39	0.57
1:1:54:VAL:O	1:1:56:GLY:N	2.38	0.57
4:4:69:ILE:HG22	4:4:70:ILE:H	1.70	0.57
5:A:258:LEU:O	5:A:280:PHE:CE1	2.58	0.57
5:A:281:LEU:HD22	20:A:1772:CLA:CMA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:746:THR:HG1	20:A:1811:CLA:CGD	2.14	0.57
20:A:1779:CLA:C4B	22:A:1805:BCR:H15C	2.34	0.57
20:A:1787:CLA:H142	20:A:1801:CLA:H43	1.86	0.57
20:A:1795:CLA:O2A	20:A:1795:CLA:C4	2.52	0.57
6:B:127:ILE:HD13	6:B:193:HIS:CE1	2.40	0.57
6:B:432:HIS:CE1	20:B:1762:CLA:NB	2.64	0.57
6:B:564:ARG:NE	7:C:64:SER:OG	2.38	0.57
22:B:1780:BCR:H351	20:B:1787:CLA:H111	1.85	0.57
24:B:1783:LMG:H111	24:B:1783:LMG:HC91	1.87	0.57
7:C:52:LYS:C	7:C:54:CYS:N	2.56	0.57
8:D:49:THR:OG1	8:D:74:LEU:HD12	2.05	0.57
20:4:1204:CLA:HBD	20:4:1204:CLA:HBA2	1.87	0.57
5:A:123:VAL:HB	5:A:129:GLN:OE1	2.04	0.57
5:A:402:ILE:C	5:A:404:GLY:H	2.07	0.57
5:A:464:ASN:H	5:A:464:ASN:ND2	2.02	0.57
5:A:547:PHE:O	5:A:551:VAL:CG1	2.46	0.57
5:A:744:ALA:HB2	22:A:1807:BCR:H391	0.67	0.57
20:A:1797:CLA:HMA2	20:A:1797:CLA:O2A	2.03	0.57
20:A:1811:CLA:H192	20:B:1786:CLA:C2B	2.35	0.57
20:A:1813:CLA:H2	20:A:1813:CLA:HMA1	1.87	0.57
21:A:7042:LMU:O2B	21:A:7042:LMU:C4'	2.52	0.57
6:B:212:PHE:HZ	20:B:1744:CLA:HAC1	1.69	0.57
7:C:6:LYS:N	7:C:65:VAL:HG22	2.20	0.57
8:D:31:GLY:O	8:D:32:SER:CB	2.53	0.57
9:E:32:ARG:NH2	9:E:53:VAL:HA	2.20	0.57
9:E:48:ASN:ND2	9:E:71:LYS:HZ1	2.03	0.57
12:H:36:GLN:HG2	12:H:36:GLN:O	2.04	0.57
3:3:205:GLY:CA	5:A:252:ARG:NH2	2.62	0.57
5:A:218:TRP:HA	20:A:1770:CLA:HBB2	1.85	0.57
5:A:553:VAL:HG22	22:A:1806:BCR:H401	1.86	0.57
5:A:625:TRP:HB3	5:A:637:ILE:HD11	1.86	0.57
20:A:1764:CLA:H142	22:A:1808:BCR:C13	2.35	0.57
20:A:1783:CLA:C11	22:A:1808:BCR:H353	2.35	0.57
20:A:1815:CLA:H61	20:A:1815:CLA:HMA3	1.79	0.57
6:B:48:ALA:CB	6:B:157:LEU:HD22	2.34	0.57
6:B:615:TYR:N	6:B:615:TYR:CD1	2.72	0.57
8:D:45:PHE:C	8:D:46:TYR:HD2	2.07	0.57
11:G:32:ALA:O	11:G:33:LYS:C	2.42	0.57
14:J:18:TRP:CH2	14:J:22:LEU:HD22	2.40	0.57
16:L:14:LEU:CD2	16:L:21:GLY:O	2.53	0.57
16:L:30:SER:C	16:L:32:LEU:N	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:54:VAL:O	16:L:58:LEU:HB2	2.04	0.57
20:2:1220:CLA:C6	3:3:140:LYS:HE2	2.34	0.57
3:3:199:VAL:HG22	20:3:1214:CLA:C4C	2.33	0.57
4:4:91:PHE:CD2	20:4:1205:CLA:HHD	2.40	0.57
5:A:109:TRP:HH2	5:A:154:ARG:HD3	1.69	0.57
20:A:1791:CLA:HBC2	22:A:1806:BCR:C3	2.22	0.57
21:A:7032:LMU:H12	21:A:7032:LMU:H2O2	1.66	0.57
6:B:34:HIS:O	6:B:36:ASP:N	2.37	0.57
6:B:305:LEU:O	6:B:306:GLU:C	2.44	0.57
6:B:399:ASN:O	6:B:401:GLU:N	2.38	0.57
20:B:1745:CLA:H2A	20:B:1745:CLA:O1D	2.05	0.57
20:B:1753:CLA:H71	20:B:1753:CLA:H2	1.82	0.57
20:B:1767:CLA:HBC3	20:B:1767:CLA:CMC	2.25	0.57
8:D:39:LYS:HG3	8:D:43:GLU:HG2	1.87	0.57
17:N:80:ASN:OD1	17:N:82:PHE:CA	2.53	0.57
20:2:1218:CLA:H2	20:2:1218:CLA:C1B	2.34	0.56
4:4:124:TYR:HB2	4:4:143:PHE:HD1	1.62	0.56
5:A:265:GLY:CA	5:A:272:LEU:HD21	2.35	0.56
5:A:298:ASP:OD2	5:A:298:ASP:N	2.38	0.56
21:A:7016:LMU:H21	21:A:7016:LMU:H61	1.86	0.56
6:B:257:ILE:HA	6:B:272:ASP:OD2	2.05	0.56
6:B:262:HIS:O	6:B:265:THR:O	2.23	0.56
6:B:493:TRP:CB	20:B:1765:CLA:HED2	2.35	0.56
6:B:542:ARG:NH2	8:D:141:VAL:O	2.38	0.56
6:B:545:LYS:CD	6:B:546:LEU:H	2.18	0.56
8:D:99:GLN:OE1	8:D:101:TYR:OH	2.22	0.56
8:D:101:TYR:CE1	8:D:114:PRO:HD3	2.40	0.56
10:F:50:LYS:O	10:F:52:ARG:C	2.43	0.56
10:F:76:ASP:O	10:F:78:ARG:N	2.38	0.56
15:K:55:PHE:N	15:K:55:PHE:CD1	2.73	0.56
16:L:17:ASP:OD1	16:L:17:ASP:O	2.23	0.56
17:N:80:ASN:C	17:N:82:PHE:N	2.59	0.56
20:1:1188:CLA:HMC1	20:1:1188:CLA:CBC	2.31	0.56
20:2:1215:CLA:C4	20:2:1220:CLA:HBC1	2.34	0.56
4:4:104:ARG:CA	4:4:107:GLN:HB2	2.19	0.56
5:A:207:LEU:HA	5:A:211:LEU:HB2	1.86	0.56
5:A:284:ARG:NH1	5:A:507:ALA:HB1	2.19	0.56
5:A:435:VAL:HA	5:A:438:HIS:CE1	2.40	0.56
5:A:583:GLY:O	5:A:585:GLY:N	2.38	0.56
20:A:1796:CLA:H71	20:A:1813:CLA:H171	1.86	0.56
6:B:224:PRO:O	6:B:226:LEU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:553:PHE:O	6:B:555:TYR:N	2.38	0.56
20:B:1738:CLA:H71	24:B:1783:LMG:H381	1.86	0.56
7:C:31:TRP:CB	7:C:39:ILE:HG21	2.34	0.56
16:L:14:LEU:HD21	16:L:20:ILE:HG22	1.87	0.56
16:L:65:VAL:H	16:L:67:PRO:HD2	1.70	0.56
17:N:76:LYS:CG	17:N:77:CYS:H	2.07	0.56
2:2:56:MET:SD	2:2:169:LEU:HA	2.45	0.56
3:3:194:ILE:HA	3:3:197:TYR:CE1	2.40	0.56
5:A:146:THR:HA	5:A:391:THR:HG23	1.85	0.56
5:A:309:LEU:O	5:A:310:PHE:CB	2.52	0.56
5:A:567:ARG:NH2	8:D:82:GLN:OE1	2.37	0.56
20:A:1759:CLA:HMB1	20:A:1767:CLA:H18	1.87	0.56
20:A:1784:CLA:H51	22:A:1804:BCR:H331	1.87	0.56
20:A:1796:CLA:C19	14:J:19:PHE:CD2	2.88	0.56
21:A:7016:LMU:C3	21:A:7016:LMU:C9	2.62	0.56
6:B:189:ALA:CB	20:B:1758:CLA:C20	2.66	0.56
6:B:304:ILE:HD11	20:B:1749:CLA:HED3	1.87	0.56
6:B:408:LEU:O	6:B:411:MET:HB3	2.04	0.56
6:B:481:THR:O	6:B:482:ASN:HB2	2.05	0.56
6:B:500:ALA:CB	6:B:508:LEU:HD22	2.34	0.56
6:B:707:LEU:HD13	24:B:1783:LMG:H301	1.87	0.56
20:B:1749:CLA:HBD	20:B:1749:CLA:HBA1	1.87	0.56
20:B:1755:CLA:CHD	20:B:1755:CLA:HBC3	2.35	0.56
9:E:39:LEU:N	9:E:40:ARG:HH11	1.94	0.56
9:E:41:ARG:HG3	9:E:46:PHE:CE1	2.40	0.56
10:F:131:PHE:O	10:F:133:GLY:N	2.38	0.56
11:G:60:SER:HG	11:G:63:PRO:HB2	1.70	0.56
16:L:63:LEU:O	16:L:64:LEU:C	2.42	0.56
17:N:80:ASN:O	17:N:82:PHE:HD2	1.89	0.56
4:4:106:TRP:HE3	20:4:1207:CLA:HMA2	1.69	0.56
5:A:95:GLY:HA3	20:A:1763:CLA:C1C	2.35	0.56
5:A:544:ILE:HD11	20:A:1811:CLA:H193	1.88	0.56
5:A:578:ARG:HB2	5:A:578:ARG:NH1	2.20	0.56
5:A:702:GLU:HA	6:B:545:LYS:HE2	1.87	0.56
20:A:1776:CLA:C3C	20:A:1782:CLA:C17	2.77	0.56
20:A:1791:CLA:H3A	20:A:1797:CLA:HBB1	1.87	0.56
6:B:266:GLN:HE21	6:B:363:GLN:HG2	1.70	0.56
6:B:275:HIS:ND1	20:B:1747:CLA:HMB1	2.20	0.56
6:B:442:VAL:HG21	20:B:1763:CLA:CAC	2.32	0.56
6:B:486:LEU:O	6:B:487:ASN:HB3	2.06	0.56
6:B:559:CYS:SG	6:B:560:ASP:N	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1760:CLA:HMB2	20:B:1761:CLA:C4A	2.36	0.56
14:J:26:LEU:HA	14:J:29:ILE:HG22	1.88	0.56
5:A:40:PHE:H	5:A:44:ILE:HG21	1.71	0.56
20:A:1815:CLA:C3A	20:A:1815:CLA:CGA	2.84	0.56
6:B:144:PHE:O	6:B:144:PHE:HD2	1.86	0.56
6:B:186:SER:C	6:B:187:SER:O	2.44	0.56
6:B:266:GLN:O	6:B:267:SER:CB	2.45	0.56
6:B:444:LEU:O	6:B:445:ALA:CB	2.54	0.56
6:B:555:TYR:CE2	6:B:573:TRP:HA	2.41	0.56
6:B:722:ALA:O	6:B:726:ILE:HD12	2.06	0.56
9:E:44:TYR:CD2	9:E:45:TRP:HE3	2.23	0.56
20:J:1044:CLA:O2D	20:J:1045:CLA:C9	2.40	0.56
20:J:1044:CLA:C9	20:J:1044:CLA:H151	2.33	0.56
20:J:1045:CLA:O1D	20:J:1045:CLA:C2	2.54	0.56
15:K:43:ARG:NE	15:K:43:ARG:HA	2.21	0.56
16:L:65:VAL:N	16:L:67:PRO:HD2	2.21	0.56
17:N:45:ASN:HA	17:N:57:LYS:NZ	2.20	0.56
17:N:62:SER:O	17:N:63:ASP:CG	2.44	0.56
19:Q:1:GLC:O5	19:Q:2:FRU:H5	2.05	0.56
4:4:151:GLU:HG3	4:4:152:LYS:H	1.71	0.56
5:A:716:VAL:O	20:A:1795:CLA:HMD3	2.05	0.56
20:A:1790:CLA:C1B	22:A:1806:BCR:H333	2.36	0.56
20:A:1795:CLA:CGA	20:A:1795:CLA:C4	2.82	0.56
20:B:1753:CLA:C2A	20:B:1753:CLA:CGD	2.83	0.56
22:B:1780:BCR:C20	20:B:1786:CLA:C15	2.84	0.56
24:B:1783:LMG:H111	24:B:1783:LMG:C9	2.35	0.56
7:C:1:MET:SD	7:C:4:SER:HB2	2.45	0.56
8:D:75:LEU:HD21	16:L:19:PHE:CE2	2.41	0.56
10:F:23:LYS:O	10:F:24:LYS:NZ	2.29	0.56
11:G:33:LYS:CE	11:G:33:LYS:CA	2.62	0.56
17:N:25:THR:CG2	17:N:26:GLY:N	2.69	0.56
17:N:47:THR:HG21	17:N:54:LYS:CE	2.30	0.56
17:N:72:LYS:CD	17:N:74:LYS:H	2.19	0.56
20:1:1192:CLA:O1D	21:1:1202:LMU:O2'	2.23	0.56
5:A:59:ALA:C	5:A:61:ALA:H	2.09	0.56
5:A:500:PRO:HB3	5:A:506:GLY:HA2	1.88	0.56
5:A:704:ILE:HA	5:A:707:ILE:HG13	1.87	0.56
20:A:1761:CLA:H201	22:A:1804:BCR:C18	2.35	0.56
20:A:1761:CLA:HMC3	20:A:1785:CLA:HMA1	1.87	0.56
20:A:1794:CLA:HBC3	20:A:1794:CLA:CMC	2.25	0.56
20:A:1813:CLA:HBC2	20:A:1813:CLA:HMC1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:510:LEU:HD22	6:B:510:LEU:H	1.70	0.56
6:B:670:TYR:OH	20:B:1787:CLA:CAD	2.53	0.56
20:B:1762:CLA:H51	22:B:1779:BCR:C40	2.35	0.56
10:F:40:LEU:HD12	10:F:42:ILE:HD11	1.88	0.56
10:F:126:ALA:O	10:F:128:SER:N	2.38	0.56
19:T:1:GLC:HO2	19:T:2:FRU:C1	2.17	0.56
20:3:1218:CLA:HHD	20:3:1218:CLA:CBC	2.22	0.56
5:A:156:SER:O	5:A:158:ILE:N	2.39	0.56
5:A:223:VAL:O	5:A:228:PRO:HD3	2.05	0.56
5:A:362:LEU:HB3	5:A:406:LEU:O	2.05	0.56
5:A:409:GLY:C	5:A:411:ALA:H	2.09	0.56
21:A:7043:LMU:C1B	21:A:7043:LMU:H3O2	2.19	0.56
6:B:132:ASN:C	6:B:132:ASN:OD1	2.44	0.56
6:B:390:GLY:N	6:B:391:PRO:CD	2.69	0.56
20:B:1735:CLA:CBB	20:B:1762:CLA:H43	2.36	0.56
20:B:1735:CLA:HBC3	22:B:1778:BCR:H332	1.88	0.56
20:B:1759:CLA:H62	24:B:1783:LMG:C18	2.35	0.56
24:B:1783:LMG:C9	24:B:1783:LMG:C11	2.84	0.56
10:F:22:LEU:CB	10:F:23:LYS:HD3	2.35	0.56
2:2:53:ARG:HH22	20:2:1212:CLA:HBC1	1.70	0.56
4:4:169:GLN:NE2	4:4:169:GLN:HA	2.18	0.56
5:A:210:LEU:HD12	20:A:1769:CLA:CMB	2.35	0.56
5:A:232:PHE:CZ	5:A:242:ILE:HG22	2.40	0.56
5:A:249:ILE:HG23	5:A:251:ASN:OD1	2.06	0.56
20:A:1771:CLA:HBB1	22:A:1803:BCR:C13	2.36	0.56
20:A:1776:CLA:C1C	20:A:1782:CLA:C17	2.80	0.56
20:A:1815:CLA:CMA	20:A:1815:CLA:C2	2.83	0.56
6:B:291:TYR:O	6:B:292:ARG:O	2.24	0.56
20:B:1759:CLA:H201	20:B:1771:CLA:HBA1	1.88	0.56
20:B:1760:CLA:HED2	20:B:1760:CLA:HAA2	1.85	0.56
22:B:1775:BCR:C33	22:B:1775:BCR:C8	2.84	0.56
7:C:75:ARG:NH1	8:D:110:GLN:OE1	2.37	0.56
8:D:125:PRO:HG2	8:D:127:ARG:HD3	1.87	0.56
9:E:36:VAL:CG2	9:E:52:VAL:HG22	2.36	0.56
11:G:69:VAL:O	11:G:73:ALA:HB3	2.06	0.56
12:H:36:GLN:HE22	20:L:1166:CLA:CAD	2.19	0.56
17:N:67:LEU:CB	17:N:68:GLU:CB	2.82	0.56
18:R:36:UNK:C	18:R:38:UNK:N	2.66	0.56
20:1:1193:CLA:HBC3	20:1:1193:CLA:CMC	2.33	0.56
5:A:150:PHE:H	5:A:153:TRP:HE3	1.49	0.56
5:A:214:GLY:CA	22:A:1804:BCR:H15C	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:341:GLN:HB3	5:A:434:ARG:NH1	2.21	0.56
5:A:701:GLN:HA	5:A:701:GLN:NE2	2.21	0.56
21:A:7033:LMU:C6B	21:A:7033:LMU:C2'	2.81	0.56
6:B:321:GLY:O	6:B:325:THR:HG22	2.06	0.56
6:B:388:ALA:HA	6:B:391:PRO:CG	2.36	0.56
6:B:455:ILE:HD12	6:B:517:PHE:CZ	2.40	0.56
20:B:1756:CLA:C10	20:B:1756:CLA:H142	2.34	0.56
20:B:1765:CLA:CBB	22:B:1777:BCR:H281	2.35	0.56
20:B:1786:CLA:NB	20:B:1787:CLA:HBB2	2.20	0.56
10:F:7:PRO:HB3	10:F:60:GLY:O	2.06	0.56
10:F:80:TRP:CE3	20:F:1157:CLA:HMC2	2.38	0.56
16:L:25:THR:HB	16:L:26:PRO:HD2	1.88	0.56
3:3:49:ILE:HA	3:3:51:PRO:HD2	1.88	0.55
3:3:50:GLU:H	3:3:51:PRO:HD3	1.71	0.55
3:3:84:ILE:H	20:A:1798:CLA:H41	1.63	0.55
4:4:161:LEU:HD12	4:4:161:LEU:O	2.07	0.55
20:4:4014:CLA:HED2	20:4:4014:CLA:H2A	0.72	0.55
5:A:75:SER:HB3	5:A:354:TRP:CZ2	2.41	0.55
5:A:217:SER:HA	22:A:1803:BCR:C35	2.31	0.55
5:A:337:PRO:CD	20:A:1799:CLA:HHC	2.36	0.55
5:A:361:ASN:HD22	5:A:361:ASN:C	2.09	0.55
5:A:471:GLY:O	5:A:472:ARG:HG2	2.06	0.55
22:A:1807:BCR:H15C	20:A:1812:CLA:H151	1.88	0.55
20:A:1812:CLA:HED2	20:A:1812:CLA:C3D	2.36	0.55
21:A:7013:LMU:H41	21:A:7013:LMU:H1'	1.87	0.55
6:B:25:ILE:HG22	22:L:1169:BCR:C28	2.25	0.55
6:B:247:THR:CG2	6:B:250:ALA:CB	2.83	0.55
6:B:275:HIS:O	6:B:278:LEU:HB3	2.06	0.55
6:B:341:LEU:O	6:B:345:THR:OG1	2.17	0.55
6:B:630:GLN:HE21	6:B:731:GLY:CA	2.16	0.55
9:E:39:LEU:HA	9:E:46:PHE:CE1	2.41	0.55
11:G:5:SER:O	11:G:7:VAL:HG13	2.05	0.55
17:N:70:GLU:CB	17:N:72:LYS:H	2.15	0.55
20:1:1190:CLA:HBA1	20:1:1190:CLA:CHA	2.35	0.55
2:2:127:ASN:HB3	14:J:1:MET:O	2.06	0.55
20:2:1220:CLA:H61	3:3:140:LYS:HZ2	1.68	0.55
3:3:94:ARG:C	3:3:97:PHE:HE1	2.09	0.55
3:3:201:ALA:C	3:3:202:LEU:HD22	2.27	0.55
5:A:42:ARG:HA	5:A:44:ILE:HG12	1.88	0.55
5:A:284:ARG:HG3	5:A:295:TRP:CG	2.41	0.55
5:A:361:ASN:ND2	20:A:1761:CLA:HED1	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:374:GLN:O	5:A:376:MET:N	2.39	0.55
5:A:378:SER:OG	20:A:1782:CLA:HBC2	2.06	0.55
5:A:586:ARG:HG3	7:C:49:VAL:CG2	2.36	0.55
5:A:699:TYR:HD1	5:A:700:TRP:CD1	2.24	0.55
5:A:711:HIS:O	5:A:716:VAL:HG22	2.06	0.55
20:A:1776:CLA:H43	20:A:1779:CLA:H2	1.88	0.55
20:A:1799:CLA:O2D	20:A:1799:CLA:HBA2	2.05	0.55
6:B:197:VAL:O	6:B:198:ALA:HB2	2.07	0.55
6:B:479:SER:O	6:B:481:THR:N	2.28	0.55
6:B:586:THR:C	6:B:588:GLY:N	2.54	0.55
6:B:596:TRP:CZ3	6:B:613:SER:HB3	2.41	0.55
20:B:1754:CLA:C8	20:B:1756:CLA:H43	2.36	0.55
20:B:1768:CLA:CBC	10:F:83:PHE:CZ	2.79	0.55
9:E:48:ASN:HD21	9:E:71:LYS:NZ	2.04	0.55
17:N:1:GLY:C	17:N:2:VAL:HG13	2.23	0.55
17:N:52:LEU:HB3	17:N:53:ALA:CA	2.36	0.55
3:3:202:LEU:HB3	3:3:204:THR:HG23	1.87	0.55
5:A:240:LYS:H	5:A:243:PRO:HD3	1.70	0.55
5:A:372:VAL:O	5:A:374:GLN:N	2.39	0.55
5:A:679:PHE:HE1	5:A:749:PHE:HB2	1.70	0.55
20:A:1760:CLA:CBA	20:A:1767:CLA:H62	2.36	0.55
20:A:1781:CLA:H162	20:A:1781:CLA:C11	2.36	0.55
6:B:37:ILE:HD12	6:B:37:ILE:C	2.27	0.55
6:B:577:TYR:CE2	6:B:578:LEU:HD12	2.41	0.55
6:B:597:LYS:O	6:B:598:HIS:HB2	2.06	0.55
20:B:1768:CLA:H121	22:B:1779:BCR:H311	1.88	0.55
7:C:44:ARG:NH2	8:D:127:ARG:CB	2.66	0.55
9:E:69:PHE:CD2	9:E:70:ALA:N	2.74	0.55
9:E:73:ASN:ND2	9:E:73:ASN:C	2.60	0.55
11:G:46:ALA:CA	11:G:48:ASP:CB	2.81	0.55
22:I:1032:BCR:C3	20:I:1033:CLA:HAC2	2.12	0.55
16:L:25:THR:HB	16:L:26:PRO:CD	2.37	0.55
3:3:48:PHE:CD2	3:3:49:ILE:CG2	2.69	0.55
5:A:133:ASN:HD22	5:A:142:GLY:HA2	1.70	0.55
5:A:211:LEU:HB3	5:A:310:PHE:CD2	2.42	0.55
5:A:216:LEU:CD1	22:A:1803:BCR:H352	2.37	0.55
5:A:468:SER:HB2	5:A:476:MET:SD	2.47	0.55
5:A:545:HIS:ND1	20:A:1792:CLA:CBB	2.52	0.55
5:A:587:GLY:HA3	6:B:668:ARG:CZ	2.36	0.55
5:A:678:PHE:O	5:A:681:GLY:O	2.25	0.55
20:A:1782:CLA:H101	20:A:1782:CLA:C14	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1801:CLA:HBA1	16:L:33:ILE:HD13	1.88	0.55
21:A:7030:LMU:C9	21:A:7030:LMU:H51	2.14	0.55
21:A:7038:LMU:C1B	21:A:7038:LMU:H6'	2.18	0.55
6:B:42:LEU:O	6:B:45:ASN:N	2.39	0.55
6:B:197:VAL:O	6:B:197:VAL:HG12	2.05	0.55
6:B:361:ILE:C	6:B:362:ALA:O	2.44	0.55
6:B:378:ILE:HA	6:B:381:PHE:HB2	1.87	0.55
6:B:421:HIS:CE1	20:B:1761:CLA:C4D	2.89	0.55
6:B:646:TRP:CZ3	6:B:726:ILE:HD13	2.42	0.55
6:B:707:LEU:HD11	20:B:1759:CLA:C9	2.37	0.55
20:B:1771:CLA:CHD	23:B:1773:PQN:H18	2.36	0.55
7:C:75:ARG:NH2	8:D:110:GLN:OE1	2.35	0.55
8:D:91:ARG:NH1	8:D:119:TYR:HE1	2.05	0.55
17:N:48:GLY:HA3	17:N:49:CYS:C	2.17	0.55
19:S:1:GLC:H5	19:S:1:GLC:O2	2.06	0.55
3:3:56:TYR:HD1	3:3:185:LYS:HZ1	1.51	0.55
5:A:62:HIS:O	20:A:1785:CLA:HAA2	2.06	0.55
5:A:64:PHE:HE2	20:A:1761:CLA:HMC1	1.71	0.55
5:A:100:GLY:HA3	5:A:153:TRP:CZ3	2.42	0.55
5:A:369:THR:HG21	5:A:402:ILE:CG2	2.37	0.55
6:B:290:MET:HG3	20:B:1751:CLA:C2C	2.36	0.55
8:D:69:ARG:O	8:D:70:GLU:CB	2.54	0.55
10:F:46:MET:O	10:F:49:THR:N	2.38	0.55
20:1:1193:CLA:HBA2	20:1:1193:CLA:HMA3	1.88	0.55
3:3:205:GLY:HA3	5:A:252:ARG:NH1	2.21	0.55
5:A:88:ILE:CG2	5:A:89:ILE:N	2.70	0.55
5:A:425:THR:O	5:A:428:TYR:CE1	2.59	0.55
5:A:478:SER:C	5:A:480:THR:H	2.10	0.55
5:A:711:HIS:CG	20:A:1795:CLA:HBC1	2.39	0.55
5:A:744:ALA:CB	22:A:1807:BCR:C39	2.46	0.55
20:A:1764:CLA:O2D	20:A:1764:CLA:H2A	2.06	0.55
20:A:1787:CLA:H141	20:A:1801:CLA:H93	1.89	0.55
20:A:1788:CLA:H101	20:A:1788:CLA:H142	1.88	0.55
20:A:1796:CLA:H43	20:A:1796:CLA:ND	2.21	0.55
20:A:1801:CLA:HED1	16:L:32:LEU:CD1	2.34	0.55
6:B:75:GLU:CB	6:B:132:ASN:HD22	2.19	0.55
6:B:102:GLU:O	6:B:103:ALA:C	2.45	0.55
6:B:476:ILE:O	6:B:479:SER:OG	2.16	0.55
6:B:597:LYS:HG2	20:B:1767:CLA:HBC1	1.89	0.55
20:B:1786:CLA:H91	20:B:1787:CLA:H92	1.88	0.55
8:D:140:ASN:HA	8:D:142:SER:OG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:78:GLY:O	11:G:79:HIS:ND1	2.40	0.55
12:H:27:ASP:O	12:H:29:PRO:HD3	2.06	0.55
13:I:24:LEU:HD21	22:L:1169:BCR:H271	1.89	0.55
20:J:1043:CLA:C15	20:J:1044:CLA:HMB1	2.37	0.55
15:K:55:PHE:N	15:K:55:PHE:HD1	2.04	0.55
17:N:82:PHE:H	17:N:82:PHE:HD2	1.55	0.55
21:R:1056:LMU:O5B	21:R:1056:LMU:H5'	2.07	0.55
21:2:7006:LMU:H3'	21:2:7006:LMU:O6B	2.06	0.55
5:A:679:PHE:O	5:A:683:HIS:HB2	2.07	0.55
5:A:705:GLU:CB	6:B:545:LYS:NZ	2.69	0.55
20:A:1762:CLA:H51	20:A:1785:CLA:C4C	2.36	0.55
20:A:1781:CLA:HMA2	20:A:1782:CLA:CGA	2.36	0.55
20:A:1789:CLA:O1D	16:L:73:PRO:O	2.25	0.55
21:A:7016:LMU:C1'	21:A:7016:LMU:H31	2.36	0.55
6:B:193:HIS:HD2	20:B:1744:CLA:NC	2.05	0.55
20:B:1768:CLA:H203	22:B:1779:BCR:HC41	1.89	0.55
7:C:1:MET:H1	7:C:4:SER:CA	2.20	0.55
10:F:152:ASN:ND2	10:F:152:ASN:H	2.05	0.55
11:G:27:GLN:O	11:G:28:ARG:HB3	2.06	0.55
14:J:13:VAL:CG1	14:J:15:SER:HB2	2.37	0.55
16:L:50:LEU:HG	16:L:51:LEU:CD2	2.36	0.55
17:N:63:ASP:H	17:N:64:ASP:HB2	1.66	0.55
17:N:66:ASP:CA	17:N:67:LEU:HD12	2.33	0.55
19:U:1:GLC:HO2	19:U:2:FRU:C2	2.20	0.55
2:2:60:ALA:HA	2:2:63:PHE:CE2	2.42	0.55
20:2:1212:CLA:HBC3	20:2:1212:CLA:CMC	2.29	0.55
3:3:134:LYS:O	3:3:135:PRO:C	2.44	0.55
5:A:82:HIS:O	5:A:84:GLY:N	2.40	0.55
5:A:141:ARG:HH21	5:A:141:ARG:CG	2.14	0.55
5:A:412:ALA:O	5:A:415:ALA:HB3	2.07	0.55
5:A:532:ILE:N	5:A:533:PRO:HD3	2.21	0.55
5:A:603:PHE:HZ	5:A:693:LEU:CD2	2.20	0.55
20:A:1796:CLA:H43	20:A:1796:CLA:C4C	2.36	0.55
6:B:95:HIS:CE1	20:B:1740:CLA:HMB3	2.41	0.55
6:B:340:SER:O	6:B:344:ILE:HG13	2.07	0.55
6:B:574:ASP:OD2	6:B:706:ARG:NE	2.40	0.55
6:B:633:ASN:O	6:B:636:THR:HB	2.07	0.55
6:B:654:HIS:HE1	20:B:1785:CLA:NB	2.01	0.55
10:F:25:LEU:HD21	10:F:46:MET:HB3	1.84	0.55
13:I:19:VAL:O	13:I:23:SER:N	2.40	0.55
16:L:41:PRO:HG3	16:L:52:ARG:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:1198:CLA:C5	20:1:1198:CLA:H101	2.34	0.55
5:A:103:PHE:HE1	20:A:1763:CLA:CGD	2.17	0.55
5:A:157:GLY:O	5:A:248:PHE:HE1	1.90	0.55
20:A:1764:CLA:CMB	20:A:1765:CLA:H11	2.37	0.55
20:A:1783:CLA:H171	20:A:1783:CLA:H122	1.89	0.55
6:B:154:TRP:O	6:B:157:LEU:N	2.29	0.55
6:B:378:ILE:CA	6:B:381:PHE:HB2	2.37	0.55
6:B:575:ASP:O	6:B:579:ALA:N	2.36	0.55
13:I:12:VAL:CG2	20:I:1031:CLA:O1A	2.52	0.55
20:1:1198:CLA:H121	20:1:1198:CLA:H92	1.86	0.55
5:A:137:GLY:C	5:A:139:GLY:H	2.10	0.55
5:A:210:LEU:N	5:A:213:LEU:H	2.05	0.55
5:A:358:LEU:O	5:A:361:ASN:HB3	2.06	0.55
5:A:431:LEU:O	5:A:435:VAL:CG1	2.55	0.55
5:A:700:TRP:HZ3	20:A:1813:CLA:O1D	1.90	0.55
21:A:7019:LMU:O2'	21:A:7019:LMU:H32	2.07	0.55
6:B:486:LEU:HB2	6:B:489:GLY:O	2.07	0.55
6:B:519:VAL:HG11	6:B:593:TYR:HB2	1.89	0.55
6:B:732:LYS:HG3	6:B:734:GLY:HA2	1.87	0.55
7:C:39:ILE:HG23	7:C:40:ALA:N	2.22	0.55
7:C:74:THR:OG1	7:C:75:ARG:N	2.33	0.55
9:E:40:ARG:NH2	9:E:87:VAL:HG22	2.21	0.55
10:F:23:LYS:CA	10:F:24:LYS:NZ	2.70	0.55
11:G:18:LEU:C	11:G:21:PHE:H	2.10	0.55
12:H:25:GLY:HA3	12:H:27:ASP:CG	2.26	0.55
17:N:41:LYS:CB	17:N:42:PHE:CA	2.83	0.55
1:1:111:GLN:HA	1:1:111:GLN:HE21	1.72	0.54
20:1:1187:CLA:CMA	20:1:1187:CLA:HBA2	2.26	0.54
2:2:96:ILE:HG13	2:2:97:VAL:N	2.21	0.54
2:2:179:PHE:HD1	2:2:183:TYR:HE2	1.53	0.54
5:A:83:PHE:HA	5:A:86:LEU:HD23	1.89	0.54
5:A:158:ILE:HG23	5:A:163:GLN:NE2	2.22	0.54
5:A:541:VAL:CG1	5:A:615:HIS:CD2	2.72	0.54
5:A:584:PRO:HG2	7:C:66:ARG:HB2	1.89	0.54
10:F:24:LYS:N	10:F:26:GLN:H	2.05	0.54
11:G:19:GLY:O	11:G:22:VAL:N	2.40	0.54
15:K:69:ILE:CA	15:K:72:VAL:HG12	2.35	0.54
16:L:88:ALA:O	16:L:90:GLY:N	2.39	0.54
20:L:1505:CLA:HAA1	20:L:1505:CLA:H42	1.90	0.54
17:N:46:PHE:C	17:N:47:THR:HG23	2.17	0.54
20:R:1054:CLA:HBA2	20:R:1054:CLA:HBD	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:156:PRO:O	3:3:157:ALA:C	2.46	0.54
5:A:124:TRP:HA	5:A:124:TRP:CE3	2.42	0.54
5:A:250:LEU:O	5:A:252:ARG:HG2	2.07	0.54
5:A:368:LEU:HD12	20:A:1782:CLA:C6	2.38	0.54
5:A:394:SER:HB2	20:A:1783:CLA:CMA	2.28	0.54
5:A:479:ASP:OD1	5:A:536:THR:O	2.25	0.54
5:A:527:VAL:CG1	5:A:528:ALA:H	2.19	0.54
5:A:705:GLU:HB3	6:B:545:LYS:HZ1	1.72	0.54
20:A:1777:CLA:C2D	20:A:1778:CLA:HMB3	2.37	0.54
21:A:7009:LMU:H5B	21:A:7009:LMU:H3O2	1.69	0.54
21:A:7039:LMU:O2'	21:A:7039:LMU:C5'	2.45	0.54
6:B:14:GLN:HE21	6:B:14:GLN:H	1.55	0.54
6:B:166:SER:C	6:B:168:PHE:H	2.09	0.54
20:B:1747:CLA:CAD	20:B:1756:CLA:HBB2	2.36	0.54
20:B:1756:CLA:H72	20:B:1756:CLA:C4	2.37	0.54
22:B:1781:BCR:H342	20:H:1079:CLA:CHD	2.36	0.54
20:J:1045:CLA:CMA	20:J:1045:CLA:C2	2.84	0.54
16:L:33:ILE:HD11	16:L:36:TYR:HD1	1.72	0.54
16:L:121:THR:OG1	16:L:122:GLY:N	2.38	0.54
17:N:63:ASP:N	17:N:64:ASP:HB3	2.11	0.54
1:1:48:ARG:O	1:1:52:LEU:HB2	2.07	0.54
2:2:128:ASN:CG	14:J:3:ASP:HB3	2.28	0.54
2:2:211:LYS:HE2	2:2:211:LYS:HA	1.89	0.54
20:3:3008:CLA:CGD	20:3:3008:CLA:O1A	2.55	0.54
4:4:107:GLN:HA	20:4:1196:CLA:H2A	1.88	0.54
4:4:169:GLN:CG	20:4:1199:CLA:CAC	2.80	0.54
5:A:177:LEU:C	5:A:179:LEU:H	2.11	0.54
5:A:680:LEU:CD2	6:B:617:MET:HB2	2.37	0.54
6:B:224:PRO:HB3	6:B:227:THR:HB	1.89	0.54
6:B:625:TRP:CE3	6:B:625:TRP:C	2.81	0.54
20:B:1753:CLA:C2	20:B:1753:CLA:H72	2.32	0.54
20:B:1760:CLA:HAA2	20:B:1760:CLA:CED	2.37	0.54
8:D:124:ASN:HB3	8:D:125:PRO:CD	2.31	0.54
10:F:23:LYS:N	10:F:23:LYS:HD3	2.19	0.54
20:I:1033:CLA:O1D	20:I:1033:CLA:H2A	2.07	0.54
16:L:62:PHE:HB2	16:L:154:ALA:HB2	1.88	0.54
1:1:140:LEU:HG	1:1:142:GLU:N	2.23	0.54
2:2:169:LEU:HD23	20:2:1215:CLA:HBB2	1.87	0.54
20:2:1220:CLA:H51	20:2:1220:CLA:H102	1.88	0.54
3:3:94:ARG:C	3:3:97:PHE:CE1	2.81	0.54
3:3:106:TYR:HB3	3:3:107:TRP:HD1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3:1216:CLA:C2B	20:A:1798:CLA:H2	2.38	0.54
5:A:46:LYS:HG3	5:A:48:PRO:HB2	1.88	0.54
5:A:157:GLY:O	5:A:248:PHE:CE1	2.60	0.54
5:A:229:ILE:HG13	5:A:243:PRO:HB3	1.90	0.54
5:A:278:ALA:O	5:A:279:ASP:O	2.26	0.54
5:A:287:LEU:N	5:A:295:TRP:HE1	2.05	0.54
20:A:1765:CLA:H51	22:A:1808:BCR:C10	2.36	0.54
20:A:1769:CLA:HMA2	20:A:1769:CLA:C1	2.37	0.54
20:A:1783:CLA:H43	20:A:1783:CLA:CGA	2.36	0.54
6:B:284:PHE:CE1	20:B:1749:CLA:HHC	2.43	0.54
6:B:456:GLU:HA	6:B:514:PRO:HD3	1.90	0.54
6:B:633:ASN:HD22	6:B:636:THR:HB	1.73	0.54
6:B:715:VAL:HA	6:B:718:ILE:HG22	1.90	0.54
20:B:1787:CLA:CMB	20:B:1787:CLA:H41	2.37	0.54
8:D:46:TYR:CE1	8:D:80:LYS:HE2	2.34	0.54
10:F:20:GLN:O	10:F:21:ALA:HB3	2.05	0.54
17:N:50:GLN:OE1	17:N:51:ASP:HA	2.07	0.54
21:1:1202:LMU:C6'	21:1:1202:LMU:H1B	2.36	0.54
3:3:95:THR:HB	3:3:96:GLY:O	2.08	0.54
4:4:150:LYS:HE3	4:4:150:LYS:N	2.23	0.54
5:A:547:PHE:CE2	20:B:1787:CLA:O1A	2.59	0.54
5:A:650:ASN:O	5:A:653:LEU:N	2.31	0.54
5:A:731:ARG:O	5:A:735:VAL:HG23	2.08	0.54
21:A:7013:LMU:C1B	21:A:7013:LMU:H3O2	2.21	0.54
21:A:7041:LMU:O4'	21:A:7042:LMU:O1'	2.26	0.54
6:B:301:ILE:CG2	6:B:301:ILE:O	2.55	0.54
6:B:330:ILE:HD11	20:B:1737:CLA:H193	1.89	0.54
6:B:351:HIS:NE2	20:B:1756:CLA:NC	2.56	0.54
20:B:1754:CLA:H61	20:B:1754:CLA:CMA	2.38	0.54
20:B:1756:CLA:C7	20:B:1756:CLA:C4	2.86	0.54
20:B:1759:CLA:C20	20:B:1771:CLA:HBA1	2.37	0.54
20:B:1787:CLA:H41	20:B:1787:CLA:HMB2	1.88	0.54
7:C:19:ARG:NE	8:D:121:GLU:OE2	2.41	0.54
7:C:35:LYS:C	7:C:37:LYS:H	2.10	0.54
8:D:64:GLY:O	8:D:65:ALA:CB	2.56	0.54
16:L:14:LEU:HD22	16:L:21:GLY:O	2.07	0.54
17:N:63:ASP:N	17:N:64:ASP:HB2	2.22	0.54
4:4:128:ALA:HB2	4:4:143:PHE:CE2	2.43	0.54
5:A:23:ASP:OD1	5:A:33:GLN:CG	2.55	0.54
5:A:162:LEU:C	5:A:165:TYR:HB3	2.28	0.54
5:A:223:VAL:HA	5:A:227:LEU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:262:PHE:O	5:A:264:GLU:N	2.40	0.54
5:A:397:THR:HB	5:A:613:ILE:HG12	1.87	0.54
5:A:582:ASP:HB3	5:A:589:THR:CG2	2.38	0.54
20:A:1759:CLA:H41	20:A:1796:CLA:H8	1.89	0.54
20:A:1763:CLA:HMB1	22:A:1808:BCR:HC7	1.89	0.54
20:A:1771:CLA:HMC1	20:A:1771:CLA:CBC	2.35	0.54
6:B:16:PRO:HG3	7:C:74:THR:CG2	2.37	0.54
6:B:50:HIS:HA	6:B:53:GLN:H	1.73	0.54
6:B:475:ASP:O	6:B:479:SER:OG	2.26	0.54
20:B:1755:CLA:C7	20:B:1769:CLA:C3D	2.85	0.54
17:N:65:LEU:O	17:N:65:LEU:CG	2.54	0.54
21:R:1057:LMU:C6	21:R:1057:LMU:C1	2.76	0.54
3:3:53:TRP:HA	3:3:56:TYR:HD2	1.73	0.54
22:3:1220:BCR:C8	22:3:1220:BCR:C31	2.72	0.54
5:A:84:GLY:C	5:A:87:SER:O	2.46	0.54
5:A:207:LEU:HB3	20:A:1776:CLA:CBB	2.38	0.54
5:A:218:TRP:N	20:A:1770:CLA:HBB2	2.22	0.54
5:A:361:ASN:O	5:A:365:LEU:N	2.39	0.54
5:A:451:ILE:HD12	20:A:1788:CLA:CED	2.06	0.54
5:A:536:THR:HA	5:A:539:PHE:CB	2.38	0.54
5:A:615:HIS:CE1	20:A:1792:CLA:CBC	2.89	0.54
5:A:619:LYS:HG2	5:A:642:PHE:CE1	2.43	0.54
5:A:622:SER:OG	5:A:642:PHE:HB2	2.07	0.54
20:A:1759:CLA:H12	20:A:1796:CLA:H61	1.89	0.54
20:A:1781:CLA:HAA2	20:A:1782:CLA:OBD	2.08	0.54
6:B:76:ALA:O	6:B:79:GLN:N	2.39	0.54
6:B:310:PRO:CB	6:B:311:PRO:HD2	2.36	0.54
6:B:492:ILE:HD13	6:B:492:ILE:N	2.13	0.54
20:B:1747:CLA:H112	20:B:1765:CLA:H3A	1.90	0.54
20:B:1751:CLA:HMA3	20:B:1752:CLA:C4D	2.37	0.54
8:D:124:ASN:CB	8:D:125:PRO:CD	2.84	0.54
3:3:66:MET:HG2	3:3:195:LEU:HD11	1.88	0.54
3:3:114:PHE:CE1	20:3:1216:CLA:C3D	2.91	0.54
20:3:1219:CLA:CBC	20:3:1219:CLA:CMC	2.73	0.54
5:A:210:LEU:HD13	20:A:1769:CLA:CMB	2.31	0.54
5:A:328:LYS:CD	5:A:332:GLU:HG3	2.28	0.54
5:A:448:TRP:CD1	20:A:1788:CLA:CED	2.91	0.54
5:A:472:ARG:O	5:A:474:GLN:N	2.41	0.54
5:A:618:TRP:HB2	5:A:656:PHE:CE1	2.43	0.54
5:A:654:ARG:HA	6:B:632:ILE:HD13	1.88	0.54
5:A:706:SER:HB3	6:B:419:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1760:CLA:O2D	20:A:1760:CLA:C2A	2.55	0.54
20:A:1811:CLA:HMB3	20:A:1812:CLA:CAD	2.38	0.54
21:A:7037:LMU:C5	21:A:7037:LMU:H12	1.87	0.54
6:B:124:TRP:CZ2	6:B:135:LEU:HD22	2.43	0.54
6:B:160:LYS:HE3	6:B:161:TRP:CE2	2.43	0.54
6:B:189:ALA:HA	20:B:1745:CLA:HBB1	1.90	0.54
6:B:330:ILE:HD12	6:B:330:ILE:O	2.06	0.54
6:B:550:LYS:CG	6:B:550:LYS:O	2.55	0.54
6:B:649:MET:HE3	6:B:723:ALA:HB2	1.90	0.54
22:B:1777:BCR:H311	22:B:1777:BCR:C8	2.38	0.54
8:D:102:ARG:HH21	8:D:110:GLN:HB2	1.72	0.54
10:F:80:TRP:HB3	20:F:1157:CLA:HHC	1.90	0.54
10:F:102:ARG:CD	10:F:106:ILE:HD11	2.38	0.54
12:H:67:TYR:C	12:H:67:TYR:HD1	2.11	0.54
20:J:1043:CLA:H152	20:J:1044:CLA:CMB	2.37	0.54
15:K:67:GLY:C	15:K:68:HIS:O	2.45	0.54
16:L:39:ASN:O	16:L:52:ARG:NH2	2.24	0.54
17:N:52:LEU:HB3	17:N:53:ALA:HA	1.88	0.54
20:2:1217:CLA:H102	20:2:1217:CLA:H161	1.90	0.54
5:A:83:PHE:CE1	20:A:1769:CLA:HED1	2.43	0.54
5:A:88:ILE:HG22	5:A:89:ILE:H	1.73	0.54
5:A:308:ILE:O	5:A:311:LEU:HB2	2.07	0.54
5:A:470:LEU:HG	20:B:1740:CLA:HMC3	1.90	0.54
5:A:638:THR:OG1	5:A:641:ASN:ND2	2.40	0.54
20:A:1795:CLA:C4D	20:B:1735:CLA:HMC3	2.38	0.54
6:B:20:ARG:HH11	6:B:20:ARG:CG	2.21	0.54
6:B:120:VAL:HA	6:B:123:TRP:HE1	1.66	0.54
6:B:276:HIS:HB2	20:B:1747:CLA:C1B	2.37	0.54
6:B:363:GLN:HA	6:B:365:PHE:CE1	2.42	0.54
6:B:398:TYR:CD1	6:B:542:ARG:NH2	2.75	0.54
20:B:1739:CLA:C14	20:B:1757:CLA:H91	2.34	0.54
20:B:1762:CLA:CBB	22:B:1778:BCR:H272	2.36	0.54
22:B:1778:BCR:C33	22:B:1778:BCR:HC8	2.37	0.54
22:B:1781:BCR:HC42	20:B:1787:CLA:H142	1.88	0.54
10:F:72:ILE:HG22	10:F:73:VAL:N	2.23	0.54
12:H:14:ILE:HD11	12:H:17:THR:H	1.73	0.54
12:H:77:LEU:HB3	12:H:78:PRO:CD	2.36	0.54
13:I:2:ILE:HG13	13:I:3:ASN:OD1	2.08	0.54
16:L:58:LEU:HD11	16:L:153:TRP:HZ2	1.73	0.54
2:2:49:LEU:HB3	20:2:1215:CLA:CAC	2.37	0.54
3:3:194:ILE:HD12	20:3:1212:CLA:HMC2	1.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:255:LEU:HD11	5:A:280:PHE:HZ	1.72	0.54
5:A:316:MET:CA	5:A:317:TYR:CB	2.86	0.54
5:A:584:PRO:CB	7:C:67:VAL:HB	2.38	0.54
5:A:650:ASN:O	5:A:653:LEU:HD13	2.07	0.54
5:A:672:LEU:HD23	5:A:672:LEU:H	1.71	0.54
5:A:723:ARG:HH11	5:A:723:ARG:HG3	1.68	0.54
20:A:1779:CLA:C1C	22:A:1805:BCR:H17C	2.37	0.54
20:A:1781:CLA:C3B	22:A:1806:BCR:C21	2.86	0.54
20:A:1788:CLA:H162	22:L:1169:BCR:H362	1.88	0.54
20:A:1796:CLA:NC	20:A:1796:CLA:H41	2.23	0.54
20:A:1800:CLA:CGA	20:A:1800:CLA:C1A	2.86	0.54
6:B:25:ILE:HG22	22:L:1169:BCR:H291	1.83	0.54
6:B:117:TYR:O	6:B:367:THR:HG23	2.08	0.54
6:B:132:ASN:HA	6:B:135:LEU:HG	1.89	0.54
6:B:222:LEU:O	6:B:222:LEU:HD23	2.07	0.54
15:K:72:VAL:HG13	15:K:73:GLY:N	2.23	0.54
17:N:59:PRO:C	17:N:61:LEU:O	2.46	0.54
1:1:89:VAL:HB	1:1:90:PRO:CD	2.30	0.53
4:4:118:ASP:H	4:4:119:PRO:CD	2.21	0.53
5:A:224:HIS:HE1	20:A:1771:CLA:C4C	2.20	0.53
5:A:253:ASP:O	5:A:256:ALA:CB	2.56	0.53
5:A:591:GLN:OE1	5:A:600:LEU:HD21	2.08	0.53
20:A:1760:CLA:HBB2	20:A:1762:CLA:CAD	2.38	0.53
6:B:373:THR:O	6:B:377:TYR:N	2.31	0.53
6:B:427:LEU:HB3	20:B:1762:CLA:HED1	1.91	0.53
6:B:463:ILE:O	6:B:464:GLN:CB	2.56	0.53
6:B:573:TRP:O	6:B:577:TYR:N	2.31	0.53
6:B:603:ARG:NH1	6:B:732:LYS:HB3	2.18	0.53
20:B:1738:CLA:HBB	20:B:1759:CLA:HBB2	1.90	0.53
22:B:1780:BCR:C33	22:B:1780:BCR:C8	2.85	0.53
11:G:31:MET:O	11:G:34:GLN:N	2.37	0.53
16:L:48:ASN:HB2	16:L:50:LEU:HD22	1.90	0.53
17:N:62:SER:C	17:N:66:ASP:H	2.10	0.53
20:1:1191:CLA:CAB	20:1:1197:CLA:CHD	2.87	0.53
4:4:107:GLN:O	20:4:1196:CLA:CMA	2.55	0.53
5:A:78:VAL:O	5:A:82:HIS:CB	2.55	0.53
5:A:148:GLY:C	5:A:149:PHE:O	2.43	0.53
5:A:242:ILE:HG12	5:A:243:PRO:HG3	1.90	0.53
5:A:291:THR:O	5:A:293:GLY:N	2.36	0.53
5:A:389:TYR:CE1	5:A:625:TRP:CG	2.96	0.53
5:A:629:ASN:HD21	5:A:633:VAL:CG2	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1816:CLA:H2	20:A:1816:CLA:O1A	2.07	0.53
21:A:7023:LMU:O4'	21:A:7023:LMU:C1B	2.55	0.53
21:A:7039:LMU:H4'	21:A:7039:LMU:H6B	1.71	0.53
6:B:416:GLU:CD	6:B:416:GLU:H	2.10	0.53
6:B:476:ILE:HG22	6:B:479:SER:OG	2.09	0.53
6:B:594:TRP:HD1	6:B:595:HIS:HB2	1.73	0.53
20:B:1755:CLA:HED2	20:B:1756:CLA:CAD	2.37	0.53
20:B:1758:CLA:H62	22:B:1776:BCR:H321	1.90	0.53
20:B:1768:CLA:C12	22:B:1779:BCR:H311	2.38	0.53
3:3:194:ILE:HG13	20:3:1212:CLA:HMC2	1.85	0.53
5:A:29:THR:OG1	5:A:31:PHE:N	2.42	0.53
5:A:253:ASP:O	5:A:256:ALA:HB3	2.09	0.53
5:A:420:ARG:HG2	5:A:421:ASP:N	2.22	0.53
5:A:447:ASN:ND2	6:B:678:LEU:CD2	2.71	0.53
5:A:520:LEU:HD22	21:A:1809:LMU:O1'	2.08	0.53
5:A:690:LEU:HD21	6:B:661:PHE:HE1	1.74	0.53
20:A:1762:CLA:HBA2	20:A:1762:CLA:HED2	1.90	0.53
6:B:302:LYS:O	6:B:303:TYR:CB	2.35	0.53
6:B:533:ILE:O	6:B:537:GLY:N	2.30	0.53
10:F:128:SER:O	10:F:130:LEU:HD23	2.08	0.53
11:G:13:GLY:O	11:G:16:LEU:HB2	2.07	0.53
16:L:123:ARG:O	16:L:124:LYS:HE3	2.08	0.53
17:N:37:PHE:CD2	17:N:37:PHE:N	2.75	0.53
2:2:103:GLY:HA2	20:2:1222:CLA:CBB	2.38	0.53
3:3:56:TYR:O	3:3:60:ILE:HD12	2.07	0.53
5:A:491:TRP:HE1	20:A:1792:CLA:C1	2.19	0.53
20:A:1760:CLA:HBC3	20:A:1760:CLA:CHD	2.37	0.53
20:A:1780:CLA:OBD	20:A:1780:CLA:C9	2.42	0.53
6:B:15:ASP:O	6:B:20:ARG:CG	2.57	0.53
6:B:78:VAL:HG23	6:B:78:VAL:O	2.08	0.53
6:B:310:PRO:O	20:B:1772:CLA:CHD	2.57	0.53
6:B:336:LEU:CD1	20:B:1754:CLA:HBB1	2.37	0.53
6:B:437:TYR:CG	6:B:616:LEU:HD22	2.42	0.53
6:B:732:LYS:HG3	6:B:733:PHE:O	2.06	0.53
20:B:1740:CLA:H193	20:B:1771:CLA:C4	2.39	0.53
20:B:1746:CLA:HBC2	20:B:1746:CLA:CHD	2.27	0.53
9:E:86:GLU:CG	9:E:87:VAL:N	2.30	0.53
9:E:88:GLU:O	9:E:90:VAL:HG23	2.08	0.53
10:F:117:LYS:N	10:F:118:GLU:OE2	2.41	0.53
10:F:126:ALA:O	10:F:128:SER:OG	2.17	0.53
16:L:66:GLY:HA2	16:L:69:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:87:ALA:O	16:L:89:ALA:N	2.42	0.53
2:2:120:ASN:HA	14:J:5:LYS:CD	2.39	0.53
3:3:49:ILE:HG13	3:3:52:LYS:HB2	1.90	0.53
5:A:131:ILE:HG21	6:B:446:PHE:HA	1.90	0.53
5:A:473:PRO:O	5:A:474:GLN:C	2.47	0.53
5:A:559:GLY:HA2	5:A:597:HIS:ND1	2.23	0.53
20:A:1794:CLA:HMC1	20:A:1794:CLA:CBC	2.28	0.53
22:A:1805:BCR:H382	22:A:1805:BCR:C23	2.11	0.53
6:B:406:ASN:C	6:B:406:ASN:HD22	2.11	0.53
6:B:493:TRP:CH2	20:B:1747:CLA:H122	2.43	0.53
6:B:596:TRP:O	6:B:597:LYS:CB	2.55	0.53
20:B:1735:CLA:H191	10:F:104:TYR:CG	2.43	0.53
20:B:1735:CLA:H52	20:B:1735:CLA:C4C	2.39	0.53
7:C:74:THR:OG1	7:C:80:ALA:HB3	2.07	0.53
8:D:86:LEU:HD13	8:D:90:LEU:HG	1.90	0.53
10:F:123:VAL:HG21	10:F:128:SER:OG	2.08	0.53
17:N:42:PHE:H	17:N:43:PRO:HD2	1.71	0.53
4:4:127:PRO:HB2	4:4:143:PHE:CE1	2.44	0.53
5:A:160:SER:O	5:A:163:GLN:CG	2.38	0.53
5:A:281:LEU:HB2	5:A:301:HIS:HD2	1.73	0.53
5:A:382:TYR:HE2	20:A:1784:CLA:HED3	1.72	0.53
20:A:1762:CLA:O1A	20:A:1785:CLA:HMB2	2.09	0.53
20:A:1789:CLA:HBC3	20:A:1789:CLA:CMC	2.38	0.53
21:A:7023:LMU:H91	21:A:7023:LMU:C1	2.31	0.53
6:B:20:ARG:HH11	6:B:20:ARG:CB	2.20	0.53
6:B:75:GLU:HB2	6:B:132:ASN:HD22	1.72	0.53
6:B:167:TRP:CZ2	20:B:1741:CLA:HMA1	2.43	0.53
6:B:233:TYR:HB3	6:B:254:ILE:O	2.09	0.53
6:B:338:LEU:O	6:B:339:ALA:HB3	2.08	0.53
6:B:681:ALA:O	6:B:684:ARG:N	2.33	0.53
22:B:1781:BCR:H272	22:I:1032:BCR:H352	1.89	0.53
7:C:5:VAL:C	7:C:65:VAL:CG2	2.69	0.53
8:D:28:ILE:O	8:D:66:ALA:HB3	2.09	0.53
8:D:75:LEU:HD22	8:D:76:LYS:H	1.74	0.53
10:F:61:LEU:CD2	10:F:69:PRO:HB2	2.31	0.53
11:G:19:GLY:HA2	11:G:22:VAL:H	1.74	0.53
12:H:25:GLY:CA	12:H:27:ASP:CB	2.75	0.53
13:I:11:LEU:HD11	22:I:1032:BCR:C10	2.38	0.53
16:L:56:VAL:CA	20:L:1167:CLA:HED2	2.34	0.53
4:4:119:PRO:HG2	4:4:120:ILE:H	1.74	0.53
20:A:1759:CLA:C1	20:A:1796:CLA:H2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1783:CLA:C17	20:A:1783:CLA:H122	2.37	0.53
6:B:174:ARG:HH12	20:B:1754:CLA:CMD	2.21	0.53
6:B:503:GLU:HB3	6:B:507:SER:CA	2.39	0.53
6:B:580:VAL:CG1	6:B:710:LEU:HD21	2.38	0.53
6:B:668:ARG:HH12	6:B:672:GLN:HG2	1.72	0.53
10:F:2:ILE:HG22	10:F:3:ALA:H	1.74	0.53
10:F:104:TYR:O	10:F:104:TYR:HD2	1.89	0.53
20:L:1167:CLA:HAC2	22:L:1169:BCR:HC42	1.89	0.53
18:R:26:UNK:O	18:R:28:UNK:CA	2.57	0.53
2:2:66:GLU:O	2:2:69:THR:HG23	2.09	0.53
4:4:104:ARG:NH1	4:4:105:ARG:HB2	2.16	0.53
5:A:40:PHE:N	5:A:44:ILE:HG21	2.24	0.53
5:A:55:TRP:CD2	5:A:729:GLN:NE2	2.77	0.53
5:A:114:THR:O	5:A:525:ASN:ND2	2.42	0.53
5:A:184:PHE:CE2	20:A:1766:CLA:C2D	2.92	0.53
5:A:567:ARG:NH2	5:A:567:ARG:HB3	2.23	0.53
6:B:91:ILE:HD11	6:B:104:PHE:CE2	2.44	0.53
6:B:188:LEU:HG	6:B:189:ALA:N	2.24	0.53
6:B:196:HIS:NE2	20:B:1745:CLA:ND	2.56	0.53
6:B:294:ASN:CB	11:G:36:PRO:HD2	2.36	0.53
9:E:48:ASN:C	9:E:48:ASN:OD1	2.46	0.53
9:E:50:GLY:HA3	9:E:69:PHE:HB2	1.91	0.53
10:F:58:LYS:O	10:F:60:GLY:N	2.42	0.53
12:H:65:LEU:HD11	16:L:90:GLY:HA2	1.90	0.53
13:I:29:GLU:HA	13:I:29:GLU:OE2	2.09	0.53
14:J:19:PHE:O	14:J:23:ALA:HB3	2.08	0.53
20:K:1142:CLA:HBC3	20:K:1142:CLA:HHD	1.91	0.53
17:N:58:VAL:CG1	17:N:59:PRO:CD	2.87	0.53
17:N:69:CYS:O	17:N:72:LYS:CD	2.57	0.53
20:1:1192:CLA:CGD	21:1:1202:LMU:O2'	2.57	0.53
20:1:1200:CLA:CMA	20:1:1200:CLA:HBA2	2.33	0.53
4:4:136:GLY:O	4:4:137:ILE:HB	2.09	0.53
4:4:154:ILE:O	4:4:157:GLY:N	2.33	0.53
4:4:154:ILE:CG1	4:4:155:ALA:N	2.68	0.53
5:A:293:GLY:O	5:A:294:LEU:HB3	2.08	0.53
5:A:442:ILE:HG23	20:A:1786:CLA:CMC	2.31	0.53
5:A:641:ASN:HD22	5:A:641:ASN:H	1.57	0.53
5:A:710:ALA:CB	20:B:1735:CLA:HED2	2.39	0.53
20:A:1800:CLA:H92	22:L:1169:BCR:C32	2.36	0.53
6:B:172:GLU:C	6:B:176:ASN:HB2	2.29	0.53
20:B:1739:CLA:H2	20:B:1739:CLA:H71	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1780:BCR:C19	20:B:1786:CLA:C15	2.80	0.53
8:D:40:ALA:HA	8:D:44:GLU:O	2.08	0.53
8:D:87:GLY:H	8:D:90:LEU:H	1.57	0.53
10:F:96:TRP:HZ2	20:F:1155:CLA:CAB	2.22	0.53
11:G:47:GLY:N	11:G:48:ASP:HA	2.17	0.53
11:G:85:ILE:O	11:G:86:LEU:HB2	2.09	0.53
22:I:1032:BCR:C2	20:I:1033:CLA:C4C	2.66	0.53
17:N:46:PHE:O	17:N:47:THR:CB	2.56	0.53
1:1:144:LYS:NZ	20:1:1187:CLA:OBD	2.36	0.53
2:2:40:SER:O	2:2:42:ARG:N	2.40	0.53
20:2:1212:CLA:HBC2	20:2:1212:CLA:CMC	2.32	0.53
3:3:74:ALA:CB	20:3:1215:CLA:C1D	2.86	0.53
5:A:216:LEU:CD1	22:A:1803:BCR:C35	2.86	0.53
5:A:453:LEU:CB	5:A:547:PHE:HB2	2.34	0.53
20:A:1782:CLA:O1D	20:A:1782:CLA:CBA	2.46	0.53
20:A:1812:CLA:H152	20:A:1812:CLA:H101	1.90	0.53
6:B:308:HIS:HD1	6:B:309:ILE:N	2.06	0.53
6:B:462:TRP:CZ3	20:B:1764:CLA:CBC	2.92	0.53
10:F:23:LYS:CA	10:F:24:LYS:HZ3	2.22	0.53
10:F:92:TYR:C	10:F:92:TYR:CD2	2.81	0.53
14:J:25:LEU:HA	14:J:28:GLU:HB2	1.91	0.53
22:L:1169:BCR:H331	22:L:1169:BCR:C8	2.38	0.53
17:N:45:ASN:CA	17:N:57:LYS:NZ	2.72	0.53
1:1:29:LEU:O	1:1:31:GLU:N	2.42	0.52
4:4:128:ALA:HB2	4:4:143:PHE:CZ	2.44	0.52
5:A:44:ILE:O	5:A:45:ALA:C	2.47	0.52
5:A:158:ILE:HG23	5:A:163:GLN:HE22	1.74	0.52
20:A:1776:CLA:C9	22:A:1805:BCR:H371	2.22	0.52
21:A:7027:LMU:C6B	21:A:7027:LMU:C2B	2.87	0.52
6:B:415:LYS:CG	6:B:416:GLU:OE2	2.57	0.52
20:B:1786:CLA:CBB	20:B:1787:CLA:C1B	2.80	0.52
7:C:39:ILE:CG1	7:C:40:ALA:N	2.64	0.52
11:G:69:VAL:O	11:G:73:ALA:CB	2.58	0.52
12:H:67:TYR:C	12:H:67:TYR:CD1	2.83	0.52
18:R:32:UNK:CB	18:R:33:UNK:CA	2.76	0.52
1:1:140:LEU:HD23	1:1:140:LEU:H	1.73	0.52
2:2:126:PRO:O	2:2:127:ASN:HB2	2.09	0.52
2:2:181:HIS:NE2	20:2:1214:CLA:C2D	2.73	0.52
20:2:1224:CLA:H151	20:2:1224:CLA:C8	2.38	0.52
3:3:208:PRO:HB3	3:3:210:GLN:CD	2.29	0.52
20:4:1198:CLA:HMC1	20:4:1198:CLA:HBC3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:214:GLY:O	5:A:215:SER:CB	2.56	0.52
5:A:334:HIS:HB3	20:A:1777:CLA:HMA1	1.90	0.52
5:A:733:VAL:HG11	20:A:1796:CLA:C1D	2.39	0.52
20:A:1789:CLA:H172	20:A:1793:CLA:H202	1.91	0.52
20:A:1797:CLA:H2A	20:A:1797:CLA:O1A	1.98	0.52
20:A:1797:CLA:O1A	20:A:1797:CLA:CED	2.57	0.52
6:B:46:ILE:CD1	20:B:1737:CLA:H192	2.40	0.52
6:B:295:PHE:O	11:G:33:LYS:HB2	2.08	0.52
6:B:297:ILE:HG21	11:G:21:PHE:HZ	1.75	0.52
6:B:596:TRP:O	6:B:597:LYS:HB3	2.08	0.52
6:B:616:LEU:O	6:B:619:TRP:HB2	2.08	0.52
20:B:1738:CLA:C4	24:B:1783:LMG:H321	2.39	0.52
20:B:1755:CLA:CGA	20:B:1769:CLA:HAA1	2.38	0.52
20:B:1764:CLA:C1D	20:B:1765:CLA:HBB2	2.39	0.52
8:D:86:LEU:CD1	8:D:90:LEU:HG	2.39	0.52
9:E:40:ARG:H	9:E:46:PHE:HE1	1.56	0.52
10:F:44:ALA:HB1	10:F:48:LYS:HB3	1.91	0.52
11:G:44:PHE:H	11:G:45:GLU:HB3	1.73	0.52
15:K:31:ASN:H	15:K:32:ARG:NH1	2.07	0.52
15:K:32:ARG:NE	15:K:32:ARG:HA	2.24	0.52
16:L:66:GLY:C	20:L:1168:CLA:HMC3	2.29	0.52
3:3:114:PHE:HE1	20:3:1216:CLA:C3D	2.22	0.52
5:A:32:GLU:HG3	5:A:33:GLN:N	2.24	0.52
5:A:144:GLN:CG	5:A:145:ILE:H	2.22	0.52
5:A:187:HIS:NE2	20:A:1767:CLA:C4C	2.50	0.52
5:A:697:ARG:C	5:A:699:TYR:N	2.62	0.52
20:A:1762:CLA:C7	20:A:1762:CLA:H2	2.38	0.52
6:B:124:TRP:HD1	6:B:124:TRP:C	2.11	0.52
6:B:203:ARG:HB3	6:B:270:LEU:HD12	1.91	0.52
6:B:207:VAL:O	6:B:208:ARG:O	2.27	0.52
6:B:378:ILE:HG22	6:B:379:ALA:N	2.24	0.52
6:B:475:ASP:HA	6:B:480:SER:C	2.30	0.52
6:B:696:LYS:NZ	8:D:39:LYS:HE3	2.25	0.52
20:B:1762:CLA:CBB	22:B:1778:BCR:C23	2.87	0.52
20:B:1770:CLA:HBC2	20:B:1770:CLA:HMC1	1.91	0.52
8:D:122:LYS:NZ	8:D:124:ASN:OD1	2.43	0.52
11:G:48:ASP:HB3	11:G:49:THR:HG21	1.87	0.52
16:L:66:GLY:N	16:L:67:PRO:CD	2.72	0.52
3:3:49:ILE:CG1	3:3:52:LYS:HB2	2.39	0.52
3:3:52:LYS:C	3:3:56:TYR:HD2	2.10	0.52
4:4:126:LEU:N	4:4:127:PRO:CD	2.70	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:223:VAL:CG1	5:A:224:HIS:N	2.72	0.52
20:A:1788:CLA:H152	22:L:1169:BCR:H363	1.90	0.52
20:A:1790:CLA:C3D	20:A:1791:CLA:CAC	2.87	0.52
22:A:1807:BCR:H17C	20:A:1812:CLA:H172	1.91	0.52
21:A:7036:LMU:H6E	21:A:7036:LMU:C1B	2.39	0.52
6:B:127:ILE:CG1	6:B:193:HIS:HE1	2.22	0.52
6:B:488:ALA:HB1	20:B:1766:CLA:C1C	2.40	0.52
6:B:525:LEU:HD22	6:B:529:THR:OG1	2.09	0.52
6:B:544:SER:O	6:B:546:LEU:N	2.42	0.52
6:B:564:ARG:NH2	7:C:66:ARG:HH12	2.07	0.52
10:F:22:LEU:C	10:F:25:LEU:HD13	2.29	0.52
17:N:65:LEU:C	17:N:66:ASP:OD2	2.48	0.52
17:N:67:LEU:CD1	17:N:67:LEU:N	2.53	0.52
2:2:120:ASN:CA	14:J:5:LYS:CD	2.86	0.52
20:2:1218:CLA:HBA1	21:2:7003:LMU:H51	1.91	0.52
5:A:353:SER:O	5:A:354:TRP:CB	2.57	0.52
5:A:408:VAL:HG21	5:A:602:LEU:HG	1.90	0.52
5:A:618:TRP:O	5:A:618:TRP:CD1	2.62	0.52
5:A:703:LEU:O	5:A:707:ILE:HG12	2.09	0.52
20:A:1759:CLA:H12	20:A:1796:CLA:C6	2.40	0.52
6:B:98:GLN:O	6:B:98:GLN:NE2	2.43	0.52
6:B:143:LEU:C	6:B:145:LEU:N	2.62	0.52
6:B:545:LYS:HG2	9:E:74:TYR:CE2	2.44	0.52
6:B:551:LYS:O	6:B:553:PHE:CE2	2.62	0.52
6:B:551:LYS:CD	8:D:143:PRO:HA	2.39	0.52
20:B:1753:CLA:H12	20:B:1753:CLA:CAA	2.23	0.52
20:B:1762:CLA:CBB	22:B:1778:BCR:H23C	2.39	0.52
7:C:69:LEU:HD23	7:C:70:TRP:N	2.24	0.52
8:D:113:HIS:HD2	8:D:118:VAL:HG21	1.72	0.52
13:I:8:PHE:CE1	20:I:1031:CLA:H43	2.44	0.52
13:I:17:PRO:O	13:I:18:ALA:C	2.48	0.52
2:2:74:LEU:O	2:2:75:ASN:HB2	2.10	0.52
3:3:60:ILE:HA	3:3:63:ARG:HD2	1.92	0.52
5:A:40:PHE:HZ	5:A:56:ASN:HB3	1.73	0.52
5:A:163:GLN:O	5:A:166:CYS:SG	2.67	0.52
5:A:265:GLY:HA2	5:A:272:LEU:HD21	1.92	0.52
5:A:389:TYR:CD1	5:A:625:TRP:CG	2.97	0.52
5:A:631:GLN:O	5:A:632:GLY:C	2.48	0.52
5:A:656:PHE:O	5:A:659:ALA:N	2.42	0.52
20:A:1779:CLA:NB	22:A:1805:BCR:H15C	2.24	0.52
21:A:7010:LMU:H3'	21:A:7010:LMU:C2B	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7042:LMU:C6'	21:A:7042:LMU:C4	2.88	0.52
6:B:330:ILE:O	6:B:330:ILE:CD1	2.58	0.52
20:B:1753:CLA:HMD2	20:B:1754:CLA:HBB2	1.89	0.52
8:D:36:LEU:HD21	8:D:45:PHE:CZ	2.44	0.52
10:F:96:TRP:CE3	10:F:134:PHE:N	2.78	0.52
11:G:45:GLU:CA	11:G:49:THR:CG2	2.76	0.52
12:H:23:VAL:O	12:H:24:TYR:C	2.48	0.52
17:N:42:PHE:N	17:N:43:PRO:HD3	2.22	0.52
17:N:76:LYS:O	17:N:77:CYS:O	2.27	0.52
1:1:25:ASP:N	6:B:314:ARG:HH22	1.99	0.52
2:2:64:ILE:HG13	2:2:68:LEU:HD13	1.91	0.52
3:3:132:TRP:CZ3	3:3:155:GLU:OE1	2.57	0.52
4:4:107:GLN:C	20:4:1196:CLA:HMA3	2.02	0.52
5:A:331:LEU:CD1	5:A:346:LEU:CB	2.61	0.52
5:A:438:HIS:HB2	5:A:441:ALA:HB3	1.92	0.52
5:A:680:LEU:HD21	6:B:617:MET:HB2	1.91	0.52
21:A:7036:LMU:H22	21:A:7036:LMU:C9	2.38	0.52
6:B:546:LEU:HD11	6:B:567:THR:CG2	2.38	0.52
20:B:1735:CLA:HBC3	20:B:1735:CLA:HHD	1.92	0.52
20:B:1736:CLA:CHD	22:I:1032:BCR:H401	2.40	0.52
9:E:90:VAL:O	9:E:91:ALA:O	2.28	0.52
12:H:34:SER:OG	12:H:36:GLN:NE2	2.42	0.52
12:H:47:PHE:CD2	16:L:141:GLY:HA2	2.45	0.52
16:L:58:LEU:HA	16:L:146:GLY:O	2.10	0.52
18:R:39:UNK:CA	18:R:41:UNK:CB	2.88	0.52
19:O:2:FRU:O1	19:O:2:FRU:C5	2.56	0.52
2:2:126:PRO:HD2	2:2:129:LYS:HB2	1.90	0.52
3:3:47:GLY:C	3:3:49:ILE:H	2.10	0.52
5:A:242:ILE:HG12	5:A:243:PRO:CG	2.39	0.52
5:A:310:PHE:H	5:A:313:ALA:HB3	1.74	0.52
5:A:361:ASN:OD1	20:A:1761:CLA:OBD	2.28	0.52
5:A:365:LEU:CD2	20:A:1761:CLA:CED	2.67	0.52
5:A:378:SER:OG	5:A:378:SER:O	2.28	0.52
5:A:527:VAL:HG13	5:A:528:ALA:H	1.75	0.52
5:A:707:ILE:C	5:A:711:HIS:HD2	2.13	0.52
5:A:709:TRP:CZ3	6:B:417:ALA:HA	2.45	0.52
20:A:1764:CLA:HBB2	20:A:1765:CLA:C4D	2.39	0.52
20:A:1788:CLA:C15	22:L:1169:BCR:H361	2.38	0.52
20:B:1738:CLA:H43	24:B:1783:LMG:H321	1.92	0.52
22:B:1780:BCR:C19	20:B:1786:CLA:H112	2.29	0.52
8:D:31:GLY:O	8:D:32:SER:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:28:ARG:CG	11:G:29:GLU:HB2	2.39	0.52
12:H:58:ILE:CD1	16:L:97:MET:SD	2.84	0.52
16:L:8:TYR:HE1	16:L:11:ILE:CG2	2.20	0.52
17:N:5:GLU:OE2	17:N:6:TYR:CA	2.57	0.52
17:N:70:GLU:O	17:N:72:LYS:N	2.40	0.52
3:3:104:TYR:CB	3:3:106:TYR:H	2.22	0.52
3:3:106:TYR:CB	3:3:107:TRP:CD1	2.92	0.52
4:4:91:PHE:O	4:4:95:PHE:CD1	2.63	0.52
4:4:106:TRP:NE1	20:4:1196:CLA:HED3	2.19	0.52
5:A:375:HIS:HE1	20:A:1782:CLA:NC	2.07	0.52
5:A:435:VAL:O	5:A:438:HIS:ND1	2.39	0.52
5:A:455:PHE:CD1	20:A:1788:CLA:HMA2	2.44	0.52
20:A:1799:CLA:CED	20:A:1799:CLA:CBA	2.88	0.52
6:B:8:PHE:O	6:B:35:ASP:CG	2.48	0.52
6:B:87:ILE:O	6:B:121:TYR:HE2	1.92	0.52
6:B:304:ILE:CD1	20:B:1749:CLA:CED	2.86	0.52
6:B:326:ILE:O	6:B:326:ILE:HG12	2.09	0.52
6:B:513:GLY:O	6:B:515:GLY:N	2.42	0.52
6:B:546:LEU:HD12	6:B:570:ILE:HD13	1.91	0.52
16:L:5:LYS:N	16:L:6:PRO:CD	2.73	0.52
20:1:1193:CLA:HAA2	20:1:1193:CLA:CBD	2.40	0.52
2:2:189:ILE:O	2:2:190:ASP:HB3	2.10	0.52
4:4:154:ILE:CD1	20:4:1202:CLA:CHA	2.84	0.52
5:A:149:PHE:O	5:A:150:PHE:HB2	2.09	0.52
5:A:299:ILE:HD11	20:A:1774:CLA:HMA3	1.91	0.52
5:A:351:THR:O	20:A:1780:CLA:H201	2.10	0.52
5:A:701:GLN:OE1	9:E:74:TYR:CE1	2.63	0.52
20:A:1776:CLA:CAA	20:A:1780:CLA:HBB2	2.38	0.52
20:A:1783:CLA:CGA	20:A:1783:CLA:C1A	2.88	0.52
20:A:1815:CLA:CGA	20:A:1815:CLA:H3A	2.33	0.52
6:B:70:TRP:HB3	6:B:136:TYR:OH	2.08	0.52
20:B:1755:CLA:H52	20:B:1769:CLA:HBD	1.91	0.52
20:B:1755:CLA:C2B	22:B:1777:BCR:C35	2.88	0.52
20:B:1786:CLA:C12	20:B:1786:CLA:H71	2.39	0.52
11:G:14:LEU:HG	11:G:14:LEU:O	2.09	0.52
12:H:20:GLN:C	12:H:22:ASP:HB3	2.31	0.52
20:H:1079:CLA:HMA2	20:H:1079:CLA:C1	2.39	0.52
16:L:33:ILE:O	16:L:36:TYR:N	2.43	0.52
3:3:194:ILE:CG1	20:3:1212:CLA:CMC	2.84	0.51
20:3:1219:CLA:O1A	20:3:1219:CLA:C3A	2.58	0.51
4:4:161:LEU:O	4:4:162:ALA:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:40:PHE:H	5:A:44:ILE:CG2	2.23	0.51
5:A:197:GLN:OE1	5:A:351:THR:O	2.28	0.51
5:A:209:GLY:C	5:A:213:LEU:HB2	2.30	0.51
5:A:473:PRO:C	5:A:475:ASP:N	2.61	0.51
20:A:1779:CLA:ND	22:A:1805:BCR:C19	2.73	0.51
20:A:1781:CLA:CBA	20:A:1794:CLA:CED	2.81	0.51
6:B:729:THR:O	6:B:729:THR:CG2	2.29	0.51
11:G:13:GLY:C	11:G:16:LEU:HG	2.31	0.51
11:G:43:HIS:O	11:G:45:GLU:CA	2.57	0.51
22:I:1032:BCR:C40	22:I:1032:BCR:C38	2.75	0.51
17:N:44:GLU:C	17:N:46:PHE:H	2.13	0.51
1:1:42:SER:HA	1:1:45:ILE:HG12	1.92	0.51
2:2:53:ARG:O	2:2:57:LEU:HB3	2.10	0.51
20:2:1212:CLA:CGA	20:2:1212:CLA:C3A	2.87	0.51
3:3:153:SER:OG	3:3:154:GLY:N	2.43	0.51
3:3:157:ALA:O	3:3:158:TYR:CD2	2.63	0.51
4:4:154:ILE:CG1	4:4:155:ALA:H	2.16	0.51
5:A:316:MET:CA	5:A:317:TYR:HD1	2.20	0.51
5:A:379:MET:SD	5:A:512:SER:HB2	2.50	0.51
5:A:466:THR:O	5:A:470:LEU:CG	2.59	0.51
5:A:584:PRO:HB2	7:C:67:VAL:HB	1.92	0.51
5:A:603:PHE:CZ	5:A:735:VAL:HG22	2.45	0.51
5:A:747:TRP:HB2	20:A:1783:CLA:HBB1	1.92	0.51
20:A:1787:CLA:HMB1	20:A:1800:CLA:HAA2	1.92	0.51
20:A:1813:CLA:H93	6:B:431:PHE:CD1	2.46	0.51
21:A:7026:LMU:O3'	21:A:7026:LMU:C2B	2.56	0.51
21:A:7043:LMU:H102	21:A:7043:LMU:H61	1.80	0.51
6:B:273:VAL:O	6:B:277:HIS:CD2	2.62	0.51
6:B:274:ALA:O	6:B:278:LEU:HB2	2.09	0.51
6:B:323:TYR:CD1	20:B:1754:CLA:CBC	2.93	0.51
6:B:362:ALA:C	6:B:364:ASP:H	2.14	0.51
6:B:440:ASN:ND2	6:B:453:ILE:O	2.44	0.51
6:B:531:THR:CG2	20:B:1755:CLA:HMC2	2.07	0.51
6:B:536:LYS:O	6:B:537:GLY:C	2.48	0.51
6:B:551:LYS:HE2	8:D:143:PRO:CA	2.39	0.51
6:B:593:TYR:CZ	20:B:1767:CLA:HBC2	2.45	0.51
6:B:626:LEU:O	6:B:627:ASN:HB2	2.10	0.51
6:B:715:VAL:O	6:B:719:PHE:N	2.33	0.51
20:B:1768:CLA:C6	22:B:1779:BCR:C32	2.87	0.51
7:C:9:ASP:CB	25:C:1083:SF4:S3	2.98	0.51
8:D:43:GLU:HG3	8:D:44:GLU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:149:LEU:HD23	10:F:153:ASN:ND2	2.24	0.51
12:H:32:TYR:OH	16:L:44:ARG:NE	2.22	0.51
18:R:39:UNK:CA	18:R:42:UNK:CB	2.85	0.51
5:A:183:TRP:O	5:A:185:HIS:N	2.44	0.51
5:A:211:LEU:HB3	5:A:310:PHE:CE2	2.44	0.51
5:A:224:HIS:HE1	20:A:1771:CLA:CHD	2.22	0.51
5:A:430:ASP:H	5:A:433:ASP:CG	2.13	0.51
5:A:588:GLY:N	6:B:668:ARG:NH1	2.57	0.51
20:A:1773:CLA:H12	20:A:1773:CLA:C4A	2.41	0.51
6:B:55:ALA:HB1	6:B:150:LEU:HD12	1.91	0.51
6:B:190:TRP:HE3	20:B:1744:CLA:CAB	2.23	0.51
6:B:247:THR:O	6:B:248:GLN:O	2.27	0.51
6:B:563:GLY:C	6:B:564:ARG:O	2.46	0.51
20:B:1755:CLA:H11	20:B:1769:CLA:HBD	1.92	0.51
7:C:31:TRP:HD1	7:C:32:GLY:N	2.08	0.51
12:H:77:LEU:HB3	12:H:78:PRO:HD2	1.93	0.51
16:L:96:SER:HG	16:L:143:PHE:HD2	1.50	0.51
16:L:163:LEU:O	16:L:164:PRO:O	2.29	0.51
17:N:34:THR:C	17:N:36:GLU:N	2.64	0.51
17:N:38:GLY:HA3	17:N:46:PHE:CD1	2.46	0.51
17:N:42:PHE:CD1	17:N:43:PRO:CA	2.93	0.51
17:N:61:LEU:HG	17:N:62:SER:N	2.14	0.51
17:N:63:ASP:OD1	17:N:66:ASP:OD2	2.29	0.51
18:R:38:UNK:O	18:R:42:UNK:C	2.59	0.51
4:4:95:PHE:CZ	20:4:1208:CLA:C1C	2.94	0.51
4:4:171:ASN:O	4:4:172:VAL:CB	2.58	0.51
5:A:356:ALA:O	5:A:360:ILE:HG22	2.10	0.51
5:A:393:LEU:O	5:A:397:THR:CG2	2.55	0.51
5:A:619:LYS:O	5:A:621:GLN:N	2.43	0.51
5:A:630:ASP:C	5:A:632:GLY:N	2.60	0.51
20:A:1781:CLA:CHC	22:A:1806:BCR:H371	2.39	0.51
21:A:7017:LMU:O3'	21:A:7017:LMU:C1B	2.55	0.51
6:B:130:ARG:CG	6:B:130:ARG:NH1	2.71	0.51
6:B:202:SER:CB	6:B:270:LEU:HD21	2.41	0.51
6:B:231:ASN:OD1	11:G:5:SER:HB2	2.10	0.51
6:B:292:ARG:NE	6:B:297:ILE:O	2.44	0.51
6:B:337:ALA:O	6:B:339:ALA:O	2.29	0.51
6:B:529:THR:HA	6:B:532:LEU:HD23	1.91	0.51
6:B:724:PHE:CE1	20:B:1785:CLA:HMD1	2.45	0.51
8:D:58:PHE:CD2	8:D:59:GLU:N	2.78	0.51
12:H:70:ALA:O	12:H:71:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:1043:CLA:HED3	20:J:1043:CLA:NA	2.12	0.51
17:N:53:ALA:HB3	17:N:55:GLN:NE2	2.25	0.51
2:2:59:ALA:HB1	2:2:172:LEU:HD22	1.91	0.51
20:2:1220:CLA:H62	3:3:140:LYS:HZ3	1.74	0.51
3:3:63:ARG:NH2	3:3:189:LEU:HD23	2.19	0.51
5:A:224:HIS:CE1	20:A:1771:CLA:NC	2.78	0.51
5:A:281:LEU:HD22	20:A:1772:CLA:HMA3	1.93	0.51
5:A:335:LYS:CG	5:A:336:GLY:N	2.60	0.51
6:B:18:THR:O	6:B:21:ILE:N	2.31	0.51
6:B:160:LYS:HG3	6:B:161:TRP:N	2.20	0.51
6:B:188:LEU:HG	6:B:189:ALA:H	1.75	0.51
6:B:309:ILE:HD12	6:B:312:GLY:HA3	1.92	0.51
6:B:556:SER:O	24:B:1783:LMG:HC2	2.11	0.51
6:B:599:ILE:O	6:B:734:GLY:C	2.48	0.51
20:B:1786:CLA:C14	20:H:1079:CLA:HBC3	2.40	0.51
7:C:1:MET:SD	7:C:4:SER:OG	2.68	0.51
10:F:73:VAL:HG11	10:F:83:PHE:HB2	1.90	0.51
11:G:96:SER:C	11:G:98:PHE:H	2.13	0.51
16:L:128:ASP:CG	16:L:129:GLN:N	2.63	0.51
17:N:69:CYS:O	17:N:70:GLU:O	2.28	0.51
1:1:32:VAL:HG12	1:1:36:LEU:HD12	1.92	0.51
1:1:160:GLY:C	20:1:1189:CLA:HBB2	2.31	0.51
3:3:116:PHE:O	3:3:120:LEU:HB2	2.10	0.51
5:A:130:GLU:HG3	10:F:45:THR:HG21	1.92	0.51
5:A:187:HIS:CD2	20:A:1767:CLA:C1C	2.94	0.51
5:A:207:LEU:HA	5:A:211:LEU:CB	2.40	0.51
5:A:536:THR:HA	5:A:539:PHE:HB3	1.93	0.51
5:A:725:LEU:N	5:A:725:LEU:HD12	2.26	0.51
20:A:1788:CLA:H11	20:A:1800:CLA:H43	1.92	0.51
21:A:7030:LMU:C6'	21:A:7030:LMU:H2'	2.41	0.51
6:B:17:THR:HA	6:B:696:LYS:N	2.26	0.51
6:B:44:GLN:CD	6:B:163:PRO:HB2	2.30	0.51
6:B:74:PHE:C	6:B:76:ALA:H	2.13	0.51
6:B:700:LEU:N	6:B:700:LEU:CD2	2.73	0.51
6:B:730:SER:O	6:B:731:GLY:O	2.29	0.51
20:B:1740:CLA:H143	20:B:1757:CLA:H18	1.93	0.51
20:B:1755:CLA:OBD	20:B:1767:CLA:HBB1	2.11	0.51
7:C:5:VAL:HB	7:C:65:VAL:HG22	1.91	0.51
7:C:12:ILE:O	7:C:38:GLN:HG2	2.10	0.51
7:C:51:CYS:N	25:C:1082:SF4:S2	2.78	0.51
7:C:73:THR:OG1	7:C:76:SER:OG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:30:ALA:O	16:L:18:PRO:CB	2.54	0.51
11:G:28:ARG:HH21	11:G:29:GLU:N	2.06	0.51
20:J:1045:CLA:C2	20:J:1045:CLA:HMA2	2.41	0.51
16:L:108:LYS:C	16:L:108:LYS:HE2	2.31	0.51
18:R:37:UNK:O	18:R:42:UNK:O	2.29	0.51
3:3:85:PRO:HB2	3:3:104:TYR:HA	1.91	0.51
5:A:63:ASP:HA	20:A:1785:CLA:HED2	1.92	0.51
5:A:450:CYS:O	5:A:453:LEU:O	2.28	0.51
5:A:509:ALA:O	5:A:510:SER:OG	2.17	0.51
5:A:701:GLN:OE1	9:E:74:TYR:HE1	1.93	0.51
20:A:1782:CLA:H143	20:A:1782:CLA:C10	2.40	0.51
20:A:1816:CLA:H2	20:A:1816:CLA:C7	2.41	0.51
6:B:197:VAL:O	6:B:198:ALA:CB	2.59	0.51
6:B:375:HIS:CE1	20:B:1758:CLA:NC	2.76	0.51
6:B:464:GLN:OE1	6:B:469:LYS:CD	2.55	0.51
6:B:606:VAL:C	6:B:608:GLN:H	2.14	0.51
6:B:710:LEU:C	6:B:712:HIS:H	2.12	0.51
8:D:50:TRP:N	8:D:50:TRP:CD1	2.79	0.51
9:E:40:ARG:N	9:E:46:PHE:HE1	2.09	0.51
10:F:23:LYS:O	10:F:24:LYS:HE2	2.08	0.51
10:F:50:LYS:C	10:F:52:ARG:N	2.63	0.51
10:F:91:LEU:O	10:F:94:ALA:O	2.28	0.51
11:G:32:ALA:C	11:G:34:GLN:N	2.64	0.51
15:K:69:ILE:O	15:K:70:MET:O	2.29	0.51
16:L:60:HIS:HD2	20:L:1167:CLA:CED	2.24	0.51
16:L:102:TYR:C	16:L:104:ILE:H	2.14	0.51
16:L:123:ARG:C	16:L:124:LYS:HE3	2.31	0.51
17:N:72:LYS:HZ3	17:N:74:LYS:HA	1.76	0.51
2:2:179:PHE:HD1	2:2:183:TYR:CE2	2.28	0.51
5:A:439:ARG:HG2	5:A:562:PHE:CE2	2.45	0.51
20:A:1800:CLA:HMB2	20:L:1167:CLA:CBC	2.38	0.51
21:A:7039:LMU:O6B	21:A:7039:LMU:O3'	2.29	0.51
6:B:271:THR:OG1	6:B:272:ASP:N	2.43	0.51
6:B:290:MET:O	6:B:290:MET:HG2	2.10	0.51
6:B:305:LEU:O	6:B:308:HIS:N	2.25	0.51
6:B:376:GLN:HB3	6:B:587:ILE:HD12	1.93	0.51
6:B:420:SER:O	6:B:424:TRP:N	2.35	0.51
6:B:428:PHE:HA	20:B:1762:CLA:O1D	2.11	0.51
6:B:486:LEU:HD12	20:B:1765:CLA:OBD	2.10	0.51
6:B:549:ASP:OD1	7:C:63:LEU:HB3	2.11	0.51
6:B:560:ASP:OD1	7:C:52:LYS:NZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1752:CLA:O1A	11:G:54:TYR:OH	2.28	0.51
11:G:38:GLN:O	11:G:40:GLY:O	2.28	0.51
22:I:1032:BCR:H403	22:I:1032:BCR:H271	1.92	0.51
17:N:4:GLU:C	17:N:4:GLU:CD	2.70	0.51
17:N:35:VAL:HG12	17:N:37:PHE:CE1	2.45	0.51
17:N:47:THR:O	17:N:48:GLY:O	2.29	0.51
17:N:51:ASP:OD2	17:N:51:ASP:N	2.30	0.51
18:R:27:UNK:C	18:R:29:UNK:N	2.74	0.51
18:R:30:UNK:O	18:R:32:UNK:N	2.43	0.51
19:Z:1:GLC:O6	19:Z:2:FRU:O5	2.29	0.51
20:1:1198:CLA:HAA2	20:1:1198:CLA:HBD	1.93	0.51
2:2:77:PRO:O	17:N:3:ILE:HD12	2.10	0.51
20:2:1215:CLA:HED2	20:2:1220:CLA:HBB1	1.92	0.51
20:3:3011:CLA:H172	20:3:3011:CLA:C12	2.30	0.51
5:A:104:SER:HG	5:A:161:GLU:CD	2.14	0.51
5:A:401:TRP:CZ3	5:A:609:ILE:HB	2.45	0.51
5:A:584:PRO:HG3	6:B:559:CYS:SG	2.50	0.51
5:A:685:VAL:O	5:A:688:PHE:HB3	2.11	0.51
20:A:1770:CLA:C4B	22:A:1803:BCR:C20	2.87	0.51
20:A:1783:CLA:H92	22:A:1807:BCR:H373	1.92	0.51
20:A:1783:CLA:HBD	20:A:1783:CLA:HAA1	1.92	0.51
20:A:1787:CLA:H93	16:L:36:TYR:HE1	1.76	0.51
6:B:92:TRP:CZ2	13:I:6:SER:HB2	2.45	0.51
6:B:167:TRP:HB2	11:G:41:MET:HE3	1.91	0.51
6:B:387:PHE:O	6:B:391:PRO:HG3	2.10	0.51
20:B:1735:CLA:HBB2	20:B:1735:CLA:C11	2.41	0.51
20:B:1755:CLA:HBD	20:B:1767:CLA:HMB3	1.92	0.51
7:C:12:ILE:HG21	7:C:39:ILE:C	2.31	0.51
7:C:34:CYS:SG	7:C:39:ILE:HD12	2.51	0.51
8:D:48:ILE:HG12	8:D:49:THR:N	2.23	0.51
10:F:53:PHE:C	10:F:55:ASN:N	2.63	0.51
10:F:80:TRP:CH2	20:F:1156:CLA:HAC2	2.46	0.51
10:F:124:PRO:C	10:F:126:ALA:H	2.14	0.51
11:G:33:LYS:O	11:G:34:GLN:O	2.28	0.51
12:H:26:SER:O	12:H:27:ASP:O	2.29	0.51
20:J:1043:CLA:CHD	20:J:1043:CLA:CBC	2.85	0.51
17:N:45:ASN:CA	17:N:57:LYS:HZ2	2.24	0.51
5:A:592:VAL:O	5:A:597:HIS:CD2	2.64	0.51
5:A:685:VAL:HG12	5:A:741:GLY:CA	2.40	0.51
5:A:746:THR:O	5:A:750:PHE:N	2.38	0.51
5:A:750:PHE:O	5:A:752:ALA:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1808:BCR:C39	22:A:1808:BCR:C23	2.66	0.51
6:B:185:VAL:CG2	22:B:1775:BCR:H272	2.41	0.51
6:B:561:GLY:HA3	7:C:52:LYS:CB	2.41	0.51
20:F:1156:CLA:O1D	20:F:1156:CLA:H2A	2.11	0.51
11:G:7:VAL:HG23	11:G:8:ILE:H	1.64	0.51
20:J:1044:CLA:OBD	20:J:1045:CLA:C4	2.54	0.51
17:N:27:ALA:O	17:N:28:ASN:O	2.29	0.51
17:N:42:PHE:HD1	17:N:43:PRO:CA	2.24	0.51
17:N:45:ASN:ND2	17:N:45:ASN:O	2.44	0.51
17:N:62:SER:O	17:N:66:ASP:OD2	2.29	0.51
17:N:82:PHE:N	17:N:82:PHE:HD2	2.08	0.51
3:3:86:GLN:CB	3:3:88:THR:HB	2.37	0.50
3:3:92:TRP:O	3:3:95:THR:HG23	2.11	0.50
3:3:182:LYS:O	3:3:185:LYS:HB3	2.11	0.50
5:A:23:ASP:HA	5:A:24:ARG:HD2	1.87	0.50
5:A:118:PRO:HB3	5:A:150:PHE:CD2	2.46	0.50
5:A:327:ILE:O	5:A:328:LYS:O	2.29	0.50
5:A:379:MET:SD	5:A:511:THR:O	2.69	0.50
5:A:462:ILE:HG21	20:A:1789:CLA:CMC	2.41	0.50
20:A:1776:CLA:HMC1	20:A:1776:CLA:HBC2	1.92	0.50
20:A:1781:CLA:HED2	20:A:1781:CLA:HAA1	1.92	0.50
20:A:1791:CLA:HBD	20:A:1791:CLA:HAA1	1.94	0.50
21:A:7016:LMU:H71	21:A:7016:LMU:H111	1.92	0.50
6:B:231:ASN:O	6:B:233:TYR:N	2.44	0.50
6:B:436:LEU:O	6:B:437:TYR:CB	2.59	0.50
6:B:440:ASN:CG	6:B:614:THR:O	2.49	0.50
6:B:626:LEU:HD12	6:B:627:ASN:N	2.26	0.50
6:B:726:ILE:C	6:B:728:SER:H	2.13	0.50
7:C:7:ILE:CG2	7:C:65:VAL:HG21	2.42	0.50
7:C:9:ASP:HB3	25:C:1083:SF4:S3	2.51	0.50
7:C:28:MET:SD	8:D:122:LYS:O	2.70	0.50
8:D:132:LEU:HD23	8:D:133:ASN:O	2.10	0.50
17:N:49:CYS:O	17:N:51:ASP:O	2.29	0.50
17:N:49:CYS:O	17:N:50:GLN:O	2.30	0.50
17:N:62:SER:O	17:N:66:ASP:OD1	2.29	0.50
18:R:38:UNK:C	18:R:42:UNK:C	2.89	0.50
3:3:74:ALA:CB	3:3:75:PRO:HD3	2.26	0.50
4:4:160:MET:CG	20:4:1201:CLA:CBB	2.87	0.50
5:A:23:ASP:OD1	5:A:23:ASP:O	2.29	0.50
5:A:212:GLY:C	5:A:214:GLY:H	2.14	0.50
5:A:227:LEU:HD23	5:A:231:GLN:NE2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:274:TRP:NE1	5:A:277:TYR:CE2	2.79	0.50
5:A:329:ASP:O	5:A:332:GLU:O	2.29	0.50
5:A:665:ILE:HD13	6:B:621:ARG:HG3	1.93	0.50
5:A:741:GLY:O	5:A:743:ILE:N	2.44	0.50
20:A:1789:CLA:H172	20:A:1793:CLA:C20	2.41	0.50
20:A:1796:CLA:H62	20:A:1813:CLA:C19	2.41	0.50
20:A:1799:CLA:CED	20:A:1799:CLA:HBA1	2.41	0.50
20:A:1800:CLA:H61	20:A:1800:CLA:C11	2.40	0.50
6:B:77:TRP:CE2	6:B:81:PRO:HB3	2.46	0.50
6:B:182:LEU:HA	20:B:1743:CLA:HMB2	1.93	0.50
6:B:295:PHE:HE2	11:G:38:GLN:NE2	2.09	0.50
6:B:392:ILE:HD13	20:B:1759:CLA:HED1	1.92	0.50
6:B:393:PHE:CE1	6:B:394:PHE:CE2	2.99	0.50
6:B:648:TRP:CZ2	20:B:1786:CLA:H62	2.46	0.50
20:B:1768:CLA:C12	22:B:1779:BCR:H312	2.33	0.50
7:C:29:ILE:CG2	8:D:126:GLY:CA	2.89	0.50
9:E:69:PHE:HD2	9:E:71:LYS:HG2	1.77	0.50
20:K:1146:CLA:HBC2	20:K:1146:CLA:CMC	2.20	0.50
17:N:62:SER:O	17:N:63:ASP:OD1	2.29	0.50
18:R:35:UNK:O	18:R:42:UNK:O	2.30	0.50
1:1:54:VAL:C	1:1:56:GLY:H	2.15	0.50
20:1:1188:CLA:HED2	20:1:1188:CLA:CAD	2.42	0.50
2:2:56:MET:HG2	2:2:172:LEU:HB2	1.93	0.50
3:3:157:ALA:O	3:3:158:TYR:CB	2.59	0.50
3:3:182:LYS:O	3:3:182:LYS:HG2	2.12	0.50
20:4:4014:CLA:HAA2	20:4:4014:CLA:HBD	1.94	0.50
5:A:89:ILE:O	5:A:93:LEU:HG	2.11	0.50
5:A:281:LEU:CD2	20:A:1772:CLA:HMA2	2.41	0.50
5:A:462:ILE:HG21	20:A:1789:CLA:HMC3	1.94	0.50
5:A:672:LEU:C	5:A:674:ALA:H	2.08	0.50
20:A:1770:CLA:CAB	22:A:1803:BCR:H19C	2.33	0.50
20:A:1781:CLA:H162	20:A:1781:CLA:H111	1.93	0.50
21:A:7020:LMU:O6'	21:A:7020:LMU:O1B	2.29	0.50
21:A:7022:LMU:O3B	21:A:7022:LMU:O6B	2.30	0.50
21:A:7023:LMU:C1B	21:A:7023:LMU:H4O1	2.23	0.50
6:B:31:PHE:O	6:B:32:GLU:C	2.49	0.50
6:B:54:LEU:HD11	20:B:1743:CLA:HBA2	1.91	0.50
6:B:343:VAL:CG1	20:B:1756:CLA:H2	2.41	0.50
6:B:535:VAL:HG13	6:B:536:LYS:H	1.76	0.50
20:B:1759:CLA:C9	24:B:1783:LMG:H311	2.42	0.50
9:E:63:TYR:HA	9:E:83:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:80:ASN:HB3	9:E:82:TYR:CE2	2.46	0.50
10:F:28:SER:O	10:F:29:LEU:O	2.29	0.50
15:K:58:ALA:HB1	20:K:1085:CLA:HMD3	1.92	0.50
20:K:1142:CLA:O1D	20:K:1142:CLA:H2A	2.11	0.50
17:N:80:ASN:O	17:N:80:ASN:OD1	2.30	0.50
18:R:44:UNK:O	18:R:45:UNK:O	2.30	0.50
19:O:1:GLC:O6	19:O:2:FRU:H5	2.10	0.50
2:2:182:ILE:O	2:2:205:PHE:HB3	2.11	0.50
20:2:1213:CLA:CHD	20:2:1213:CLA:CBC	2.88	0.50
3:3:64:TYR:HB2	20:3:1218:CLA:H42	1.87	0.50
3:3:86:GLN:HB2	3:3:88:THR:N	2.26	0.50
22:3:1220:BCR:H361	20:A:1798:CLA:H92	1.92	0.50
4:4:164:LEU:O	4:4:165:GLY:C	2.50	0.50
5:A:38:GLY:O	5:A:39:HIS:HB3	2.11	0.50
5:A:341:GLN:O	5:A:344:LYS:HB2	2.12	0.50
5:A:409:GLY:C	5:A:411:ALA:N	2.65	0.50
5:A:571:ASP:OD2	8:D:88:THR:HG21	2.12	0.50
5:A:685:VAL:CG1	5:A:741:GLY:HA2	2.41	0.50
5:A:734:GLY:O	5:A:736:THR:N	2.45	0.50
20:A:1762:CLA:HBA2	20:A:1762:CLA:CED	2.41	0.50
20:A:1781:CLA:H43	20:A:1793:CLA:HBA1	1.92	0.50
20:A:1791:CLA:HMA2	20:A:1797:CLA:CHC	2.42	0.50
6:B:136:TYR:O	6:B:140:ILE:HD11	2.12	0.50
6:B:681:ALA:O	6:B:683:GLU:N	2.45	0.50
20:B:1735:CLA:HAA1	20:B:1735:CLA:HBD	1.93	0.50
8:D:113:HIS:N	8:D:114:PRO:CD	2.74	0.50
10:F:144:LEU:HG	10:F:145:LEU:HD23	1.94	0.50
11:G:21:PHE:O	11:G:23:PHE:N	2.44	0.50
11:G:43:HIS:O	11:G:45:GLU:OE1	2.29	0.50
22:I:1032:BCR:H291	22:L:1169:BCR:H281	1.92	0.50
16:L:99:LEU:HD11	22:L:1169:BCR:C7	2.40	0.50
17:N:5:GLU:OE2	17:N:6:TYR:N	2.45	0.50
17:N:58:VAL:HG12	17:N:59:PRO:HD3	1.93	0.50
17:N:82:PHE:N	17:N:82:PHE:CD2	2.78	0.50
20:2:1215:CLA:H43	20:2:1220:CLA:CBC	2.33	0.50
20:4:1196:CLA:O2D	20:4:1196:CLA:OBD	2.30	0.50
5:A:88:ILE:C	5:A:90:PHE:N	2.63	0.50
5:A:163:GLN:C	5:A:165:TYR:N	2.64	0.50
5:A:354:TRP:O	5:A:358:LEU:N	2.44	0.50
5:A:472:ARG:NE	5:A:474:GLN:HG3	2.15	0.50
5:A:655:ASP:O	5:A:660:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1776:CLA:H101	20:A:1779:CLA:H93	1.94	0.50
20:A:1781:CLA:HHB	22:A:1806:BCR:H363	1.88	0.50
6:B:50:HIS:CA	6:B:53:GLN:HB2	2.41	0.50
6:B:560:ASP:HB2	7:C:66:ARG:CZ	2.40	0.50
8:D:116:ASP:HB3	8:D:127:ARG:HH12	1.75	0.50
8:D:120:PRO:O	8:D:121:GLU:HB3	2.11	0.50
8:D:131:GLY:O	8:D:132:LEU:HB2	2.10	0.50
9:E:85:ASP:O	9:E:85:ASP:OD1	2.30	0.50
10:F:83:PHE:C	10:F:86:PRO:HD2	2.32	0.50
15:K:40:LEU:O	15:K:41:GLU:HG3	2.12	0.50
16:L:123:ARG:HB3	16:L:126:GLN:CG	2.41	0.50
16:L:136:TRP:O	16:L:140:THR:HG23	2.12	0.50
17:N:59:PRO:O	17:N:61:LEU:O	2.29	0.50
18:R:38:UNK:O	18:R:39:UNK:O	2.30	0.50
2:2:63:PHE:CD1	2:2:64:ILE:N	2.80	0.50
3:3:106:TYR:CD2	3:3:107:TRP:CG	2.99	0.50
3:3:109:ASP:O	3:3:110:SER:O	2.28	0.50
5:A:72:GLU:HB3	5:A:76:ARG:NH2	2.27	0.50
5:A:216:LEU:O	5:A:219:ALA:N	2.44	0.50
5:A:334:HIS:HB3	20:A:1777:CLA:HMA3	1.93	0.50
5:A:620:MET:SD	5:A:624:VAL:HG21	2.52	0.50
5:A:733:VAL:CG1	20:A:1796:CLA:C3D	2.89	0.50
5:A:746:THR:OG1	20:A:1811:CLA:O1D	2.19	0.50
20:A:1773:CLA:H51	20:A:1782:CLA:HMB1	1.94	0.50
20:A:1811:CLA:HMB3	20:A:1812:CLA:HMD1	1.94	0.50
21:A:7016:LMU:H112	21:A:7016:LMU:H72	1.91	0.50
21:A:7021:LMU:C6	21:A:7021:LMU:C2	2.72	0.50
6:B:290:MET:HG3	20:B:1751:CLA:HMC3	1.94	0.50
6:B:320:LYS:O	6:B:322:LEU:N	2.44	0.50
6:B:382:ILE:O	6:B:385:GLY:N	2.42	0.50
6:B:662:MET:HE2	23:B:1773:PQN:H2M3	1.93	0.50
23:B:1773:PQN:C29	24:B:1783:LMG:H201	2.41	0.50
20:B:1787:CLA:HMC1	20:B:1787:CLA:HBC2	1.93	0.50
7:C:11:CYS:C	7:C:13:GLY:H	2.14	0.50
9:E:89:GLU:O	9:E:90:VAL:CB	2.59	0.50
11:G:43:HIS:O	11:G:45:GLU:N	2.45	0.50
17:N:46:PHE:O	17:N:47:THR:OG1	2.30	0.50
20:R:1054:CLA:HED3	20:R:1054:CLA:C4D	2.36	0.50
5:A:51:THR:CG2	20:A:1795:CLA:HBB1	2.06	0.50
5:A:208:ALA:HA	5:A:310:PHE:C	2.28	0.50
5:A:254:LEU:C	5:A:256:ALA:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:364:MET:O	5:A:368:LEU:HB2	2.11	0.50
5:A:462:ILE:CG2	20:A:1789:CLA:HMC3	2.42	0.50
5:A:571:ASP:HB3	7:C:53:ARG:HH12	1.76	0.50
5:A:594:ALA:O	5:A:598:VAL:HG23	2.11	0.50
20:A:1765:CLA:CHA	20:A:1765:CLA:CBA	2.89	0.50
20:A:1776:CLA:H18	22:A:1805:BCR:H383	1.94	0.50
20:A:1786:CLA:CBB	20:A:1794:CLA:HBB2	2.40	0.50
6:B:406:ASN:C	6:B:406:ASN:ND2	2.65	0.50
6:B:595:HIS:CE1	6:B:599:ILE:HD11	2.46	0.50
20:B:1756:CLA:H101	22:B:1777:BCR:H14C	1.93	0.50
20:B:1757:CLA:CGA	20:B:1757:CLA:H3A	2.36	0.50
22:B:1775:BCR:C8	22:B:1775:BCR:H331	2.41	0.50
7:C:72:GLU:O	7:C:73:THR:O	2.29	0.50
7:C:73:THR:O	7:C:76:SER:OG	2.30	0.50
8:D:24:THR:O	8:D:24:THR:OG1	2.30	0.50
8:D:33:THR:HG23	16:L:23:LEU:HD12	1.94	0.50
8:D:41:GLN:HG3	16:L:125:LYS:HZ2	1.77	0.50
8:D:46:TYR:HD1	8:D:80:LYS:HB3	1.76	0.50
11:G:16:LEU:CD2	11:G:68:ILE:HG21	2.42	0.50
11:G:19:GLY:C	11:G:21:PHE:HA	2.32	0.50
16:L:48:ASN:CB	16:L:49:PRO:HD2	2.34	0.50
19:Z:1:GLC:O6	19:Z:2:FRU:O2	2.30	0.50
20:2:1212:CLA:O1A	20:2:1212:CLA:C4A	2.59	0.50
3:3:80:LYS:HD3	3:3:105:ASN:HB3	1.91	0.50
3:3:84:ILE:O	3:3:84:ILE:HD13	2.12	0.50
5:A:93:LEU:O	5:A:97:TYR:HD2	1.94	0.50
5:A:394:SER:OG	5:A:395:LEU:N	2.44	0.50
5:A:519:ASP:C	5:A:520:LEU:HG	2.31	0.50
5:A:588:GLY:HA3	6:B:668:ARG:HB3	1.93	0.50
5:A:635:THR:O	5:A:635:THR:HG22	2.12	0.50
5:A:654:ARG:HH21	6:B:637:PRO:HD2	1.76	0.50
21:A:7022:LMU:H5'	21:A:7022:LMU:H2O2	1.76	0.50
6:B:160:LYS:O	6:B:162:LYS:N	2.44	0.50
6:B:190:TRP:CD2	20:B:1748:CLA:HMD3	2.47	0.50
6:B:655:LEU:HD22	20:B:1771:CLA:CAB	2.41	0.50
20:B:1764:CLA:HMC3	20:B:1767:CLA:H2	1.94	0.50
24:B:1783:LMG:HC91	24:B:1783:LMG:C11	2.40	0.50
7:C:31:TRP:CD1	7:C:32:GLY:N	2.80	0.50
9:E:88:GLU:O	9:E:90:VAL:CG2	2.59	0.50
9:E:88:GLU:O	9:E:90:VAL:N	2.44	0.50
11:G:68:ILE:HD12	11:G:68:ILE:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:92:GLY:O	11:G:93:TYR:O	2.30	0.50
16:L:115:ALA:N	16:L:116:PRO:CD	2.70	0.50
16:L:160:VAL:O	16:L:161:LEU:O	2.29	0.50
17:N:47:THR:O	17:N:52:LEU:O	2.30	0.50
18:R:34:UNK:O	18:R:36:UNK:O	2.30	0.50
19:O:1:GLC:O6	19:O:2:FRU:C5	2.60	0.50
1:1:45:ILE:HG22	1:1:48:ARG:HD2	1.94	0.50
4:4:108:ASP:OD1	4:4:120:ILE:HG12	2.11	0.50
5:A:24:ARG:O	5:A:25:ASP:O	2.29	0.50
5:A:249:ILE:N	5:A:251:ASN:OD1	2.45	0.50
5:A:332:GLU:HA	5:A:344:LYS:HG2	1.93	0.50
5:A:398:HIS:HD2	20:A:1783:CLA:ND	2.09	0.50
5:A:430:ASP:O	5:A:434:ARG:HB2	2.12	0.50
5:A:744:ALA:HA	5:A:747:TRP:HB3	1.93	0.50
20:A:1787:CLA:H12	6:B:686:PRO:HG2	1.92	0.50
21:A:7023:LMU:O4'	21:A:7023:LMU:O1B	2.29	0.50
6:B:141:PHE:O	6:B:144:PHE:N	2.45	0.50
6:B:346:SER:O	6:B:350:GLN:N	2.43	0.50
6:B:586:THR:O	6:B:589:TRP:N	2.44	0.50
6:B:707:LEU:HD12	6:B:711:VAL:CG2	2.42	0.50
20:B:1741:CLA:HAA2	20:B:1741:CLA:H12	1.94	0.50
20:B:1746:CLA:HMA2	20:B:1746:CLA:O2A	2.12	0.50
20:B:1755:CLA:HED1	20:B:1756:CLA:HMD2	1.88	0.50
20:B:1758:CLA:H171	22:B:1775:BCR:H363	1.93	0.50
10:F:25:LEU:O	10:F:26:GLN:O	2.30	0.50
16:L:112:PRO:O	16:L:113:SER:HB3	2.12	0.50
18:R:35:UNK:O	18:R:36:UNK:O	2.30	0.50
20:2:1212:CLA:CGA	20:2:1212:CLA:H43	2.34	0.49
3:3:84:ILE:N	20:A:1798:CLA:C3	2.62	0.49
4:4:35:GLU:O	4:4:37:LEU:N	2.34	0.49
5:A:438:HIS:HB2	5:A:441:ALA:CB	2.42	0.49
5:A:462:ILE:HD13	20:B:1786:CLA:H72	1.93	0.49
5:A:527:VAL:HG12	5:A:528:ALA:N	2.27	0.49
21:A:7036:LMU:O5B	21:A:7036:LMU:O6'	2.30	0.49
21:A:7042:LMU:H5'	21:A:7042:LMU:C2B	2.41	0.49
6:B:122:GLN:O	6:B:126:THR:CB	2.59	0.49
6:B:353:TYR:HB2	6:B:594:TRP:HH2	1.77	0.49
6:B:441:ASP:OD1	6:B:617:MET:HB3	2.12	0.49
6:B:655:LEU:CD2	20:B:1771:CLA:CAB	2.90	0.49
20:B:1735:CLA:H2A	20:B:1735:CLA:CED	2.27	0.49
20:B:1735:CLA:CBC	22:B:1778:BCR:C33	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1736:CLA:HBC2	20:B:1736:CLA:HMC1	1.94	0.49
17:N:42:PHE:O	17:N:43:PRO:O	2.29	0.49
17:N:59:PRO:O	17:N:66:ASP:OD1	2.30	0.49
18:R:38:UNK:O	18:R:42:UNK:O	2.30	0.49
19:M:1:GLC:O2	19:M:2:FRU:O4	2.30	0.49
19:Z:1:GLC:C1	19:Z:2:FRU:O3	2.60	0.49
2:2:206:ALA:O	2:2:207:ALA:CB	2.59	0.49
3:3:157:ALA:O	3:3:158:TYR:HD2	1.95	0.49
4:4:150:LYS:HG2	4:4:150:LYS:O	2.12	0.49
5:A:249:ILE:HD13	5:A:250:LEU:HB2	1.93	0.49
5:A:369:THR:HG21	5:A:402:ILE:HG22	1.92	0.49
5:A:441:ALA:HA	5:A:444:SER:HB3	1.94	0.49
5:A:575:LEU:CD1	5:A:576:GLY:H	2.25	0.49
5:A:668:TYR:CE1	6:B:445:ALA:HB2	2.47	0.49
20:A:1781:CLA:HAA1	20:A:1781:CLA:HBD	1.93	0.49
6:B:661:PHE:HB3	20:B:1787:CLA:HMC1	1.93	0.49
6:B:707:LEU:HD11	20:B:1759:CLA:H91	1.93	0.49
20:B:1755:CLA:C4A	20:B:1769:CLA:HAA2	2.42	0.49
7:C:72:GLU:C	7:C:73:THR:O	2.46	0.49
10:F:123:VAL:HG13	14:J:7:TYR:N	2.26	0.49
11:G:37:GLU:O	11:G:38:GLN:O	2.29	0.49
11:G:58:LEU:O	11:G:60:SER:N	2.44	0.49
15:K:24:PHE:HB3	15:K:52:PRO:CG	2.40	0.49
1:1:160:GLY:C	1:1:162:CYS:H	2.14	0.49
3:3:86:GLN:HB2	3:3:88:THR:H	1.76	0.49
4:4:124:TYR:HA	4:4:145:PRO:HD3	1.94	0.49
5:A:648:THR:O	5:A:649:ILE:HG22	2.12	0.49
20:A:1784:CLA:H52	20:A:1784:CLA:CMD	2.42	0.49
20:A:1817:CLA:HAA1	20:A:1817:CLA:CGD	2.43	0.49
21:A:7032:LMU:O5B	21:A:7032:LMU:O1'	2.29	0.49
21:A:7037:LMU:O1B	21:A:7037:LMU:O2'	2.30	0.49
6:B:232:LEU:HD21	6:B:235:GLN:OE1	2.12	0.49
6:B:292:ARG:HH22	20:B:1750:CLA:HED1	1.76	0.49
6:B:509:PHE:CD2	6:B:509:PHE:N	2.81	0.49
6:B:667:TRP:O	6:B:669:GLY:N	2.45	0.49
20:B:1759:CLA:HMD2	24:B:1783:LMG:H341	1.95	0.49
20:B:1768:CLA:C16	22:B:1779:BCR:H311	2.38	0.49
9:E:55:VAL:CG2	9:E:65:VAL:HB	2.40	0.49
10:F:116:GLN:O	10:F:118:GLU:N	2.45	0.49
12:H:45:ALA:C	12:H:48:THR:H	2.09	0.49
14:J:22:LEU:O	14:J:23:ALA:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:1045:CLA:O1D	20:J:1045:CLA:O1A	2.30	0.49
21:K:1086:LMU:O6B	21:K:1086:LMU:O4'	2.30	0.49
17:N:38:GLY:O	17:N:39:SER:O	2.30	0.49
20:R:1054:CLA:CED	20:R:1054:CLA:C4D	2.90	0.49
5:A:393:LEU:HD13	5:A:750:PHE:CE1	2.45	0.49
20:A:1783:CLA:O1D	20:A:1783:CLA:H2A	2.12	0.49
20:A:1793:CLA:HMB2	20:A:1794:CLA:C2D	2.42	0.49
21:A:7013:LMU:O5B	21:A:7013:LMU:O3'	2.29	0.49
6:B:48:ALA:HB3	6:B:157:LEU:HD22	1.93	0.49
6:B:50:HIS:HB2	6:B:53:GLN:HB2	1.94	0.49
6:B:289:LEU:HA	20:B:1750:CLA:O1D	2.12	0.49
20:B:1750:CLA:HMA1	11:G:21:PHE:CG	2.47	0.49
8:D:72:PRO:HB2	8:D:74:LEU:HB2	1.95	0.49
11:G:47:GLY:N	11:G:48:ASP:HB3	2.10	0.49
20:G:1099:CLA:HBC3	20:G:1099:CLA:CHD	2.42	0.49
12:H:54:LEU:CD1	12:H:55:LYS:HG3	2.42	0.49
20:J:1044:CLA:O2D	20:J:1044:CLA:OBD	2.29	0.49
16:L:78:GLU:HG3	16:L:78:GLU:O	2.13	0.49
1:1:161:PHE:O	1:1:164:GLN:HB2	2.12	0.49
2:2:98:GLU:O	2:2:102:ILE:HG12	2.12	0.49
3:3:98:ILE:O	17:N:63:ASP:C	2.46	0.49
5:A:298:ASP:O	5:A:301:HIS:N	2.45	0.49
5:A:549:ILE:O	5:A:552:THR:O	2.30	0.49
5:A:694:PHE:HZ	6:B:661:PHE:CD1	2.30	0.49
5:A:729:GLN:HE21	20:A:1796:CLA:HMD1	1.77	0.49
20:A:1774:CLA:H8	20:A:1774:CLA:CBB	2.43	0.49
20:A:1781:CLA:C3B	22:A:1806:BCR:C37	2.90	0.49
22:A:1805:BCR:C38	22:A:1805:BCR:C23	2.74	0.49
6:B:193:HIS:CD2	20:B:1744:CLA:NB	2.80	0.49
6:B:278:LEU:HD12	20:B:1746:CLA:HMA1	1.90	0.49
6:B:377:TYR:O	6:B:378:ILE:HB	2.13	0.49
6:B:521:HIS:CE1	20:B:1768:CLA:C4A	2.96	0.49
6:B:535:VAL:CG2	6:B:539:LEU:HD23	2.42	0.49
20:B:1762:CLA:HMD2	20:B:1762:CLA:H13	1.94	0.49
10:F:17:ARG:O	10:F:18:GLU:C	2.51	0.49
10:F:151:ASP:HA	10:F:154:PHE:CB	2.43	0.49
11:G:42:SER:OG	11:G:43:HIS:O	2.30	0.49
16:L:5:LYS:N	16:L:6:PRO:HD3	2.28	0.49
17:N:38:GLY:C	17:N:39:SER:O	2.49	0.49
17:N:45:ASN:O	17:N:46:PHE:O	2.30	0.49
17:N:60:PHE:N	17:N:61:LEU:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:2:FRU:O6	19:Z:2:FRU:O1	2.30	0.49
3:3:133:ALA:O	3:3:134:LYS:HB2	2.12	0.49
4:4:48:GLY:N	4:4:161:LEU:HD23	2.27	0.49
20:4:1196:CLA:HBD	20:4:1196:CLA:HAA1	1.93	0.49
5:A:44:ILE:O	5:A:46:LYS:CA	2.60	0.49
5:A:79:PHE:HZ	5:A:185:HIS:HE2	1.57	0.49
5:A:141:ARG:HG3	5:A:141:ARG:NH2	2.16	0.49
5:A:302:HIS:HE1	20:A:1774:CLA:C1B	2.25	0.49
5:A:354:TRP:CZ2	20:A:1780:CLA:H171	2.48	0.49
5:A:464:ASN:O	5:A:468:SER:N	2.40	0.49
5:A:497:ALA:HA	5:A:510:SER:OG	2.12	0.49
5:A:538:ASP:O	5:A:542:HIS:HB2	2.11	0.49
5:A:569:ILE:HB	5:A:572:LYS:HG3	1.94	0.49
5:A:598:VAL:O	5:A:598:VAL:HG12	2.13	0.49
20:A:1783:CLA:C20	22:A:1808:BCR:C16	2.88	0.49
20:A:1797:CLA:O1A	20:A:1797:CLA:O2D	2.30	0.49
21:A:7021:LMU:O3B	21:A:7021:LMU:H6'1	2.10	0.49
6:B:492:ILE:O	6:B:493:TRP:HB2	2.13	0.49
6:B:606:VAL:C	6:B:608:GLN:N	2.64	0.49
20:B:1740:CLA:C9	22:B:1781:BCR:H361	2.41	0.49
20:B:1751:CLA:HMA3	20:B:1752:CLA:C3D	2.42	0.49
20:B:1753:CLA:H43	20:B:1753:CLA:CHA	2.38	0.49
20:B:1758:CLA:H62	22:B:1776:BCR:C32	2.43	0.49
20:B:1758:CLA:H172	22:B:1775:BCR:H363	1.94	0.49
8:D:75:LEU:HD21	16:L:19:PHE:CE1	2.48	0.49
20:1:1191:CLA:CHC	20:1:1197:CLA:HBC1	2.43	0.49
2:2:59:ALA:HB3	2:2:172:LEU:HD13	1.94	0.49
2:2:192:LEU:HG	2:2:193:PHE:H	1.78	0.49
3:3:158:TYR:CB	3:3:159:PRO:HD2	2.22	0.49
20:3:1217:CLA:C2A	20:3:3011:CLA:HHD	2.43	0.49
4:4:36:ASN:HB2	4:4:39:TRP:CG	2.48	0.49
4:4:146:THR:HG22	4:4:147:LEU:HD12	1.93	0.49
5:A:68:THR:O	5:A:70:ASP:N	2.43	0.49
5:A:90:PHE:HE2	5:A:178:MET:SD	2.34	0.49
5:A:259:TYR:HB3	5:A:260:PRO:CD	2.31	0.49
5:A:402:ILE:HD11	20:A:1784:CLA:CBB	2.40	0.49
5:A:411:ALA:O	5:A:412:ALA:C	2.51	0.49
5:A:435:VAL:HA	5:A:438:HIS:HE1	1.76	0.49
5:A:473:PRO:C	5:A:475:ASP:H	2.16	0.49
5:A:705:GLU:HG2	6:B:545:LYS:HZ2	1.76	0.49
20:A:1795:CLA:NC	20:B:1735:CLA:HBC2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:304:ILE:HG22	20:B:1752:CLA:O1D	2.10	0.49
6:B:356:PRO:HB2	6:B:361:ILE:CG2	2.43	0.49
6:B:419:ILE:C	6:B:420:SER:OG	2.47	0.49
6:B:580:VAL:HG11	6:B:710:LEU:HD21	1.94	0.49
7:C:15:THR:N	7:C:17:CYS:SG	2.85	0.49
9:E:52:VAL:HA	9:E:67:VAL:HA	1.95	0.49
10:F:22:LEU:HB2	10:F:23:LYS:HD3	1.94	0.49
10:F:26:GLN:O	10:F:28:SER:OG	2.29	0.49
11:G:8:ILE:O	11:G:8:ILE:CG1	2.56	0.49
12:H:40:PHE:O	12:H:43:PHE:N	2.46	0.49
17:N:77:CYS:O	17:N:79:SER:O	2.29	0.49
3:3:129:PHE:O	3:3:129:PHE:CD1	2.66	0.49
4:4:192:THR:HG22	4:4:193:ILE:N	2.26	0.49
5:A:188:LYS:O	5:A:190:ALA:N	2.46	0.49
5:A:283:PHE:O	5:A:284:ARG:NH1	2.45	0.49
5:A:338:PHE:CE1	20:A:1799:CLA:HBB1	2.48	0.49
5:A:366:GLY:O	5:A:403:GLY:HA2	2.12	0.49
5:A:681:GLY:C	5:A:683:HIS:H	2.15	0.49
22:A:1807:BCR:C15	20:A:1812:CLA:H151	2.43	0.49
21:A:7033:LMU:O2'	21:A:7033:LMU:O6B	2.29	0.49
6:B:255:LEU:HD12	20:B:1746:CLA:O2D	2.13	0.49
6:B:255:LEU:N	6:B:255:LEU:HD23	2.28	0.49
6:B:517:PHE:O	6:B:517:PHE:CG	2.61	0.49
6:B:662:MET:O	6:B:663:PHE:C	2.50	0.49
6:B:681:ALA:O	6:B:682:HIS:C	2.51	0.49
23:B:1773:PQN:H141	22:B:1780:BCR:H331	1.94	0.49
7:C:7:ILE:HA	7:C:60:THR:OG1	2.13	0.49
20:K:1085:CLA:C1B	20:K:1142:CLA:OBD	2.61	0.49
2:2:116:PRO:O	2:2:131:THR:HB	2.13	0.49
2:2:124:ILE:HD12	2:2:129:LYS:O	2.13	0.49
4:4:106:TRP:HA	4:4:109:ILE:HG13	1.94	0.49
5:A:368:LEU:HD12	20:A:1782:CLA:H61	1.93	0.49
5:A:382:TYR:HB2	5:A:385:LEU:HD11	1.94	0.49
5:A:589:THR:HG22	5:A:589:THR:O	2.13	0.49
20:A:1761:CLA:C4	22:A:1804:BCR:C31	2.90	0.49
20:A:1774:CLA:HAC2	22:A:1804:BCR:H352	1.95	0.49
20:A:1776:CLA:HBC2	20:A:1782:CLA:H18	1.93	0.49
20:A:1779:CLA:CAB	22:A:1805:BCR:H353	2.34	0.49
21:A:7038:LMU:C1B	21:A:7038:LMU:C6'	2.90	0.49
6:B:29:HIS:CE1	20:B:1759:CLA:H43	2.48	0.49
6:B:247:THR:HB	6:B:248:GLN:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1759:CLA:HBC3	20:B:1759:CLA:CMC	2.37	0.49
20:B:1786:CLA:H71	20:B:1786:CLA:H122	1.95	0.49
10:F:104:TYR:CD2	10:F:104:TYR:C	2.86	0.49
11:G:46:ALA:N	11:G:48:ASP:CG	2.60	0.49
17:N:61:LEU:HD21	17:N:64:ASP:N	2.28	0.49
1:1:142:GLU:OE1	20:1:1187:CLA:HMD3	2.13	0.49
5:A:73:GLU:HA	5:A:76:ARG:HD2	1.94	0.49
5:A:92:TRP:CD1	20:A:1763:CLA:CBB	2.96	0.49
5:A:683:HIS:O	20:A:1812:CLA:HAA2	2.13	0.49
20:A:1779:CLA:NC	22:A:1805:BCR:C17	2.75	0.49
6:B:224:PRO:HB3	6:B:227:THR:CB	2.43	0.49
6:B:317:ARG:NH2	6:B:410:ARG:HG2	2.28	0.49
6:B:420:SER:H	6:B:422:LEU:H	1.61	0.49
6:B:564:ARG:CZ	7:C:64:SER:OG	2.61	0.49
6:B:568:CYS:O	6:B:570:ILE:HG23	2.12	0.49
20:B:1736:CLA:HBC3	20:B:1759:CLA:H41	1.95	0.49
20:B:1747:CLA:O1D	20:B:1748:CLA:HMA1	2.12	0.49
20:B:1771:CLA:H51	23:B:1773:PQN:H251	1.93	0.49
8:D:28:ILE:O	8:D:66:ALA:CB	2.61	0.49
8:D:67:ILE:O	8:D:68:MET:HG3	2.12	0.49
10:F:28:SER:O	10:F:30:LYS:O	2.29	0.49
13:I:4:LEU:HG	13:I:4:LEU:O	2.13	0.49
16:L:126:GLN:O	16:L:127:PRO:O	2.31	0.49
20:L:1167:CLA:CAC	22:L:1169:BCR:HC42	2.43	0.49
17:N:61:LEU:O	17:N:62:SER:O	2.30	0.49
20:2:1215:CLA:H43	20:2:1220:CLA:HHD	1.95	0.48
4:4:91:PHE:HA	4:4:94:GLU:HB3	1.95	0.48
4:4:121:PHE:CD1	4:4:143:PHE:CE2	3.01	0.48
5:A:58:HIS:CE1	20:A:1759:CLA:C4D	2.96	0.48
5:A:396:PHE:CD1	5:A:396:PHE:O	2.65	0.48
5:A:506:GLY:O	5:A:507:ALA:HB3	2.12	0.48
6:B:299:HIS:NE2	6:B:304:ILE:HG21	2.28	0.48
6:B:385:GLY:N	20:B:1759:CLA:HBC3	2.28	0.48
6:B:461:GLN:N	6:B:512:ILE:HD12	2.28	0.48
6:B:510:LEU:H	6:B:510:LEU:CD2	2.25	0.48
6:B:601:LEU:O	6:B:601:LEU:HD22	2.12	0.48
6:B:646:TRP:CZ3	6:B:726:ILE:CD1	2.96	0.48
20:B:1755:CLA:O2D	20:B:1756:CLA:OBD	2.30	0.48
10:F:104:TYR:HD2	10:F:104:TYR:C	2.16	0.48
11:G:17:PHE:O	11:G:20:ARG:CB	2.57	0.48
20:1:1187:CLA:HBA1	20:1:1187:CLA:CMA	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:1200:CLA:HBA2	20:1:1200:CLA:HMA3	1.94	0.48
2:2:120:ASN:ND2	14:J:5:LYS:CD	2.75	0.48
20:3:3008:CLA:O1A	20:3:3008:CLA:O2D	2.30	0.48
5:A:104:SER:OG	5:A:161:GLU:OE1	2.31	0.48
5:A:165:TYR:O	5:A:165:TYR:HD2	1.95	0.48
5:A:176:GLY:O	5:A:180:PHE:HB2	2.13	0.48
5:A:415:ALA:HB2	5:A:560:VAL:HG12	1.94	0.48
5:A:484:LEU:N	5:A:485:GLN:OE1	2.40	0.48
5:A:661:ALA:O	5:A:665:ILE:HG13	2.13	0.48
5:A:679:PHE:CE2	5:A:683:HIS:CD2	2.98	0.48
20:A:1764:CLA:HBC3	20:A:1764:CLA:HHD	1.95	0.48
20:A:1793:CLA:C1B	20:A:1794:CLA:HMD3	2.43	0.48
21:A:7032:LMU:H2B	21:A:7032:LMU:C4	2.43	0.48
6:B:67:HIS:O	6:B:88:ALA:O	2.31	0.48
6:B:145:LEU:HD22	6:B:148:ILE:HD12	1.94	0.48
6:B:228:GLY:HA3	11:G:8:ILE:HB	1.95	0.48
6:B:295:PHE:CE2	11:G:38:GLN:NE2	2.81	0.48
6:B:302:LYS:HD3	11:G:49:THR:HA	1.94	0.48
6:B:317:ARG:HD3	6:B:410:ARG:HG2	1.95	0.48
6:B:471:THR:CG2	6:B:502:ASN:ND2	2.76	0.48
6:B:531:THR:O	6:B:535:VAL:CG1	2.54	0.48
6:B:570:ILE:O	6:B:570:ILE:HG13	2.13	0.48
6:B:724:PHE:CD1	20:B:1785:CLA:HMD1	2.49	0.48
20:B:1762:CLA:CBB	22:B:1778:BCR:C26	2.92	0.48
20:B:1762:CLA:C5	22:B:1779:BCR:C40	2.91	0.48
20:B:1770:CLA:HBA1	22:L:1169:BCR:H362	1.94	0.48
20:B:1787:CLA:O2A	20:B:1787:CLA:C3A	2.57	0.48
8:D:101:TYR:CD1	8:D:114:PRO:CD	2.95	0.48
9:E:41:ARG:NE	9:E:46:PHE:CZ	2.81	0.48
11:G:16:LEU:CD1	11:G:17:PHE:CE2	2.93	0.48
12:H:42:THR:O	12:H:45:ALA:N	2.47	0.48
16:L:56:VAL:HG22	20:L:1167:CLA:HED2	1.95	0.48
16:L:96:SER:OG	16:L:143:PHE:CD2	2.60	0.48
17:N:47:THR:OG1	17:N:52:LEU:O	2.30	0.48
1:1:57:ILE:HG23	1:1:58:LEU:N	2.19	0.48
4:4:137:ILE:HG22	4:4:138:PHE:HD2	1.77	0.48
5:A:24:ARG:O	5:A:25:ASP:C	2.50	0.48
5:A:131:ILE:HG23	5:A:132:LEU:N	2.29	0.48
5:A:242:ILE:HD13	5:A:242:ILE:N	2.28	0.48
5:A:553:VAL:O	5:A:557:LEU:HB2	2.12	0.48
5:A:574:ASN:OD1	5:A:574:ASN:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:578:ARG:O	5:A:593:SER:OG	2.27	0.48
5:A:580:PRO:HB3	5:A:727:ILE:HG21	1.94	0.48
5:A:684:PHE:HB2	20:A:1812:CLA:HAA1	1.95	0.48
20:A:1764:CLA:HAA2	20:A:1783:CLA:HED3	1.95	0.48
20:A:1782:CLA:HBD	20:A:1782:CLA:CBA	2.43	0.48
20:A:1788:CLA:H152	22:L:1169:BCR:H361	1.93	0.48
20:A:1811:CLA:HBB2	20:A:1812:CLA:HED1	1.95	0.48
21:A:7040:LMU:O6B	21:A:7040:LMU:O4'	2.29	0.48
6:B:22:TRP:HA	6:B:25:ILE:HD11	1.93	0.48
6:B:86:PRO:C	6:B:115:ASN:HB3	2.34	0.48
6:B:124:TRP:HZ2	6:B:135:LEU:HB2	1.78	0.48
6:B:247:THR:O	6:B:248:GLN:C	2.51	0.48
6:B:331:HIS:CE1	6:B:392:ILE:CG2	2.92	0.48
6:B:389:HIS:HE1	20:B:1759:CLA:NC	2.12	0.48
6:B:577:TYR:CE1	6:B:706:ARG:HB3	2.48	0.48
20:B:1747:CLA:H8	20:B:1765:CLA:HMA1	1.94	0.48
20:B:1762:CLA:HBB2	22:B:1778:BCR:C25	2.43	0.48
8:D:34:GLY:HA3	8:D:62:THR:HB	1.94	0.48
8:D:118:VAL:HG13	8:D:119:TYR:H	1.76	0.48
9:E:43:SER:CB	9:E:82:TYR:HE1	2.22	0.48
11:G:34:GLN:O	11:G:36:PRO:HD3	2.12	0.48
17:N:52:LEU:CB	17:N:53:ALA:CA	2.91	0.48
17:N:84:LYS:HZ2	17:N:84:LYS:HG2	1.43	0.48
19:U:2:FRU:O2	19:U:2:FRU:O4	2.30	0.48
20:1:1197:CLA:OBD	20:1:1197:CLA:CMD	2.54	0.48
3:3:94:ARG:CB	3:3:97:PHE:HE1	2.26	0.48
20:4:1199:CLA:CBA	20:F:1157:CLA:H42	2.43	0.48
5:A:53:TRP:CA	5:A:56:ASN:HB2	2.38	0.48
5:A:103:PHE:HD2	5:A:103:PHE:H	1.60	0.48
5:A:172:LEU:O	5:A:175:ALA:O	2.31	0.48
5:A:331:LEU:CD2	5:A:343:HIS:C	2.62	0.48
5:A:657:LEU:HD13	20:A:1811:CLA:H93	1.96	0.48
5:A:679:PHE:O	5:A:683:HIS:CB	2.62	0.48
6:B:272:ASP:C	6:B:274:ALA:H	2.17	0.48
6:B:502:ASN:OD1	6:B:511:THR:HG21	2.13	0.48
20:B:1785:CLA:H193	20:B:1785:CLA:H161	1.52	0.48
12:H:70:ALA:O	12:H:71:ASN:CB	2.61	0.48
15:K:4:GLY:HA2	15:K:7:THR:CB	2.42	0.48
16:L:11:ILE:O	16:L:12:GLN:HG3	2.13	0.48
19:U:2:FRU:O6	19:U:2:FRU:O3	2.30	0.48
5:A:40:PHE:N	5:A:44:ILE:CG2	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:151:GLN:HA	5:A:154:ARG:HG2	1.95	0.48
5:A:284:ARG:HB2	5:A:298:ASP:OD1	2.12	0.48
5:A:351:THR:CA	20:A:1780:CLA:H191	2.43	0.48
5:A:385:LEU:O	5:A:386:ALA:HB3	2.13	0.48
5:A:567:ARG:HH11	8:D:35:GLY:N	2.11	0.48
5:A:618:TRP:CZ2	5:A:655:ASP:HB3	2.48	0.48
5:A:693:LEU:HD23	5:A:734:GLY:HA3	1.96	0.48
5:A:697:ARG:NH1	5:A:724:ALA:HB3	2.27	0.48
20:A:1768:CLA:C4D	20:A:1769:CLA:HMC3	2.43	0.48
20:A:1788:CLA:CBC	20:A:1793:CLA:CBC	2.91	0.48
6:B:110:LEU:CD1	6:B:111:GLY:H	2.19	0.48
6:B:396:ARG:HH11	20:B:1759:CLA:HED2	1.79	0.48
6:B:447:GLY:O	6:B:449:PRO:CD	2.62	0.48
7:C:28:MET:HA	7:C:38:GLN:HB2	1.95	0.48
14:J:21:SER:O	14:J:22:LEU:C	2.52	0.48
17:N:83:TRP:O	17:N:83:TRP:CE3	2.64	0.48
19:M:1:GLC:H2	19:M:2:FRU:O5	2.13	0.48
19:Q:1:GLC:O4	19:Q:2:FRU:O2	2.29	0.48
19:W:1:GLC:O2	19:W:2:FRU:O5	2.29	0.48
2:2:57:LEU:O	2:2:60:ALA:HB3	2.13	0.48
3:3:83:LEU:C	20:A:1798:CLA:H43	2.32	0.48
4:4:118:ASP:H	4:4:119:PRO:HD2	1.77	0.48
5:A:73:GLU:HA	5:A:76:ARG:HB2	1.95	0.48
5:A:159:THR:O	5:A:163:GLN:OE1	2.31	0.48
5:A:258:LEU:HG	5:A:280:PHE:CD1	2.48	0.48
5:A:312:ILE:O	5:A:313:ALA:CB	2.61	0.48
5:A:312:ILE:O	5:A:313:ALA:HB2	2.13	0.48
5:A:330:ILE:O	5:A:330:ILE:CG2	2.61	0.48
5:A:430:ASP:HA	5:A:434:ARG:HH21	1.78	0.48
5:A:630:ASP:O	5:A:632:GLY:N	2.46	0.48
21:A:7030:LMU:C2'	21:A:7030:LMU:H6E	2.37	0.48
6:B:21:ILE:N	6:B:21:ILE:HD12	2.29	0.48
6:B:36:ASP:O	6:B:41:ARG:CZ	2.62	0.48
6:B:58:PHE:CE2	6:B:145:LEU:HD12	2.47	0.48
6:B:124:TRP:CE2	6:B:129:LEU:HD22	2.48	0.48
6:B:180:SER:CB	6:B:288:GLY:HA3	2.41	0.48
6:B:238:SER:OG	6:B:239:SER:N	2.46	0.48
6:B:348:VAL:HG21	20:B:1758:CLA:HHD	1.94	0.48
6:B:462:TRP:HZ3	20:B:1764:CLA:HBC1	1.77	0.48
6:B:690:LEU:HD21	16:L:129:GLN:HA	1.95	0.48
22:B:1780:BCR:H331	22:B:1780:BCR:C8	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:22:LEU:CD1	10:F:22:LEU:N	2.32	0.48
10:F:23:LYS:O	10:F:24:LYS:CE	2.61	0.48
16:L:9:GLN:HG3	16:L:10:VAL:H	1.79	0.48
17:N:61:LEU:O	17:N:66:ASP:OD1	2.30	0.48
1:1:45:ILE:CD1	20:1:1195:CLA:CMD	2.91	0.48
20:1:1188:CLA:HMA2	20:1:1188:CLA:HBA1	1.96	0.48
20:3:1218:CLA:CHD	20:3:1218:CLA:CBC	2.75	0.48
5:A:185:HIS:O	5:A:187:HIS:N	2.47	0.48
5:A:308:ILE:HG13	20:A:1772:CLA:HBB1	1.95	0.48
5:A:499:ALA:N	5:A:500:PRO:CD	2.76	0.48
5:A:665:ILE:C	5:A:665:ILE:CD1	2.82	0.48
5:A:705:GLU:O	5:A:708:VAL:N	2.46	0.48
20:A:1783:CLA:C10	22:A:1807:BCR:C37	2.87	0.48
22:A:1807:BCR:H17C	20:A:1812:CLA:C17	2.44	0.48
21:A:7013:LMU:H22	21:A:7013:LMU:O5'	2.13	0.48
6:B:390:GLY:CA	22:B:1777:BCR:HC22	2.43	0.48
6:B:464:GLN:CG	6:B:469:LYS:HD3	2.43	0.48
6:B:503:GLU:CB	6:B:507:SER:HB2	2.42	0.48
20:B:1737:CLA:HAC1	20:B:1759:CLA:HMA1	1.94	0.48
20:B:1741:CLA:HBD	20:B:1741:CLA:C1	2.43	0.48
20:B:1751:CLA:HMD2	22:B:1774:BCR:C32	2.43	0.48
22:B:1779:BCR:C33	20:F:1156:CLA:HMA1	2.43	0.48
8:D:96:ILE:O	8:D:97:LYS:HB2	2.13	0.48
10:F:19:LYS:O	10:F:23:LYS:HB2	2.13	0.48
11:G:19:GLY:N	11:G:21:PHE:H	2.11	0.48
11:G:44:PHE:C	11:G:46:ALA:HB2	2.34	0.48
11:G:57:LEU:O	11:G:61:ASN:OD1	2.31	0.48
17:N:61:LEU:HG	17:N:64:ASP:HB2	1.95	0.48
19:O:2:FRU:O1	19:O:2:FRU:O6	2.30	0.48
5:A:127:VAL:CG2	20:A:1765:CLA:HBB2	2.44	0.48
5:A:159:THR:O	5:A:160:SER:CB	2.62	0.48
5:A:169:ILE:O	5:A:173:VAL:HG13	2.14	0.48
5:A:185:HIS:O	5:A:188:LYS:HG3	2.14	0.48
5:A:229:ILE:HG12	5:A:243:PRO:CB	2.42	0.48
5:A:679:PHE:O	5:A:679:PHE:CD2	2.67	0.48
21:A:7013:LMU:H42	21:A:7013:LMU:H11	1.54	0.48
21:A:7042:LMU:H91	21:A:7042:LMU:H121	1.49	0.48
6:B:178:HIS:C	6:B:180:SER:N	2.65	0.48
6:B:309:ILE:HD11	6:B:313:GLY:H	1.79	0.48
6:B:479:SER:C	6:B:481:THR:H	2.15	0.48
6:B:577:TYR:CD1	6:B:706:ARG:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:672:GLN:CA	6:B:672:GLN:NE2	2.59	0.48
7:C:17:CYS:SG	7:C:18:VAL:N	2.87	0.48
10:F:113:LYS:NZ	10:F:115:THR:HG21	2.28	0.48
12:H:23:VAL:O	12:H:23:VAL:HG13	2.13	0.48
2:2:56:MET:HA	2:2:59:ALA:HB3	1.96	0.48
20:4:1201:CLA:CMA	20:4:1201:CLA:O2A	2.61	0.48
5:A:53:TRP:HA	5:A:56:ASN:CG	2.34	0.48
5:A:229:ILE:O	5:A:229:ILE:HG22	2.14	0.48
5:A:529:LEU:H	5:A:529:LEU:HD12	1.79	0.48
20:A:1762:CLA:H51	20:A:1785:CLA:NC	2.29	0.48
20:A:1774:CLA:H203	20:A:1782:CLA:HAA1	1.95	0.48
20:A:1791:CLA:CMA	20:A:1797:CLA:CBB	2.92	0.48
20:A:1796:CLA:H11	20:A:1796:CLA:C4D	2.44	0.48
6:B:290:MET:HB2	20:B:1751:CLA:HMC3	1.96	0.48
6:B:353:TYR:CD1	6:B:594:TRP:HZ3	2.30	0.48
6:B:486:LEU:HD13	20:B:1765:CLA:HMD3	1.96	0.48
6:B:587:ILE:HA	6:B:587:ILE:HD13	1.68	0.48
20:B:1740:CLA:H192	22:B:1781:BCR:H19C	1.96	0.48
9:E:69:PHE:CG	9:E:70:ALA:N	2.81	0.48
11:G:43:HIS:C	11:G:45:GLU:CB	2.61	0.48
18:R:38:UNK:O	18:R:39:UNK:C	2.62	0.48
20:3:1219:CLA:O1D	20:3:1219:CLA:OBD	2.30	0.48
5:A:364:MET:CE	20:A:1782:CLA:H2	2.44	0.48
20:A:1762:CLA:HED2	20:A:1762:CLA:H12	1.94	0.48
20:A:1783:CLA:H162	20:A:1783:CLA:H193	1.75	0.48
20:A:1788:CLA:HBC1	20:A:1793:CLA:HBC2	1.95	0.48
21:A:7037:LMU:O6B	21:A:7037:LMU:O4'	2.29	0.48
6:B:628:SER:O	6:B:629:SER:C	2.51	0.48
20:B:1744:CLA:H71	20:B:1744:CLA:H111	1.41	0.48
7:C:30:PRO:HB3	7:C:37:LYS:O	2.14	0.48
8:D:132:LEU:O	8:D:135:ARG:O	2.32	0.48
9:E:38:ILE:HB	9:E:46:PHE:O	2.14	0.48
9:E:41:ARG:CD	9:E:46:PHE:CZ	2.97	0.48
12:H:75:ASP:CB	12:H:77:LEU:HG	2.43	0.48
14:J:36:ALA:O	14:J:37:LEU:HB2	2.13	0.48
16:L:57:GLY:HA3	16:L:146:GLY:HA3	1.96	0.48
19:Q:2:FRU:O3	19:Q:2:FRU:O1	2.30	0.48
3:3:195:LEU:HA	3:3:198:PHE:HB2	1.96	0.47
20:3:1218:CLA:H121	20:3:1218:CLA:C9	2.28	0.47
20:4:4014:CLA:H2A	20:4:4014:CLA:O1A	2.14	0.47
5:A:182:GLY:C	20:A:1767:CLA:HAC1	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:338:PHE:O	5:A:339:THR:O	2.31	0.47
5:A:502:THR:C	5:A:504:ALA:N	2.68	0.47
5:A:539:PHE:HE2	5:A:543:HIS:CE1	2.31	0.47
5:A:558:LYS:HZ2	6:B:674:LEU:CB	2.24	0.47
5:A:606:TYR:OH	20:A:1811:CLA:HED3	2.14	0.47
5:A:703:LEU:HD13	5:A:707:ILE:HD11	1.96	0.47
22:A:1804:BCR:C8	22:A:1804:BCR:H311	2.44	0.47
20:A:1816:CLA:HED1	20:A:1816:CLA:O1A	2.03	0.47
21:A:7016:LMU:O6'	21:A:7016:LMU:H1'	1.90	0.47
21:A:7031:LMU:H4'	21:A:7031:LMU:H3B	1.95	0.47
6:B:335:GLY:HA2	6:B:338:LEU:HB2	1.96	0.47
6:B:339:ALA:O	6:B:340:SER:CB	2.62	0.47
6:B:600:THR:O	6:B:605:ASN:O	2.32	0.47
6:B:693:TRP:CD1	20:B:1770:CLA:HMD3	2.48	0.47
10:F:22:LEU:HB3	10:F:25:LEU:HD13	1.96	0.47
12:H:20:GLN:HB2	12:H:22:ASP:CB	2.39	0.47
16:L:36:TYR:O	16:L:37:LEU:CB	2.59	0.47
2:2:103:GLY:CA	20:2:1222:CLA:CBB	2.89	0.47
20:2:1213:CLA:HAA2	20:2:1218:CLA:HED2	1.94	0.47
3:3:181:LEU:HD13	3:3:184:VAL:CG2	2.44	0.47
20:3:1215:CLA:HHC	20:3:1218:CLA:H11	1.95	0.47
20:3:1218:CLA:O2D	20:3:1218:CLA:OBD	2.31	0.47
4:4:105:ARG:O	4:4:109:ILE:HG13	2.14	0.47
5:A:23:ASP:CB	5:A:24:ARG:CZ	2.80	0.47
5:A:650:ASN:O	5:A:654:ARG:N	2.36	0.47
20:A:1762:CLA:HAA2	20:A:1762:CLA:HBD	1.96	0.47
20:A:1781:CLA:HBB2	20:A:1794:CLA:C3A	2.43	0.47
22:A:1807:BCR:C35	20:A:1812:CLA:H41	2.44	0.47
21:A:7039:LMU:O2'	21:A:7039:LMU:O1B	2.29	0.47
6:B:81:PRO:HG2	6:B:360:PHE:CE1	2.49	0.47
6:B:292:ARG:CZ	6:B:297:ILE:H	2.27	0.47
6:B:414:HIS:NE2	20:B:1760:CLA:NA	2.63	0.47
20:B:1742:CLA:H61	20:B:1742:CLA:C1	2.43	0.47
22:B:1781:BCR:H342	20:H:1079:CLA:HHD	1.95	0.47
10:F:43:LYS:N	10:F:43:LYS:HE3	2.29	0.47
11:G:20:ARG:NH2	11:G:61:ASN:CA	2.77	0.47
11:G:80:ILE:HD12	11:G:80:ILE:O	2.14	0.47
3:3:83:LEU:HD13	20:3:1216:CLA:C3B	2.44	0.47
21:3:7005:LMU:H101	21:3:7005:LMU:H62	1.96	0.47
5:A:197:GLN:NE2	5:A:351:THR:O	2.47	0.47
5:A:347:TYR:HE1	5:A:417:PHE:HZ	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:680:LEU:CG	6:B:617:MET:HB2	2.44	0.47
20:A:1774:CLA:HBB2	20:A:1774:CLA:H8	1.97	0.47
6:B:96:PHE:HZ	6:B:104:PHE:CE2	2.32	0.47
6:B:427:LEU:C	20:B:1762:CLA:HED2	2.35	0.47
20:B:1735:CLA:HBB1	20:B:1762:CLA:H43	1.96	0.47
20:B:1738:CLA:O1D	20:B:1738:CLA:C2A	2.55	0.47
20:B:1755:CLA:O1A	20:B:1769:CLA:HAA1	2.15	0.47
20:B:1766:CLA:HBA2	20:B:1766:CLA:H3A	1.70	0.47
20:B:1770:CLA:H91	22:B:1781:BCR:H333	1.95	0.47
7:C:31:TRP:CD1	7:C:31:TRP:C	2.87	0.47
9:E:43:SER:HB2	9:E:82:TYR:CE1	2.36	0.47
10:F:123:VAL:O	10:F:126:ALA:N	2.47	0.47
11:G:80:ILE:O	11:G:81:VAL:O	2.31	0.47
16:L:23:LEU:O	16:L:25:THR:N	2.47	0.47
17:N:70:GLU:HB3	17:N:72:LYS:HA	1.94	0.47
19:O:1:GLC:O5	19:O:2:FRU:O5	2.30	0.47
19:W:1:GLC:O5	19:W:2:FRU:O5	2.30	0.47
1:1:33:PRO:HG2	1:1:137:PRO:HG3	1.96	0.47
20:1:1197:CLA:C4	20:1:1198:CLA:O1D	2.62	0.47
2:2:181:HIS:CD2	20:2:1214:CLA:ND	2.82	0.47
4:4:36:ASN:HB2	4:4:39:TRP:CD2	2.48	0.47
5:A:337:PRO:HD2	20:A:1799:CLA:HHC	1.95	0.47
5:A:733:VAL:HG11	20:A:1796:CLA:C3D	2.43	0.47
5:A:747:TRP:HB2	20:A:1783:CLA:CBB	2.45	0.47
20:A:1796:CLA:H192	14:J:19:PHE:HD2	1.79	0.47
6:B:167:TRP:CG	6:B:167:TRP:O	2.67	0.47
6:B:459:PHE:CD2	20:B:1768:CLA:C3D	2.97	0.47
6:B:653:GLY:HA3	6:B:720:THR:OG1	2.13	0.47
20:B:1739:CLA:C9	20:B:1739:CLA:CBB	2.68	0.47
9:E:37:LYS:N	9:E:49:VAL:HG13	2.29	0.47
10:F:152:ASN:HD22	10:F:152:ASN:N	2.12	0.47
2:2:98:GLU:CD	20:2:1223:CLA:CHD	2.83	0.47
3:3:59:ILE:HB	3:3:63:ARG:HH21	1.79	0.47
4:4:58:MET:O	4:4:60:LEU:HD23	2.14	0.47
4:4:94:GLU:OE2	20:4:1208:CLA:NB	2.47	0.47
5:A:197:GLN:HE22	5:A:351:THR:CB	2.22	0.47
5:A:434:ARG:O	5:A:437:ARG:N	2.47	0.47
5:A:452:PHE:O	5:A:456:HIS:ND1	2.28	0.47
5:A:599:PHE:CZ	5:A:731:ARG:HB3	2.47	0.47
20:A:1761:CLA:H161	20:A:1761:CLA:H141	1.64	0.47
20:A:1800:CLA:HMC3	20:B:1770:CLA:ND	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7033:LMU:O6B	21:A:7033:LMU:O3'	2.29	0.47
6:B:31:PHE:O	6:B:37:ILE:HG21	2.13	0.47
6:B:125:TYR:CE1	6:B:130:ARG:NH1	2.83	0.47
6:B:361:ILE:O	6:B:361:ILE:HG22	2.14	0.47
6:B:475:ASP:HA	6:B:480:SER:CA	2.45	0.47
6:B:697:PRO:HB3	20:B:1770:CLA:CBC	2.41	0.47
20:B:1740:CLA:HED1	20:I:1031:CLA:HMA2	1.96	0.47
20:B:1764:CLA:O1D	20:B:1764:CLA:H2A	2.15	0.47
20:B:1764:CLA:CMD	20:B:1765:CLA:C1C	2.92	0.47
22:B:1778:BCR:C33	22:B:1778:BCR:C8	2.91	0.47
16:L:65:VAL:C	16:L:67:PRO:CD	2.83	0.47
16:L:95:LEU:O	16:L:99:LEU:HD13	2.13	0.47
17:N:58:VAL:CG1	17:N:59:PRO:HD3	2.44	0.47
19:M:1:GLC:O2	19:M:2:FRU:O5	2.30	0.47
1:1:39:TYR:HB2	20:1:1196:CLA:OBD	2.12	0.47
2:2:161:THR:HG22	2:2:165:LYS:HD2	1.96	0.47
21:2:7006:LMU:H3'	21:2:7006:LMU:H5B	1.95	0.47
21:3:7005:LMU:O3'	21:3:7005:LMU:H1B	2.12	0.47
5:A:70:ASP:O	5:A:71:LEU:O	2.33	0.47
5:A:420:ARG:HB3	5:A:420:ARG:CZ	2.45	0.47
5:A:553:VAL:CG2	22:A:1806:BCR:H401	2.43	0.47
21:A:7020:LMU:O6'	21:A:7020:LMU:O2B	2.32	0.47
6:B:292:ARG:NH1	6:B:293:THR:H	2.13	0.47
6:B:560:ASP:CB	7:C:66:ARG:NE	2.61	0.47
6:B:631:LEU:HG	6:B:632:ILE:HG23	1.97	0.47
20:B:1785:CLA:H3A	20:B:1785:CLA:HBA2	1.40	0.47
7:C:6:LYS:O	7:C:63:LEU:HD21	2.14	0.47
7:C:63:LEU:CG	7:C:64:SER:N	2.51	0.47
9:E:83:ALA:O	9:E:85:ASP:N	2.47	0.47
11:G:30:ASN:ND2	11:G:31:MET:O	2.48	0.47
16:L:46:ALA:CB	16:L:52:ARG:NH2	2.77	0.47
17:N:68:GLU:O	17:N:69:CYS:HB2	2.13	0.47
17:N:81:VAL:C	17:N:83:TRP:N	2.68	0.47
18:R:46:UNK:CB	18:R:47:UNK:CA	2.92	0.47
2:2:98:GLU:OE1	20:2:1223:CLA:CHD	2.63	0.47
3:3:166:PRO:HB2	3:3:167:LEU:H	1.54	0.47
20:3:3011:CLA:H93	20:3:3011:CLA:H52	1.97	0.47
4:4:91:PHE:O	4:4:94:GLU:HB3	2.14	0.47
4:4:95:PHE:HZ	20:4:1208:CLA:C4C	2.25	0.47
4:4:118:ASP:OD2	4:4:123:GLN:HB2	2.15	0.47
5:A:78:VAL:O	5:A:82:HIS:CD2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:81:ALA:CA	20:A:1760:CLA:HMA1	2.38	0.47
5:A:210:LEU:CD1	20:A:1769:CLA:HHB	2.45	0.47
5:A:302:HIS:CD2	20:A:1773:CLA:NB	2.82	0.47
5:A:302:HIS:HD2	20:A:1773:CLA:NB	2.11	0.47
5:A:377:TYR:HD1	5:A:616:PHE:HE1	1.59	0.47
5:A:392:GLN:CG	5:A:392:GLN:O	2.63	0.47
5:A:409:GLY:O	5:A:411:ALA:N	2.47	0.47
5:A:449:VAL:CG2	20:A:1794:CLA:HMC3	2.44	0.47
5:A:457:SER:OG	5:A:544:ILE:HA	2.15	0.47
5:A:508:THR:O	5:A:509:ALA:HB3	2.14	0.47
5:A:553:VAL:N	5:A:556:LEU:HD12	2.26	0.47
5:A:568:LEU:O	5:A:586:ARG:HD3	2.14	0.47
5:A:603:PHE:CE1	5:A:735:VAL:HA	2.50	0.47
5:A:669:GLY:H	6:B:445:ALA:CA	2.21	0.47
20:A:1782:CLA:OBD	20:A:1782:CLA:O2D	2.32	0.47
20:A:1786:CLA:HMB2	20:A:1787:CLA:C3D	2.45	0.47
20:A:1813:CLA:H2	20:A:1813:CLA:CMA	2.44	0.47
21:A:7027:LMU:H31	21:A:7027:LMU:H62	1.62	0.47
21:A:7033:LMU:H2B	21:A:7033:LMU:H6E	1.96	0.47
21:A:7039:LMU:H6'2	21:A:7039:LMU:H1B	1.40	0.47
21:A:7041:LMU:H82	21:A:7041:LMU:H111	1.48	0.47
6:B:415:LYS:HG2	6:B:416:GLU:OE2	2.13	0.47
6:B:448:THR:O	6:B:448:THR:OG1	2.31	0.47
6:B:535:VAL:CG1	6:B:536:LYS:N	2.76	0.47
6:B:720:THR:O	6:B:724:PHE:N	2.48	0.47
6:B:732:LYS:CD	6:B:734:GLY:CA	2.93	0.47
20:B:1758:CLA:H62	22:B:1776:BCR:HC7	1.96	0.47
22:B:1776:BCR:H15C	22:B:1776:BCR:H351	1.80	0.47
7:C:12:ILE:N	7:C:12:ILE:CD1	2.73	0.47
7:C:14:CYS:SG	7:C:17:CYS:SG	3.13	0.47
7:C:25:VAL:HA	7:C:43:PRO:CD	2.45	0.47
8:D:36:LEU:HB2	16:L:19:PHE:O	2.14	0.47
10:F:136:TRP:HB2	10:F:139:ALA:CB	2.45	0.47
11:G:28:ARG:HG2	11:G:29:GLU:HB2	1.96	0.47
11:G:64:VAL:HG13	11:G:67:ASN:HB2	1.94	0.47
11:G:79:HIS:NE2	11:G:82:ALA:HB2	2.30	0.47
12:H:19:GLY:O	12:H:20:GLN:HB2	2.15	0.47
13:I:7:LEU:HD12	22:I:1032:BCR:H333	0.83	0.47
13:I:9:VAL:H	13:I:10:PRO:CD	2.27	0.47
13:I:12:VAL:HG21	20:I:1031:CLA:CGA	2.45	0.47
16:L:5:LYS:HE2	16:L:5:LYS:CA	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:63:LEU:O	16:L:65:VAL:N	2.48	0.47
16:L:99:LEU:O	16:L:136:TRP:HZ3	1.98	0.47
16:L:101:MET:SD	16:L:104:ILE:HG12	2.55	0.47
20:L:1166:CLA:HHD	20:L:1166:CLA:HBC2	1.96	0.47
17:N:47:THR:O	17:N:48:GLY:C	2.52	0.47
1:1:38:ARG:HA	1:1:41:GLU:HG3	1.97	0.47
2:2:189:ILE:O	2:2:190:ASP:CB	2.63	0.47
20:3:1218:CLA:O1D	20:3:1218:CLA:HAA2	2.15	0.47
4:4:124:TYR:O	4:4:125:SER:HB2	2.15	0.47
20:4:1200:CLA:HAA2	20:4:1200:CLA:HBD	1.97	0.47
5:A:41:SER:O	5:A:44:ILE:CA	2.61	0.47
5:A:132:LEU:HD13	5:A:671:SER:O	2.15	0.47
5:A:144:GLN:C	5:A:145:ILE:HG12	2.36	0.47
5:A:248:PHE:HD2	5:A:248:PHE:N	1.93	0.47
5:A:467:MET:HE1	5:A:475:ASP:O	2.15	0.47
5:A:539:PHE:C	5:A:539:PHE:CD2	2.88	0.47
5:A:605:MET:O	5:A:608:SER:N	2.48	0.47
5:A:628:ILE:HG13	5:A:632:GLY:CA	2.42	0.47
20:A:1772:CLA:H93	20:A:1772:CLA:H61	1.58	0.47
20:A:1787:CLA:HBB1	20:A:1793:CLA:C19	2.39	0.47
20:A:1787:CLA:C9	20:A:1801:CLA:H2	2.44	0.47
6:B:182:LEU:HD13	20:B:1743:CLA:HHB	1.97	0.47
6:B:183:PHE:HB3	6:B:284:PHE:HD2	1.80	0.47
6:B:269:TRP:CD1	6:B:497:TRP:HH2	2.33	0.47
6:B:289:LEU:O	20:B:1751:CLA:HMC1	2.15	0.47
6:B:311:PRO:HD3	20:B:1772:CLA:C3C	2.44	0.47
6:B:459:PHE:CD2	20:B:1768:CLA:C2D	2.98	0.47
6:B:471:THR:HB	6:B:472:TYR:CE1	2.50	0.47
6:B:478:LEU:O	6:B:479:SER:HB3	2.15	0.47
20:B:1752:CLA:HBA2	20:B:1752:CLA:H3A	1.46	0.47
20:B:1753:CLA:O1D	20:B:1753:CLA:OBD	2.31	0.47
7:C:66:ARG:NH2	7:C:66:ARG:CG	2.69	0.47
8:D:58:PHE:HE2	8:D:60:MET:HA	1.80	0.47
8:D:89:ARG:O	8:D:92:SER:N	2.48	0.47
8:D:138:GLY:O	8:D:140:ASN:N	2.48	0.47
10:F:116:GLN:C	10:F:118:GLU:N	2.58	0.47
16:L:123:ARG:HB3	16:L:126:GLN:HG3	1.96	0.47
17:N:6:TYR:HD2	17:N:6:TYR:HA	1.68	0.47
17:N:70:GLU:CA	17:N:72:LYS:H	2.26	0.47
3:3:127:ARG:C	3:3:129:PHE:H	2.18	0.47
3:3:171:LYS:HE3	3:3:171:LYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:189:LEU:C	3:3:191:MET:H	2.18	0.47
4:4:76:TYR:HB2	20:4:1204:CLA:CGD	2.45	0.47
5:A:202:MET:HB3	20:A:1780:CLA:HMD3	1.97	0.47
5:A:241:GLU:OE1	5:A:241:GLU:O	2.32	0.47
20:A:1781:CLA:H11	20:A:1794:CLA:CAD	2.45	0.47
21:A:7031:LMU:H21	21:A:7031:LMU:H52	1.70	0.47
6:B:30:ASP:O	6:B:34:HIS:HD2	1.98	0.47
6:B:63:GLY:HA2	6:B:66:PHE:HB3	1.97	0.47
6:B:211:ASN:ND2	6:B:214:ASP:OD1	2.48	0.47
6:B:431:PHE:HE2	20:B:1762:CLA:CED	2.28	0.47
6:B:454:LEU:HD12	6:B:454:LEU:H	1.80	0.47
6:B:647:ALA:O	6:B:651:LEU:HD22	2.15	0.47
6:B:724:PHE:CE2	20:B:1785:CLA:CMD	2.98	0.47
20:B:1749:CLA:H61	20:B:1749:CLA:H41	1.66	0.47
20:B:1756:CLA:H122	22:B:1777:BCR:C12	2.45	0.47
20:B:1767:CLA:HMC1	20:B:1767:CLA:CBC	2.24	0.47
20:B:1785:CLA:HMB3	20:B:1786:CLA:CAD	2.44	0.47
7:C:29:ILE:HG23	8:D:126:GLY:CA	2.39	0.47
7:C:70:TRP:O	7:C:71:HIS:C	2.53	0.47
7:C:77:MET:C	7:C:79:LEU:H	2.12	0.47
16:L:55:GLU:HG3	20:L:1166:CLA:C1A	2.45	0.47
18:R:34:UNK:CB	18:R:35:UNK:CA	2.80	0.47
1:1:135:LYS:HB3	1:1:136:ASP:H	1.54	0.47
20:1:1190:CLA:CMC	20:1:1196:CLA:CAC	2.92	0.47
20:1:1200:CLA:HMC1	20:4:1198:CLA:CMB	2.44	0.47
3:3:141:GLN:O	3:3:142:TYR:HB2	2.14	0.47
3:3:164:PHE:O	3:3:165:ASN:C	2.53	0.47
3:3:197:TYR:OH	20:3:1212:CLA:CHC	2.63	0.47
5:A:298:ASP:O	5:A:300:ALA:N	2.48	0.47
5:A:417:PHE:CD1	5:A:417:PHE:C	2.89	0.47
5:A:581:CYS:HB3	5:A:590:CYS:O	2.14	0.47
5:A:629:ASN:CG	5:A:630:ASP:N	2.68	0.47
20:A:1774:CLA:H71	20:A:1774:CLA:CAB	2.45	0.47
20:A:1795:CLA:OBD	10:F:105:LEU:HD11	2.15	0.47
6:B:9:SER:HA	6:B:35:ASP:OD1	2.15	0.47
6:B:135:LEU:O	6:B:135:LEU:HD12	2.15	0.47
6:B:230:TRP:O	6:B:231:ASN:C	2.52	0.47
6:B:309:ILE:HG22	6:B:319:HIS:CD2	2.50	0.47
6:B:580:VAL:HG11	6:B:710:LEU:HD11	1.97	0.47
20:B:1753:CLA:C10	20:B:1753:CLA:C15	2.55	0.47
10:F:95:GLY:O	10:F:99:TRP:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:137:PRO:O	10:F:139:ALA:N	2.47	0.47
12:H:76:VAL:HG22	12:H:76:VAL:O	2.15	0.47
14:J:15:SER:HA	14:J:18:TRP:HB3	1.97	0.47
1:1:40:LYS:O	1:1:44:LEU:HG	2.15	0.46
3:3:58:GLU:HG2	20:3:1217:CLA:C1D	2.45	0.46
3:3:63:ARG:NH1	3:3:189:LEU:H	2.13	0.46
5:A:99:HIS:C	5:A:101:ALA:H	2.17	0.46
5:A:109:TRP:HA	5:A:116:ILE:CG1	2.44	0.46
5:A:185:HIS:O	5:A:186:TYR:C	2.53	0.46
5:A:354:TRP:O	5:A:357:GLN:N	2.48	0.46
5:A:603:PHE:CZ	5:A:693:LEU:CD2	2.98	0.46
5:A:613:ILE:HG22	5:A:614:PHE:N	2.29	0.46
5:A:636:HIS:O	5:A:637:ILE:C	2.53	0.46
5:A:660:GLN:HE21	5:A:660:GLN:H	1.62	0.46
20:A:1761:CLA:HMB3	20:A:1762:CLA:HAA1	1.97	0.46
6:B:293:THR:C	6:B:294:ASN:CG	2.66	0.46
6:B:350:GLN:O	6:B:353:TYR:CD1	2.69	0.46
6:B:377:TYR:O	6:B:378:ILE:CB	2.62	0.46
6:B:387:PHE:HE2	20:B:1755:CLA:HHC	1.79	0.46
6:B:552:ASP:OD1	6:B:553:PHE:HD2	1.98	0.46
6:B:556:SER:CA	6:B:558:PRO:HD2	2.45	0.46
20:B:1758:CLA:H101	22:B:1776:BCR:C34	2.43	0.46
22:B:1779:BCR:H371	22:B:1779:BCR:H24C	1.52	0.46
7:C:81:TYR:N	7:C:81:TYR:CD1	2.83	0.46
8:D:48:ILE:CG1	8:D:49:THR:N	2.77	0.46
9:E:88:GLU:O	9:E:89:GLU:C	2.53	0.46
11:G:37:GLU:O	11:G:38:GLN:C	2.52	0.46
15:K:52:PRO:O	15:K:56:THR:HG22	2.15	0.46
15:K:69:ILE:HG12	15:K:72:VAL:HG12	1.96	0.46
16:L:40:LEU:HD12	16:L:40:LEU:H	1.80	0.46
16:L:56:VAL:HG13	20:L:1167:CLA:HED3	1.94	0.46
20:1:1188:CLA:HMA2	20:1:1188:CLA:CGA	2.45	0.46
3:3:56:TYR:HD1	3:3:185:LYS:CE	2.29	0.46
5:A:83:PHE:CE2	5:A:185:HIS:CD2	3.03	0.46
5:A:218:TRP:CZ3	20:A:1770:CLA:HMB3	2.50	0.46
5:A:223:VAL:HG12	5:A:224:HIS:H	1.79	0.46
5:A:265:GLY:HA3	5:A:272:LEU:HD21	1.97	0.46
5:A:281:LEU:CD2	20:A:1772:CLA:CMA	2.94	0.46
5:A:616:PHE:O	5:A:620:MET:HB2	2.15	0.46
5:A:733:VAL:HG12	5:A:737:HIS:CE1	2.50	0.46
20:A:1781:CLA:H93	22:A:1806:BCR:C10	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1782:CLA:H111	20:A:1782:CLA:H151	1.56	0.46
20:A:1791:CLA:HMA2	20:A:1797:CLA:CBB	2.45	0.46
20:A:1796:CLA:HBD	20:A:1796:CLA:HAA1	1.97	0.46
6:B:127:ILE:O	6:B:128:GLY:C	2.53	0.46
6:B:154:TRP:O	6:B:155:LEU:C	2.53	0.46
6:B:292:ARG:NH2	20:B:1750:CLA:HED1	2.31	0.46
6:B:594:TRP:CD1	6:B:595:HIS:N	2.83	0.46
6:B:596:TRP:HZ3	6:B:613:SER:CB	2.28	0.46
6:B:732:LYS:C	6:B:733:PHE:O	2.53	0.46
22:B:1779:BCR:HC8	22:B:1779:BCR:H311	1.97	0.46
24:B:1783:LMG:H111	24:B:1783:LMG:O8	2.15	0.46
10:F:34:ASP:O	10:F:34:ASP:OD2	2.33	0.46
10:F:41:ALA:O	10:F:44:ALA:O	2.33	0.46
17:N:28:ASN:CA	17:N:30:ALA:H	2.28	0.46
17:N:59:PRO:CA	17:N:66:ASP:OD1	2.63	0.46
17:N:80:ASN:C	17:N:80:ASN:OD1	2.54	0.46
18:R:6:UNK:CB	18:R:10:UNK:CB	2.92	0.46
1:1:29:LEU:C	1:1:33:PRO:HD3	2.36	0.46
5:A:86:LEU:HD22	5:A:86:LEU:H	1.81	0.46
5:A:110:LEU:CD1	5:A:239:PRO:HG2	2.38	0.46
5:A:154:ARG:O	5:A:155:ALA:C	2.54	0.46
5:A:281:LEU:C	5:A:283:PHE:N	2.68	0.46
5:A:426:THR:HG23	5:A:428:TYR:OH	2.15	0.46
5:A:452:PHE:CD2	5:A:456:HIS:CE1	3.03	0.46
20:A:1776:CLA:HMC1	20:A:1776:CLA:HBC3	1.95	0.46
20:A:1776:CLA:H43	20:A:1779:CLA:C2	2.45	0.46
20:A:1776:CLA:HMC2	20:A:1782:CLA:H193	1.96	0.46
20:A:1778:CLA:HAA1	15:K:32:ARG:NE	2.30	0.46
20:A:1790:CLA:H3A	20:A:1790:CLA:HBA2	1.53	0.46
20:A:1815:CLA:CBC	20:A:1815:CLA:CMC	2.89	0.46
21:A:7016:LMU:O6'	21:A:7016:LMU:H31	2.13	0.46
21:A:7039:LMU:O3'	21:A:7039:LMU:O5'	2.29	0.46
6:B:164:SER:HB2	6:B:167:TRP:CE3	2.50	0.46
6:B:172:GLU:O	6:B:173:SER:C	2.54	0.46
6:B:176:ASN:ND2	6:B:293:THR:OG1	2.47	0.46
6:B:334:LEU:HA	20:B:1737:CLA:HMD3	1.97	0.46
6:B:596:TRP:CZ3	6:B:613:SER:CB	2.98	0.46
6:B:719:PHE:CZ	20:B:1757:CLA:H71	2.50	0.46
6:B:721:TYR:HA	6:B:724:PHE:HB3	1.96	0.46
20:B:1756:CLA:CED	20:B:1764:CLA:CBB	2.91	0.46
20:B:1764:CLA:H3A	20:B:1764:CLA:HBA2	1.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1767:CLA:O2D	20:B:1767:CLA:OBD	2.33	0.46
10:F:131:PHE:C	10:F:133:GLY:N	2.68	0.46
11:G:34:GLN:O	11:G:36:PRO:N	2.47	0.46
15:K:74:ILE:CG2	15:K:75:VAL:HG22	2.37	0.46
20:K:1085:CLA:HBC2	20:K:1085:CLA:CMC	2.41	0.46
17:N:53:ALA:O	17:N:54:LYS:CB	2.62	0.46
17:N:62:SER:OG	17:N:66:ASP:HB3	2.15	0.46
19:W:2:FRU:H62	19:W:2:FRU:H12	1.83	0.46
4:4:106:TRP:CG	20:4:1196:CLA:HED2	2.50	0.46
5:A:76:ARG:C	5:A:186:TYR:HD2	2.19	0.46
5:A:249:ILE:CG2	5:A:251:ASN:OD1	2.64	0.46
5:A:308:ILE:HG21	20:A:1772:CLA:HMC2	1.98	0.46
5:A:350:LEU:HA	5:A:350:LEU:HD23	1.51	0.46
5:A:361:ASN:ND2	5:A:361:ASN:C	2.68	0.46
5:A:385:LEU:O	5:A:386:ALA:HB2	2.13	0.46
5:A:458:PHE:C	5:A:458:PHE:CD1	2.89	0.46
5:A:740:LEU:HD13	20:A:1796:CLA:HMA1	1.98	0.46
21:A:7017:LMU:H1B	21:A:7017:LMU:H6'2	1.44	0.46
6:B:395:ILE:HG22	6:B:551:LYS:HG3	1.97	0.46
6:B:396:ARG:NH1	20:B:1759:CLA:HED2	2.30	0.46
6:B:442:VAL:O	6:B:446:PHE:HB2	2.16	0.46
6:B:454:LEU:HD22	10:F:70:HIS:CD2	2.50	0.46
22:B:1775:BCR:H15C	22:B:1775:BCR:H351	1.71	0.46
7:C:52:LYS:C	7:C:54:CYS:H	2.17	0.46
8:D:77:LEU:HA	8:D:77:LEU:HD23	1.66	0.46
10:F:80:TRP:CH2	20:F:1156:CLA:CAC	2.98	0.46
11:G:20:ARG:NH1	11:G:64:VAL:C	2.69	0.46
11:G:57:LEU:O	11:G:57:LEU:HD22	2.16	0.46
12:H:57:LEU:HD13	12:H:57:LEU:C	2.36	0.46
12:H:62:GLY:O	13:I:15:LEU:HD22	2.15	0.46
20:H:1079:CLA:HMB1	13:I:9:VAL:HG13	1.97	0.46
17:N:59:PRO:HG2	17:N:73:ASP:O	2.15	0.46
1:1:44:LEU:O	1:1:48:ARG:N	2.49	0.46
3:3:165:ASN:HD22	3:3:165:ASN:HA	1.59	0.46
5:A:131:ILE:HD13	6:B:447:GLY:HA3	1.97	0.46
5:A:531:PRO:O	5:A:532:ILE:HG23	2.15	0.46
5:A:550:HIS:C	5:A:552:THR:O	2.53	0.46
5:A:720:THR:O	5:A:720:THR:CG2	2.62	0.46
20:A:1816:CLA:CED	20:A:1816:CLA:CAA	2.92	0.46
21:A:7020:LMU:O6'	21:A:7020:LMU:O5B	2.30	0.46
21:A:7021:LMU:H1'	21:A:7021:LMU:C4	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:280:ILE:HD13	20:B:1748:CLA:HBB2	1.96	0.46
6:B:348:VAL:HG22	20:B:1758:CLA:HMD3	1.97	0.46
6:B:717:TYR:O	20:B:1785:CLA:HED3	2.15	0.46
9:E:60:LYS:CG	9:E:61:THR:N	2.72	0.46
12:H:66:THR:N	12:H:69:SER:HB3	2.29	0.46
20:K:1142:CLA:HBC3	20:K:1142:CLA:CHD	2.46	0.46
21:R:1056:LMU:H71	21:R:1056:LMU:H102	1.68	0.46
3:3:74:ALA:CB	20:3:1215:CLA:ND	2.78	0.46
5:A:205:HIS:ND1	20:A:1769:CLA:HMC2	2.30	0.46
5:A:207:LEU:CD1	20:A:1776:CLA:HBB2	2.46	0.46
5:A:208:ALA:HB2	5:A:314:GLY:CA	2.38	0.46
20:A:1762:CLA:H11	20:A:1785:CLA:O2A	2.16	0.46
20:A:1797:CLA:H143	20:A:1797:CLA:H111	1.73	0.46
21:A:7010:LMU:O3'	21:A:7010:LMU:C2B	2.64	0.46
21:A:7036:LMU:O5B	21:A:7036:LMU:C5'	2.62	0.46
6:B:22:TRP:CZ2	20:B:1770:CLA:HMB1	2.51	0.46
6:B:255:LEU:HA	6:B:271:THR:HB	1.98	0.46
6:B:256:THR:HG22	6:B:271:THR:OG1	2.16	0.46
20:B:1755:CLA:CAD	20:B:1767:CLA:CBB	2.91	0.46
11:G:16:LEU:HB2	11:G:17:PHE:CD2	2.51	0.46
11:G:30:ASN:ND2	11:G:34:GLN:H	2.14	0.46
11:G:50:ARG:HB2	11:G:51:ALA:HB2	1.96	0.46
20:H:1079:CLA:H41	16:L:87:ALA:HB1	1.98	0.46
20:K:1085:CLA:HBD	20:K:1085:CLA:HAA2	1.97	0.46
20:K:1142:CLA:HBD	20:K:1142:CLA:HAA2	1.96	0.46
16:L:108:LYS:HD3	16:L:132:SER:HB3	1.98	0.46
17:N:59:PRO:CB	17:N:75:TYR:CE1	2.96	0.46
18:R:1:UNK:O	18:R:2:UNK:O	2.34	0.46
2:2:68:LEU:HD21	20:2:1217:CLA:C17	2.42	0.46
3:3:84:ILE:O	3:3:84:ILE:HG23	2.16	0.46
5:A:218:TRP:HZ3	20:A:1770:CLA:HMB3	1.80	0.46
5:A:365:LEU:HD22	20:A:1761:CLA:HED3	1.91	0.46
5:A:462:ILE:HD13	20:B:1786:CLA:H93	1.97	0.46
20:A:1779:CLA:CBB	22:A:1805:BCR:H352	2.29	0.46
20:A:1787:CLA:C4	16:L:33:ILE:CG1	2.93	0.46
20:A:1796:CLA:H143	20:A:1796:CLA:H111	1.72	0.46
20:A:1797:CLA:HAA2	20:A:1797:CLA:HBD	1.96	0.46
6:B:399:ASN:O	6:B:399:ASN:OD1	2.34	0.46
6:B:544:SER:O	6:B:547:MET:C	2.54	0.46
20:B:1739:CLA:H162	20:B:1757:CLA:H192	1.97	0.46
20:B:1771:CLA:H2	23:B:1773:PQN:H251	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:1773:PQN:H143	22:B:1780:BCR:H322	1.97	0.46
20:B:1785:CLA:HMB3	20:B:1786:CLA:OBD	2.16	0.46
10:F:37:ALA:N	10:F:38:PRO:HD3	2.31	0.46
11:G:28:ARG:CG	11:G:29:GLU:CB	2.94	0.46
22:I:1032:BCR:H11C	22:I:1032:BCR:H341	1.72	0.46
16:L:126:GLN:N	16:L:127:PRO:CD	2.78	0.46
16:L:158:MET:CG	16:L:159:TYR:N	2.75	0.46
2:2:55:ALA:HB3	2:2:56:MET:HE2	1.96	0.46
3:3:56:TYR:HD1	3:3:185:LYS:NZ	2.12	0.46
3:3:162:PRO:HG2	3:3:164:PHE:CG	2.50	0.46
4:4:107:GLN:HA	20:4:1196:CLA:C2A	2.46	0.46
20:4:1204:CLA:HBA2	20:4:1204:CLA:CBD	2.46	0.46
5:A:265:GLY:HA2	5:A:272:LEU:CD2	2.46	0.46
5:A:401:TRP:CB	20:A:1783:CLA:HMC3	2.46	0.46
5:A:660:GLN:O	5:A:661:ALA:HB3	2.15	0.46
20:A:1781:CLA:CED	20:A:1782:CLA:HMD2	2.38	0.46
20:A:1783:CLA:H202	22:A:1808:BCR:C16	2.46	0.46
20:A:1795:CLA:C2C	20:B:1735:CLA:HBC2	2.45	0.46
20:A:1796:CLA:H62	20:A:1813:CLA:C17	2.46	0.46
6:B:31:PHE:HB2	6:B:42:LEU:HD12	1.97	0.46
6:B:322:LEU:O	6:B:326:ILE:HG22	2.16	0.46
6:B:527:LEU:CD1	6:B:586:THR:HG21	2.43	0.46
6:B:568:CYS:C	6:B:570:ILE:HG23	2.36	0.46
6:B:645:VAL:HA	20:B:1740:CLA:HAC1	1.97	0.46
20:B:1743:CLA:H192	20:B:1748:CLA:OBD	2.16	0.46
20:B:1748:CLA:C15	20:B:1749:CLA:H71	2.46	0.46
20:B:1771:CLA:HHD	23:B:1773:PQN:H18	1.97	0.46
8:D:102:ARG:NH2	8:D:110:GLN:HB2	2.30	0.46
8:D:146:VAL:HG21	8:D:152:GLN:HG3	1.98	0.46
10:F:26:GLN:O	10:F:28:SER:N	2.48	0.46
10:F:44:ALA:C	10:F:46:MET:N	2.69	0.46
11:G:39:ASN:HA	11:G:40:GLY:O	2.16	0.46
11:G:66:PHE:O	11:G:69:VAL:HG12	2.16	0.46
14:J:2:ARG:HH11	14:J:2:ARG:CG	2.29	0.46
2:2:91:THR:O	2:2:94:LEU:HB3	2.15	0.46
2:2:206:ALA:O	2:2:207:ALA:HB3	2.16	0.46
4:4:98:SER:HA	4:4:101:VAL:HG12	1.98	0.46
4:4:142:ASN:O	4:4:143:PHE:HB2	2.16	0.46
5:A:68:THR:C	5:A:70:ASP:N	2.68	0.46
5:A:258:LEU:O	5:A:259:TYR:HB2	2.15	0.46
5:A:258:LEU:HG	5:A:280:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:296:LEU:C	5:A:298:ASP:N	2.67	0.46
5:A:302:HIS:O	5:A:306:ILE:CG1	2.51	0.46
5:A:313:ALA:C	5:A:315:HIS:H	2.19	0.46
5:A:606:TYR:HH	20:A:1811:CLA:HED3	1.81	0.46
5:A:660:GLN:O	5:A:661:ALA:HB2	2.14	0.46
20:A:1761:CLA:H161	20:A:1761:CLA:H202	1.63	0.46
6:B:138:GLY:H	6:B:140:ILE:HG12	1.80	0.46
6:B:224:PRO:CA	6:B:227:THR:OG1	2.63	0.46
6:B:244:PHE:C	6:B:244:PHE:CD2	2.89	0.46
6:B:290:MET:SD	6:B:291:TYR:CE1	3.08	0.46
20:B:1745:CLA:HMA1	22:B:1776:BCR:H372	1.98	0.46
12:H:53:LEU:HG	12:H:54:LEU:N	2.22	0.46
17:N:27:ALA:O	17:N:28:ASN:C	2.54	0.46
17:N:62:SER:HB3	17:N:66:ASP:N	2.30	0.46
3:3:106:TYR:O	3:3:107:TRP:C	2.54	0.46
3:3:112:THR:C	3:3:114:PHE:N	2.69	0.46
3:3:188:ARG:HA	3:3:191:MET:HB2	1.97	0.46
5:A:47:GLY:O	10:F:115:THR:HB	2.16	0.46
5:A:316:MET:CA	5:A:317:TYR:CD1	2.99	0.46
5:A:355:HIS:ND1	5:A:416:ILE:HG22	2.24	0.46
5:A:434:ARG:O	5:A:435:VAL:C	2.54	0.46
5:A:457:SER:HG	5:A:544:ILE:HA	1.80	0.46
5:A:637:ILE:H	5:A:637:ILE:HG12	1.52	0.46
5:A:708:VAL:N	5:A:711:HIS:HD2	2.14	0.46
20:A:1763:CLA:HBA2	20:A:1763:CLA:H3A	1.48	0.46
20:A:1781:CLA:H93	22:A:1806:BCR:H10C	1.98	0.46
6:B:15:ASP:OD2	6:B:15:ASP:C	2.55	0.46
6:B:500:ALA:C	6:B:501:ILE:HG12	2.36	0.46
6:B:530:THR:HG22	20:B:1755:CLA:CMC	2.46	0.46
6:B:638:LEU:HD22	6:B:638:LEU:N	2.31	0.46
20:B:1743:CLA:H41	20:B:1748:CLA:CBC	2.46	0.46
22:B:1774:BCR:H15C	22:B:1774:BCR:H351	1.77	0.46
10:F:115:THR:O	10:F:116:GLN:CB	2.63	0.46
10:F:124:PRO:O	10:F:125:LEU:HB2	2.15	0.46
11:G:43:HIS:CA	11:G:44:PHE:CB	2.62	0.46
17:N:42:PHE:N	17:N:43:PRO:CD	2.58	0.46
3:3:132:TRP:HZ3	3:3:155:GLU:CD	1.82	0.45
4:4:169:GLN:HE22	20:4:1199:CLA:CHD	2.26	0.45
5:A:64:PHE:CE1	5:A:74:ILE:HG22	2.51	0.45
5:A:98:PHE:HD1	5:A:99:HIS:CD2	2.33	0.45
5:A:316:MET:HA	5:A:317:TYR:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:678:PHE:CZ	20:A:1783:CLA:H142	2.51	0.45
5:A:685:VAL:CG1	5:A:741:GLY:CA	2.94	0.45
5:A:693:LEU:HD11	5:A:738:TYR:HD1	1.78	0.45
5:A:709:TRP:O	5:A:712:ASN:N	2.49	0.45
20:A:1761:CLA:H3A	20:A:1761:CLA:HBA1	1.66	0.45
20:A:1790:CLA:C2B	22:A:1806:BCR:H333	2.46	0.45
20:A:1795:CLA:C6	10:F:121:ILE:HD12	2.46	0.45
20:A:1799:CLA:HBA2	20:A:1799:CLA:CED	2.46	0.45
20:A:1800:CLA:HMC3	20:B:1770:CLA:C1D	2.46	0.45
6:B:125:TYR:HE1	6:B:130:ARG:NH1	2.14	0.45
6:B:551:LYS:HG2	6:B:552:ASP:H	1.79	0.45
20:B:1755:CLA:H11	20:B:1769:CLA:CAD	2.45	0.45
20:B:1755:CLA:C2B	22:B:1777:BCR:H352	2.46	0.45
9:E:58:ASP:OD1	9:E:58:ASP:N	2.30	0.45
13:I:8:PHE:HE1	22:I:1032:BCR:C9	2.28	0.45
1:1:85:LEU:HD13	1:1:85:LEU:H	1.82	0.45
20:2:1215:CLA:C3	20:2:1220:CLA:HBC3	2.42	0.45
3:3:66:MET:CE	3:3:69:ALA:HB3	2.46	0.45
3:3:90:LEU:HD12	3:3:90:LEU:N	2.31	0.45
4:4:106:TRP:C	4:4:108:ASP:H	2.19	0.45
4:4:156:ASN:O	4:4:160:MET:HG3	2.17	0.45
4:4:161:LEU:O	4:4:162:ALA:CB	2.64	0.45
5:A:126:ILE:O	5:A:129:GLN:HB2	2.16	0.45
5:A:193:LEU:O	5:A:195:TRP:N	2.50	0.45
5:A:257:GLN:O	5:A:258:LEU:CB	2.64	0.45
5:A:358:LEU:HD11	5:A:413:HIS:HB2	1.90	0.45
20:A:1767:CLA:H202	20:A:1767:CLA:H152	1.98	0.45
6:B:50:HIS:HB3	20:B:1737:CLA:CHB	2.47	0.45
6:B:80:ASP:HA	6:B:81:PRO:HD3	1.56	0.45
6:B:216:LEU:O	6:B:218:TYR:O	2.34	0.45
6:B:527:LEU:CD1	20:B:1755:CLA:C1D	2.88	0.45
6:B:557:PHE:CD2	6:B:557:PHE:O	2.69	0.45
20:B:1735:CLA:HBC1	22:B:1778:BCR:C33	2.46	0.45
20:B:1748:CLA:CGA	20:B:1748:CLA:C4A	2.94	0.45
8:D:31:GLY:CA	16:L:13:PRO:HB3	2.44	0.45
8:D:137:ILE:H	8:D:137:ILE:HG13	1.44	0.45
9:E:60:LYS:HG3	9:E:61:THR:OG1	2.16	0.45
11:G:48:ASP:CB	11:G:49:THR:CB	2.92	0.45
16:L:63:LEU:HD13	16:L:64:LEU:HG	1.98	0.45
17:N:42:PHE:CG	17:N:43:PRO:N	2.80	0.45
20:1:1197:CLA:HAA2	20:1:1197:CLA:CB	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:50:VAL:O	2:2:50:VAL:HG12	2.17	0.45
3:3:73:ILE:O	20:3:1215:CLA:C3D	2.65	0.45
5:A:374:GLN:O	5:A:377:TYR:CD2	2.64	0.45
5:A:672:LEU:HD23	5:A:673:SER:H	1.80	0.45
20:A:1759:CLA:HBC3	20:A:1759:CLA:HHD	1.99	0.45
20:A:1764:CLA:ND	20:A:1783:CLA:C4	2.79	0.45
20:A:1781:CLA:CBB	20:A:1794:CLA:HMA1	2.47	0.45
20:A:1783:CLA:H191	20:A:1812:CLA:H13	1.98	0.45
20:A:1793:CLA:HMB2	20:A:1794:CLA:C1D	2.46	0.45
20:A:1798:CLA:H11	20:A:1798:CLA:H52	1.75	0.45
6:B:77:TRP:O	6:B:81:PRO:HG3	2.17	0.45
6:B:176:ASN:ND2	6:B:291:TYR:O	2.48	0.45
6:B:180:SER:O	6:B:181:GLY:C	2.54	0.45
6:B:221:GLY:C	6:B:223:GLY:N	2.69	0.45
6:B:470:THR:OG1	6:B:501:ILE:HG23	2.16	0.45
6:B:573:TRP:O	6:B:576:PHE:HB3	2.16	0.45
6:B:700:LEU:HD23	6:B:700:LEU:H	1.80	0.45
20:B:1738:CLA:H91	20:B:1738:CLA:H161	1.97	0.45
23:B:1773:PQN:H2M1	23:B:1773:PQN:H111	1.67	0.45
8:D:26:SER:N	8:D:27:PRO:HD3	2.30	0.45
10:F:23:LYS:HB3	10:F:24:LYS:NZ	2.19	0.45
16:L:50:LEU:HD23	16:L:51:LEU:H	1.81	0.45
16:L:63:LEU:CD2	16:L:64:LEU:N	2.75	0.45
20:L:1168:CLA:HHD	20:L:1168:CLA:HBC2	1.88	0.45
19:V:1:GLC:HO2	19:V:2:FRU:H3	1.68	0.45
20:1:1198:CLA:H91	20:1:1198:CLA:H122	1.98	0.45
4:4:107:GLN:C	20:4:1196:CLA:HMA1	2.24	0.45
20:4:1201:CLA:HAA2	20:4:1201:CLA:O2D	2.14	0.45
5:A:70:ASP:O	5:A:71:LEU:C	2.54	0.45
5:A:107:GLU:O	5:A:110:LEU:HG	2.17	0.45
5:A:205:HIS:CG	20:A:1769:CLA:HMC2	2.51	0.45
5:A:284:ARG:HG3	5:A:295:TRP:CB	2.47	0.45
5:A:374:GLN:C	5:A:376:MET:N	2.68	0.45
5:A:680:LEU:HD21	6:B:617:MET:SD	2.55	0.45
5:A:707:ILE:HG22	5:A:711:HIS:CD2	2.49	0.45
5:A:707:ILE:HG12	5:A:707:ILE:H	1.53	0.45
5:A:714:LEU:HD13	22:B:1779:BCR:H393	1.92	0.45
20:A:1764:CLA:HBB2	20:A:1765:CLA:C3D	2.47	0.45
20:A:1781:CLA:HMB3	22:A:1806:BCR:C17	2.46	0.45
20:A:1792:CLA:O1A	20:A:1792:CLA:C2	2.64	0.45
6:B:260:GLY:HA2	6:B:497:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:535:VAL:O	6:B:539:LEU:HB2	2.17	0.45
6:B:652:PHE:CZ	6:B:656:VAL:HG21	2.52	0.45
20:B:1737:CLA:H92	20:B:1754:CLA:O1A	2.17	0.45
10:F:145:LEU:C	10:F:146:ASN:ND2	2.70	0.45
16:L:40:LEU:CB	16:L:41:PRO:HD3	2.38	0.45
17:N:44:GLU:HB3	17:N:45:ASN:H	1.43	0.45
17:N:45:ASN:CG	17:N:57:LYS:NZ	2.70	0.45
19:M:1:GLC:C2	19:M:1:GLC:C6	2.87	0.45
2:2:70:LYS:HG3	2:2:73:ILE:HG12	1.95	0.45
20:2:1213:CLA:O2D	20:2:1213:CLA:OBD	2.35	0.45
4:4:101:VAL:C	4:4:104:ARG:HD3	2.37	0.45
5:A:53:TRP:HA	5:A:56:ASN:ND2	2.32	0.45
5:A:73:GLU:O	5:A:76:ARG:HB2	2.16	0.45
5:A:425:THR:O	5:A:427:ARG:CD	2.65	0.45
5:A:493:GLN:OE1	5:A:534:LEU:HD11	2.16	0.45
5:A:539:PHE:O	5:A:539:PHE:CD2	2.65	0.45
5:A:678:PHE:HZ	20:A:1783:CLA:H142	1.82	0.45
5:A:680:LEU:N	5:A:680:LEU:HD22	2.31	0.45
20:A:1778:CLA:CGD	20:A:1778:CLA:HAA2	2.47	0.45
20:A:1781:CLA:H43	20:A:1793:CLA:CBA	2.47	0.45
6:B:53:GLN:NE2	20:B:1736:CLA:HBB1	2.30	0.45
6:B:319:HIS:O	6:B:320:LYS:O	2.34	0.45
6:B:398:TYR:O	8:D:143:PRO:HG2	2.16	0.45
6:B:431:PHE:HE2	20:B:1762:CLA:HED3	1.81	0.45
6:B:439:HIS:NE2	6:B:443:MET:SD	2.89	0.45
20:B:1747:CLA:H12	20:B:1747:CLA:NA	2.31	0.45
20:B:1755:CLA:CAB	20:B:1769:CLA:HMA1	2.47	0.45
7:C:44:ARG:NH2	8:D:127:ARG:NE	2.63	0.45
8:D:113:HIS:HD2	8:D:113:HIS:O	2.00	0.45
9:E:83:ALA:O	9:E:86:GLU:CG	2.50	0.45
11:G:57:LEU:O	11:G:57:LEU:CD2	2.64	0.45
11:G:62:ASP:CB	11:G:63:PRO:HD3	2.42	0.45
17:N:38:GLY:HA3	17:N:46:PHE:HD1	1.80	0.45
19:M:2:FRU:O4	19:M:2:FRU:O2	2.35	0.45
19:U:1:GLC:HO2	19:U:2:FRU:H11	1.80	0.45
3:3:164:PHE:HD1	3:3:164:PHE:HA	1.71	0.45
20:4:1198:CLA:HBC3	20:4:1198:CLA:CMC	2.46	0.45
5:A:73:GLU:O	5:A:76:ARG:CA	2.64	0.45
5:A:141:ARG:CD	10:F:40:LEU:H	2.30	0.45
5:A:207:LEU:HD11	5:A:313:ALA:HB1	1.98	0.45
5:A:347:TYR:HE1	5:A:417:PHE:CZ	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:397:THR:HB	5:A:613:ILE:HG13	1.97	0.45
5:A:476:MET:O	5:A:477:PHE:HB2	2.17	0.45
5:A:645:SER:O	5:A:651:GLY:HA3	2.16	0.45
5:A:701:GLN:O	5:A:703:LEU:N	2.49	0.45
20:A:1781:CLA:CMA	20:A:1782:CLA:CGA	2.94	0.45
20:A:1815:CLA:H3A	20:A:1815:CLA:HBA1	1.74	0.45
6:B:212:PHE:CE1	20:B:1744:CLA:HHD	2.36	0.45
6:B:323:TYR:O	6:B:327:ASN:HB2	2.17	0.45
6:B:513:GLY:O	6:B:516:ASP:OD1	2.35	0.45
20:B:1762:CLA:NB	10:F:90:PHE:CE1	2.85	0.45
7:C:18:VAL:HB	7:C:58:CYS:HB2	1.99	0.45
8:D:99:GLN:HG2	8:D:101:TYR:CE2	2.52	0.45
8:D:132:LEU:HD12	8:D:136:SER:OG	2.17	0.45
9:E:36:VAL:HG23	9:E:52:VAL:HG22	1.99	0.45
9:E:62:ARG:O	9:E:83:ALA:CB	2.65	0.45
10:F:102:ARG:NH1	10:F:106:ILE:HD12	2.31	0.45
10:F:149:LEU:CD2	10:F:153:ASN:HD21	2.29	0.45
11:G:34:GLN:O	11:G:36:PRO:CD	2.65	0.45
12:H:75:ASP:HB3	12:H:77:LEU:HG	1.99	0.45
14:J:7:TYR:HB3	14:J:8:LEU:H	1.61	0.45
14:J:31:ARG:HH22	20:J:1043:CLA:C3B	2.10	0.45
17:N:7:LEU:O	17:N:8:GLU:HB2	2.16	0.45
1:1:34:ALA:O	1:1:38:ARG:N	2.39	0.45
1:1:89:VAL:O	11:G:77:ILE:HD13	2.16	0.45
2:2:96:ILE:HG13	2:2:97:VAL:H	1.80	0.45
3:3:94:ARG:HG2	3:3:97:PHE:CD1	2.52	0.45
5:A:347:TYR:CE1	5:A:417:PHE:HZ	2.34	0.45
5:A:499:ALA:O	5:A:501:GLY:N	2.38	0.45
20:A:1786:CLA:H2A	16:L:25:THR:HG21	1.99	0.45
22:A:1805:BCR:H11C	22:A:1805:BCR:H341	1.71	0.45
22:A:1807:BCR:H341	22:A:1807:BCR:H11C	1.72	0.45
21:A:7022:LMU:O3B	21:A:7022:LMU:H6'2	2.13	0.45
6:B:167:TRP:O	6:B:167:TRP:CD2	2.70	0.45
6:B:188:LEU:HD21	22:B:1775:BCR:H281	1.99	0.45
6:B:347:LEU:HD13	6:B:351:HIS:ND1	2.29	0.45
6:B:467:HIS:NE2	20:B:1764:CLA:CHA	2.80	0.45
6:B:540:ASP:N	6:B:540:ASP:OD1	2.48	0.45
6:B:707:LEU:CD1	24:B:1783:LMG:H301	2.47	0.45
6:B:708:VAL:C	6:B:710:LEU:O	2.55	0.45
20:B:1735:CLA:HBC3	20:B:1735:CLA:CHD	2.46	0.45
20:B:1738:CLA:CBC	20:B:1757:CLA:CMD	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:139:LYS:HZ3	9:E:41:ARG:NH1	2.15	0.45
21:L:1171:LMU:H52	21:L:1171:LMU:H82	1.78	0.45
17:N:2:VAL:O	17:N:2:VAL:CG2	2.63	0.45
1:1:184:PRO:HA	1:1:185:TRP:O	2.16	0.45
20:2:1224:CLA:H111	20:2:1224:CLA:H71	1.59	0.45
5:A:83:PHE:HA	5:A:86:LEU:CD2	2.47	0.45
5:A:555:ILE:H	5:A:555:ILE:HG12	1.46	0.45
5:A:709:TRP:CE3	5:A:710:ALA:N	2.85	0.45
20:A:1767:CLA:C4A	20:A:1767:CLA:CBA	2.94	0.45
20:A:1768:CLA:O1D	20:A:1769:CLA:HMC1	2.17	0.45
20:A:1779:CLA:NB	22:A:1805:BCR:C15	2.79	0.45
20:A:1816:CLA:HED3	20:A:1816:CLA:H72	1.98	0.45
6:B:47:PHE:CZ	6:B:51:PHE:HE1	2.35	0.45
6:B:198:ALA:H	6:B:200:PRO:HG2	1.82	0.45
6:B:216:LEU:O	6:B:217:PRO:C	2.55	0.45
6:B:279:ALA:HA	20:B:1746:CLA:HMA1	1.99	0.45
6:B:514:PRO:HG2	10:F:70:HIS:CE1	2.51	0.45
6:B:518:LEU:O	6:B:521:HIS:N	2.42	0.45
6:B:623:TYR:H	6:B:626:LEU:HB3	1.81	0.45
20:B:1755:CLA:C2	20:B:1768:CLA:HBA2	2.46	0.45
22:B:1775:BCR:HC8	22:B:1775:BCR:H331	1.96	0.45
20:B:1787:CLA:H202	20:B:1787:CLA:H162	1.72	0.45
7:C:17:CYS:O	7:C:58:CYS:HB2	2.16	0.45
7:C:81:TYR:N	7:C:81:TYR:HD1	2.15	0.45
10:F:152:ASN:ND2	10:F:152:ASN:N	2.64	0.45
11:G:16:LEU:CA	11:G:68:ILE:HG13	2.45	0.45
11:G:33:LYS:O	11:G:34:GLN:HG2	2.15	0.45
14:J:26:LEU:H	14:J:28:GLU:H	1.65	0.45
20:R:1055:CLA:H122	21:R:1056:LMU:O4'	2.17	0.45
20:4:4014:CLA:HBC3	20:4:4014:CLA:CMC	2.12	0.45
5:A:72:GLU:HB2	5:A:73:GLU:H	1.56	0.45
5:A:82:HIS:CE1	20:A:1761:CLA:HAA1	2.51	0.45
5:A:260:PRO:HG3	5:A:277:TYR:CZ	2.51	0.45
5:A:365:LEU:HD23	20:A:1761:CLA:HED2	1.91	0.45
5:A:593:SER:O	5:A:594:ALA:HB2	2.16	0.45
5:A:614:PHE:HE1	20:A:1811:CLA:H62	1.82	0.45
5:A:656:PHE:O	5:A:658:TRP:N	2.50	0.45
5:A:663:GLN:OE1	5:A:753:ARG:NE	2.50	0.45
6:B:29:HIS:HB2	20:B:1759:CLA:HBA1	1.99	0.45
6:B:461:GLN:HE21	6:B:461:GLN:HB3	1.63	0.45
6:B:558:PRO:HB3	6:B:706:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:560:ASP:O	25:B:1784:SF4:S3	2.75	0.45
22:B:1780:BCR:C38	22:B:1780:BCR:C23	2.74	0.45
10:F:62:LEU:HG	10:F:72:ILE:HD11	1.96	0.45
20:K:1085:CLA:HMB1	20:K:1142:CLA:HED2	1.90	0.45
16:L:154:ALA:O	16:L:155:CYS:C	2.55	0.45
17:N:45:ASN:O	17:N:46:PHE:C	2.50	0.45
3:3:111:TYR:HB2	3:3:112:THR:H	1.68	0.45
5:A:73:GLU:O	5:A:74:ILE:C	2.55	0.45
5:A:327:ILE:O	5:A:328:LYS:C	2.55	0.45
5:A:463:HIS:NE2	5:A:467:MET:SD	2.90	0.45
5:A:541:VAL:HG12	5:A:545:HIS:NE2	2.32	0.45
5:A:684:PHE:HD2	5:A:685:VAL:CA	2.29	0.45
20:A:1759:CLA:H12	20:A:1796:CLA:C5	2.47	0.45
20:A:1760:CLA:HMC3	20:A:1762:CLA:CED	2.47	0.45
20:A:1776:CLA:H121	22:A:1806:BCR:H23C	1.98	0.45
20:A:1797:CLA:H62	20:A:1797:CLA:H41	1.45	0.45
6:B:218:TYR:HB3	6:B:219:PRO:HD2	1.99	0.45
6:B:304:ILE:CD1	20:B:1749:CLA:HED3	2.47	0.45
6:B:347:LEU:HD21	6:B:351:HIS:CE1	2.40	0.45
6:B:493:TRP:CZ2	20:B:1747:CLA:H122	2.52	0.45
20:B:1749:CLA:HBA1	20:B:1749:CLA:CHA	2.46	0.45
7:C:9:ASP:HB2	25:C:1083:SF4:S3	2.57	0.45
8:D:139:LYS:HG2	8:D:141:VAL:HG22	1.98	0.45
12:H:24:TYR:HB3	12:H:25:GLY:H	1.60	0.45
12:H:29:PRO:O	12:H:30:SER:OG	2.30	0.45
12:H:40:PHE:O	12:H:41:GLU:C	2.56	0.45
14:J:31:ARG:O	14:J:34:PRO:HG3	2.17	0.45
22:L:1169:BCR:H11C	22:L:1169:BCR:H341	1.83	0.45
1:1:57:ILE:CG2	1:1:58:LEU:H	2.19	0.44
2:2:131:THR:HG23	2:2:132:GLY:N	2.30	0.44
5:A:132:LEU:O	5:A:143:ILE:HB	2.17	0.44
5:A:187:HIS:CE1	20:A:1767:CLA:CHA	2.96	0.44
5:A:400:MET:HE3	5:A:612:VAL:HG11	1.99	0.44
5:A:462:ILE:O	5:A:466:THR:OG1	2.33	0.44
5:A:488:PHE:CZ	5:A:533:PRO:HB3	2.52	0.44
20:A:1780:CLA:HMD2	20:A:1780:CLA:C14	2.33	0.44
22:A:1803:BCR:C12	22:A:1803:BCR:C34	2.88	0.44
21:A:7032:LMU:H81	21:A:7032:LMU:H52	1.36	0.44
6:B:17:THR:OG1	6:B:18:THR:N	2.50	0.44
6:B:275:HIS:HD2	20:B:1746:CLA:HMA3	1.83	0.44
6:B:318:GLY:HA3	6:B:405:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:679:ALA:O	6:B:683:GLU:OE2	2.35	0.44
20:B:1738:CLA:HBA1	20:B:1738:CLA:H3A	1.71	0.44
8:D:74:LEU:O	8:D:74:LEU:HG	2.16	0.44
14:J:21:SER:O	14:J:23:ALA:N	2.50	0.44
17:N:22:LEU:HD23	17:N:22:LEU:O	2.17	0.44
21:R:1056:LMU:H22	21:R:1056:LMU:O2'	2.17	0.44
3:3:49:ILE:CG1	3:3:52:LYS:CB	2.94	0.44
3:3:114:PHE:CE1	20:3:1216:CLA:C4D	3.01	0.44
21:3:7005:LMU:H1'	21:3:7005:LMU:H6D	1.74	0.44
5:A:113:PRO:O	5:A:115:HIS:CD2	2.70	0.44
5:A:122:VAL:HG22	5:A:142:GLY:CA	2.47	0.44
5:A:163:GLN:C	5:A:165:TYR:H	2.19	0.44
5:A:251:ASN:O	5:A:253:ASP:HB3	2.17	0.44
5:A:436:LEU:C	5:A:438:HIS:O	2.56	0.44
5:A:451:ILE:HD13	20:A:1788:CLA:HED1	1.98	0.44
5:A:472:ARG:O	5:A:474:GLN:CB	2.65	0.44
5:A:665:ILE:HD12	5:A:666:GLN:N	2.32	0.44
5:A:680:LEU:HB3	20:A:1812:CLA:C2	2.47	0.44
20:A:1759:CLA:HBC3	20:A:1759:CLA:CHD	2.47	0.44
20:A:1762:CLA:C7	20:A:1762:CLA:C2	2.95	0.44
20:A:1786:CLA:HMB2	20:A:1787:CLA:C4D	2.48	0.44
22:A:1804:BCR:C31	22:A:1804:BCR:C8	2.95	0.44
6:B:343:VAL:HG11	20:B:1756:CLA:H2	1.98	0.44
6:B:415:LYS:HG3	6:B:416:GLU:OE2	2.17	0.44
6:B:564:ARG:HH12	7:C:63:LEU:HA	1.82	0.44
6:B:629:SER:O	6:B:630:GLN:C	2.54	0.44
20:B:1738:CLA:CBB	20:B:1758:CLA:HHC	2.47	0.44
20:B:1747:CLA:HBA2	20:B:1747:CLA:H3A	1.33	0.44
20:B:1756:CLA:H202	20:B:1756:CLA:H162	1.64	0.44
23:B:1773:PQN:H142	23:B:1773:PQN:C2M	2.46	0.44
22:B:1778:BCR:H372	10:F:93:ILE:HG22	1.99	0.44
7:C:62:PHE:CE2	9:E:42:GLU:CD	2.82	0.44
8:D:41:GLN:CD	8:D:41:GLN:C	2.76	0.44
8:D:93:LYS:CB	8:D:93:LYS:HZ2	2.27	0.44
10:F:13:GLN:HG3	10:F:66:ASP:H	1.83	0.44
11:G:16:LEU:CD1	11:G:17:PHE:CZ	3.00	0.44
15:K:27:ALA:HB1	15:K:28:PRO:HD3	1.96	0.44
16:L:107:PHE:CB	16:L:109:GLU:OE1	2.62	0.44
21:1:7004:LMU:H11	21:1:7004:LMU:H2O2	1.74	0.44
20:2:1218:CLA:CGA	20:2:1218:CLA:C1A	2.96	0.44
3:3:86:GLN:HB2	3:3:88:THR:CA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:103:ILE:HG23	20:4:1207:CLA:HMB3	2.00	0.44
4:4:104:ARG:HE	4:4:105:ARG:N	2.15	0.44
5:A:49:ASP:HB2	5:A:720:THR:HA	1.98	0.44
5:A:223:VAL:CG1	5:A:224:HIS:H	2.29	0.44
5:A:369:THR:O	5:A:372:VAL:HG23	2.18	0.44
5:A:432:LEU:O	5:A:435:VAL:N	2.50	0.44
5:A:514:THR:HA	5:A:530:LEU:O	2.17	0.44
5:A:581:CYS:HB2	5:A:590:CYS:O	2.16	0.44
5:A:705:GLU:CG	6:B:545:LYS:HZ2	2.31	0.44
5:A:732:ALA:HB1	20:A:1796:CLA:HED2	1.99	0.44
20:A:1764:CLA:H111	22:A:1808:BCR:C10	2.47	0.44
20:A:1766:CLA:HBB2	20:A:1769:CLA:HMA3	1.98	0.44
20:A:1773:CLA:C4C	20:A:1773:CLA:H62	2.47	0.44
20:A:1788:CLA:HED1	20:A:1800:CLA:O1A	2.16	0.44
20:A:1800:CLA:H93	22:L:1169:BCR:H321	1.97	0.44
22:A:1803:BCR:C31	22:A:1803:BCR:C8	2.67	0.44
21:A:7010:LMU:H22	21:A:7010:LMU:H51	1.40	0.44
21:A:7033:LMU:H61	21:A:7033:LMU:H31	1.59	0.44
6:B:120:VAL:HG22	6:B:123:TRP:HE1	1.83	0.44
6:B:158:GLN:O	6:B:159:PRO:O	2.36	0.44
6:B:194:LEU:O	6:B:199:ILE:HG13	2.17	0.44
6:B:353:TYR:C	6:B:355:LEU:N	2.70	0.44
6:B:535:VAL:CG1	6:B:536:LYS:H	2.30	0.44
7:C:53:ARG:O	7:C:55:GLU:O	2.36	0.44
10:F:24:LYS:N	10:F:24:LYS:HE3	2.25	0.44
20:F:1157:CLA:OBD	20:F:1157:CLA:O2D	2.31	0.44
11:G:60:SER:O	11:G:62:ASP:N	2.50	0.44
12:H:42:THR:HG22	12:H:45:ALA:CB	2.44	0.44
14:J:2:ARG:HH22	14:J:8:LEU:HD22	1.81	0.44
16:L:65:VAL:C	16:L:69:VAL:HG22	2.36	0.44
18:R:5:UNK:O	18:R:6:UNK:CB	2.65	0.44
21:1:1202:LMU:O5B	21:1:1202:LMU:H5'	2.15	0.44
3:3:93:PHE:HD2	3:3:95:THR:N	2.12	0.44
4:4:35:GLU:HB2	4:4:36:ASN:H	1.52	0.44
5:A:64:PHE:CD1	5:A:74:ILE:HG22	2.53	0.44
5:A:79:PHE:CD2	5:A:185:HIS:CD2	2.97	0.44
5:A:143:ILE:HG12	20:A:1764:CLA:HBC2	2.00	0.44
5:A:174:PHE:HE2	20:A:1761:CLA:H152	1.79	0.44
5:A:430:ASP:C	5:A:432:LEU:H	2.21	0.44
5:A:711:HIS:CB	5:A:717:ALA:HB2	2.41	0.44
20:A:1817:CLA:O1D	20:A:1817:CLA:HAA1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7020:LMU:C6'	21:A:7020:LMU:C1B	2.95	0.44
21:A:7033:LMU:C6B	21:A:7033:LMU:H2O2	2.19	0.44
6:B:57:ILE:HG22	6:B:58:PHE:CD1	2.52	0.44
6:B:60:TRP:CD1	20:B:1738:CLA:HBC1	2.52	0.44
6:B:431:PHE:CE2	20:B:1762:CLA:CED	3.00	0.44
6:B:693:TRP:CZ2	6:B:697:PRO:HG3	2.52	0.44
6:B:710:LEU:O	6:B:712:HIS:N	2.51	0.44
6:B:718:ILE:HD11	20:B:1757:CLA:HHC	1.99	0.44
20:B:1738:CLA:CBC	20:B:1757:CLA:HMD3	2.48	0.44
20:B:1768:CLA:HBD	20:B:1768:CLA:HAA1	1.99	0.44
7:C:28:MET:HB2	8:D:121:GLU:HA	1.99	0.44
7:C:58:CYS:HA	7:C:59:PRO:HD2	1.65	0.44
8:D:21:ASP:HB3	8:D:22:PRO:HD3	1.99	0.44
8:D:94:TYR:O	8:D:95:LYS:NZ	2.33	0.44
8:D:139:LYS:NZ	9:E:41:ARG:NH1	2.65	0.44
9:E:69:PHE:CE2	9:E:70:ALA:HB3	2.53	0.44
10:F:33:ALA:C	10:F:35:ASP:H	2.20	0.44
10:F:104:TYR:OH	10:F:121:ILE:HA	2.17	0.44
12:H:11:LEU:HD22	12:H:11:LEU:HA	1.85	0.44
20:L:1166:CLA:H3A	20:L:1166:CLA:HBA2	1.54	0.44
17:N:59:PRO:HA	17:N:66:ASP:OD1	2.16	0.44
1:1:27:LEU:H	6:B:314:ARG:HH12	1.66	0.44
2:2:37:ASP:HA	2:2:38:PRO:HD3	1.85	0.44
5:A:55:TRP:CH2	20:A:1795:CLA:HMB1	2.53	0.44
5:A:316:MET:HA	5:A:317:TYR:CD1	2.52	0.44
5:A:349:ILE:HD13	5:A:422:TYR:HB3	1.99	0.44
5:A:472:ARG:HG2	6:B:97:GLY:HA3	2.00	0.44
5:A:575:LEU:H	5:A:575:LEU:HD12	1.82	0.44
20:A:1760:CLA:HBA2	20:A:1767:CLA:C6	2.47	0.44
20:A:1767:CLA:H171	20:A:1767:CLA:H141	1.98	0.44
20:A:1774:CLA:ND	20:A:1784:CLA:H72	2.33	0.44
21:A:7030:LMU:H42	21:A:7030:LMU:H11	1.76	0.44
21:A:7043:LMU:C7	21:A:7043:LMU:H111	2.22	0.44
6:B:74:PHE:C	6:B:76:ALA:N	2.70	0.44
6:B:183:PHE:HE1	20:B:1743:CLA:H71	1.83	0.44
6:B:290:MET:HA	20:B:1751:CLA:C3C	2.47	0.44
6:B:365:PHE:HB3	6:B:602:TRP:CZ2	2.52	0.44
6:B:509:PHE:N	6:B:509:PHE:HD2	2.15	0.44
6:B:544:SER:N	6:B:547:MET:O	2.47	0.44
6:B:590:VAL:O	6:B:593:TYR:HB3	2.18	0.44
6:B:673:GLU:O	6:B:676:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:694:ARG:HE	16:L:105:ALA:CA	2.28	0.44
6:B:700:LEU:N	23:B:1773:PQN:O4	2.44	0.44
20:B:1735:CLA:H61	22:B:1778:BCR:H12C	1.99	0.44
20:B:1741:CLA:H51	20:B:1741:CLA:H8	1.59	0.44
20:B:1763:CLA:H3A	20:B:1763:CLA:HBA1	1.67	0.44
22:B:1775:BCR:H11C	22:B:1775:BCR:H341	1.70	0.44
7:C:60:THR:HG21	7:C:64:SER:HB3	1.98	0.44
10:F:72:ILE:O	10:F:73:VAL:HG12	2.18	0.44
11:G:28:ARG:NH2	11:G:28:ARG:CG	2.72	0.44
14:J:10:VAL:CG2	14:J:14:LEU:HD12	2.47	0.44
20:J:1044:CLA:C4	20:J:1044:CLA:C8	2.76	0.44
16:L:61:GLY:O	16:L:63:LEU:N	2.51	0.44
16:L:95:LEU:HA	16:L:98:CYS:CB	2.42	0.44
19:Z:1:GLC:O2	19:Z:1:GLC:O4	2.29	0.44
1:1:45:ILE:CD1	20:1:1195:CLA:HMD2	2.38	0.44
1:1:141:GLU:O	1:1:143:LEU:O	2.36	0.44
20:1:1188:CLA:HMA2	20:1:1188:CLA:CBA	2.48	0.44
20:2:1213:CLA:CHD	20:2:1213:CLA:H42	2.48	0.44
20:2:1220:CLA:H51	20:2:1220:CLA:H11	1.85	0.44
3:3:50:GLU:OE1	3:3:54:LEU:HB2	2.17	0.44
5:A:363:ALA:O	5:A:367:SER:CB	2.65	0.44
5:A:377:TYR:CD1	5:A:616:PHE:CE1	3.04	0.44
5:A:400:MET:CE	5:A:612:VAL:HG11	2.48	0.44
20:A:1764:CLA:H161	20:A:1785:CLA:C20	2.48	0.44
20:A:1765:CLA:HBC3	20:A:1765:CLA:CMC	2.48	0.44
20:A:1787:CLA:H161	20:A:1787:CLA:H122	1.60	0.44
20:A:1787:CLA:O1A	6:B:686:PRO:HD3	2.18	0.44
22:A:1805:BCR:C8	22:A:1805:BCR:H321	2.48	0.44
21:A:7016:LMU:H72	21:A:7016:LMU:H42	1.51	0.44
21:A:7039:LMU:H112	21:A:7039:LMU:H82	1.38	0.44
21:A:7042:LMU:H61	21:A:7042:LMU:H31	1.48	0.44
6:B:103:ALA:HA	6:B:105:THR:O	2.18	0.44
6:B:154:TRP:CD1	6:B:154:TRP:C	2.91	0.44
6:B:167:TRP:HD1	11:G:41:MET:HE1	1.82	0.44
6:B:288:GLY:O	6:B:289:LEU:HB2	2.17	0.44
6:B:395:ILE:H	6:B:395:ILE:HG13	1.72	0.44
6:B:668:ARG:NH1	6:B:672:GLN:HG2	2.32	0.44
6:B:726:ILE:C	6:B:728:SER:N	2.70	0.44
20:B:1747:CLA:H2	20:B:1756:CLA:HBB1	1.98	0.44
22:B:1774:BCR:H343	11:G:21:PHE:CE1	2.51	0.44
26:B:8057:UNL:O1'	26:B:8057:UNL:O3'	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:41:GLN:HG3	16:L:125:LYS:NZ	2.33	0.44
9:E:44:TYR:HB3	9:E:45:TRP:CZ3	2.53	0.44
11:G:58:LEU:HB2	11:G:59:LYS:H	1.42	0.44
20:J:1045:CLA:CBA	20:J:1045:CLA:CHA	2.87	0.44
17:N:62:SER:OG	17:N:66:ASP:HA	2.18	0.44
17:N:72:LYS:HD2	17:N:72:LYS:HA	1.57	0.44
2:2:189:ILE:H	2:2:189:ILE:CD1	2.20	0.44
3:3:86:GLN:CB	3:3:88:THR:H	2.31	0.44
3:3:111:TYR:HB2	3:3:112:THR:HG22	2.00	0.44
5:A:203:LEU:O	5:A:207:LEU:HD23	2.17	0.44
5:A:301:HIS:NE2	20:A:1772:CLA:CHA	2.81	0.44
5:A:334:HIS:CB	20:A:1777:CLA:HMA3	2.48	0.44
5:A:458:PHE:C	5:A:460:LEU:N	2.70	0.44
5:A:461:TYR:CD2	5:A:649:ILE:HD12	2.52	0.44
5:A:680:LEU:HG	6:B:617:MET:HB2	1.98	0.44
20:A:1780:CLA:HBC2	20:A:1780:CLA:HMC1	1.98	0.44
20:A:1793:CLA:HBD	20:A:1793:CLA:HAA1	1.99	0.44
22:A:1806:BCR:H11C	22:A:1806:BCR:H341	1.71	0.44
21:A:7009:LMU:H3'	21:A:7009:LMU:O6B	2.18	0.44
6:B:141:PHE:CG	20:B:1744:CLA:H12	2.53	0.44
6:B:332:PHE:HE1	6:B:408:LEU:CD2	2.30	0.44
6:B:431:PHE:CE2	20:B:1762:CLA:HED3	2.53	0.44
6:B:431:PHE:CD2	20:B:1762:CLA:HMA3	2.52	0.44
7:C:26:LEU:O	7:C:43:PRO:HB3	2.18	0.44
7:C:77:MET:C	7:C:79:LEU:N	2.69	0.44
8:D:113:HIS:CD2	8:D:113:HIS:O	2.70	0.44
8:D:152:GLN:HA	8:D:153:PRO:HD2	1.73	0.44
10:F:84:ILE:HD13	10:F:84:ILE:N	2.33	0.44
11:G:92:GLY:O	11:G:94:ASP:OD1	2.36	0.44
20:H:1079:CLA:H2A	20:H:1079:CLA:O1D	2.17	0.44
15:K:47:ILE:HG23	15:K:48:GLN:N	2.28	0.44
1:1:105:ILE:O	1:1:105:ILE:HG22	2.18	0.44
1:1:137:PRO:O	1:1:139:LYS:N	2.51	0.44
2:2:186:THR:O	2:2:187:GLY:C	2.56	0.44
3:3:132:TRP:CE3	3:3:155:GLU:HG2	2.26	0.44
20:3:1219:CLA:H2A	20:3:1219:CLA:CED	2.48	0.44
20:3:3011:CLA:H62	20:3:3011:CLA:H41	1.73	0.44
4:4:38:ARG:O	4:4:39:TRP:CD1	2.68	0.44
5:A:42:ARG:O	5:A:44:ILE:HG13	2.17	0.44
5:A:173:VAL:O	5:A:175:ALA:O	2.36	0.44
5:A:212:GLY:O	5:A:214:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:554:LEU:CD2	20:B:1787:CLA:O2D	2.66	0.44
5:A:560:VAL:O	5:A:563:ALA:HB2	2.16	0.44
5:A:665:ILE:O	6:B:621:ARG:HD3	2.18	0.44
20:A:1768:CLA:HAA1	20:A:1768:CLA:HBD	1.98	0.44
20:A:1782:CLA:H91	20:A:1782:CLA:H112	1.61	0.44
20:A:1792:CLA:HBD	20:A:1792:CLA:HBA1	1.99	0.44
20:A:1793:CLA:H71	20:A:1793:CLA:H112	1.70	0.44
20:A:1796:CLA:C4	20:A:1796:CLA:C4C	2.94	0.44
6:B:5:ILE:CB	6:B:6:PRO:CD	2.86	0.44
6:B:67:HIS:CD2	6:B:71:GLN:HE22	2.35	0.44
6:B:309:ILE:HA	6:B:310:PRO:HD3	1.82	0.44
6:B:353:TYR:CB	6:B:594:TRP:CH2	3.00	0.44
6:B:535:VAL:HG23	6:B:539:LEU:HD23	1.98	0.44
20:B:1743:CLA:C14	20:B:1748:CLA:H2	2.39	0.44
20:B:1744:CLA:H3A	20:B:1744:CLA:HBA2	1.58	0.44
20:B:1749:CLA:C2	20:B:1754:CLA:H92	2.47	0.44
22:B:1777:BCR:C38	22:B:1777:BCR:C23	2.66	0.44
24:B:1783:LMG:O3	7:C:70:TRP:HZ2	1.88	0.44
9:E:46:PHE:CD2	9:E:47:LYS:N	2.86	0.44
10:F:61:LEU:HD23	10:F:69:PRO:HB3	1.96	0.44
16:L:151:VAL:O	16:L:154:ALA:HB3	2.17	0.44
18:R:8:UNK:CB	20:R:1054:CLA:O2D	2.66	0.44
18:R:34:UNK:C	18:R:36:UNK:O	2.66	0.44
3:3:92:TRP:CZ2	5:A:250:LEU:HB2	2.51	0.44
5:A:144:GLN:HG3	5:A:145:ILE:H	1.82	0.44
5:A:388:ASP:OD1	5:A:391:THR:HB	2.18	0.44
5:A:596:ASP:HA	5:A:599:PHE:CB	2.39	0.44
20:A:1811:CLA:H122	20:A:1811:CLA:H162	1.68	0.44
21:A:7032:LMU:C1B	21:A:7032:LMU:C1	2.96	0.44
6:B:120:VAL:C	6:B:123:TRP:HD1	2.20	0.44
6:B:196:HIS:CE1	20:B:1745:CLA:C4D	3.00	0.44
6:B:457:PRO:O	6:B:460:ALA:HB3	2.18	0.44
6:B:564:ARG:NH1	7:C:63:LEU:HA	2.33	0.44
6:B:727:ALA:O	6:B:728:SER:OG	2.29	0.44
20:B:1768:CLA:HBB2	20:B:1768:CLA:C8	2.42	0.44
10:F:89:LEU:HD12	10:F:89:LEU:HA	1.88	0.44
11:G:16:LEU:HD12	11:G:17:PHE:CZ	2.51	0.44
12:H:25:GLY:HA3	12:H:27:ASP:OD2	2.11	0.44
16:L:123:ARG:NE	16:L:123:ARG:CA	2.72	0.44
2:2:161:THR:HA	2:2:165:LYS:HB2	2.00	0.43
5:A:92:TRP:CD1	20:A:1763:CLA:HBB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:220:ARG:O	5:A:221:HIS:CB	2.62	0.43
5:A:570:PRO:C	5:A:572:LYS:H	2.21	0.43
5:A:631:GLN:HG2	5:A:633:VAL:HG13	1.98	0.43
5:A:651:GLY:O	5:A:655:ASP:HB2	2.18	0.43
20:A:1783:CLA:H18	20:A:1783:CLA:H122	1.99	0.43
20:A:1801:CLA:H41	20:A:1801:CLA:H62	1.63	0.43
21:A:7037:LMU:H1B	21:A:7037:LMU:H4B	1.50	0.43
6:B:458:ILE:HD11	20:F:1156:CLA:HED1	2.00	0.43
6:B:460:ALA:O	6:B:462:TRP:N	2.51	0.43
6:B:583:MET:O	6:B:583:MET:CE	2.66	0.43
6:B:714:SER:O	6:B:718:ILE:HG22	2.18	0.43
20:B:1762:CLA:C4B	10:F:90:PHE:CE1	3.01	0.43
8:D:79:ARG:H	8:D:82:GLN:HE21	1.63	0.43
8:D:125:PRO:HG2	8:D:127:ARG:HH11	1.82	0.43
16:L:92:VAL:HG11	16:L:147:GLY:CA	2.47	0.43
17:N:42:PHE:CD1	17:N:43:PRO:CD	3.01	0.43
17:N:69:CYS:O	17:N:72:LYS:HD2	2.17	0.43
17:N:84:LYS:HA	17:N:85:TRP:HA	1.46	0.43
18:R:27:UNK:O	18:R:29:UNK:C	2.65	0.43
18:R:50:UNK:HA	18:R:51:UNK:HA	1.70	0.43
1:1:74:TRP:CZ3	1:1:81:GLN:HA	2.54	0.43
20:3:1219:CLA:HBC3	20:3:1219:CLA:CMC	2.12	0.43
4:4:83:TYR:HB3	4:4:84:PHE:H	1.64	0.43
4:4:143:PHE:O	4:4:144:ALA:CB	2.65	0.43
20:4:1204:CLA:H41	20:4:1204:CLA:C8	2.48	0.43
5:A:25:ASP:HB3	5:A:26:PRO:HD3	2.00	0.43
5:A:34:TRP:O	5:A:35:ALA:CB	2.66	0.43
5:A:222:GLN:O	5:A:227:LEU:HD12	2.19	0.43
5:A:478:SER:HB2	5:A:481:ALA:H	1.83	0.43
5:A:558:LYS:HZ1	6:B:674:LEU:HD23	1.82	0.43
5:A:567:ARG:HH11	8:D:34:GLY:C	2.22	0.43
5:A:569:ILE:HG12	5:A:586:ARG:NH1	2.33	0.43
5:A:705:GLU:O	5:A:706:SER:C	2.57	0.43
5:A:711:HIS:NE2	20:A:1795:CLA:CBC	2.79	0.43
20:A:1772:CLA:H121	20:A:1772:CLA:H8	1.87	0.43
20:A:1781:CLA:HMB3	22:A:1806:BCR:C19	2.48	0.43
20:A:1793:CLA:O1A	20:A:1793:CLA:CBD	2.67	0.43
22:A:1807:BCR:C8	20:A:1813:CLA:H142	2.48	0.43
6:B:141:PHE:O	6:B:142:LEU:C	2.57	0.43
6:B:434:LEU:O	6:B:438:VAL:HG13	2.18	0.43
6:B:560:ASP:CG	7:C:66:ARG:CZ	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:75:ARG:NH1	8:D:46:TYR:OH	2.51	0.43
8:D:29:PHE:HA	8:D:66:ALA:HB2	2.00	0.43
8:D:94:TYR:O	8:D:95:LYS:HB3	2.18	0.43
10:F:123:VAL:CB	10:F:126:ALA:O	2.66	0.43
11:G:10:LEU:HD23	11:G:13:GLY:HA3	2.00	0.43
16:L:43:TYR:O	16:L:44:ARG:CB	2.63	0.43
16:L:127:PRO:O	16:L:128:ASP:O	2.37	0.43
2:2:55:ALA:HB3	2:2:56:MET:CE	2.48	0.43
3:3:50:GLU:OE2	3:3:54:LEU:HD13	2.17	0.43
3:3:84:ILE:N	20:A:1798:CLA:H51	2.33	0.43
20:3:1218:CLA:H3A	20:3:1218:CLA:HBA2	1.69	0.43
4:4:102:GLU:C	4:4:104:ARG:H	2.21	0.43
4:4:117:GLN:HB3	4:4:121:PHE:CE2	2.53	0.43
20:4:1201:CLA:HBC3	20:4:1201:CLA:CHD	2.48	0.43
5:A:310:PHE:H	5:A:313:ALA:CB	2.32	0.43
5:A:390:ALA:HA	5:A:393:LEU:HD21	1.98	0.43
5:A:568:LEU:HD21	5:A:586:ARG:HB3	1.99	0.43
20:A:1817:CLA:CMC	20:A:1817:CLA:CBC	2.81	0.43
21:A:7038:LMU:O6'	21:A:7038:LMU:O1B	2.30	0.43
6:B:297:ILE:HG21	11:G:21:PHE:CZ	2.54	0.43
6:B:365:PHE:HB3	6:B:602:TRP:CH2	2.53	0.43
6:B:460:ALA:O	6:B:463:ILE:N	2.52	0.43
6:B:556:SER:HA	6:B:558:PRO:HD3	2.00	0.43
6:B:621:ARG:HE	6:B:621:ARG:HB3	1.57	0.43
6:B:626:LEU:O	6:B:627:ASN:CB	2.66	0.43
6:B:651:LEU:HB3	20:B:1786:CLA:C1	2.48	0.43
20:B:1758:CLA:H3A	20:B:1758:CLA:HBA2	1.55	0.43
8:D:40:ALA:O	8:D:45:PHE:CD2	2.71	0.43
9:E:69:PHE:HD2	9:E:71:LYS:H	1.61	0.43
9:E:80:ASN:OD1	9:E:81:ASN:N	2.49	0.43
10:F:51:LYS:O	10:F:53:PHE:N	2.46	0.43
13:I:25:PHE:CE2	13:I:28:VAL:HG21	2.53	0.43
16:L:33:ILE:HG23	16:L:34:ALA:N	2.34	0.43
16:L:77:THR:OG1	16:L:82:ALA:HB3	2.19	0.43
17:N:62:SER:CB	17:N:66:ASP:HA	2.48	0.43
2:2:171:MET:SD	2:2:172:LEU:HG	2.57	0.43
2:2:211:LYS:HA	2:2:211:LYS:CE	2.48	0.43
20:2:1215:CLA:HED2	20:2:1220:CLA:CBB	2.48	0.43
4:4:119:PRO:HG2	4:4:120:ILE:HG13	2.01	0.43
4:4:143:PHE:O	4:4:144:ALA:HB2	2.19	0.43
20:4:1196:CLA:H62	20:4:1196:CLA:H41	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:27:ILE:C	5:A:28:LYS:HG3	2.24	0.43
5:A:213:LEU:O	22:A:1804:BCR:C17	2.66	0.43
5:A:363:ALA:N	5:A:410:ALA:CB	2.81	0.43
5:A:400:MET:HG3	5:A:609:ILE:HG23	2.00	0.43
5:A:539:PHE:HE2	5:A:543:HIS:HE1	1.66	0.43
5:A:656:PHE:O	5:A:657:LEU:C	2.57	0.43
20:A:1776:CLA:HBA1	20:A:1780:CLA:CBB	2.48	0.43
20:A:1783:CLA:C11	22:A:1808:BCR:C35	2.96	0.43
20:A:1784:CLA:H52	20:A:1784:CLA:HMD2	2.00	0.43
20:A:1796:CLA:H41	20:A:1796:CLA:C1C	2.48	0.43
21:A:7026:LMU:H1B	21:A:7026:LMU:H4B	1.07	0.43
6:B:385:GLY:CA	20:B:1759:CLA:HBC3	2.48	0.43
6:B:659:THR:OG1	20:B:1787:CLA:C3B	2.67	0.43
6:B:662:MET:O	6:B:664:LEU:N	2.52	0.43
23:B:1773:PQN:H192	22:B:1780:BCR:HC8	1.97	0.43
8:D:56:GLN:OE1	8:D:94:TYR:CE2	2.71	0.43
9:E:42:GLU:CG	9:E:43:SER:N	2.70	0.43
9:E:65:VAL:HG23	9:E:66:VAL:O	2.19	0.43
10:F:63:CYS:CA	10:F:69:PRO:HA	2.45	0.43
11:G:60:SER:O	11:G:61:ASN:C	2.56	0.43
12:H:53:LEU:CG	12:H:54:LEU:N	2.77	0.43
17:N:25:THR:HG22	17:N:26:GLY:N	2.33	0.43
17:N:25:THR:HG22	17:N:26:GLY:H	1.83	0.43
17:N:40:CYS:N	17:N:41:LYS:CA	2.81	0.43
1:I:180:HIS:O	4:I:88:SER:OG	2.27	0.43
5:A:128:GLY:HA3	6:B:446:PHE:HD2	1.80	0.43
5:A:249:ILE:C	5:A:251:ASN:N	2.65	0.43
5:A:284:ARG:CZ	5:A:284:ARG:CA	2.91	0.43
5:A:370:ILE:CG2	5:A:400:MET:CA	2.87	0.43
5:A:379:MET:HE2	5:A:379:MET:HB2	1.80	0.43
5:A:503:THR:HG21	20:A:1791:CLA:NB	2.33	0.43
5:A:506:GLY:O	5:A:507:ALA:CB	2.66	0.43
5:A:603:PHE:CE2	6:B:665:ILE:HG21	2.54	0.43
20:A:1761:CLA:H122	22:A:1803:BCR:C39	2.48	0.43
20:A:1796:CLA:ND	20:A:1796:CLA:H11	2.33	0.43
22:A:1807:BCR:C12	20:A:1812:CLA:H122	2.48	0.43
21:A:7030:LMU:H1'	21:A:7030:LMU:H6D	1.18	0.43
6:B:57:ILE:HG12	20:B:1738:CLA:HMC2	2.00	0.43
6:B:144:PHE:O	6:B:148:ILE:HD11	2.18	0.43
6:B:183:PHE:HB3	6:B:284:PHE:CD2	2.53	0.43
6:B:190:TRP:CE2	20:B:1748:CLA:CMD	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:351:HIS:HB3	20:B:1747:CLA:CED	2.35	0.43
6:B:458:ILE:HG13	6:B:459:PHE:CD1	2.54	0.43
6:B:473:GLY:O	6:B:474:PHE:HB3	2.19	0.43
6:B:589:TRP:CD1	20:B:1785:CLA:H152	2.54	0.43
6:B:674:LEU:O	6:B:678:LEU:HB2	2.18	0.43
20:B:1750:CLA:NA	20:B:1750:CLA:O2A	2.52	0.43
7:C:5:VAL:CA	7:C:65:VAL:HG22	2.46	0.43
8:D:92:SER:O	8:D:93:LYS:HG3	2.19	0.43
10:F:53:PHE:O	10:F:55:ASN:N	2.52	0.43
10:F:116:GLN:HA	10:F:118:GLU:OE1	2.18	0.43
12:H:77:LEU:HD23	12:H:78:PRO:CD	2.48	0.43
13:I:15:LEU:HD12	13:I:18:ALA:HB3	2.00	0.43
16:L:49:PRO:HG3	16:L:131:GLN:NE2	2.34	0.43
16:L:107:PHE:HA	16:L:133:ALA:HB2	2.00	0.43
2:2:124:ILE:HG22	2:2:124:ILE:O	2.18	0.43
5:A:98:PHE:O	5:A:99:HIS:CD2	2.71	0.43
5:A:680:LEU:HB3	20:A:1812:CLA:C1	2.48	0.43
5:A:703:LEU:O	5:A:707:ILE:CG1	2.67	0.43
5:A:725:LEU:HD21	20:A:1796:CLA:HMD3	1.99	0.43
20:A:1763:CLA:CHC	22:A:1808:BCR:H333	2.49	0.43
20:A:1783:CLA:C20	22:A:1808:BCR:C15	2.95	0.43
6:B:179:LEU:O	6:B:284:PHE:O	2.36	0.43
6:B:289:LEU:CD2	20:B:1750:CLA:C1A	2.96	0.43
6:B:361:ILE:O	6:B:362:ALA:O	2.36	0.43
6:B:458:ILE:HD11	20:F:1156:CLA:CED	2.48	0.43
6:B:672:GLN:HE22	6:B:698:VAL:HA	1.84	0.43
20:B:1736:CLA:HBA2	20:B:1736:CLA:H3A	1.53	0.43
20:B:1744:CLA:H143	20:B:1744:CLA:H162	1.75	0.43
20:B:1750:CLA:H43	20:B:1750:CLA:C1C	2.49	0.43
20:B:1757:CLA:H193	20:B:1757:CLA:H161	1.88	0.43
22:B:1781:BCR:C34	20:H:1079:CLA:CHD	2.96	0.43
9:E:37:LYS:CB	9:E:49:VAL:HG22	2.47	0.43
9:E:65:VAL:CG2	9:E:66:VAL:O	2.66	0.43
10:F:151:ASP:O	10:F:154:PHE:N	2.52	0.43
17:N:53:ALA:O	17:N:54:LYS:CG	2.67	0.43
20:R:1054:CLA:H62	20:R:1054:CLA:H41	1.87	0.43
2:2:117:GLY:O	2:2:119:VAL:HG22	2.18	0.43
20:2:1220:CLA:C11	3:3:137:SER:OG	2.67	0.43
21:2:7006:LMU:H71	21:2:7006:LMU:H41	1.81	0.43
20:3:1218:CLA:O1D	20:3:1218:CLA:CAA	2.66	0.43
4:4:105:ARG:O	4:4:108:ASP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:163:GLN:O	5:A:165:TYR:N	2.51	0.43
5:A:281:LEU:HD21	20:A:1772:CLA:HMA2	1.99	0.43
5:A:347:TYR:CE1	5:A:417:PHE:CZ	3.06	0.43
5:A:378:SER:HG	5:A:512:SER:HG	1.65	0.43
5:A:479:ASP:HA	5:A:536:THR:CG2	2.46	0.43
5:A:530:LEU:HD11	5:A:624:VAL:HA	2.01	0.43
5:A:606:TYR:HB2	5:A:739:LEU:HD22	2.00	0.43
5:A:620:MET:C	5:A:623:ASP:O	2.57	0.43
5:A:682:ALA:HA	5:A:685:VAL:HG12	1.99	0.43
20:A:1776:CLA:H111	20:A:1776:CLA:C16	2.47	0.43
21:A:7039:LMU:H1B	21:A:7039:LMU:H4B	1.58	0.43
6:B:190:TRP:O	6:B:191:ALA:C	2.57	0.43
6:B:203:ARG:CG	6:B:204:GLY:N	2.70	0.43
6:B:594:TRP:HD1	6:B:595:HIS:N	2.16	0.43
6:B:680:TRP:O	6:B:681:ALA:O	2.37	0.43
20:B:1771:CLA:C2	23:B:1773:PQN:H251	2.49	0.43
8:D:46:TYR:N	8:D:46:TYR:HD2	2.13	0.43
9:E:73:ASN:ND2	9:E:78:SER:HB2	2.33	0.43
9:E:88:GLU:O	9:E:90:VAL:HA	2.14	0.43
12:H:63:SER:O	12:H:67:TYR:HB3	2.17	0.43
17:N:47:THR:CG2	17:N:54:LYS:HZ2	2.16	0.43
17:N:72:LYS:HZ2	17:N:74:LYS:HG2	1.59	0.43
4:4:152:LYS:HD2	4:4:152:LYS:HA	1.81	0.43
20:4:1199:CLA:HAA1	20:F:1157:CLA:H12	2.00	0.43
5:A:57:LEU:HD22	5:A:58:HIS:CD2	2.54	0.43
5:A:208:ALA:CA	5:A:310:PHE:O	2.43	0.43
5:A:249:ILE:CD1	5:A:250:LEU:HB2	2.48	0.43
5:A:499:ALA:CB	20:A:1790:CLA:O2D	2.66	0.43
5:A:552:THR:O	5:A:553:VAL:HB	2.19	0.43
5:A:648:THR:HG23	5:A:650:ASN:H	1.83	0.43
5:A:655:ASP:O	5:A:659:ALA:HB3	2.18	0.43
20:A:1764:CLA:H161	20:A:1764:CLA:H122	1.73	0.43
20:A:1767:CLA:HBC3	20:A:1767:CLA:CMC	2.37	0.43
20:A:1789:CLA:HMD2	6:B:95:HIS:HD2	1.84	0.43
20:A:1793:CLA:HBC2	20:A:1793:CLA:HMC1	2.00	0.43
20:A:1811:CLA:HBB1	6:B:624:LEU:HD11	2.00	0.43
21:A:7016:LMU:O6'	21:A:7016:LMU:H41	2.17	0.43
21:A:7019:LMU:H101	21:A:7019:LMU:H72	1.67	0.43
21:A:7026:LMU:H82	21:A:7026:LMU:C4	2.29	0.43
21:A:7032:LMU:H22	21:A:7032:LMU:C6B	2.44	0.43
21:A:7034:LMU:H5'	21:A:7034:LMU:H1B	1.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:91:ILE:HD12	20:B:1740:CLA:HMD3	2.00	0.43
6:B:278:LEU:CD1	20:B:1746:CLA:HMA2	2.42	0.43
6:B:414:HIS:CD2	6:B:414:HIS:O	2.71	0.43
6:B:421:HIS:O	20:B:1769:CLA:HMC3	2.18	0.43
6:B:555:TYR:HE2	6:B:573:TRP:HD1	1.67	0.43
6:B:715:VAL:O	6:B:719:PHE:HB2	2.18	0.43
20:B:1736:CLA:H2A	20:B:1736:CLA:O1D	2.18	0.43
20:B:1755:CLA:HBB1	20:B:1769:CLA:HBB	1.95	0.43
7:C:12:ILE:HD12	7:C:12:ILE:H	1.81	0.43
10:F:22:LEU:CB	10:F:25:LEU:HD13	2.48	0.43
10:F:52:ARG:N	10:F:52:ARG:HD2	2.33	0.43
12:H:27:ASP:O	12:H:29:PRO:CD	2.67	0.43
16:L:64:LEU:CD2	16:L:91:LEU:HD22	2.48	0.43
1:1:55:PRO:HA	1:1:58:LEU:HB2	2.01	0.43
1:1:161:PHE:CD1	20:1:1189:CLA:CBB	3.01	0.43
5:A:48:PRO:HB3	9:E:72:VAL:HG22	2.01	0.43
5:A:141:ARG:HE	10:F:40:LEU:H	1.67	0.43
5:A:545:HIS:HB3	20:A:1792:CLA:CBB	2.30	0.43
5:A:551:VAL:HG21	5:A:604:TRP:CZ2	2.54	0.43
5:A:554:LEU:HD21	20:B:1787:CLA:O2D	2.18	0.43
20:A:1759:CLA:O1A	20:A:1796:CLA:H52	2.19	0.43
6:B:42:LEU:O	6:B:43:TYR:O	2.37	0.43
6:B:175:LEU:O	6:B:179:LEU:CG	2.66	0.43
23:B:1773:PQN:H2M1	23:B:1773:PQN:C14	2.47	0.43
8:D:75:LEU:HD11	16:L:19:PHE:CD1	2.54	0.43
8:D:83:CYS:O	8:D:83:CYS:SG	2.77	0.43
8:D:84:LEU:HD12	8:D:100:PHE:CZ	2.50	0.43
8:D:149:THR:O	8:D:151:LYS:N	2.51	0.43
9:E:44:TYR:HD2	9:E:45:TRP:HE3	1.66	0.43
11:G:42:SER:HG	11:G:45:GLU:CB	2.31	0.43
11:G:88:THR:HG23	11:G:91:ASN:O	2.18	0.43
14:J:32:PHE:HE2	14:J:33:PHE:CE1	2.37	0.43
14:J:32:PHE:CE2	14:J:33:PHE:CZ	3.05	0.43
15:K:51:ASP:CB	15:K:52:PRO:CD	2.91	0.43
20:L:1505:CLA:HAA2	20:L:1505:CLA:HBD	2.00	0.43
3:3:192:LEU:C	3:3:194:ILE:H	2.23	0.43
4:4:70:ILE:O	4:4:72:VAL:N	2.52	0.43
4:4:73:PRO:O	4:4:74:LYS:HB2	2.19	0.43
5:A:78:VAL:O	5:A:82:HIS:CG	2.72	0.43
5:A:105:ASN:HB3	5:A:150:PHE:HZ	1.84	0.43
5:A:154:ARG:NH2	5:A:233:LEU:CD1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:154:ARG:NE	5:A:154:ARG:HA	2.33	0.43
5:A:304:LEU:CD2	20:A:1772:CLA:CBB	2.70	0.43
5:A:361:ASN:O	5:A:364:MET:N	2.52	0.43
5:A:413:HIS:CG	5:A:416:ILE:HD12	2.54	0.43
20:A:1778:CLA:HAA1	15:K:32:ARG:HD3	2.01	0.43
20:A:1796:CLA:HBA2	20:A:1796:CLA:H3A	1.48	0.43
20:A:1797:CLA:H71	20:A:1797:CLA:C12	2.09	0.43
21:A:7042:LMU:H4'	21:A:7042:LMU:H1'	1.56	0.43
6:B:17:THR:CA	6:B:696:LYS:H	2.31	0.43
6:B:114:ASN:O	6:B:115:ASN:OD1	2.37	0.43
6:B:400:PRO:HG2	8:D:141:VAL:C	2.39	0.43
6:B:661:PHE:O	6:B:665:ILE:N	2.51	0.43
6:B:662:MET:HB3	6:B:663:PHE:H	1.55	0.43
20:B:1767:CLA:HAA1	20:B:1768:CLA:HAA2	2.00	0.43
8:D:126:GLY:C	8:D:127:ARG:CG	2.86	0.43
10:F:104:TYR:N	10:F:129:LEU:HD13	2.34	0.43
11:G:48:ASP:HB3	11:G:49:THR:CB	2.44	0.43
11:G:62:ASP:HB2	11:G:63:PRO:CD	2.45	0.43
14:J:10:VAL:HG13	14:J:14:LEU:CG	2.42	0.43
17:N:78:GLY:O	17:N:82:PHE:CE2	2.72	0.43
3:3:194:ILE:HG13	20:3:1212:CLA:C2C	2.49	0.42
5:A:40:PHE:CD1	5:A:40:PHE:O	2.72	0.42
5:A:114:THR:HG1	5:A:525:ASN:HB2	1.77	0.42
5:A:219:ALA:O	5:A:222:GLN:N	2.48	0.42
20:A:1772:CLA:HBD	20:A:1772:CLA:HAA1	2.00	0.42
6:B:167:TRP:CD1	11:G:41:MET:CE	3.02	0.42
6:B:182:LEU:HG	6:B:183:PHE:H	1.84	0.42
6:B:182:LEU:HG	6:B:183:PHE:N	2.33	0.42
6:B:188:LEU:CD1	20:B:1745:CLA:CBB	2.92	0.42
6:B:332:PHE:HE1	6:B:408:LEU:HD21	1.85	0.42
6:B:393:PHE:CE2	6:B:398:TYR:HB2	2.54	0.42
6:B:685:THR:HA	6:B:686:PRO:HD3	1.92	0.42
20:B:1758:CLA:H122	22:B:1775:BCR:C14	2.49	0.42
22:B:1777:BCR:H351	22:B:1777:BCR:H15C	1.82	0.42
20:B:1785:CLA:H11	20:B:1785:CLA:HAA2	2.01	0.42
21:L:1171:LMU:H81	21:L:1171:LMU:O6'	2.18	0.42
3:3:49:ILE:O	3:3:49:ILE:HG23	2.19	0.42
3:3:84:ILE:CA	20:A:1798:CLA:C5	2.86	0.42
3:3:127:ARG:HG2	3:3:131:ASP:OD1	2.18	0.42
20:3:3011:CLA:H101	20:3:3011:CLA:H142	2.01	0.42
4:4:103:ILE:HG13	20:4:1197:CLA:CMD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:86:LEU:HA	5:A:89:ILE:HD12	2.00	0.42
5:A:96:MET:N	5:A:98:PHE:O	2.51	0.42
5:A:149:PHE:C	5:A:151:GLN:N	2.71	0.42
5:A:227:LEU:O	5:A:231:GLN:HB2	2.18	0.42
5:A:654:ARG:HG3	5:A:655:ASP:N	2.33	0.42
5:A:700:TRP:CE2	23:A:1802:PQN:H2M3	2.53	0.42
5:A:723:ARG:H	20:A:1795:CLA:CBB	2.31	0.42
5:A:748:ALA:O	5:A:749:PHE:C	2.57	0.42
20:A:1773:CLA:H3A	20:A:1773:CLA:HBA2	1.24	0.42
20:A:1789:CLA:C4	16:L:64:LEU:CD2	2.93	0.42
20:A:1792:CLA:CBA	20:A:1792:CLA:CBD	2.97	0.42
20:A:1812:CLA:H122	20:A:1812:CLA:C9	2.46	0.42
6:B:172:GLU:O	6:B:176:ASN:N	2.51	0.42
6:B:440:ASN:OD1	6:B:452:GLN:NE2	2.52	0.42
6:B:531:THR:O	6:B:535:VAL:N	2.49	0.42
6:B:724:PHE:CZ	20:B:1785:CLA:HMD1	2.54	0.42
20:B:1741:CLA:HBD	20:B:1741:CLA:CGA	2.49	0.42
20:B:1747:CLA:HMC2	20:B:1747:CLA:H141	2.01	0.42
8:D:20:LEU:O	8:D:21:ASP:C	2.58	0.42
9:E:40:ARG:N	9:E:46:PHE:CE1	2.82	0.42
10:F:26:GLN:HB3	10:F:27:ALA:H	1.69	0.42
10:F:99:TRP:CZ3	10:F:140:ALA:HB2	2.55	0.42
10:F:128:SER:C	10:F:130:LEU:HD23	2.40	0.42
22:I:1032:BCR:C39	22:L:1169:BCR:C40	2.96	0.42
22:L:1170:BCR:H342	22:L:1170:BCR:HC7	1.53	0.42
17:N:4:GLU:OE2	17:N:5:GLU:N	2.52	0.42
1:1:181:LEU:O	1:1:182:ALA:HB2	2.19	0.42
20:1:1189:CLA:O1A	20:1:1189:CLA:C2	2.66	0.42
20:2:1212:CLA:CBC	20:2:1212:CLA:CMC	2.63	0.42
20:3:1219:CLA:HAA2	20:3:1219:CLA:HBD	2.00	0.42
5:A:29:THR:OG1	5:A:31:PHE:HB2	2.19	0.42
5:A:64:PHE:HZ	5:A:77:LYS:CE	2.32	0.42
5:A:173:VAL:HG23	5:A:174:PHE:N	2.34	0.42
5:A:306:ILE:O	5:A:309:LEU:N	2.52	0.42
5:A:343:HIS:O	5:A:346:LEU:HB2	2.19	0.42
5:A:388:ASP:O	5:A:390:ALA:N	2.52	0.42
5:A:515:TRP:CZ2	20:A:1782:CLA:HMC3	2.54	0.42
5:A:541:VAL:O	5:A:544:ILE:HG22	2.18	0.42
5:A:588:GLY:N	6:B:668:ARG:CD	2.73	0.42
5:A:591:GLN:HA	5:A:591:GLN:NE2	2.26	0.42
5:A:693:LEU:CD2	5:A:734:GLY:HA3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:694:PHE:CZ	6:B:661:PHE:CD1	3.07	0.42
20:A:1764:CLA:CGA	20:A:1783:CLA:H11	2.49	0.42
20:A:1779:CLA:HBC1	22:A:1805:BCR:H393	2.02	0.42
20:A:1815:CLA:HMA1	20:A:1815:CLA:C5	2.49	0.42
6:B:25:ILE:H	6:B:25:ILE:HG13	1.56	0.42
6:B:175:LEU:HD11	20:B:1749:CLA:CMA	2.49	0.42
6:B:176:ASN:ND2	6:B:292:ARG:O	2.52	0.42
6:B:260:GLY:O	6:B:262:HIS:NE2	2.51	0.42
6:B:262:HIS:HA	6:B:263:PRO:HD2	1.92	0.42
6:B:278:LEU:O	6:B:279:ALA:C	2.58	0.42
6:B:393:PHE:CZ	6:B:398:TYR:CD2	3.07	0.42
6:B:674:LEU:C	6:B:674:LEU:CD1	2.88	0.42
20:B:1745:CLA:C4B	22:B:1774:BCR:H291	2.49	0.42
20:B:1751:CLA:HBA2	20:B:1752:CLA:O1A	2.18	0.42
20:B:1757:CLA:H71	20:B:1757:CLA:H41	2.01	0.42
20:B:1768:CLA:CBB	20:B:1768:CLA:C9	2.54	0.42
20:B:1770:CLA:H191	13:I:21:MET:CE	2.49	0.42
10:F:96:TRP:HZ3	10:F:134:PHE:CB	2.21	0.42
11:G:60:SER:C	11:G:62:ASP:N	2.71	0.42
16:L:12:GLN:HA	16:L:13:PRO:HD3	1.82	0.42
20:L:1168:CLA:O1D	20:L:1168:CLA:CAA	2.63	0.42
19:U:1:GLC:O5	19:U:2:FRU:O4	2.36	0.42
1:1:25:ASP:CB	1:1:26:PRO:CD	2.97	0.42
20:2:1217:CLA:H41	20:2:1217:CLA:H72	2.01	0.42
3:3:66:MET:HE1	3:3:69:ALA:HB3	2.01	0.42
4:4:106:TRP:HE3	20:4:1207:CLA:HMA1	1.84	0.42
4:4:193:ILE:CG2	4:4:194:VAL:H	2.29	0.42
5:A:59:ALA:C	5:A:61:ALA:N	2.72	0.42
5:A:97:TYR:HA	5:A:153:TRP:HZ2	1.85	0.42
5:A:179:LEU:O	5:A:179:LEU:HD13	2.19	0.42
5:A:281:LEU:HB2	5:A:301:HIS:CD2	2.52	0.42
5:A:374:GLN:C	5:A:376:MET:H	2.21	0.42
5:A:422:TYR:N	5:A:422:TYR:HD1	2.11	0.42
5:A:536:THR:HA	5:A:539:PHE:HB2	2.01	0.42
5:A:570:PRO:C	5:A:572:LYS:N	2.72	0.42
20:A:1800:CLA:H201	16:L:64:LEU:CG	2.50	0.42
22:A:1804:BCR:H15C	22:A:1804:BCR:H351	1.81	0.42
20:A:1815:CLA:H61	20:A:1815:CLA:H2	1.82	0.42
6:B:8:PHE:CD2	6:B:34:HIS:ND1	2.87	0.42
6:B:123:TRP:CZ3	20:B:1743:CLA:C19	2.99	0.42
6:B:632:ILE:C	6:B:634:GLY:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1764:CLA:ND	20:B:1765:CLA:CBB	2.82	0.42
20:B:1787:CLA:CGA	20:B:1787:CLA:C3A	2.92	0.42
8:D:151:LYS:NZ	8:D:151:LYS:HB3	2.33	0.42
10:F:22:LEU:HA	10:F:25:LEU:CD1	2.49	0.42
11:G:5:SER:O	11:G:7:VAL:CG1	2.67	0.42
11:G:28:ARG:HG2	11:G:29:GLU:CB	2.50	0.42
11:G:75:GLY:O	11:G:80:ILE:HG23	2.19	0.42
20:K:1146:CLA:C3A	20:K:1146:CLA:CGA	2.96	0.42
19:X:1:GLC:C5	19:X:2:FRU:H12	2.47	0.42
1:1:60:PRO:O	1:1:61:GLU:HB3	2.19	0.42
1:1:113:SER:O	1:1:114:MET:HG3	2.20	0.42
20:2:1217:CLA:OBD	20:2:1217:CLA:HED2	2.19	0.42
5:A:90:PHE:HB3	5:A:175:ALA:HB2	2.01	0.42
5:A:164:LEU:HA	5:A:167:THR:CG2	2.46	0.42
5:A:183:TRP:C	5:A:185:HIS:H	2.23	0.42
5:A:382:TYR:CD2	20:A:1784:CLA:HED3	2.54	0.42
5:A:729:GLN:O	5:A:732:ALA:HB3	2.19	0.42
20:A:1759:CLA:H42	20:A:1796:CLA:C8	2.46	0.42
20:A:1787:CLA:H72	20:A:1801:CLA:CBA	2.50	0.42
20:A:1789:CLA:H41	20:A:1789:CLA:H61	1.64	0.42
21:A:7016:LMU:H6'	21:A:7016:LMU:H12	1.84	0.42
21:A:7021:LMU:H22	21:A:7021:LMU:O6'	2.14	0.42
21:A:7037:LMU:H12	21:A:7037:LMU:H41	1.45	0.42
6:B:145:LEU:HA	6:B:145:LEU:HD22	1.83	0.42
6:B:199:ILE:N	6:B:200:PRO:HD2	2.34	0.42
6:B:269:TRP:CG	6:B:497:TRP:HH2	2.37	0.42
6:B:336:LEU:HD13	20:B:1754:CLA:CBB	2.48	0.42
6:B:470:THR:H	6:B:501:ILE:HG23	1.84	0.42
6:B:477:PRO:O	6:B:478:LEU:HD22	2.19	0.42
6:B:505:SER:O	6:B:506:ASN:HB3	2.19	0.42
6:B:542:ARG:HH21	8:D:143:PRO:HG3	1.80	0.42
6:B:603:ARG:HB3	6:B:734:GLY:H	1.84	0.42
6:B:641:ASN:HB3	6:B:642:SER:H	1.72	0.42
20:B:1737:CLA:HMC3	20:B:1759:CLA:H3A	2.00	0.42
20:B:1759:CLA:HHD	24:B:1783:LMG:H352	2.01	0.42
24:B:1783:LMG:H292	24:B:1783:LMG:H112	2.00	0.42
15:K:35:THR:HG23	15:K:36:ALA:H	1.84	0.42
16:L:62:PHE:HE2	20:L:1168:CLA:H2A	1.84	0.42
16:L:99:LEU:HB3	16:L:140:THR:HG21	2.02	0.42
20:L:1166:CLA:H11	20:L:1166:CLA:C4D	2.49	0.42
17:N:62:SER:HA	17:N:64:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:1056:LMU:H62	21:R:1056:LMU:H32	1.69	0.42
21:2:7006:LMU:H3'	21:2:7006:LMU:C6B	2.50	0.42
3:3:182:LYS:O	3:3:186:ASN:N	2.33	0.42
22:3:1220:BCR:H11C	22:3:1220:BCR:H341	1.56	0.42
4:4:70:ILE:HG13	4:4:71:ASN:N	2.35	0.42
5:A:299:ILE:HD12	5:A:299:ILE:HA	1.69	0.42
5:A:372:VAL:HG22	20:A:1774:CLA:C4	2.49	0.42
5:A:419:VAL:HG21	5:A:577:PHE:HB2	2.01	0.42
5:A:467:MET:HE1	5:A:475:ASP:C	2.40	0.42
5:A:650:ASN:C	5:A:652:TRP:N	2.71	0.42
20:A:1774:CLA:HBA2	20:A:1774:CLA:H3A	1.72	0.42
20:A:1792:CLA:HBA2	20:A:1792:CLA:CBD	2.49	0.42
22:A:1805:BCR:H351	22:A:1805:BCR:H15C	1.84	0.42
22:A:1806:BCR:H15C	22:A:1806:BCR:H351	1.87	0.42
21:A:1810:LMU:H41	21:A:1810:LMU:H12	1.71	0.42
6:B:16:PRO:HG3	7:C:74:THR:HG22	2.01	0.42
6:B:242:HIS:CE1	6:B:244:PHE:HA	2.55	0.42
6:B:274:ALA:HA	6:B:277:HIS:HB2	2.00	0.42
6:B:354:SER:OG	20:B:1756:CLA:HBC3	2.19	0.42
6:B:494:LEU:HD12	20:B:1765:CLA:CED	2.48	0.42
6:B:543:GLY:HA3	6:B:548:PRO:O	2.20	0.42
6:B:561:GLY:H	7:C:66:ARG:HB3	1.85	0.42
6:B:649:MET:CG	22:B:1780:BCR:H272	2.49	0.42
6:B:684:ARG:HD3	6:B:684:ARG:HA	1.74	0.42
20:B:1738:CLA:H192	20:B:1757:CLA:H141	2.02	0.42
20:B:1739:CLA:HMB3	20:I:1031:CLA:HMA1	2.00	0.42
20:B:1765:CLA:CBB	22:B:1777:BCR:C28	2.98	0.42
7:C:27:GLU:OE1	7:C:40:ALA:HB3	2.19	0.42
8:D:41:GLN:NE2	8:D:42:VAL:HA	2.34	0.42
9:E:87:VAL:C	9:E:89:GLU:N	2.67	0.42
12:H:36:GLN:O	12:H:36:GLN:CG	2.68	0.42
16:L:65:VAL:O	16:L:69:VAL:N	2.53	0.42
16:L:135:GLY:HA2	16:L:138:LYS:HE2	2.02	0.42
16:L:149:SER:C	16:L:151:VAL:N	2.72	0.42
18:R:38:UNK:C	18:R:42:UNK:CA	2.97	0.42
19:T:1:GLC:O2	19:T:2:FRU:O1	2.29	0.42
19:Z:1:GLC:HO6	19:Z:2:FRU:C2	2.31	0.42
20:1:1200:CLA:HBA1	20:1:1200:CLA:H3A	1.42	0.42
5:A:79:PHE:CE2	5:A:185:HIS:CG	2.93	0.42
5:A:82:HIS:CE1	20:A:1761:CLA:C1A	3.02	0.42
5:A:150:PHE:O	5:A:151:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:408:VAL:O	5:A:411:ALA:HB3	2.20	0.42
5:A:579:PHE:HA	5:A:580:PRO:HD2	1.66	0.42
5:A:648:THR:C	5:A:650:ASN:H	2.23	0.42
20:A:1763:CLA:HMB2	22:A:1808:BCR:H342	2.01	0.42
20:A:1777:CLA:HBA2	20:A:1777:CLA:H3A	1.63	0.42
20:A:1778:CLA:HED2	20:A:1778:CLA:CBA	2.49	0.42
20:A:1788:CLA:H192	20:B:1770:CLA:HMB2	2.01	0.42
20:A:1800:CLA:CGA	20:A:1800:CLA:CHA	2.98	0.42
6:B:454:LEU:HD13	10:F:69:PRO:O	2.15	0.42
8:D:49:THR:C	8:D:50:TRP:HD1	2.23	0.42
9:E:36:VAL:CG2	9:E:52:VAL:CG2	2.97	0.42
10:F:44:ALA:O	10:F:46:MET:HG2	2.20	0.42
10:F:78:ARG:O	10:F:80:TRP:CD1	2.69	0.42
10:F:126:ALA:HB1	10:F:129:LEU:HD12	2.02	0.42
11:G:32:ALA:O	11:G:34:GLN:C	2.57	0.42
16:L:98:CYS:SG	22:L:1169:BCR:C12	3.08	0.42
21:2:7003:LMU:H22	21:2:7003:LMU:O2'	2.20	0.42
21:2:7006:LMU:C2	21:2:7006:LMU:H2'	2.48	0.42
3:3:96:GLY:C	3:3:97:PHE:CG	2.92	0.42
4:4:60:LEU:HG	4:4:61:PRO:HD3	2.02	0.42
5:A:132:LEU:HD23	6:B:446:PHE:HE1	1.85	0.42
5:A:163:GLN:HA	5:A:166:CYS:SG	2.60	0.42
5:A:210:LEU:N	5:A:213:LEU:N	2.68	0.42
5:A:244:LEU:H	5:A:244:LEU:HD12	1.85	0.42
5:A:315:HIS:HB2	20:A:1778:CLA:HBC1	2.02	0.42
5:A:500:PRO:HA	5:A:504:ALA:HB1	2.01	0.42
5:A:575:LEU:HD13	5:A:576:GLY:H	1.85	0.42
20:A:1777:CLA:H52	20:A:1777:CLA:C1C	2.50	0.42
21:A:7041:LMU:H1B	21:A:7041:LMU:H4B	1.52	0.42
6:B:216:LEU:HD22	6:B:218:TYR:H	1.85	0.42
6:B:587:ILE:O	6:B:587:ILE:CG2	2.67	0.42
6:B:661:PHE:O	6:B:662:MET:O	2.37	0.42
20:B:1743:CLA:HHD	20:B:1743:CLA:HAC2	1.84	0.42
8:D:133:ASN:C	8:D:134:MET:SD	2.94	0.42
9:E:69:PHE:CD2	9:E:71:LYS:N	2.82	0.42
11:G:20:ARG:NH2	11:G:61:ASN:C	2.73	0.42
11:G:45:GLU:C	11:G:49:THR:CG2	2.62	0.42
11:G:50:ARG:HB2	11:G:51:ALA:CA	2.50	0.42
12:H:50:ARG:NH1	12:H:53:LEU:C	2.63	0.42
15:K:24:PHE:CB	15:K:52:PRO:HG2	2.43	0.42
21:K:1086:LMU:H52	20:K:1146:CLA:HMD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:149:SER:C	16:L:151:VAL:H	2.23	0.42
17:N:45:ASN:HA	17:N:57:LYS:HZ3	1.84	0.42
3:3:52:LYS:O	3:3:56:TYR:CB	2.68	0.42
3:3:106:TYR:CB	3:3:107:TRP:HD1	2.32	0.42
3:3:207:GLY:O	3:3:208:PRO:C	2.58	0.42
20:4:1209:CLA:C3D	20:4:1209:CLA:O1D	2.57	0.42
5:A:90:PHE:CD1	20:A:1761:CLA:H91	2.53	0.42
5:A:98:PHE:CD1	5:A:98:PHE:C	2.93	0.42
5:A:163:GLN:CG	5:A:164:LEU:N	2.82	0.42
5:A:204:ASN:HA	5:A:314:GLY:O	2.20	0.42
5:A:277:TYR:CD2	5:A:278:ALA:N	2.88	0.42
5:A:452:PHE:HE1	20:A:1793:CLA:CAB	2.27	0.42
5:A:621:GLN:HG2	5:A:637:ILE:CD1	2.39	0.42
5:A:664:VAL:HG11	5:A:749:PHE:HA	2.01	0.42
21:A:7037:LMU:C6'	21:A:7037:LMU:H3O2	2.20	0.42
6:B:175:LEU:HD11	20:B:1749:CLA:HMA1	2.02	0.42
6:B:269:TRP:HA	6:B:269:TRP:CE3	2.55	0.42
6:B:373:THR:C	6:B:376:GLN:H	2.23	0.42
6:B:503:GLU:CA	6:B:507:SER:HB2	2.50	0.42
6:B:588:GLY:O	6:B:592:PHE:CB	2.51	0.42
20:B:1753:CLA:H43	20:B:1753:CLA:C2A	2.41	0.42
8:D:100:PHE:O	8:D:113:HIS:HB2	2.20	0.42
10:F:96:TRP:CZ3	10:F:134:PHE:N	2.87	0.42
10:F:131:PHE:O	10:F:132:ARG:C	2.56	0.42
14:J:38:THR:O	14:J:39:PHE:CB	2.68	0.42
21:R:1057:LMU:H1B	21:R:1057:LMU:H3'	1.31	0.42
19:U:2:FRU:O3	19:U:2:FRU:O1	2.30	0.42
2:2:70:LYS:O	2:2:73:ILE:N	2.52	0.42
2:2:103:GLY:HA2	20:2:1222:CLA:CAB	2.49	0.42
3:3:83:LEU:C	20:A:1798:CLA:C4	2.88	0.42
3:3:94:ARG:CA	3:3:97:PHE:HE1	2.33	0.42
4:4:52:MET:C	4:4:54:GLY:H	2.23	0.42
4:4:193:ILE:CG2	14:J:42:PHE:CD1	2.87	0.42
5:A:51:THR:OG1	20:A:1795:CLA:CAB	2.68	0.42
5:A:210:LEU:HD23	5:A:211:LEU:N	2.35	0.42
5:A:302:HIS:HE2	20:A:1774:CLA:HMB3	1.84	0.42
5:A:368:LEU:HD12	20:A:1782:CLA:H62	2.01	0.42
5:A:372:VAL:HG22	20:A:1774:CLA:H41	2.01	0.42
5:A:672:LEU:H	5:A:672:LEU:CD2	2.33	0.42
20:A:1777:CLA:O2D	20:A:1777:CLA:OBD	2.38	0.42
23:A:1802:PQN:H251	20:B:1735:CLA:HMC1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:7026:LMU:O3B	19:Z:2:FRU:C6	2.58	0.42
6:B:199:ILE:HG22	6:B:203:ARG:CZ	2.50	0.42
6:B:310:PRO:CG	6:B:311:PRO:CD	2.87	0.42
6:B:350:GLN:HG3	6:B:372:TYR:HE1	1.84	0.42
6:B:541:ALA:HB2	6:B:572:ALA:CB	2.50	0.42
6:B:593:TYR:CD1	20:B:1767:CLA:HMC2	2.55	0.42
6:B:693:TRP:CD1	20:B:1770:CLA:CMD	3.03	0.42
6:B:721:TYR:N	20:B:1785:CLA:O1D	2.53	0.42
20:B:1756:CLA:H201	20:B:1769:CLA:C2	2.50	0.42
20:B:1758:CLA:C19	22:B:1776:BCR:H14C	2.50	0.42
7:C:5:VAL:HG23	7:C:65:VAL:HG21	1.23	0.42
10:F:44:ALA:O	10:F:46:MET:N	2.52	0.42
11:G:43:HIS:C	11:G:45:GLU:CA	2.88	0.42
14:J:31:ARG:HH21	20:J:1043:CLA:C3B	2.32	0.42
16:L:64:LEU:CA	16:L:67:PRO:HG2	2.46	0.42
17:N:29:PHE:O	17:N:33:TYR:N	2.53	0.42
17:N:72:LYS:HB3	17:N:74:LYS:HB2	1.98	0.42
2:2:163:GLU:O	2:2:167:GLY:N	2.52	0.41
2:2:197:LEU:HD21	5:A:162:LEU:CD2	2.45	0.41
3:3:114:PHE:HD1	20:3:1216:CLA:CHA	2.31	0.41
20:3:1218:CLA:CAA	20:3:1218:CLA:CBD	2.98	0.41
20:3:3011:CLA:H71	20:3:3011:CLA:H112	1.55	0.41
20:3:3011:CLA:HBA2	20:3:3011:CLA:H11	1.91	0.41
4:4:127:PRO:C	4:4:143:PHE:HZ	2.22	0.41
5:A:87:SER:HA	5:A:90:PHE:HB2	2.02	0.41
5:A:92:TRP:C	5:A:94:SER:H	2.22	0.41
5:A:159:THR:OG1	5:A:239:PRO:HB3	2.20	0.41
5:A:183:TRP:C	5:A:185:HIS:N	2.74	0.41
5:A:207:LEU:HD11	5:A:313:ALA:CB	2.50	0.41
5:A:254:LEU:HD13	5:A:254:LEU:HA	1.66	0.41
5:A:302:HIS:NE2	20:A:1774:CLA:HMB3	2.34	0.41
5:A:345:GLY:C	5:A:347:TYR:N	2.66	0.41
5:A:538:ASP:O	5:A:542:HIS:CD2	2.73	0.41
5:A:681:GLY:O	5:A:682:ALA:HB3	2.19	0.41
20:A:1761:CLA:C4B	20:A:1785:CLA:HMB2	2.50	0.41
20:A:1781:CLA:CED	20:A:1781:CLA:HAA1	2.50	0.41
20:A:1795:CLA:H43	10:F:121:ILE:HD13	2.01	0.41
20:A:1816:CLA:CGD	20:A:1816:CLA:C2A	2.88	0.41
6:B:120:VAL:O	6:B:123:TRP:HD1	2.02	0.41
6:B:518:LEU:O	6:B:519:VAL:C	2.59	0.41
6:B:691:ILE:HA	16:L:102:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1749:CLA:HBB2	20:B:1754:CLA:C4	2.48	0.41
20:B:1753:CLA:H161	20:B:1753:CLA:H141	1.65	0.41
9:E:36:VAL:CG1	9:E:87:VAL:HG11	2.49	0.41
10:F:147:GLY:O	10:F:149:LEU:O	2.38	0.41
11:G:46:ALA:C	11:G:48:ASP:CB	2.82	0.41
11:G:83:TYR:O	11:G:83:TYR:CD1	2.72	0.41
11:G:93:TYR:CB	11:G:94:ASP:HB2	2.43	0.41
14:J:2:ARG:HB3	14:J:7:TYR:CE1	2.55	0.41
3:3:84:ILE:H	20:A:1798:CLA:C5	2.30	0.41
3:3:88:THR:H	22:3:1220:BCR:H383	1.79	0.41
3:3:111:TYR:HB2	3:3:112:THR:CG2	2.51	0.41
5:A:21:LEU:O	5:A:21:LEU:HD13	2.16	0.41
5:A:35:ALA:O	5:A:36:LYS:HB2	2.20	0.41
5:A:67:HIS:O	5:A:68:THR:HB	2.21	0.41
5:A:599:PHE:CD1	5:A:600:LEU:HD23	2.36	0.41
5:A:620:MET:HG3	5:A:625:TRP:CD2	2.54	0.41
5:A:662:SER:HA	5:A:665:ILE:CD1	2.50	0.41
5:A:677:LEU:HD11	6:B:442:VAL:HG13	2.01	0.41
5:A:690:LEU:HD22	6:B:661:PHE:HE1	1.84	0.41
20:A:1767:CLA:H72	20:A:1767:CLA:H111	1.50	0.41
20:A:1774:CLA:HMB2	20:A:1774:CLA:H2	2.02	0.41
21:A:7033:LMU:C2'	21:A:7033:LMU:O6B	2.68	0.41
21:A:7042:LMU:H71	21:A:7042:LMU:H11	2.00	0.41
6:B:75:GLU:HB2	6:B:132:ASN:CB	2.42	0.41
6:B:292:ARG:NE	6:B:292:ARG:CA	2.65	0.41
6:B:392:ILE:CD1	20:B:1759:CLA:O2D	2.68	0.41
6:B:429:LEU:HD11	20:B:1768:CLA:CMB	2.50	0.41
22:B:1780:BCR:H353	20:B:1787:CLA:H122	2.02	0.41
8:D:48:ILE:HA	8:D:100:PHE:HB3	2.01	0.41
8:D:53:PRO:HB2	8:D:54:LYS:H	1.63	0.41
11:G:28:ARG:HG3	11:G:29:GLU:CB	2.50	0.41
11:G:79:HIS:CG	11:G:79:HIS:O	2.72	0.41
17:N:57:LYS:O	17:N:60:PHE:HD1	2.00	0.41
1:1:38:ARG:O	1:1:41:GLU:HB2	2.21	0.41
21:1:7004:LMU:C1B	21:1:7004:LMU:O3'	2.68	0.41
20:2:1220:CLA:C4	3:3:140:LYS:HE2	2.46	0.41
3:3:153:SER:C	3:3:161:GLY:HA2	2.41	0.41
4:4:104:ARG:HB2	4:4:107:GLN:HE21	1.85	0.41
5:A:75:SER:HB3	5:A:354:TRP:HZ2	1.83	0.41
5:A:177:LEU:HD22	5:A:177:LEU:HA	1.90	0.41
5:A:207:LEU:CB	20:A:1776:CLA:CBB	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:499:ALA:HB3	20:A:1790:CLA:CED	2.50	0.41
5:A:547:PHE:CD1	5:A:547:PHE:C	2.90	0.41
5:A:733:VAL:HG13	20:A:1796:CLA:C3D	2.50	0.41
21:A:7032:LMU:H31	21:A:7032:LMU:H4B	2.03	0.41
6:B:378:ILE:H	6:B:381:PHE:HD1	1.69	0.41
6:B:534:LEU:CD2	6:B:579:ALA:HB2	2.50	0.41
6:B:625:TRP:C	6:B:625:TRP:CD2	2.92	0.41
6:B:658:ALA:O	6:B:661:PHE:CD2	2.69	0.41
6:B:707:LEU:HD23	24:B:1783:LMG:H132	2.02	0.41
20:B:1737:CLA:HBA1	20:B:1743:CLA:HBA1	2.02	0.41
20:B:1737:CLA:H162	20:B:1743:CLA:OBD	2.20	0.41
20:B:1760:CLA:H3A	20:B:1760:CLA:HBA2	1.49	0.41
20:B:1768:CLA:H161	20:B:1768:CLA:H203	1.91	0.41
16:L:68:PHE:CD1	16:L:68:PHE:N	2.89	0.41
17:N:45:ASN:HA	17:N:57:LYS:HZ2	1.84	0.41
17:N:72:LYS:CD	17:N:74:LYS:HG3	2.43	0.41
1:1:34:ALA:O	1:1:35:ASN:C	2.59	0.41
1:1:51:MET:SD	1:1:54:VAL:HB	2.61	0.41
20:2:1213:CLA:CHD	20:2:1213:CLA:C4	2.98	0.41
20:2:1213:CLA:HBA2	20:2:1213:CLA:H3A	1.80	0.41
21:2:7003:LMU:H3B	19:T:2:FRU:O4	2.20	0.41
20:3:1215:CLA:C3B	20:3:1218:CLA:H11	2.50	0.41
4:4:107:GLN:O	20:4:1196:CLA:HMA1	2.20	0.41
4:4:193:ILE:CG2	4:4:194:VAL:N	2.83	0.41
5:A:113:PRO:C	5:A:115:HIS:N	2.71	0.41
5:A:536:THR:O	5:A:537:ALA:HB3	2.20	0.41
5:A:561:LEU:HA	5:A:561:LEU:HD23	1.76	0.41
5:A:667:SER:O	5:A:667:SER:OG	2.38	0.41
5:A:705:GLU:OE1	5:A:708:VAL:HG12	2.20	0.41
21:A:7039:LMU:H92	21:A:7039:LMU:H61	1.71	0.41
6:B:32:GLU:N	6:B:42:LEU:HD13	2.36	0.41
6:B:190:TRP:CE3	20:B:1744:CLA:HBB2	2.51	0.41
6:B:340:SER:CA	20:B:1756:CLA:H51	2.29	0.41
6:B:707:LEU:O	6:B:710:LEU:CB	2.68	0.41
20:B:1764:CLA:HMD2	20:B:1765:CLA:CMC	2.50	0.41
22:B:1779:BCR:C5	20:F:1156:CLA:HMA1	2.50	0.41
11:G:24:PHE:HB3	11:G:28:ARG:HH11	1.86	0.41
20:J:1045:CLA:H93	20:J:1045:CLA:H61	1.63	0.41
16:L:33:ILE:O	16:L:35:TRP:N	2.53	0.41
17:N:9:LYS:HB3	17:N:9:LYS:HE2	1.86	0.41
17:N:72:LYS:CB	17:N:74:LYS:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:158:TYR:C	3:3:160:GLY:N	2.70	0.41
4:4:150:LYS:H	4:4:150:LYS:CE	2.33	0.41
4:4:160:MET:HG2	20:4:1201:CLA:HBB2	2.02	0.41
5:A:88:ILE:O	5:A:92:TRP:N	2.44	0.41
5:A:156:SER:HB2	5:A:159:THR:H	1.86	0.41
5:A:277:TYR:HD2	5:A:278:ALA:N	2.19	0.41
5:A:405:PHE:O	20:A:1785:CLA:HMC1	2.20	0.41
5:A:553:VAL:O	5:A:557:LEU:CB	2.68	0.41
5:A:697:ARG:CD	6:B:566:GLY:O	2.67	0.41
5:A:749:PHE:CG	20:A:1811:CLA:HMD1	2.55	0.41
20:A:1759:CLA:HBB2	20:A:1760:CLA:C1C	2.50	0.41
20:A:1776:CLA:HMB2	20:A:1780:CLA:HMA3	2.02	0.41
20:A:1813:CLA:H162	20:A:1813:CLA:H203	1.79	0.41
21:A:7016:LMU:H1'	21:A:7016:LMU:H6D	1.43	0.41
6:B:174:ARG:HH12	20:B:1754:CLA:HMD2	1.85	0.41
6:B:332:PHE:CE1	6:B:408:LEU:HD21	2.55	0.41
6:B:393:PHE:CZ	6:B:398:TYR:HD2	2.37	0.41
6:B:416:GLU:CD	6:B:416:GLU:N	2.74	0.41
6:B:448:THR:OG1	6:B:451:LYS:HB2	2.20	0.41
7:C:42:ALA:O	8:D:129:GLY:HA3	2.21	0.41
7:C:55:GLU:HG3	7:C:60:THR:HG22	2.02	0.41
10:F:23:LYS:HD2	10:F:23:LYS:HA	1.60	0.41
10:F:65:SER:C	10:F:67:GLY:H	2.23	0.41
10:F:104:TYR:OH	10:F:122:ASP:N	2.34	0.41
13:I:8:PHE:CD1	20:I:1031:CLA:H12	2.54	0.41
20:K:1146:CLA:HMA2	20:K:1146:CLA:H43	2.01	0.41
16:L:10:VAL:HG13	16:L:12:GLN:HE22	1.86	0.41
16:L:90:GLY:O	16:L:94:ILE:N	2.49	0.41
16:L:127:PRO:C	16:L:128:ASP:O	2.59	0.41
17:N:6:TYR:H	17:N:8:GLU:HA	1.85	0.41
17:N:32:ALA:CB	17:N:35:VAL:HA	2.50	0.41
2:2:187:GLY:O	2:2:189:ILE:HG12	2.20	0.41
20:2:1212:CLA:CGA	20:2:1212:CLA:C4A	2.99	0.41
20:3:1219:CLA:H61	20:3:1219:CLA:H41	1.54	0.41
5:A:74:ILE:O	5:A:78:VAL:HG13	2.20	0.41
5:A:358:LEU:HD11	5:A:413:HIS:CD2	2.53	0.41
5:A:378:SER:OG	20:A:1782:CLA:CBC	2.69	0.41
5:A:412:ALA:CB	5:A:598:VAL:HG11	2.33	0.41
5:A:509:ALA:O	5:A:510:SER:CB	2.68	0.41
5:A:523:VAL:HG13	5:A:524:GLY:N	2.36	0.41
20:A:1764:CLA:HBA2	20:A:1764:CLA:H3A	1.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:1781:CLA:C5	20:A:1782:CLA:CED	2.86	0.41
22:A:1807:BCR:C39	22:A:1807:BCR:C23	2.74	0.41
21:A:1810:LMU:H1'	21:A:1810:LMU:H21	1.60	0.41
21:A:7038:LMU:H62	21:A:7038:LMU:H91	1.93	0.41
6:B:174:ARG:C	6:B:176:ASN:H	2.24	0.41
6:B:334:LEU:HB2	20:B:1737:CLA:CMD	2.46	0.41
6:B:377:TYR:OH	6:B:717:TYR:HE1	2.04	0.41
23:B:1773:PQN:H161	23:B:1773:PQN:H141	1.42	0.41
7:C:74:THR:HB	7:C:80:ALA:HB2	1.97	0.41
8:D:102:ARG:CZ	8:D:110:GLN:HB2	2.50	0.41
10:F:100:VAL:C	10:F:103:SER:HG	2.23	0.41
12:H:54:LEU:O	12:H:54:LEU:HD22	2.21	0.41
15:K:59:ASP:HA	15:K:62:ALA:HB3	2.01	0.41
16:L:33:ILE:HG13	16:L:37:LEU:HD21	2.03	0.41
16:L:68:PHE:H	16:L:68:PHE:HD1	1.68	0.41
16:L:127:PRO:O	16:L:128:ASP:C	2.59	0.41
16:L:159:TYR:CG	16:L:159:TYR:O	2.74	0.41
17:N:69:CYS:O	17:N:72:LYS:HE3	2.20	0.41
18:R:27:UNK:C	18:R:29:UNK:C	2.98	0.41
19:W:1:GLC:C1	19:W:1:GLC:HO6	2.33	0.41
3:3:205:GLY:CA	5:A:252:ARG:NH1	2.79	0.41
20:4:1204:CLA:CHD	20:4:1204:CLA:HBC2	2.51	0.41
5:A:126:ILE:H	5:A:126:ILE:HG13	1.59	0.41
5:A:225:VAL:C	5:A:228:PRO:HD2	2.41	0.41
5:A:396:PHE:CE2	5:A:616:PHE:CB	2.94	0.41
5:A:436:LEU:O	5:A:438:HIS:O	2.37	0.41
5:A:452:PHE:HB2	20:A:1788:CLA:OBD	2.21	0.41
20:A:1761:CLA:H41	22:A:1804:BCR:C31	2.51	0.41
6:B:70:TRP:HD1	6:B:70:TRP:H	1.67	0.41
6:B:112:PRO:O	6:B:113:VAL:HG13	2.21	0.41
6:B:307:ALA:O	6:B:308:HIS:O	2.38	0.41
6:B:475:ASP:CB	6:B:480:SER:HA	2.51	0.41
6:B:534:LEU:HD21	6:B:579:ALA:HB2	2.01	0.41
6:B:707:LEU:HG	6:B:708:VAL:N	2.36	0.41
20:B:1743:CLA:H11	22:B:1775:BCR:C10	2.51	0.41
20:B:1764:CLA:ND	20:B:1765:CLA:HBB2	2.35	0.41
22:B:1781:BCR:H342	22:B:1781:BCR:HC7	1.63	0.41
7:C:60:THR:HG21	7:C:63:LEU:O	2.18	0.41
7:C:69:LEU:O	7:C:71:HIS:N	2.53	0.41
8:D:112:LEU:N	8:D:114:PRO:HG2	2.36	0.41
20:J:1044:CLA:HED2	20:J:1045:CLA:C2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:46:ALA:N	16:L:52:ARG:HH12	2.18	0.41
16:L:123:ARG:C	16:L:124:LYS:HD3	2.41	0.41
17:N:57:LYS:CG	17:N:58:VAL:N	2.26	0.41
2:2:211:LYS:HG2	3:3:113:LEU:HD11	2.01	0.41
3:3:47:GLY:O	3:3:48:PHE:CD2	2.74	0.41
3:3:49:ILE:CA	3:3:51:PRO:HD2	2.51	0.41
3:3:112:THR:HG1	3:3:113:LEU:H	1.60	0.41
3:3:120:LEU:O	3:3:123:PHE:HB3	2.21	0.41
3:3:158:TYR:CB	3:3:159:PRO:CD	2.82	0.41
4:4:34:PRO:HB2	4:4:137:ILE:HA	2.02	0.41
4:4:114:SER:O	4:4:116:ASN:N	2.54	0.41
5:A:34:TRP:O	5:A:35:ALA:HB3	2.21	0.41
5:A:112:ASP:N	5:A:113:PRO:HD3	2.36	0.41
5:A:132:LEU:HD21	5:A:674:ALA:HB2	2.03	0.41
5:A:349:ILE:CD1	5:A:422:TYR:HB3	2.51	0.41
5:A:462:ILE:CG2	20:A:1789:CLA:CMC	2.99	0.41
5:A:558:LYS:HZ1	6:B:674:LEU:HB3	1.81	0.41
5:A:583:GLY:O	5:A:589:THR:HB	2.21	0.41
5:A:690:LEU:O	5:A:694:PHE:N	2.42	0.41
5:A:705:GLU:HG2	6:B:545:LYS:NZ	2.36	0.41
20:A:1774:CLA:H8	20:A:1774:CLA:H152	2.02	0.41
20:A:1776:CLA:H112	20:A:1776:CLA:H91	1.83	0.41
20:A:1784:CLA:C4C	22:A:1804:BCR:H333	2.50	0.41
20:A:1795:CLA:O1A	20:A:1795:CLA:C2	2.68	0.41
20:A:1800:CLA:H152	22:L:1170:BCR:C35	2.47	0.41
21:A:7026:LMU:H81	21:A:7026:LMU:C4	2.40	0.41
21:A:7043:LMU:O3B	21:A:7043:LMU:H6'2	2.21	0.41
6:B:11:GLY:CA	7:C:71:HIS:CD2	2.94	0.41
6:B:22:TRP:HA	6:B:25:ILE:CD1	2.51	0.41
6:B:180:SER:OG	6:B:285:LEU:HA	2.20	0.41
6:B:301:ILE:O	6:B:301:ILE:HG23	2.21	0.41
6:B:336:LEU:CD1	20:B:1754:CLA:CBB	2.99	0.41
6:B:387:PHE:CB	6:B:534:LEU:HD13	2.50	0.41
6:B:447:GLY:C	6:B:449:PRO:HD3	2.40	0.41
6:B:527:LEU:O	20:B:1769:CLA:HMA3	2.20	0.41
6:B:568:CYS:HB3	6:B:569:ASP:H	1.67	0.41
6:B:710:LEU:HD22	6:B:710:LEU:HA	1.94	0.41
7:C:51:CYS:HB2	7:C:53:ARG:H	1.85	0.41
8:D:111:TYR:CD2	8:D:114:PRO:CG	3.04	0.41
11:G:18:LEU:HD23	11:G:18:LEU:N	2.36	0.41
12:H:55:LYS:O	12:H:56:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:1:MET:O	13:I:2:ILE:CG2	2.59	0.41
16:L:14:LEU:HD21	16:L:21:GLY:O	2.20	0.41
16:L:15:ASN:N	16:L:24:GLU:OE1	2.54	0.41
17:N:11:LYS:HE2	17:N:11:LYS:HB3	1.85	0.41
21:R:1056:LMU:H6D	21:R:1056:LMU:C5B	2.50	0.41
1:1:74:TRP:CH2	1:1:81:GLN:HA	2.56	0.41
1:1:143:LEU:HB2	1:1:144:LYS:HZ3	1.85	0.41
2:2:181:HIS:CE1	20:2:1214:CLA:C4D	3.04	0.41
3:3:56:TYR:CD1	3:3:185:LYS:NZ	2.84	0.41
4:4:52:MET:HE3	4:4:156:ASN:HB3	2.03	0.41
5:A:124:TRP:HA	5:A:124:TRP:HE3	1.84	0.41
5:A:131:ILE:HD13	6:B:446:PHE:O	2.21	0.41
5:A:158:ILE:HA	5:A:243:PRO:O	2.20	0.41
5:A:338:PHE:CD2	5:A:338:PHE:C	2.94	0.41
5:A:379:MET:CE	20:A:1782:CLA:HMC2	2.51	0.41
5:A:527:VAL:HG12	5:A:528:ALA:O	2.21	0.41
5:A:541:VAL:HA	5:A:544:ILE:HG22	2.03	0.41
5:A:714:LEU:CD1	20:B:1735:CLA:HMA1	2.51	0.41
5:A:747:TRP:CE3	22:A:1807:BCR:H402	2.53	0.41
20:A:1764:CLA:H112	20:A:1783:CLA:H91	2.01	0.41
20:A:1781:CLA:HBB2	20:A:1794:CLA:CMA	2.50	0.41
20:A:1781:CLA:H202	20:A:1781:CLA:H161	1.85	0.41
22:A:1807:BCR:H371	22:A:1807:BCR:H24C	1.79	0.41
6:B:126:THR:HG21	6:B:358:TYR:HD1	1.86	0.41
6:B:138:GLY:O	6:B:139:ALA:C	2.59	0.41
6:B:185:VAL:HG22	22:B:1775:BCR:H272	2.03	0.41
6:B:213:LEU:HD12	6:B:214:ASP:H	1.85	0.41
6:B:289:LEU:CD2	22:B:1774:BCR:H352	2.49	0.41
6:B:290:MET:HG3	20:B:1751:CLA:CMC	2.50	0.41
6:B:309:ILE:CD1	6:B:312:GLY:HA3	2.51	0.41
6:B:325:THR:HG21	6:B:403:ASN:HD21	1.86	0.41
6:B:366:THR:C	6:B:368:GLN:N	2.74	0.41
6:B:393:PHE:CE2	6:B:398:TYR:HD2	2.38	0.41
6:B:416:GLU:O	6:B:420:SER:OG	2.39	0.41
6:B:603:ARG:HB2	6:B:732:LYS:HD3	2.03	0.41
6:B:693:TRP:HE1	20:B:1770:CLA:HHD	1.86	0.41
20:B:1736:CLA:HMC3	20:B:1738:CLA:OBD	2.21	0.41
20:B:1742:CLA:HMC2	22:B:1775:BCR:H373	2.00	0.41
20:B:1752:CLA:H72	20:B:1752:CLA:HBB1	1.99	0.41
20:B:1768:CLA:HBC1	10:F:83:PHE:CE1	2.49	0.41
20:B:1768:CLA:H62	20:B:1768:CLA:H101	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:3:HIS:ND1	7:C:69:LEU:HD12	2.36	0.41
8:D:70:GLU:OE1	8:D:71:GLY:O	2.39	0.41
9:E:37:LYS:HD2	9:E:47:LYS:HE3	2.03	0.41
10:F:39:ALA:O	10:F:42:ILE:CG2	2.69	0.41
11:G:80:ILE:O	11:G:81:VAL:C	2.59	0.41
13:I:20:ALA:O	13:I:24:LEU:N	2.54	0.41
20:J:1043:CLA:CHA	20:J:1043:CLA:HED2	2.45	0.41
16:L:112:PRO:O	16:L:113:SER:CB	2.68	0.41
17:N:45:ASN:ND2	17:N:54:LYS:CD	2.73	0.41
17:N:45:ASN:CG	17:N:57:LYS:HZ1	2.17	0.41
17:N:53:ALA:C	17:N:54:LYS:HD2	2.41	0.41
17:N:57:LYS:O	17:N:58:VAL:C	2.58	0.41
17:N:72:LYS:CA	17:N:73:ASP:C	2.89	0.41
20:1:1191:CLA:CMC	20:1:1194:CLA:CHD	2.70	0.41
3:3:50:GLU:HG3	3:3:51:PRO:N	2.35	0.41
3:3:84:ILE:N	3:3:85:PRO:HD3	2.36	0.41
3:3:189:LEU:C	3:3:191:MET:N	2.74	0.41
20:3:1218:CLA:O1A	20:3:1218:CLA:H2	2.21	0.41
5:A:57:LEU:O	5:A:61:ALA:HB2	2.21	0.41
5:A:77:LYS:NZ	20:A:1760:CLA:CED	2.84	0.41
5:A:242:ILE:CG1	5:A:243:PRO:HD3	2.44	0.41
5:A:277:TYR:HD2	5:A:279:ASP:H	1.68	0.41
5:A:344:LYS:HB3	5:A:344:LYS:HE2	1.90	0.41
5:A:586:ARG:H	7:C:49:VAL:HG22	1.86	0.41
5:A:607:ASN:HD22	5:A:607:ASN:HA	1.68	0.41
5:A:630:ASP:C	5:A:632:GLY:H	2.22	0.41
5:A:663:GLN:OE1	5:A:753:ARG:CZ	2.69	0.41
20:A:1764:CLA:HBC3	20:A:1764:CLA:CHD	2.50	0.41
20:A:1789:CLA:HBC2	20:H:1079:CLA:HBC1	2.03	0.41
20:A:1795:CLA:HBA1	20:A:1795:CLA:H3A	1.68	0.41
20:A:1796:CLA:HAC1	23:A:1802:PQN:H152	2.03	0.41
22:A:1805:BCR:C8	22:A:1805:BCR:C32	2.98	0.41
21:A:7020:LMU:H92	21:A:7020:LMU:H62	1.25	0.41
6:B:52:GLY:O	6:B:56:ILE:HG12	2.21	0.41
6:B:54:LEU:HD11	20:B:1743:CLA:CBA	2.51	0.41
6:B:58:PHE:HE2	6:B:145:LEU:HD12	1.86	0.41
6:B:122:GLN:HB2	6:B:358:TYR:HB3	2.01	0.41
6:B:266:GLN:NE2	6:B:363:GLN:HG2	2.35	0.41
6:B:556:SER:CA	6:B:558:PRO:CD	2.99	0.41
6:B:557:PHE:HE2	7:C:66:ARG:NE	2.16	0.41
20:B:1736:CLA:C4C	22:I:1032:BCR:H401	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:1755:CLA:H3A	20:B:1755:CLA:HBA2	1.40	0.41
23:B:1773:PQN:H192	22:B:1780:BCR:C9	2.47	0.41
21:B:1782:LMU:H3'	21:B:1782:LMU:H1B	1.49	0.41
7:C:62:PHE:CZ	9:E:42:GLU:CB	3.04	0.41
8:D:93:LYS:HB3	8:D:93:LYS:HZ2	1.80	0.41
10:F:17:ARG:NE	10:F:17:ARG:CA	2.83	0.41
10:F:47:GLU:N	10:F:50:LYS:HB2	2.36	0.41
10:F:96:TRP:HE3	10:F:134:PHE:N	2.16	0.41
10:F:144:LEU:CD1	10:F:149:LEU:HD13	2.51	0.41
10:F:151:ASP:OD2	10:F:154:PHE:CG	2.73	0.41
11:G:17:PHE:CD2	11:G:17:PHE:N	2.88	0.41
11:G:20:ARG:NH2	11:G:61:ASN:HA	2.36	0.41
16:L:104:ILE:C	16:L:104:ILE:HD12	2.42	0.41
20:R:1055:CLA:C11	21:R:1056:LMU:O4'	2.67	0.41
4:4:127:PRO:HB2	4:4:143:PHE:HE1	1.83	0.40
20:4:1201:CLA:CGD	20:4:1201:CLA:C2A	2.97	0.40
5:A:40:PHE:O	5:A:40:PHE:CG	2.74	0.40
5:A:392:GLN:O	5:A:392:GLN:CD	2.60	0.40
5:A:604:TRP:O	5:A:605:MET:C	2.60	0.40
5:A:650:ASN:HD22	6:B:635:ILE:CD1	2.34	0.40
5:A:733:VAL:CG1	20:A:1796:CLA:C4D	2.99	0.40
20:A:1766:CLA:HBB1	20:A:1769:CLA:NA	2.36	0.40
20:A:1793:CLA:H151	20:A:1793:CLA:H18	1.76	0.40
20:A:1796:CLA:C7	20:A:1813:CLA:H171	2.51	0.40
6:B:17:THR:HA	6:B:696:LYS:CB	2.51	0.40
6:B:197:VAL:HG22	6:B:207:VAL:HG11	2.03	0.40
6:B:262:HIS:ND1	6:B:265:THR:O	2.42	0.40
6:B:330:ILE:HA	6:B:333:GLN:NE2	2.36	0.40
6:B:522:ALA:O	6:B:589:TRP:HE3	2.04	0.40
6:B:696:LYS:HB2	6:B:696:LYS:HE2	1.83	0.40
20:B:1755:CLA:H42	20:B:1768:CLA:CBA	2.51	0.40
22:B:1776:BCR:C8	22:B:1776:BCR:C33	2.86	0.40
11:G:58:LEU:HA	11:G:61:ASN:OD1	2.21	0.40
12:H:45:ALA:HA	12:H:48:THR:OG1	2.21	0.40
15:K:10:ILE:HG23	15:K:13:THR:OG1	2.21	0.40
17:N:4:GLU:OE2	17:N:5:GLU:CB	2.62	0.40
17:N:58:VAL:O	17:N:59:PRO:C	2.59	0.40
21:R:1056:LMU:O2'	21:R:1056:LMU:C2	2.69	0.40
1:1:18:ALA:N	1:1:19:PRO:HD2	2.36	0.40
2:2:167:GLY:O	2:2:171:MET:N	2.53	0.40
5:A:472:ARG:HH22	16:L:74:LEU:CD2	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:575:LEU:HD13	5:A:579:PHE:HB3	2.03	0.40
5:A:714:LEU:HB2	5:A:716:VAL:HG13	2.02	0.40
5:A:733:VAL:HG11	20:A:1796:CLA:C4D	2.51	0.40
20:A:1816:CLA:O2D	20:A:1816:CLA:HBA2	2.19	0.40
6:B:91:ILE:CG2	20:B:1740:CLA:CAD	2.96	0.40
6:B:228:GLY:HA3	11:G:8:ILE:HD13	2.02	0.40
6:B:362:ALA:HA	6:B:365:PHE:H	1.85	0.40
6:B:488:ALA:HB2	20:B:1766:CLA:C3C	2.51	0.40
20:B:1762:CLA:C7	22:B:1779:BCR:H402	2.50	0.40
22:B:1774:BCR:H11C	22:B:1774:BCR:H341	1.73	0.40
7:C:73:THR:HB	7:C:74:THR:H	1.17	0.40
8:D:109:VAL:O	8:D:110:GLN:HG3	2.21	0.40
10:F:123:VAL:O	10:F:126:ALA:CA	2.69	0.40
11:G:24:PHE:C	11:G:26:PHE:N	2.71	0.40
11:G:44:PHE:HA	11:G:46:ALA:HB2	2.03	0.40
21:K:1086:LMU:H122	21:K:1086:LMU:H91	1.27	0.40
16:L:14:LEU:CA	16:L:24:GLU:HG3	2.41	0.40
20:L:1166:CLA:HED2	20:L:1166:CLA:CAA	2.48	0.40
1:1:136:ASP:HB2	1:1:140:LEU:HB3	2.03	0.40
20:2:1220:CLA:H92	20:2:1220:CLA:H52	0.61	0.40
3:3:92:TRP:O	3:3:95:THR:CG2	2.68	0.40
4:4:38:ARG:NH1	4:4:38:ARG:CG	2.70	0.40
4:4:94:GLU:OE2	20:4:1208:CLA:C1B	2.69	0.40
4:4:106:TRP:HB3	20:4:1196:CLA:HED2	2.03	0.40
4:4:119:PRO:CG	4:4:120:ILE:H	2.34	0.40
5:A:36:LYS:HA	5:A:37:PRO:HD3	1.97	0.40
5:A:316:MET:CA	5:A:317:TYR:HB2	2.39	0.40
5:A:430:ASP:O	5:A:432:LEU:N	2.55	0.40
5:A:639:ALA:O	5:A:640:GLY:C	2.59	0.40
20:A:1789:CLA:HAA2	16:L:71:ALA:O	2.21	0.40
21:A:7031:LMU:H4'	21:A:7031:LMU:C3B	2.46	0.40
21:A:7042:LMU:H52	21:A:7042:LMU:H81	1.58	0.40
6:B:139:ALA:O	6:B:141:PHE:N	2.54	0.40
6:B:140:ILE:HD13	6:B:140:ILE:N	2.32	0.40
6:B:160:LYS:HB2	6:B:160:LYS:NZ	2.32	0.40
6:B:167:TRP:HD1	11:G:41:MET:CE	2.34	0.40
6:B:381:PHE:HA	6:B:583:MET:SD	2.62	0.40
6:B:387:PHE:O	6:B:391:PRO:CD	2.67	0.40
6:B:471:THR:HG23	6:B:502:ASN:HD21	1.83	0.40
24:B:1783:LMG:C11	24:B:1783:LMG:O8	2.69	0.40
8:D:47:VAL:O	8:D:100:PHE:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:152:GLN:O	8:D:154:TYR:N	2.55	0.40
11:G:42:SER:OG	11:G:45:GLU:CG	2.69	0.40
11:G:67:ASN:HA	11:G:70:ASP:CG	2.40	0.40
13:I:8:PHE:CE1	22:I:1032:BCR:C9	3.04	0.40
1:1:28:GLY:CA	20:1:1199:CLA:C3C	2.95	0.40
1:1:142:GLU:O	1:1:143:LEU:HB2	2.21	0.40
20:1:1189:CLA:O1A	20:1:1189:CLA:HMA2	2.22	0.40
2:2:126:PRO:CG	2:2:129:LYS:HB2	2.51	0.40
4:4:38:ARG:HG3	4:4:39:TRP:N	2.27	0.40
4:4:121:PHE:HD1	4:4:143:PHE:CE2	2.40	0.40
4:4:124:TYR:HB3	4:4:127:PRO:HG2	2.03	0.40
5:A:44:ILE:H	5:A:44:ILE:HG13	1.59	0.40
5:A:334:HIS:CD2	20:A:1777:CLA:NB	2.90	0.40
5:A:375:HIS:CE1	20:A:1782:CLA:C1C	3.04	0.40
5:A:396:PHE:CE2	5:A:616:PHE:CD1	3.09	0.40
5:A:413:HIS:HA	5:A:416:ILE:HD12	2.03	0.40
5:A:457:SER:O	5:A:544:ILE:CD1	2.64	0.40
5:A:652:TRP:CE2	20:A:1811:CLA:H142	2.56	0.40
5:A:698:GLY:CA	6:B:570:ILE:HG21	2.52	0.40
5:A:704:ILE:HG12	20:A:1795:CLA:CMC	2.52	0.40
20:A:1785:CLA:HBD	20:A:1785:CLA:HAA1	2.03	0.40
20:A:1801:CLA:HMA3	16:L:27:VAL:CA	2.19	0.40
22:A:1808:BCR:C8	22:A:1808:BCR:H311	2.51	0.40
21:A:1809:LMU:H22	21:A:1809:LMU:H51	1.66	0.40
21:A:7036:LMU:H101	21:A:7036:LMU:H72	1.68	0.40
6:B:98:GLN:N	6:B:99:PRO:HD2	2.37	0.40
6:B:122:GLN:HG3	6:B:361:ILE:CG1	2.44	0.40
6:B:193:HIS:O	6:B:194:LEU:C	2.57	0.40
6:B:303:TYR:H	6:B:306:GLU:HB2	1.85	0.40
6:B:355:LEU:HD21	20:B:1756:CLA:HMC2	2.03	0.40
6:B:429:LEU:HD23	6:B:429:LEU:HA	1.66	0.40
6:B:462:TRP:CZ3	20:B:1764:CLA:HBC1	2.55	0.40
6:B:557:PHE:N	6:B:558:PRO:HD3	2.31	0.40
6:B:583:MET:O	6:B:583:MET:HE2	2.21	0.40
20:B:1786:CLA:H141	20:H:1079:CLA:HBC3	2.02	0.40
7:C:63:LEU:CD1	7:C:65:VAL:H	2.35	0.40
9:E:34:SER:O	9:E:35:LYS:CB	2.66	0.40
10:F:125:LEU:O	10:F:126:ALA:HB3	2.21	0.40
11:G:20:ARG:NH2	11:G:61:ASN:O	2.55	0.40
11:G:44:PHE:CA	11:G:46:ALA:HB2	2.50	0.40
17:N:54:LYS:HD2	17:N:54:LYS:HA	1.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:64:ASP:HB3	17:N:65:LEU:H	1.44	0.40
1:1:26:PRO:HD2	6:B:314:ARG:NH1	2.36	0.40
20:1:1192:CLA:H41	20:1:1192:CLA:H62	1.78	0.40
2:2:51:HIS:O	2:2:54:TRP:HB2	2.22	0.40
3:3:157:ALA:HB1	3:3:158:TYR:CD2	2.57	0.40
3:3:172:ASP:H	3:3:173:GLU:CB	2.34	0.40
3:3:205:GLY:HA2	5:A:252:ARG:HH12	1.85	0.40
4:4:142:ASN:O	4:4:143:PHE:CB	2.69	0.40
5:A:97:TYR:HA	5:A:153:TRP:CZ2	2.57	0.40
5:A:150:PHE:N	5:A:153:TRP:HE3	2.19	0.40
5:A:158:ILE:HG21	20:A:1770:CLA:O1D	2.21	0.40
5:A:173:VAL:HG23	5:A:174:PHE:H	1.86	0.40
5:A:193:LEU:HA	5:A:196:PHE:HE2	1.82	0.40
5:A:193:LEU:O	5:A:196:PHE:CD2	2.75	0.40
5:A:567:ARG:CB	5:A:567:ARG:HH21	2.35	0.40
5:A:581:CYS:HB2	5:A:590:CYS:C	2.42	0.40
5:A:686:TRP:C	5:A:688:PHE:H	2.24	0.40
20:A:1776:CLA:H92	22:A:1805:BCR:H373	0.43	0.40
20:A:1779:CLA:CAB	22:A:1805:BCR:H15C	2.52	0.40
20:A:1781:CLA:CBB	20:A:1794:CLA:CMA	3.00	0.40
20:A:1789:CLA:H3A	20:A:1789:CLA:HBA1	1.84	0.40
22:A:1807:BCR:C17	20:A:1812:CLA:H172	2.51	0.40
21:A:7013:LMU:C1B	21:A:7013:LMU:O3'	2.66	0.40
6:B:151:LEU:HD23	6:B:151:LEU:HA	1.91	0.40
6:B:178:HIS:CE1	20:B:1743:CLA:NC	2.85	0.40
6:B:227:THR:HG1	11:G:97:PHE:HD2	1.68	0.40
6:B:347:LEU:O	6:B:351:HIS:HB2	2.21	0.40
6:B:471:THR:O	6:B:472:TYR:C	2.60	0.40
7:C:49:VAL:O	25:C:1082:SF4:S2	2.79	0.40
9:E:36:VAL:HG11	9:E:87:VAL:HG11	2.04	0.40
11:G:50:ARG:CB	11:G:51:ALA:CA	2.99	0.40
12:H:77:LEU:CD2	12:H:78:PRO:HD2	2.52	0.40
17:N:67:LEU:CB	17:N:68:GLU:HB3	2.48	0.40

All (25) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:31:MET:CE	17:N:85:TRP:NE1[2_546]	0.92	1.28
4:4:130:GLU:C	16:L:159:TYR:OH[1_655]	1.18	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:31:MET:CE	17:N:85:TRP:CE2[2_546]	1.19	1.01
20:1:1193:CLA:O2D	20:K:1142:CLA:O2A[1_654]	1.34	0.86
4:4:130:GLU:CA	16:L:159:TYR:OH[1_655]	1.43	0.77
11:G:31:MET:SD	17:N:85:TRP:CE2[2_546]	1.46	0.74
4:4:121:PHE:CE2	16:L:78:GLU:OE2[1_655]	1.48	0.72
4:4:130:GLU:O	16:L:159:TYR:OH[1_655]	1.50	0.70
11:G:31:MET:SD	17:N:85:TRP:CD2[2_546]	1.65	0.55
4:4:126:LEU:O	16:L:78:GLU:N[1_655]	1.77	0.43
4:4:129:GLY:CA	16:L:77:THR:O[1_655]	1.87	0.33
1:1:78:PRO:O	3:3:45:THR:CG2[1_554]	1.89	0.31
11:G:31:MET:CE	17:N:85:TRP:CZ2[2_546]	1.92	0.28
20:1:1193:CLA:CED	20:K:1142:CLA:O2A[1_654]	1.94	0.26
11:G:31:MET:SD	17:N:85:TRP:CZ2[2_546]	1.95	0.25
4:4:121:PHE:CD2	16:L:78:GLU:OE1[1_655]	1.99	0.21
4:4:128:ALA:N	16:L:76:ASN:O[1_655]	2.02	0.18
4:4:121:PHE:CE2	16:L:78:GLU:CD[1_655]	2.11	0.09
11:G:31:MET:CE	17:N:85:TRP:CD1[2_546]	2.11	0.09
4:4:121:PHE:CD2	16:L:78:GLU:CD[1_655]	2.12	0.08
4:4:127:PRO:C	16:L:76:ASN:O[1_655]	2.13	0.07
6:B:205:GLU:OE2	15:K:23:ARG:NH1[1_554]	2.15	0.05
21:2:1225:LMU:O2B	20:A:1791:CLA:CMB[1_655]	2.18	0.02
4:4:121:PHE:CD2	16:L:78:GLU:OE2[1_655]	2.18	0.02
4:4:121:PHE:CZ	16:L:78:GLU:OE2[1_655]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	161/241 (67%)	83 (52%)	43 (27%)	35 (22%)	0	0
2	2	174/269 (65%)	88 (51%)	56 (32%)	30 (17%)	0	1
3	3	156/276 (56%)	78 (50%)	43 (28%)	35 (22%)	0	0
4	4	164/251 (65%)	79 (48%)	47 (29%)	38 (23%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	726/758 (96%)	334 (46%)	200 (28%)	192 (26%)	0	0
6	B	731/734 (100%)	361 (49%)	189 (26%)	181 (25%)	0	0
7	C	79/81 (98%)	23 (29%)	29 (37%)	27 (34%)	0	0
8	D	136/212 (64%)	48 (35%)	42 (31%)	46 (34%)	0	0
9	E	63/143 (44%)	29 (46%)	14 (22%)	20 (32%)	0	0
10	F	152/231 (66%)	67 (44%)	44 (29%)	41 (27%)	0	0
11	G	93/167 (56%)	35 (38%)	28 (30%)	30 (32%)	0	0
12	H	67/144 (46%)	28 (42%)	15 (22%)	24 (36%)	0	0
13	I	28/40 (70%)	10 (36%)	11 (39%)	7 (25%)	0	0
14	J	40/44 (91%)	19 (48%)	11 (28%)	10 (25%)	0	0
15	K	82/131 (63%)	49 (60%)	15 (18%)	18 (22%)	0	0
16	L	159/216 (74%)	66 (42%)	47 (30%)	46 (29%)	0	0
17	N	83/170 (49%)	22 (26%)	19 (23%)	42 (51%)	0	0
All	All	3094/4108 (75%)	1419 (46%)	853 (28%)	822 (27%)	0	0

All (822) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	25	ASP
1	1	29	LEU
1	1	30	GLY
1	1	35	ASN
1	1	58	LEU
1	1	90	PRO
1	1	118	PRO
1	1	130	PRO
1	1	137	PRO
1	1	161	PHE
1	1	183	ASP
1	1	184	PRO
2	2	37	ASP
2	2	42	ARG
2	2	70	LYS
2	2	71	LEU
2	2	73	ILE
2	2	125	PHE
2	2	127	ASN

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Mol	Chain	Res	Type
2	2	149	GLY
2	2	188	PRO
2	2	189	ILE
2	2	190	ASP
2	2	200	PRO
2	2	204	ILE
2	2	206	ALA
3	3	48	PHE
3	3	49	ILE
3	3	85	PRO
3	3	97	PHE
3	3	107	TRP
3	3	108	ALA
3	3	110	SER
3	3	111	TYR
3	3	113	LEU
3	3	134	LYS
3	3	135	PRO
3	3	142	TYR
3	3	158	TYR
3	3	159	PRO
3	3	164	PHE
3	3	166	PRO
3	3	167	LEU
3	3	172	ASP
3	3	206	VAL
3	3	210	GLN
4	4	34	PRO
4	4	36	ASN
4	4	83	TYR
4	4	115	VAL
4	4	119	PRO
4	4	125	SER
4	4	143	PHE
4	4	144	ALA
4	4	172	VAL
4	4	188	PRO
5	A	22	VAL
5	A	28	LYS
5	A	29	THR
5	A	30	SER
5	A	35	ALA

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Mol	Chain	Res	Type
5	A	36	LYS
5	A	40	PHE
5	A	60	ASP
5	A	67	HIS
5	A	69	SER
5	A	71	LEU
5	A	82	HIS
5	A	83	PHE
5	A	88	ILE
5	A	99	HIS
5	A	104	SER
5	A	155	ALA
5	A	156	SER
5	A	157	GLY
5	A	158	ILE
5	A	159	THR
5	A	160	SER
5	A	175	ALA
5	A	193	LEU
5	A	205	HIS
5	A	221	HIS
5	A	237	VAL
5	A	244	LEU
5	A	247	GLU
5	A	250	LEU
5	A	252	ARG
5	A	258	LEU
5	A	268	PRO
5	A	279	ASP
5	A	280	PHE
5	A	281	LEU
5	A	282	THR
5	A	283	PHE
5	A	286	GLY
5	A	299	ILE
5	A	307	ALA
5	A	310	PHE
5	A	329	ASP
5	A	333	ALA
5	A	339	THR
5	A	346	LEU
5	A	349	ILE

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Mol	Chain	Res	Type
5	A	361	ASN
5	A	386	ALA
5	A	389	TYR
5	A	423	ASP
5	A	427	ARG
5	A	428	TYR
5	A	429	ASN
5	A	433	ASP
5	A	473	PRO
5	A	474	GLN
5	A	477	PHE
5	A	486	PRO
5	A	489	ALA
5	A	498	LEU
5	A	507	ALA
5	A	508	THR
5	A	509	ALA
5	A	510	SER
5	A	521	VAL
5	A	523	VAL
5	A	553	VAL
5	A	578	ARG
5	A	579	PHE
5	A	594	ALA
5	A	643	ALA
5	A	657	LEU
5	A	673	SER
5	A	679	PHE
5	A	727	ILE
5	A	735	VAL
5	A	750	PHE
5	A	751	LEU
5	A	752	ALA
5	A	757	VAL
6	B	5	ILE
6	B	6	PRO
6	B	26	ALA
6	B	35	ASP
6	B	68	VAL
6	B	69	ALA
6	B	77	TRP
6	B	80	ASP

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Mol	Chain	Res	Type
6	B	83	HIS
6	B	86	PRO
6	B	99	PRO
6	B	104	PHE
6	B	120	VAL
6	B	129	LEU
6	B	136	TYR
6	B	140	ILE
6	B	142	LEU
6	B	159	PRO
6	B	160	LYS
6	B	167	TRP
6	B	182	LEU
6	B	187	SER
6	B	198	ALA
6	B	208	ARG
6	B	231	ASN
6	B	248	GLN
6	B	265	THR
6	B	292	ARG
6	B	293	THR
6	B	294	ASN
6	B	308	HIS
6	B	310	PRO
6	B	320	LYS
6	B	321	GLY
6	B	362	ALA
6	B	375	HIS
6	B	378	ILE
6	B	382	ILE
6	B	383	MET
6	B	405	ASP
6	B	420	SER
6	B	450	GLU
6	B	479	SER
6	B	480	SER
6	B	490	ARG
6	B	494	LEU
6	B	495	PRO
6	B	505	SER
6	B	506	ASN
6	B	512	ILE

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Mol	Chain	Res	Type
6	B	528	HIS
6	B	539	LEU
6	B	545	LYS
6	B	555	TYR
6	B	569	ASP
6	B	587	ILE
6	B	599	ILE
6	B	603	ARG
6	B	610	ASN
6	B	629	SER
6	B	636	THR
6	B	639	VAL
6	B	657	TRP
6	B	661	PHE
6	B	662	MET
6	B	668	ARG
6	B	681	ALA
6	B	682	HIS
6	B	691	ILE
6	B	707	LEU
6	B	710	LEU
6	B	731	GLY
7	C	8	TYR
7	C	21	CYS
7	C	32	GLY
7	C	49	VAL
7	C	56	SER
7	C	59	PRO
7	C	62	PHE
7	C	65	VAL
7	C	66	ARG
7	C	75	ARG
8	D	32	SER
8	D	36	LEU
8	D	38	ARG
8	D	65	ALA
8	D	70	GLU
8	D	78	ALA
8	D	94	TYR
8	D	95	LYS
8	D	97	LYS
8	D	109	VAL

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Mol	Chain	Res	Type
8	D	114	PRO
8	D	115	LYS
8	D	119	TYR
8	D	120	PRO
8	D	121	GLU
8	D	124	ASN
8	D	132	LEU
8	D	139	LYS
8	D	146	VAL
8	D	151	LYS
8	D	153	PRO
9	E	35	LYS
9	E	46	PHE
9	E	53	VAL
9	E	54	ALA
9	E	60	LYS
9	E	64	PRO
9	E	65	VAL
9	E	72	VAL
9	E	73	ASN
9	E	86	GLU
9	E	87	VAL
9	E	90	VAL
10	F	2	ILE
10	F	7	PRO
10	F	12	LYS
10	F	21	ALA
10	F	25	LEU
10	F	26	GLN
10	F	31	LEU
10	F	35	ASP
10	F	38	PRO
10	F	42	ILE
10	F	47	GLU
10	F	52	ARG
10	F	54	ASP
10	F	58	LYS
10	F	59	TYR
10	F	77	GLN
10	F	109	ARG
10	F	116	GLN
10	F	127	SER

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Mol	Chain	Res	Type
10	F	130	LEU
10	F	152	ASN
10	F	153	ASN
11	G	31	MET
11	G	33	LYS
11	G	34	GLN
11	G	38	GLN
11	G	42	SER
11	G	50	ARG
11	G	59	LYS
11	G	61	ASN
11	G	70	ASP
11	G	74	TRP
11	G	81	VAL
11	G	86	LEU
11	G	87	ALA
11	G	94	ASP
12	H	15	ALA
12	H	17	THR
12	H	20	GLN
12	H	24	TYR
12	H	31	PRO
12	H	41	GLU
12	H	46	PRO
12	H	50	ARG
12	H	52	LEU
12	H	56	PHE
12	H	71	ASN
12	H	77	LEU
13	I	22	ALA
13	I	23	SER
14	J	5	LYS
14	J	6	THR
14	J	10	VAL
14	J	22	LEU
14	J	39	PHE
15	K	35	THR
15	K	41	GLU
15	K	47	ILE
15	K	51	ASP
15	K	52	PRO
15	K	68	HIS

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Mol	Chain	Res	Type
15	K	69	ILE
15	K	72	VAL
15	K	75	VAL
16	L	6	PRO
16	L	8	TYR
16	L	10	VAL
16	L	37	LEU
16	L	43	TYR
16	L	44	ARG
16	L	46	ALA
16	L	63	LEU
16	L	75	ARG
16	L	76	ASN
16	L	88	ALA
16	L	97	MET
16	L	121	THR
16	L	123	ARG
16	L	125	LYS
16	L	127	PRO
16	L	128	ASP
16	L	129	GLN
16	L	149	SER
16	L	154	ALA
16	L	158	MET
16	L	161	LEU
16	L	164	PRO
17	N	2	VAL
17	N	7	LEU
17	N	11	LYS
17	N	24	THR
17	N	27	ALA
17	N	28	ASN
17	N	40	CYS
17	N	43	PRO
17	N	45	ASN
17	N	47	THR
17	N	51	ASP
17	N	58	VAL
17	N	61	LEU
17	N	63	ASP
17	N	66	ASP
17	N	68	GLU

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Mol	Chain	Res	Type
17	N	74	LYS
17	N	75	TYR
17	N	76	LYS
17	N	77	CYS
17	N	80	ASN
17	N	82	PHE
17	N	83	TRP
1	1	178	ALA
1	1	182	ALA
1	1	185	TRP
2	2	41	LEU
2	2	128	ASN
2	2	129	LYS
2	2	193	PHE
2	2	207	ALA
3	3	52	LYS
3	3	77	ILE
3	3	95	THR
3	3	106	TYR
3	3	137	SER
3	3	162	PRO
3	3	208	PRO
4	4	58	MET
4	4	59	LEU
4	4	69	ILE
4	4	141	LEU
4	4	162	ALA
4	4	177	PRO
5	A	39	HIS
5	A	41	SER
5	A	45	ALA
5	A	57	LEU
5	A	74	ILE
5	A	96	MET
5	A	105	ASN
5	A	130	GLU
5	A	144	GLN
5	A	184	PHE
5	A	189	ALA
5	A	210	LEU
5	A	213	LEU
5	A	215	SER

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Mol	Chain	Res	Type
5	A	234	ASN
5	A	242	ILE
5	A	243	PRO
5	A	266	ALA
5	A	278	ALA
5	A	290	LEU
5	A	292	GLY
5	A	308	ILE
5	A	313	ALA
5	A	317	TYR
5	A	328	LYS
5	A	337	PRO
5	A	347	TYR
5	A	373	ALA
5	A	400	MET
5	A	421	ASP
5	A	424	PRO
5	A	431	LEU
5	A	439	ARG
5	A	446	LEU
5	A	476	MET
5	A	479	ASP
5	A	505	PRO
5	A	511	THR
5	A	514	THR
5	A	516	GLY
5	A	518	GLY
5	A	538	ASP
5	A	574	ASN
5	A	592	VAL
5	A	624	VAL
5	A	637	ILE
5	A	640	GLY
5	A	649	ILE
5	A	661	ALA
5	A	671	SER
5	A	701	GLN
5	A	742	GLY
6	B	20	ARG
6	B	42	LEU
6	B	103	ALA
6	B	105	THR

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Mol	Chain	Res	Type
6	B	115	ASN
6	B	128	GLY
6	B	153	GLY
6	B	178	HIS
6	B	188	LEU
6	B	207	VAL
6	B	222	LEU
6	B	224	PRO
6	B	230	TRP
6	B	232	LEU
6	B	234	ALA
6	B	237	PRO
6	B	247	THR
6	B	267	SER
6	B	318	GLY
6	B	330	ILE
6	B	371	LEU
6	B	437	TYR
6	B	464	GLN
6	B	469	LYS
6	B	481	THR
6	B	503	GLU
6	B	514	PRO
6	B	554	GLY
6	B	592	PHE
6	B	605	ASN
6	B	664	LEU
6	B	690	LEU
6	B	716	GLY
6	B	733	PHE
7	C	10	THR
7	C	22	PRO
7	C	61	ASP
7	C	64	SER
7	C	68	TYR
7	C	70	TRP
8	D	26	SER
8	D	31	GLY
8	D	35	GLY
8	D	53	PRO
8	D	63	GLY
8	D	110	GLN

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Mol	Chain	Res	Type
8	D	129	GLY
8	D	130	VAL
8	D	138	GLY
8	D	150	GLY
9	E	30	PRO
9	E	42	GLU
9	E	89	GLU
9	E	91	ALA
10	F	46	MET
10	F	126	ALA
10	F	138	VAL
10	F	141	TYR
11	G	22	VAL
11	G	28	ARG
11	G	46	ALA
11	G	63	PRO
11	G	80	ILE
11	G	85	ILE
11	G	93	TYR
12	H	23	VAL
12	H	34	SER
12	H	37	SER
12	H	44	ALA
12	H	75	ASP
13	I	25	PHE
14	J	23	ALA
14	J	26	LEU
14	J	37	LEU
15	K	27	ALA
15	K	32	ARG
15	K	70	MET
15	K	73	GLY
15	K	79	LYS
16	L	11	ILE
16	L	24	GLU
16	L	27	VAL
16	L	36	TYR
16	L	64	LEU
16	L	89	ALA
16	L	108	LYS
16	L	120	LEU
17	N	35	VAL

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Mol	Chain	Res	Type
17	N	42	PHE
17	N	48	GLY
17	N	54	LYS
17	N	56	LYS
17	N	69	CYS
17	N	71	GLY
17	N	78	GLY
1	1	21	ASP
1	1	57	ILE
1	1	65	TYR
1	1	124	PRO
1	1	135	LYS
1	1	138	LYS
1	1	177	LEU
1	1	179	THR
2	2	91	THR
2	2	116	PRO
2	2	148	TRP
2	2	186	THR
2	2	194	ALA
3	3	88	THR
3	3	91	PRO
3	3	153	SER
3	3	157	ALA
4	4	65	THR
4	4	71	ASN
4	4	108	ASP
4	4	122	LYS
4	4	123	GLN
4	4	148	GLU
4	4	178	PHE
5	A	31	PHE
5	A	63	ASP
5	A	73	GLU
5	A	114	THR
5	A	116	ILE
5	A	124	TRP
5	A	127	VAL
5	A	149	PHE
5	A	151	GLN
5	A	200	GLU
5	A	225	VAL

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Mol	Chain	Res	Type
5	A	263	ALA
5	A	354	TRP
5	A	355	HIS
5	A	404	GLY
5	A	426	THR
5	A	485	GLN
5	A	537	ALA
5	A	659	ALA
5	A	717	ALA
6	B	8	PHE
6	B	41	ARG
6	B	43	TYR
6	B	71	GLN
6	B	161	TRP
6	B	173	SER
6	B	179	LEU
6	B	189	ALA
6	B	223	GLY
6	B	225	LEU
6	B	228	GLY
6	B	239	SER
6	B	240	SER
6	B	270	LEU
6	B	272	ASP
6	B	273	VAL
6	B	278	LEU
6	B	281	ALA
6	B	309	ILE
6	B	400	PRO
6	B	468	GLY
6	B	474	PHE
6	B	477	PRO
6	B	482	ASN
6	B	493	TRP
6	B	501	ILE
6	B	558	PRO
6	B	732	LYS
7	C	43	PRO
8	D	55	GLU
8	D	93	LYS
8	D	128	GLN
9	E	84	LEU

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Mol	Chain	Res	Type
10	F	11	SER
10	F	34	ASP
10	F	44	ALA
10	F	53	PHE
10	F	63	CYS
10	F	114	PRO
11	G	84	TYR
11	G	89	ALA
12	H	27	ASP
12	H	45	ALA
13	I	2	ILE
14	J	9	SER
14	J	38	THR
15	K	40	LEU
15	K	48	GLN
16	L	113	SER
16	L	147	GLY
17	N	9	LYS
17	N	21	ARG
17	N	81	VAL
1	1	122	LYS
1	1	134	SER
2	2	83	GLY
2	2	141	LEU
2	2	154	GLN
3	3	75	PRO
3	3	141	GLN
3	3	156	PRO
3	3	169	PHE
4	4	38	ARG
4	4	77	ALA
4	4	114	SER
4	4	118	ASP
4	4	139	ASN
4	4	187	ASP
5	A	37	PRO
5	A	135	ASP
5	A	230	ASN
5	A	276	LYS
5	A	305	ALA
5	A	422	TYR
5	A	702	GLU

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Mol	Chain	Res	Type
5	A	738	TYR
6	B	54	LEU
6	B	164	SER
6	B	170	ASN
6	B	217	PRO
6	B	227	THR
6	B	229	GLN
6	B	335	GLY
6	B	354	SER
6	B	361	ILE
6	B	379	ALA
6	B	475	ASP
6	B	476	ILE
6	B	478	LEU
6	B	540	ASP
6	B	595	HIS
6	B	596	TRP
6	B	623	TYR
6	B	627	ASN
6	B	687	LEU
6	B	730	SER
7	C	9	ASP
7	C	12	ILE
7	C	28	MET
7	C	30	PRO
7	C	37	LYS
8	D	46	TYR
8	D	60	MET
8	D	106	SER
8	D	143	PRO
9	E	61	THR
10	F	39	ALA
10	F	83	PHE
10	F	117	LYS
10	F	128	SER
10	F	132	ARG
10	F	151	ASP
11	G	36	PRO
11	G	56	SER
11	G	96	SER
12	H	18	THR
13	I	9	VAL

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Mol	Chain	Res	Type
15	K	29	SER
16	L	48	ASN
16	L	85	SER
16	L	86	LEU
16	L	112	PRO
17	N	17	ASN
17	N	25	THR
17	N	49	CYS
17	N	70	GLU
1	1	78	PRO
1	1	84	TYR
2	2	187	GLY
4	4	88	SER
4	4	127	PRO
5	A	26	PRO
5	A	86	LEU
5	A	95	GLY
5	A	186	TYR
5	A	235	ALA
5	A	269	PHE
5	A	306	ILE
5	A	353	SER
5	A	375	HIS
5	A	410	ALA
5	A	472	ARG
5	A	503	THR
5	A	571	ASP
5	A	580	PRO
5	A	709	TRP
6	B	139	ALA
6	B	206	TYR
6	B	212	PHE
6	B	360	PHE
6	B	421	HIS
6	B	451	LYS
6	B	460	ALA
6	B	550	LYS
6	B	559	CYS
6	B	586	THR
6	B	593	TYR
6	B	598	HIS
6	B	704	GLN

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Mol	Chain	Res	Type
7	C	35	LYS
7	C	52	LYS
7	C	55	GLU
7	C	58	CYS
7	C	73	THR
8	D	22	PRO
8	D	34	GLY
8	D	40	ALA
8	D	104	PHE
8	D	125	PRO
8	D	148	PHE
9	E	52	VAL
10	F	73	VAL
10	F	102	ARG
12	H	16	ASN
12	H	74	GLN
13	I	5	PRO
16	L	50	LEU
16	L	61	GLY
16	L	135	GLY
16	L	157	LEU
17	N	34	THR
17	N	50	GLN
17	N	62	SER
1	1	32	VAL
1	1	55	PRO
1	1	99	ALA
1	1	143	LEU
1	1	160	GLY
2	2	76	THR
2	2	136	GLY
4	4	73	PRO
4	4	126	LEU
4	4	147	LEU
4	4	185	ILE
5	A	179	LEU
5	A	239	PRO
5	A	259	TYR
5	A	500	PRO
5	A	584	PRO
5	A	696	GLY
5	A	721	GLN

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Mol	Chain	Res	Type
6	B	162	LYS
6	B	219	PRO
6	B	391	PRO
6	B	472	TYR
6	B	498	LEU
6	B	630	GLN
6	B	708	VAL
10	F	37	ALA
11	G	91	ASN
12	H	72	ALA
15	K	34	ALA
16	L	69	VAL
1	1	79	GLY
1	1	145	VAL
4	4	136	GLY
5	A	48	PRO
5	A	223	VAL
5	A	229	ILE
5	A	531	PRO
5	A	570	PRO
5	A	754	ILE
6	B	94	PRO
6	B	557	PHE
6	B	711	VAL
16	L	150	GLY
17	N	59	PRO
5	A	190	ALA
5	A	716	VAL
6	B	606	VAL
8	D	67	ILE
9	E	55	VAL
11	G	64	VAL
16	L	53	GLY
16	L	72	GLY
1	1	28	GLY
8	D	28	ILE
11	G	71	VAL
13	I	12	VAL
4	4	137	ILE
4	4	168	ILE
5	A	718	PRO
6	B	87	ILE

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Mol	Chain	Res	Type
6	B	113	VAL
6	B	463	ILE
11	G	35	VAL
12	H	60	GLY
16	L	16	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	127/190 (67%)	102 (80%)	25 (20%)	1	5
2	2	140/216 (65%)	107 (76%)	33 (24%)	0	3
3	3	120/215 (56%)	82 (68%)	38 (32%)	0	1
4	4	138/201 (69%)	103 (75%)	35 (25%)	0	2
5	A	592/618 (96%)	392 (66%)	200 (34%)	0	1
6	B	598/600 (100%)	367 (61%)	231 (39%)	0	0
7	C	70/70 (100%)	40 (57%)	30 (43%)	0	0
8	D	118/173 (68%)	75 (64%)	43 (36%)	0	0
9	E	56/114 (49%)	37 (66%)	19 (34%)	0	1
10	F	127/190 (67%)	73 (58%)	54 (42%)	0	0
11	G	79/144 (55%)	46 (58%)	33 (42%)	0	0
12	H	57/115 (50%)	26 (46%)	31 (54%)	0	0
13	I	26/36 (72%)	18 (69%)	8 (31%)	0	1
14	J	36/39 (92%)	25 (69%)	11 (31%)	0	1
15	K	61/102 (60%)	43 (70%)	18 (30%)	0	1
16	L	124/169 (73%)	81 (65%)	43 (35%)	0	1
17	N	74/139 (53%)	33 (45%)	41 (55%)	0	0
All	All	2543/3331 (76%)	1650 (65%)	893 (35%)	0	1

All (893) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	27	LEU
1	1	31	GLU
1	1	49	TRP
1	1	52	LEU
1	1	57	ILE
1	1	58	LEU
1	1	59	VAL
1	1	61	GLU
1	1	84	TYR
1	1	85	LEU
1	1	93	THR
1	1	103	LEU
1	1	110	HIS
1	1	111	GLN
1	1	120	LYS
1	1	121	LYS
1	1	129	ASP
1	1	133	TYR
1	1	134	SER
1	1	136	ASP
1	1	139	LYS
1	1	152	ARG
1	1	179	THR
1	1	181	LEU
1	1	186	HIS
2	2	39	GLU
2	2	43	TRP
2	2	46	GLN
2	2	51	HIS
2	2	57	LEU
2	2	70	LYS
2	2	71	LEU
2	2	73	ILE
2	2	89	THR
2	2	94	LEU
2	2	95	PHE
2	2	100	VAL
2	2	101	PHE
2	2	109	ARG
2	2	110	TRP
2	2	113	ILE
2	2	115	ASN
2	2	119	VAL

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Mol	Chain	Res	Type
2	2	125	PHE
2	2	129	LYS
2	2	130	LEU
2	2	137	TYR
2	2	158	GLU
2	2	159	LEU
2	2	162	LYS
2	2	164	ILE
2	2	169	LEU
2	2	179	PHE
2	2	189	ILE
2	2	193	PHE
2	2	196	HIS
2	2	199	ASP
2	2	211	LYS
3	3	50	GLU
3	3	60	ILE
3	3	67	LEU
3	3	73	ILE
3	3	76	GLU
3	3	78	LEU
3	3	83	LEU
3	3	84	ILE
3	3	86	GLN
3	3	90	LEU
3	3	93	PHE
3	3	94	ARG
3	3	95	THR
3	3	97	PHE
3	3	106	TYR
3	3	107	TRP
3	3	109	ASP
3	3	111	TYR
3	3	112	THR
3	3	128	ARG
3	3	131	ASP
3	3	141	GLN
3	3	146	LEU
3	3	150	LEU
3	3	163	PHE
3	3	164	PHE
3	3	165	ASN

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Mol	Chain	Res	Type
3	3	171	LYS
3	3	185	LYS
3	3	188	ARG
3	3	191	MET
3	3	192	LEU
3	3	195	LEU
3	3	198	PHE
3	3	200	GLN
3	3	204	THR
3	3	209	TYR
3	3	210	GLN
4	4	32	GLU
4	4	33	ASP
4	4	35	GLU
4	4	38	ARG
4	4	39	TRP
4	4	50	TRP
4	4	52	MET
4	4	53	LEU
4	4	59	LEU
4	4	60	LEU
4	4	64	PHE
4	4	69	ILE
4	4	71	ASN
4	4	83	TYR
4	4	90	LEU
4	4	103	ILE
4	4	104	ARG
4	4	116	ASN
4	4	118	ASP
4	4	120	ILE
4	4	124	TYR
4	4	126	LEU
4	4	131	VAL
4	4	139	ASN
4	4	147	LEU
4	4	150	LYS
4	4	159	LEU
4	4	163	PHE
4	4	169	GLN
4	4	173	THR
4	4	175	LYS

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Mol	Chain	Res	Type
4	4	189	TRP
4	4	190	HIS
4	4	194	VAL
4	4	195	GLN
5	A	21	LEU
5	A	22	VAL
5	A	23	ASP
5	A	24	ARG
5	A	25	ASP
5	A	29	THR
5	A	30	SER
5	A	31	PHE
5	A	34	TRP
5	A	40	PHE
5	A	44	ILE
5	A	46	LYS
5	A	50	THR
5	A	52	THR
5	A	60	ASP
5	A	62	HIS
5	A	63	ASP
5	A	68	THR
5	A	69	SER
5	A	71	LEU
5	A	72	GLU
5	A	78	VAL
5	A	82	HIS
5	A	83	PHE
5	A	86	LEU
5	A	88	ILE
5	A	94	SER
5	A	102	ARG
5	A	103	PHE
5	A	107	GLU
5	A	109	TRP
5	A	111	ASN
5	A	114	THR
5	A	124	TRP
5	A	130	GLU
5	A	131	ILE
5	A	133	ASN
5	A	135	ASP

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Mol	Chain	Res	Type
5	A	141	ARG
5	A	144	GLN
5	A	164	LEU
5	A	167	THR
5	A	172	LEU
5	A	177	LEU
5	A	180	PHE
5	A	188	LYS
5	A	193	LEU
5	A	197	GLN
5	A	203	LEU
5	A	207	LEU
5	A	213	LEU
5	A	217	SER
5	A	223	VAL
5	A	224	HIS
5	A	227	LEU
5	A	230	ASN
5	A	231	GLN
5	A	232	PHE
5	A	238	ASP
5	A	242	ILE
5	A	248	PHE
5	A	249	ILE
5	A	251	ASN
5	A	253	ASP
5	A	254	LEU
5	A	255	LEU
5	A	261	SER
5	A	262	PHE
5	A	277	TYR
5	A	281	LEU
5	A	284	ARG
5	A	287	LEU
5	A	290	LEU
5	A	296	LEU
5	A	297	THR
5	A	298	ASP
5	A	299	ILE
5	A	304	LEU
5	A	308	ILE
5	A	309	LEU

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Mol	Chain	Res	Type
5	A	331	LEU
5	A	332	GLU
5	A	334	HIS
5	A	339	THR
5	A	341	GLN
5	A	352	THR
5	A	353	SER
5	A	357	GLN
5	A	358	LEU
5	A	361	ASN
5	A	368	LEU
5	A	369	THR
5	A	375	HIS
5	A	376	MET
5	A	377	TYR
5	A	379	MET
5	A	384	TYR
5	A	387	THR
5	A	391	THR
5	A	392	GLN
5	A	393	LEU
5	A	397	THR
5	A	400	MET
5	A	402	ILE
5	A	405	PHE
5	A	420	ARG
5	A	422	TYR
5	A	426	THR
5	A	427	ARG
5	A	433	ASP
5	A	434	ARG
5	A	435	VAL
5	A	438	HIS
5	A	439	ARG
5	A	440	ASP
5	A	444	SER
5	A	446	LEU
5	A	458	PHE
5	A	462	ILE
5	A	464	ASN
5	A	466	THR
5	A	477	PHE

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Mol	Chain	Res	Type
5	A	479	ASP
5	A	480	THR
5	A	488	PHE
5	A	490	GLN
5	A	495	THR
5	A	498	LEU
5	A	503	THR
5	A	520	LEU
5	A	521	VAL
5	A	529	LEU
5	A	530	LEU
5	A	532	ILE
5	A	536	THR
5	A	539	PHE
5	A	540	LEU
5	A	547	PHE
5	A	548	THR
5	A	553	VAL
5	A	554	LEU
5	A	555	ILE
5	A	557	LEU
5	A	558	LYS
5	A	561	LEU
5	A	564	ARG
5	A	567	ARG
5	A	568	LEU
5	A	569	ILE
5	A	572	LYS
5	A	575	LEU
5	A	577	PHE
5	A	578	ARG
5	A	590	CYS
5	A	591	GLN
5	A	600	LEU
5	A	605	MET
5	A	607	ASN
5	A	613	ILE
5	A	614	PHE
5	A	623	ASP
5	A	629	ASN
5	A	630	ASP
5	A	631	GLN

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Mol	Chain	Res	Type
5	A	633	VAL
5	A	637	ILE
5	A	638	THR
5	A	641	ASN
5	A	642	PHE
5	A	644	GLN
5	A	645	SER
5	A	646	SER
5	A	653	LEU
5	A	654	ARG
5	A	657	LEU
5	A	660	GLN
5	A	662	SER
5	A	663	GLN
5	A	673	SER
5	A	677	LEU
5	A	684	PHE
5	A	685	VAL
5	A	689	SER
5	A	691	MET
5	A	692	PHE
5	A	697	ARG
5	A	703	LEU
5	A	707	ILE
5	A	715	LYS
5	A	723	ARG
5	A	726	SER
5	A	727	ILE
5	A	728	VAL
5	A	733	VAL
5	A	735	VAL
5	A	736	THR
5	A	740	LEU
5	A	745	THR
5	A	751	LEU
5	A	754	ILE
6	B	3	LEU
6	B	4	ARG
6	B	5	ILE
6	B	6	PRO
6	B	9	SER
6	B	14	GLN

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Mol	Chain	Res	Type
6	B	15	ASP
6	B	17	THR
6	B	19	ARG
6	B	20	ARG
6	B	25	ILE
6	B	35	ASP
6	B	41	ARG
6	B	45	ASN
6	B	46	ILE
6	B	50	HIS
6	B	51	PHE
6	B	53	GLN
6	B	57	ILE
6	B	67	HIS
6	B	70	TRP
6	B	71	GLN
6	B	75	GLU
6	B	80	ASP
6	B	83	HIS
6	B	84	VAL
6	B	91	ILE
6	B	104	PHE
6	B	110	LEU
6	B	113	VAL
6	B	114	ASN
6	B	118	SER
6	B	121	TYR
6	B	122	GLN
6	B	123	TRP
6	B	124	TRP
6	B	127	ILE
6	B	129	LEU
6	B	130	ARG
6	B	132	ASN
6	B	134	ASP
6	B	136	TYR
6	B	137	THR
6	B	140	ILE
6	B	142	LEU
6	B	143	LEU
6	B	144	PHE
6	B	145	LEU

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Mol	Chain	Res	Type
6	B	151	LEU
6	B	154	TRP
6	B	157	LEU
6	B	160	LYS
6	B	161	TRP
6	B	164	SER
6	B	175	LEU
6	B	177	HIS
6	B	178	HIS
6	B	180	SER
6	B	188	LEU
6	B	195	VAL
6	B	199	ILE
6	B	203	ARG
6	B	206	TYR
6	B	208	ARG
6	B	210	ASN
6	B	214	ASP
6	B	216	LEU
6	B	226	LEU
6	B	229	GLN
6	B	231	ASN
6	B	232	LEU
6	B	243	LEU
6	B	246	THR
6	B	248	GLN
6	B	257	ILE
6	B	258	LEU
6	B	262	HIS
6	B	265	THR
6	B	266	GLN
6	B	269	TRP
6	B	270	LEU
6	B	271	THR
6	B	272	ASP
6	B	278	LEU
6	B	285	LEU
6	B	292	ARG
6	B	294	ASN
6	B	295	PHE
6	B	297	ILE
6	B	299	HIS

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Mol	Chain	Res	Type
6	B	300	SER
6	B	301	ILE
6	B	309	ILE
6	B	315	LEU
6	B	317	ARG
6	B	325	THR
6	B	326	ILE
6	B	330	ILE
6	B	332	PHE
6	B	348	VAL
6	B	350	GLN
6	B	352	MET
6	B	353	TYR
6	B	355	LEU
6	B	361	ILE
6	B	363	GLN
6	B	364	ASP
6	B	365	PHE
6	B	372	TYR
6	B	374	HIS
6	B	382	ILE
6	B	383	MET
6	B	384	THR
6	B	387	PHE
6	B	393	PHE
6	B	396	ARG
6	B	403	ASN
6	B	406	ASN
6	B	407	VAL
6	B	410	ARG
6	B	412	LEU
6	B	418	ILE
6	B	419	ILE
6	B	420	SER
6	B	422	LEU
6	B	423	SER
6	B	427	LEU
6	B	428	PHE
6	B	431	PHE
6	B	436	LEU
6	B	437	TYR
6	B	438	VAL

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Mol	Chain	Res	Type
6	B	440	ASN
6	B	443	MET
6	B	446	PHE
6	B	448	THR
6	B	452	GLN
6	B	454	LEU
6	B	458	ILE
6	B	461	GLN
6	B	464	GLN
6	B	471	THR
6	B	472	TYR
6	B	478	LEU
6	B	481	THR
6	B	486	LEU
6	B	492	ILE
6	B	494	LEU
6	B	501	ILE
6	B	502	ASN
6	B	504	ASN
6	B	508	LEU
6	B	509	PHE
6	B	510	LEU
6	B	512	ILE
6	B	514	PRO
6	B	516	ASP
6	B	517	PHE
6	B	521	HIS
6	B	525	LEU
6	B	527	LEU
6	B	528	HIS
6	B	532	LEU
6	B	533	ILE
6	B	539	LEU
6	B	540	ASP
6	B	544	SER
6	B	545	LYS
6	B	551	LYS
6	B	555	TYR
6	B	560	ASP
6	B	564	ARG
6	B	569	ASP
6	B	577	TYR

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Mol	Chain	Res	Type
6	B	578	LEU
6	B	580	VAL
6	B	583	MET
6	B	584	LEU
6	B	587	ILE
6	B	592	PHE
6	B	594	TRP
6	B	596	TRP
6	B	601	LEU
6	B	603	ARG
6	B	605	ASN
6	B	606	VAL
6	B	607	SER
6	B	608	GLN
6	B	611	GLU
6	B	615	TYR
6	B	616	LEU
6	B	617	MET
6	B	620	LEU
6	B	621	ARG
6	B	622	ASP
6	B	629	SER
6	B	631	LEU
6	B	633	ASN
6	B	638	LEU
6	B	640	CYS
6	B	643	LEU
6	B	645	VAL
6	B	649	MET
6	B	651	LEU
6	B	659	THR
6	B	662	MET
6	B	664	LEU
6	B	665	ILE
6	B	670	TYR
6	B	672	GLN
6	B	674	LEU
6	B	676	GLU
6	B	677	THR
6	B	682	HIS
6	B	685	THR
6	B	689	ASN

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Mol	Chain	Res	Type
6	B	690	LEU
6	B	691	ILE
6	B	692	ARG
6	B	700	LEU
6	B	702	ILE
6	B	703	VAL
6	B	710	LEU
6	B	712	HIS
6	B	715	VAL
6	B	718	ILE
6	B	719	PHE
6	B	721	TYR
6	B	725	LEU
6	B	732	LYS
6	B	733	PHE
7	C	2	SER
7	C	4	SER
7	C	7	ILE
7	C	10	THR
7	C	12	ILE
7	C	15	THR
7	C	16	GLN
7	C	18	VAL
7	C	23	THR
7	C	24	ASP
7	C	28	MET
7	C	37	LYS
7	C	38	GLN
7	C	45	THR
7	C	48	CYS
7	C	52	LYS
7	C	58	CYS
7	C	59	PRO
7	C	62	PHE
7	C	63	LEU
7	C	66	ARG
7	C	67	VAL
7	C	68	TYR
7	C	69	LEU
7	C	70	TRP
7	C	73	THR
7	C	74	THR

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Mol	Chain	Res	Type
7	C	77	MET
7	C	79	LEU
7	C	81	TYR
8	D	26	SER
8	D	28	ILE
8	D	41	GLN
8	D	44	GLU
8	D	46	TYR
8	D	47	VAL
8	D	48	ILE
8	D	49	THR
8	D	50	TRP
8	D	56	GLN
8	D	57	ILE
8	D	58	PHE
8	D	69	ARG
8	D	70	GLU
8	D	73	ASN
8	D	75	LEU
8	D	79	ARG
8	D	81	GLU
8	D	82	GLN
8	D	83	CYS
8	D	86	LEU
8	D	89	ARG
8	D	92	SER
8	D	93	LYS
8	D	95	LYS
8	D	96	ILE
8	D	98	TYR
8	D	104	PHE
8	D	105	PRO
8	D	111	TYR
8	D	116	ASP
8	D	121	GLU
8	D	122	LYS
8	D	123	VAL
8	D	127	ARG
8	D	128	GLN
8	D	134	MET
8	D	135	ARG
8	D	137	ILE

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Mol	Chain	Res	Type
8	D	139	LYS
8	D	144	ILE
8	D	147	LYS
8	D	151	LYS
9	E	31	LYS
9	E	32	ARG
9	E	35	LYS
9	E	36	VAL
9	E	39	LEU
9	E	40	ARG
9	E	42	GLU
9	E	45	TRP
9	E	47	LYS
9	E	48	ASN
9	E	55	VAL
9	E	56	ASP
9	E	58	ASP
9	E	61	THR
9	E	68	ARG
9	E	73	ASN
9	E	76	ASN
9	E	79	THR
9	E	84	LEU
10	F	8	CYS
10	F	9	LYS
10	F	12	LYS
10	F	13	GLN
10	F	14	PHE
10	F	17	ARG
10	F	18	GLU
10	F	20	GLN
10	F	23	LYS
10	F	24	LYS
10	F	25	LEU
10	F	26	GLN
10	F	28	SER
10	F	29	LEU
10	F	31	LEU
10	F	43	LYS
10	F	48	LYS
10	F	51	LYS
10	F	52	ARG

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Mol	Chain	Res	Type
10	F	53	PHE
10	F	61	LEU
10	F	71	LEU
10	F	77	GLN
10	F	78	ARG
10	F	79	HIS
10	F	83	PHE
10	F	88	ILE
10	F	91	LEU
10	F	92	TYR
10	F	93	ILE
10	F	96	TRP
10	F	100	VAL
10	F	104	TYR
10	F	106	ILE
10	F	108	ILE
10	F	110	ASP
10	F	111	GLU
10	F	113	LYS
10	F	115	THR
10	F	116	GLN
10	F	119	ILE
10	F	121	ILE
10	F	123	VAL
10	F	135	SER
10	F	136	TRP
10	F	137	PRO
10	F	138	VAL
10	F	141	TYR
10	F	142	ARG
10	F	143	GLU
10	F	146	ASN
10	F	152	ASN
10	F	153	ASN
10	F	154	PHE
11	G	7	VAL
11	G	10	LEU
11	G	12	THR
11	G	15	SER
11	G	17	PHE
11	G	18	LEU
11	G	22	VAL

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Mol	Chain	Res	Type
11	G	24	PHE
11	G	28	ARG
11	G	30	ASN
11	G	31	MET
11	G	33	LYS
11	G	39	ASN
11	G	41	MET
11	G	42	SER
11	G	43	HIS
11	G	44	PHE
11	G	45	GLU
11	G	48	ASP
11	G	49	THR
11	G	50	ARG
11	G	55	VAL
11	G	57	LEU
11	G	58	LEU
11	G	59	LYS
11	G	62	ASP
11	G	71	VAL
11	G	76	SER
11	G	83	TYR
11	G	88	THR
11	G	91	ASN
11	G	93	TYR
11	G	97	PHE
12	H	11	LEU
12	H	14	ILE
12	H	17	THR
12	H	20	GLN
12	H	21	TRP
12	H	24	TYR
12	H	30	SER
12	H	32	TYR
12	H	33	ASN
12	H	35	LEU
12	H	36	GLN
12	H	37	SER
12	H	41	GLU
12	H	42	THR
12	H	43	PHE
12	H	47	PHE

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Mol	Chain	Res	Type
12	H	48	THR
12	H	49	LYS
12	H	52	LEU
12	H	53	LEU
12	H	54	LEU
12	H	55	LYS
12	H	56	PHE
12	H	57	LEU
12	H	59	LEU
12	H	64	LEU
12	H	66	THR
12	H	67	TYR
12	H	69	SER
12	H	75	ASP
12	H	77	LEU
13	I	3	ASN
13	I	7	LEU
13	I	9	VAL
13	I	11	LEU
13	I	12	VAL
13	I	16	PHE
13	I	26	LEU
13	I	30	LYS
14	J	2	ARG
14	J	4	PHE
14	J	5	LYS
14	J	9	SER
14	J	13	VAL
14	J	14	LEU
14	J	16	THR
14	J	19	PHE
14	J	35	ASP
14	J	37	LEU
14	J	41	PHE
15	K	3	ILE
15	K	18	MET
15	K	19	LEU
15	K	20	PHE
15	K	23	ARG
15	K	32	ARG
15	K	39	LYS
15	K	40	LEU

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Mol	Chain	Res	Type
15	K	41	GLU
15	K	43	ARG
15	K	45	SER
15	K	48	GLN
15	K	52	PRO
15	K	55	PHE
15	K	68	HIS
15	K	69	ILE
15	K	70	MET
15	K	72	VAL
16	L	5	LYS
16	L	8	TYR
16	L	9	GLN
16	L	10	VAL
16	L	14	LEU
16	L	15	ASN
16	L	20	ILE
16	L	30	SER
16	L	32	LEU
16	L	38	SER
16	L	39	ASN
16	L	40	LEU
16	L	44	ARG
16	L	52	ARG
16	L	54	VAL
16	L	58	LEU
16	L	63	LEU
16	L	68	PHE
16	L	70	LYS
16	L	74	LEU
16	L	76	ASN
16	L	77	THR
16	L	79	TYR
16	L	94	ILE
16	L	97	MET
16	L	107	PHE
16	L	108	LYS
16	L	111	GLU
16	L	118	LEU
16	L	120	LEU
16	L	123	ARG
16	L	124	LYS

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Mol	Chain	Res	Type
16	L	134	ASP
16	L	136	TRP
16	L	140	THR
16	L	145	PHE
16	L	149	SER
16	L	152	THR
16	L	158	MET
16	L	159	TYR
16	L	161	LEU
16	L	164	PRO
16	L	165	TYR
17	N	4	GLU
17	N	5	GLU
17	N	6	TYR
17	N	10	SER
17	N	11	LYS
17	N	16	LEU
17	N	25	THR
17	N	28	ASN
17	N	29	PHE
17	N	33	TYR
17	N	37	PHE
17	N	39	SER
17	N	40	CYS
17	N	41	LYS
17	N	46	PHE
17	N	49	CYS
17	N	50	GLN
17	N	51	ASP
17	N	52	LEU
17	N	54	LYS
17	N	55	GLN
17	N	57	LYS
17	N	58	VAL
17	N	60	PHE
17	N	61	LEU
17	N	62	SER
17	N	64	ASP
17	N	65	LEU
17	N	66	ASP
17	N	67	LEU
17	N	68	GLU

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Mol	Chain	Res	Type
17	N	69	CYS
17	N	70	GLU
17	N	72	LYS
17	N	73	ASP
17	N	75	TYR
17	N	79	SER
17	N	81	VAL
17	N	82	PHE
17	N	83	TRP
17	N	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	46	HIS
1	1	72	GLN
1	1	111	GLN
2	2	120	ASN
2	2	128	ASN
3	3	105	ASN
3	3	126	HIS
3	3	165	ASN
4	4	71	ASN
4	4	107	GLN
4	4	111	ASN
4	4	169	GLN
5	A	33	GLN
5	A	58	HIS
5	A	99	HIS
5	A	121	GLN
5	A	129	GLN
5	A	144	GLN
5	A	187	HIS
5	A	197	GLN
5	A	224	HIS
5	A	230	ASN
5	A	231	GLN
5	A	246	HIS
5	A	302	HIS
5	A	303	HIS
5	A	361	ASN
5	A	375	HIS

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Mol	Chain	Res	Type
5	A	398	HIS
5	A	447	ASN
5	A	464	ASN
5	A	474	GLN
5	A	490	GLN
5	A	542	HIS
5	A	545	HIS
5	A	591	GLN
5	A	607	ASN
5	A	629	ASN
5	A	636	HIS
5	A	641	ASN
5	A	660	GLN
5	A	683	HIS
5	A	701	GLN
5	A	711	HIS
5	A	729	GLN
6	B	14	GLN
6	B	34	HIS
6	B	50	HIS
6	B	67	HIS
6	B	71	GLN
6	B	95	HIS
6	B	122	GLN
6	B	158	GLN
6	B	178	HIS
6	B	193	HIS
6	B	220	GLN
6	B	266	GLN
6	B	277	HIS
6	B	328	ASN
6	B	333	GLN
6	B	375	HIS
6	B	399	ASN
6	B	403	ASN
6	B	406	ASN
6	B	432	HIS
6	B	461	GLN
6	B	502	ASN
6	B	504	ASN
6	B	506	ASN
6	B	521	HIS

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Mol	Chain	Res	Type
6	B	528	HIS
6	B	595	HIS
6	B	605	ASN
6	B	608	GLN
6	B	610	ASN
6	B	630	GLN
6	B	633	ASN
6	B	641	ASN
6	B	672	GLN
6	B	712	HIS
7	C	71	HIS
8	D	41	GLN
8	D	56	GLN
8	D	73	ASN
8	D	82	GLN
8	D	128	GLN
8	D	133	ASN
8	D	152	GLN
9	E	48	ASN
9	E	73	ASN
10	F	77	GLN
10	F	116	GLN
10	F	146	ASN
10	F	152	ASN
10	F	153	ASN
11	G	27	GLN
11	G	61	ASN
11	G	67	ASN
12	H	16	ASN
12	H	33	ASN
12	H	36	GLN
12	H	71	ASN
14	J	30	ASN
15	K	80	ASN
16	L	12	GLN
16	L	15	ASN
16	L	39	ASN
16	L	48	ASN
16	L	131	GLN
17	N	45	ASN
17	N	55	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

26 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
19	GLC	M	1	19	10,10,12	1.46	3 (30%)	14,14,17	3.31	10 (71%)
19	FRU	M	2	19	11,12,12	1.06	1 (9%)	10,18,18	2.33	3 (30%)
19	GLC	O	1	19	11,11,12	0.92	0	15,15,17	3.54	8 (53%)
19	FRU	O	2	19	11,12,12	1.08	1 (9%)	10,18,18	1.70	2 (20%)
19	GLC	P	1	19	11,11,12	0.99	0	15,15,17	2.44	3 (20%)
19	FRU	P	2	19	11,12,12	1.16	2 (18%)	10,18,18	0.96	0
19	GLC	Q	1	19	11,11,12	1.19	1 (9%)	15,15,17	2.20	5 (33%)
19	FRU	Q	2	19	11,12,12	1.00	1 (9%)	10,18,18	1.76	4 (40%)
19	GLC	S	1	19	11,11,12	0.44	0	15,15,17	1.12	2 (13%)
19	FRU	S	2	19,21	11,12,12	0.67	0	10,18,18	1.12	0
19	GLC	T	1	19	11,11,12	1.07	0	15,15,17	1.64	3 (20%)
19	FRU	T	2	19	11,12,12	2.01	4 (36%)	10,18,18	2.89	4 (40%)
19	GLC	U	1	19	11,11,12	1.06	1 (9%)	15,15,17	2.67	5 (33%)
19	FRU	U	2	19	11,12,12	0.96	0	10,18,18	1.53	2 (20%)
19	GLC	V	1	19	11,11,12	1.54	2 (18%)	15,15,17	1.98	5 (33%)
19	FRU	V	2	19	11,12,12	0.90	0	10,18,18	2.00	5 (50%)
19	GLC	W	1	19	11,11,12	1.30	1 (9%)	15,15,17	2.89	9 (60%)
19	FRU	W	2	19	11,12,12	1.17	2 (18%)	10,18,18	2.10	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	GLC	X	1	19	11,11,12	1.22	1 (9%)	15,15,17	1.83	4 (26%)
19	FRU	X	2	19	11,12,12	1.56	2 (18%)	10,18,18	2.32	4 (40%)
19	GLC	Y	1	19	11,11,12	1.09	0	15,15,17	3.55	7 (46%)
19	FRU	Y	2	19	11,12,12	1.15	0	10,18,18	2.27	4 (40%)
19	GLC	Z	1	19	11,11,12	1.75	2 (18%)	15,15,17	4.50	8 (53%)
19	FRU	Z	2	19,21	11,12,12	1.06	1 (9%)	10,18,18	2.34	3 (30%)
19	GLC	a	1	19	11,11,12	1.06	1 (9%)	15,15,17	1.52	3 (20%)
19	FRU	a	2	19,12	11,12,12	1.07	0	10,18,18	2.15	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	M	1	19	-	-	0/1/1/1
19	FRU	M	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	O	1	19	-	1/2/19/22	0/1/1/1
19	FRU	O	2	19	1/1/4/4	4/5/24/24	0/1/1/1
19	GLC	P	1	19	-	2/2/19/22	0/1/1/1
19	FRU	P	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	Q	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	S	1	19	-	1/2/19/22	0/1/1/1
19	FRU	S	2	19,21	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	U	1	19	-	2/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	V	1	19	-	0/2/19/22	0/1/1/1
19	FRU	V	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	W	1	19	-	1/2/19/22	0/1/1/1
19	FRU	W	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	X	1	19	-	2/2/19/22	0/1/1/1
19	FRU	X	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Y	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Y	2	19	1/1/4/4	1/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	Z	1	19	-	0/2/19/22	0/1/1/1
19	FRU	Z	2	19,21	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	a	1	19	-	2/2/19/22	0/1/1/1
19	FRU	a	2	19,12	1/1/4/4	2/5/24/24	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	1	GLC	O5-C1	-4.10	1.37	1.43
19	T	2	FRU	O5-C2	-3.74	1.37	1.43
19	T	2	FRU	C1-C2	-3.01	1.47	1.52
19	V	1	GLC	O5-C1	-2.83	1.39	1.43
19	X	2	FRU	O2-C2	-2.70	1.36	1.40
19	P	2	FRU	O2-C2	2.67	1.45	1.40
19	V	1	GLC	O5-C5	-2.64	1.38	1.43
19	X	2	FRU	O5-C2	-2.59	1.39	1.43
19	O	2	FRU	O5-C2	-2.58	1.39	1.43
19	X	1	GLC	O5-C1	-2.47	1.39	1.43
19	M	1	GLC	O5-C5	-2.46	1.38	1.43
19	M	1	GLC	O5-C1	-2.44	1.39	1.43
19	Q	1	GLC	O5-C1	-2.42	1.39	1.43
19	Z	2	FRU	O5-C2	-2.41	1.39	1.43
19	T	2	FRU	O2-C2	-2.41	1.36	1.40
19	W	2	FRU	O5-C2	-2.37	1.39	1.43
19	P	2	FRU	C1-C2	2.32	1.56	1.52
19	W	2	FRU	O5-C5	-2.27	1.38	1.43
19	T	2	FRU	O3-C3	-2.27	1.38	1.42
19	Q	2	FRU	O5-C2	-2.18	1.39	1.43
19	Z	1	GLC	O5-C5	-2.18	1.39	1.43
19	M	1	GLC	O2-C2	-2.17	1.38	1.43
19	W	1	GLC	O5-C1	-2.17	1.40	1.43
19	U	1	GLC	C4-C5	-2.14	1.48	1.53
19	M	2	FRU	O5-C5	-2.09	1.39	1.43
19	a	1	GLC	C2-C3	-2.02	1.49	1.52

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	1	GLC	C1-O5-C5	-11.46	96.66	112.19
19	M	1	GLC	C1-C2-C3	7.92	119.40	109.67
19	P	1	GLC	C1-O5-C5	7.71	122.64	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	1	GLC	C1-O5-C5	7.50	122.35	112.19
19	Z	1	GLC	O5-C1-C2	-7.29	99.52	110.77
19	T	2	FRU	O1-C1-C2	-7.09	96.79	111.86
19	O	1	GLC	O3-C3-C2	6.96	123.32	109.99
19	Y	1	GLC	O5-C5-C6	6.83	117.92	107.20
19	U	1	GLC	O5-C5-C6	5.94	116.52	107.20
19	Z	1	GLC	C6-C5-C4	5.69	126.33	113.00
19	O	1	GLC	C3-C4-C5	-5.60	100.24	110.24
19	W	2	FRU	O1-C1-C2	-5.59	99.97	111.86
19	O	1	GLC	C2-C3-C4	-5.53	101.32	110.89
19	U	1	GLC	C6-C5-C4	-5.50	100.13	113.00
19	Z	1	GLC	C3-C4-C5	-5.27	100.84	110.24
19	Y	1	GLC	C3-C4-C5	-5.17	101.02	110.24
19	X	2	FRU	C6-C5-C4	-5.04	102.95	115.09
19	O	1	GLC	O5-C1-C2	5.01	118.50	110.77
19	M	1	GLC	O5-C5-C4	-4.97	100.60	109.52
19	W	1	GLC	O3-C3-C4	4.91	121.69	110.35
19	Z	2	FRU	O1-C1-C2	-4.86	101.53	111.86
19	Z	1	GLC	O2-C2-C3	-4.70	100.73	110.14
19	Y	1	GLC	C2-C3-C4	-4.68	102.79	110.89
19	Q	1	GLC	C3-C4-C5	-4.56	102.10	110.24
19	Z	2	FRU	O2-C2-O5	4.51	118.22	109.50
19	Q	1	GLC	C6-C5-C4	-4.50	102.47	113.00
19	U	1	GLC	C1-O5-C5	4.40	118.15	112.19
19	V	1	GLC	C1-C2-C3	-4.36	104.31	109.67
19	M	2	FRU	O4-C4-C3	-4.32	99.21	112.15
19	W	1	GLC	C1-C2-C3	-4.26	104.42	109.67
19	M	2	FRU	O2-C2-O5	-4.21	101.38	109.50
19	Y	1	GLC	O3-C3-C2	4.17	117.98	109.99
19	O	1	GLC	C1-O5-C5	4.10	117.75	112.19
19	W	1	GLC	C2-C3-C4	-4.07	103.85	110.89
19	M	2	FRU	O1-C1-C2	3.83	120.01	111.86
19	Z	1	GLC	C2-C3-C4	-3.76	104.38	110.89
19	a	2	FRU	O1-C1-C2	-3.69	104.02	111.86
19	X	1	GLC	O5-C1-C2	3.67	116.43	110.77
19	a	2	FRU	O2-C2-O5	3.65	116.56	109.50
19	M	1	GLC	O2-C2-C1	-3.65	101.69	109.15
19	X	1	GLC	C2-C3-C4	-3.54	104.77	110.89
19	Y	2	FRU	O3-C3-C4	-3.54	101.09	113.32
19	T	2	FRU	O3-C3-C4	-3.53	101.12	113.32
19	X	2	FRU	O6-C6-C5	-3.48	99.36	111.29
19	W	1	GLC	C3-C4-C5	-3.44	104.11	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	1	GLC	O5-C5-C4	-3.43	102.48	110.83
19	Y	2	FRU	O5-C5-C6	3.39	118.29	108.85
19	W	1	GLC	O6-C6-C5	-3.38	99.69	111.29
19	M	1	GLC	O3-C3-C2	3.37	116.45	109.99
19	Q	1	GLC	C2-C3-C4	-3.35	105.10	110.89
19	O	1	GLC	O4-C4-C5	3.31	117.51	109.30
19	a	2	FRU	O4-C4-C3	-3.29	102.30	112.15
19	O	1	GLC	O2-C2-C3	3.28	116.72	110.14
19	W	1	GLC	C6-C5-C4	-3.27	105.33	113.00
19	W	1	GLC	O2-C2-C3	3.27	116.69	110.14
19	Z	1	GLC	O5-C5-C4	-3.23	102.96	110.83
19	T	1	GLC	O2-C2-C1	3.21	115.73	109.15
19	V	1	GLC	C1-O5-C5	-3.18	107.88	112.19
19	a	1	GLC	O5-C5-C6	3.16	112.15	107.20
19	M	1	GLC	O5-C1-C2	3.12	115.59	110.77
19	V	2	FRU	O4-C4-C5	3.09	119.98	111.05
19	Q	2	FRU	O2-C2-O5	-3.06	103.59	109.50
19	Y	2	FRU	O1-C1-C2	-3.04	105.40	111.86
19	U	1	GLC	O4-C4-C5	-3.03	101.78	109.30
19	O	2	FRU	O2-C2-O5	3.02	115.33	109.50
19	Y	1	GLC	O3-C3-C4	-3.00	103.40	110.35
19	T	1	GLC	O5-C1-C2	2.91	115.26	110.77
19	a	1	GLC	C2-C3-C4	-2.91	105.87	110.89
19	T	2	FRU	O2-C2-O5	-2.89	103.92	109.50
19	V	1	GLC	O5-C5-C6	2.83	111.63	107.20
19	Y	2	FRU	O6-C6-C5	2.80	120.91	111.29
19	U	2	FRU	O4-C4-C5	-2.79	102.99	111.05
19	W	1	GLC	O4-C4-C3	2.72	116.64	110.35
19	S	1	GLC	O5-C5-C6	2.69	111.43	107.20
19	W	2	FRU	O2-C2-O5	2.62	114.56	109.50
19	a	1	GLC	O2-C2-C3	-2.59	104.95	110.14
19	M	1	GLC	C1-O5-C5	-2.55	106.99	112.78
19	P	1	GLC	O3-C3-C2	2.55	114.88	109.99
19	U	1	GLC	C1-C2-C3	2.55	112.80	109.67
19	X	2	FRU	O1-C1-C2	-2.54	106.46	111.86
19	Q	2	FRU	O4-C4-C5	-2.53	103.72	111.05
19	T	2	FRU	O4-C4-C3	-2.52	104.61	112.15
19	Q	2	FRU	O5-C5-C6	2.50	115.82	108.85
19	W	1	GLC	O5-C1-C2	-2.47	106.96	110.77
19	P	1	GLC	O5-C5-C4	2.45	116.78	110.83
19	T	1	GLC	C3-C4-C5	2.45	114.60	110.24
19	Z	1	GLC	O4-C4-C3	-2.44	104.70	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	2	FRU	O3-C3-C4	-2.44	104.91	113.32
19	X	2	FRU	O5-C5-C6	2.40	115.54	108.85
19	Q	1	GLC	O3-C3-C4	-2.39	104.81	110.35
19	S	1	GLC	C1-O5-C5	2.39	115.42	112.19
19	M	1	GLC	O4-C4-C5	-2.31	104.53	109.67
19	X	1	GLC	C1-O5-C5	2.31	115.32	112.19
19	M	1	GLC	O3-C3-C4	2.30	115.67	110.35
19	O	2	FRU	O1-C1-C2	-2.29	107.00	111.86
19	V	2	FRU	O4-C4-C3	-2.28	105.31	112.15
19	V	2	FRU	C6-C5-C4	2.26	120.54	115.09
19	M	1	GLC	C2-C3-C4	-2.21	107.08	110.89
19	V	2	FRU	O1-C1-C2	-2.20	107.19	111.86
19	Q	1	GLC	O5-C1-C2	-2.19	107.39	110.77
19	X	1	GLC	O2-C2-C3	-2.16	105.82	110.14
19	O	1	GLC	C6-C5-C4	2.14	118.03	113.00
19	U	2	FRU	O4-C4-C3	-2.14	105.73	112.15
19	Y	1	GLC	C6-C5-C4	-2.13	108.00	113.00
19	Q	2	FRU	C6-C5-C4	-2.12	109.98	115.09
19	Z	2	FRU	C6-C5-C4	-2.06	110.11	115.09
19	V	1	GLC	O3-C3-C2	-2.06	106.05	109.99
19	M	1	GLC	O2-C2-C3	-2.00	106.12	110.14

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	M	2	FRU	C2
19	O	2	FRU	C2
19	P	2	FRU	C2
19	Q	2	FRU	C2
19	S	2	FRU	C2
19	T	2	FRU	C2
19	U	2	FRU	C2
19	V	2	FRU	C2
19	W	2	FRU	C2
19	X	2	FRU	C2
19	Y	2	FRU	C2
19	Z	2	FRU	C2
19	a	2	FRU	C2

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	O	2	FRU	O1-C1-C2-C3
19	O	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-O5
19	U	2	FRU	O1-C1-C2-C3
19	U	2	FRU	O1-C1-C2-O2
19	U	2	FRU	O1-C1-C2-O5
19	W	2	FRU	O5-C5-C6-O6
19	Z	2	FRU	C4-C5-C6-O6
19	O	2	FRU	O5-C5-C6-O6
19	T	1	GLC	O5-C5-C6-O6
19	a	1	GLC	O5-C5-C6-O6
19	Q	1	GLC	O5-C5-C6-O6
19	Q	1	GLC	C4-C5-C6-O6
19	Z	2	FRU	O5-C5-C6-O6
19	P	1	GLC	C4-C5-C6-O6
19	P	1	GLC	O5-C5-C6-O6
19	U	1	GLC	O5-C5-C6-O6
19	T	1	GLC	C4-C5-C6-O6
19	O	2	FRU	O1-C1-C2-O5
19	V	2	FRU	O1-C1-C2-O5
19	W	2	FRU	C4-C5-C6-O6
19	Y	1	GLC	O5-C5-C6-O6
19	X	1	GLC	C4-C5-C6-O6
19	X	1	GLC	O5-C5-C6-O6
19	a	1	GLC	C4-C5-C6-O6
19	S	1	GLC	O5-C5-C6-O6
19	O	1	GLC	C4-C5-C6-O6
19	X	2	FRU	O1-C1-C2-O5
19	P	2	FRU	O5-C5-C6-O6
19	T	2	FRU	C4-C5-C6-O6
19	U	1	GLC	C4-C5-C6-O6
19	V	2	FRU	O1-C1-C2-O2
19	X	2	FRU	O1-C1-C2-O2
19	V	2	FRU	O1-C1-C2-C3
19	Y	1	GLC	C4-C5-C6-O6
19	a	2	FRU	O5-C5-C6-O6
19	P	2	FRU	O1-C1-C2-O5
19	Y	2	FRU	O1-C1-C2-O5
19	T	2	FRU	O1-C1-C2-C3
19	X	2	FRU	O1-C1-C2-C3
19	Z	2	FRU	O1-C1-C2-C3

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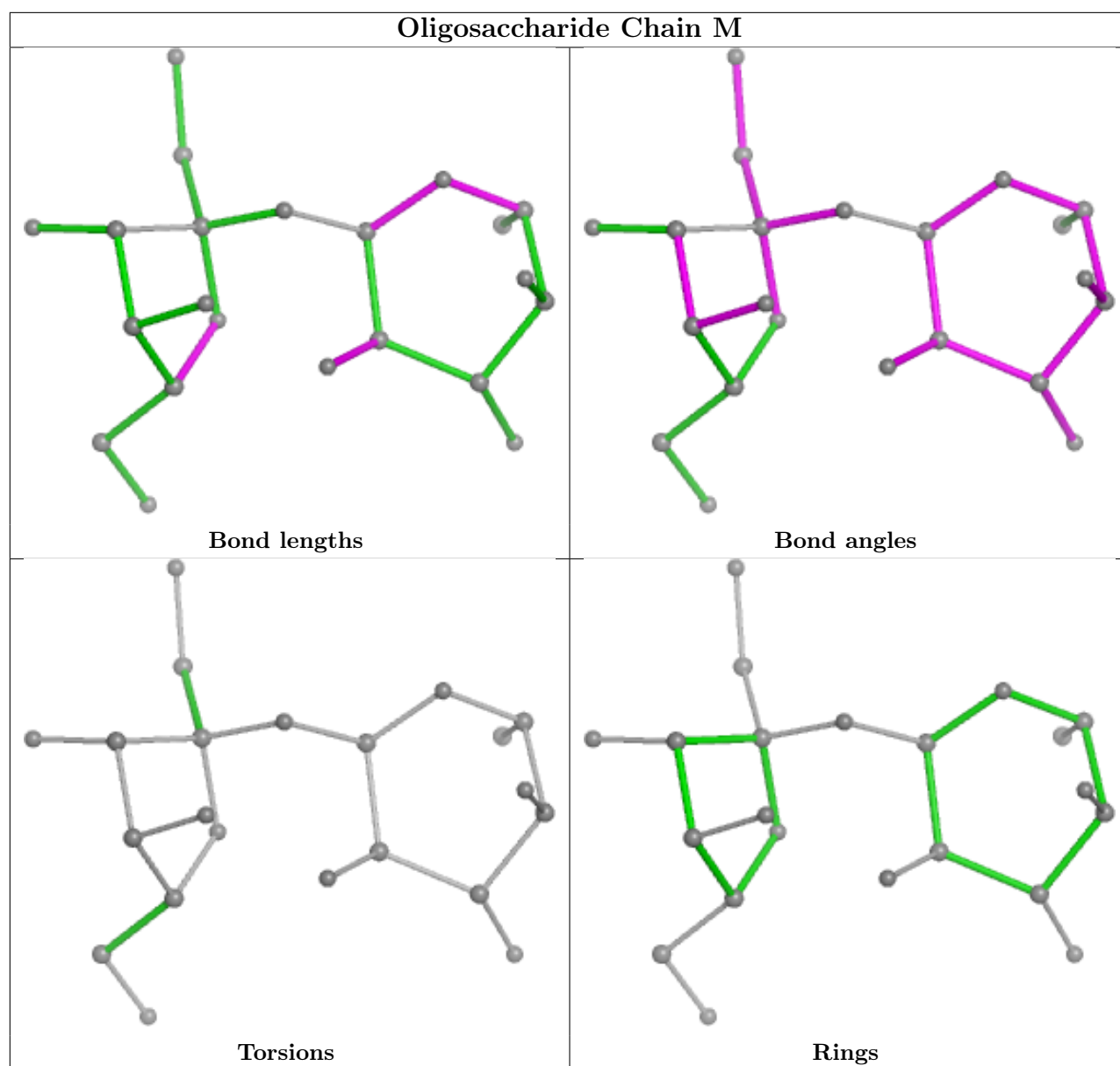
Mol	Chain	Res	Type	Atoms
19	T	2	FRU	O5-C5-C6-O6
19	W	1	GLC	C4-C5-C6-O6
19	a	2	FRU	C4-C5-C6-O6

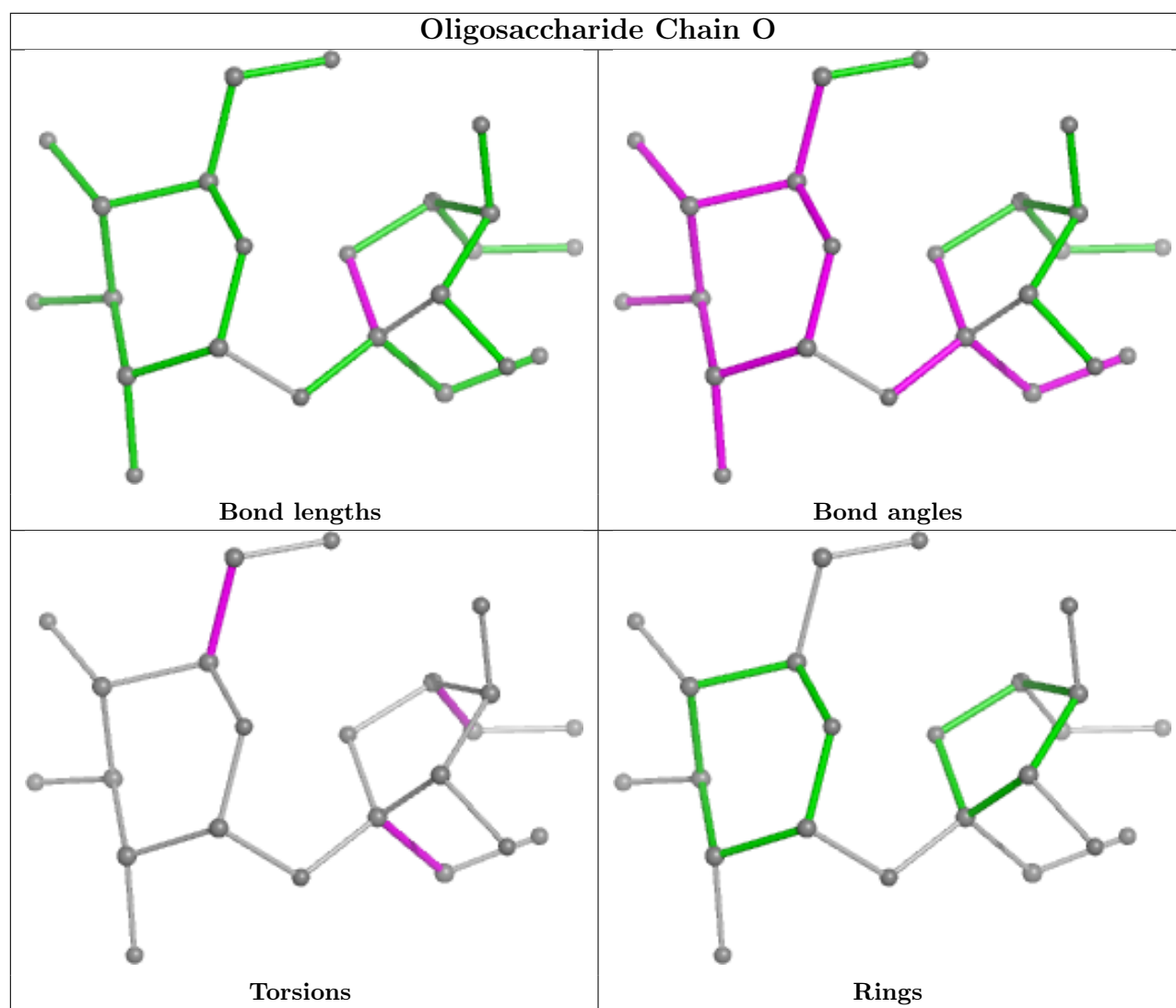
There are no ring outliers.

21 monomers are involved in 102 short contacts:

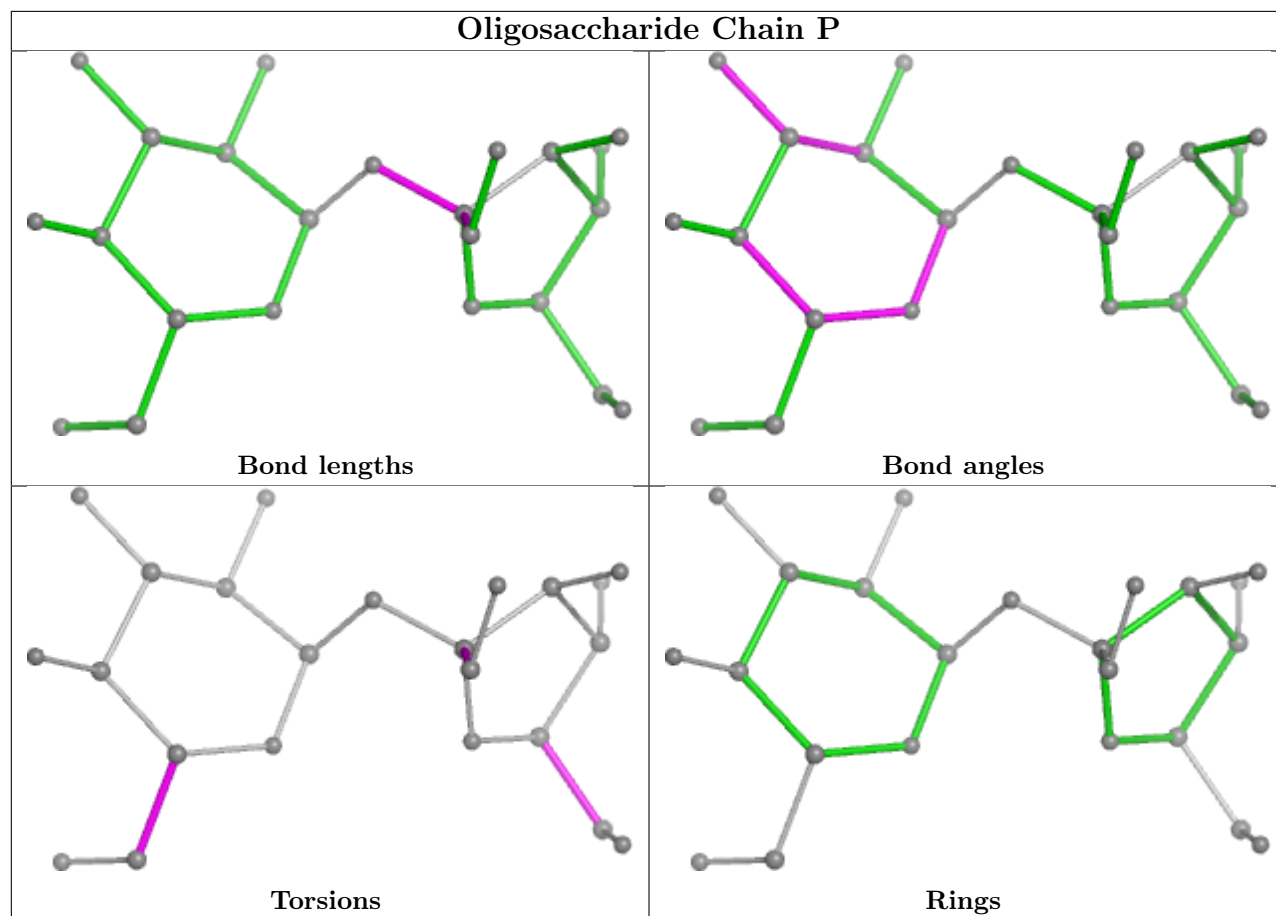
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	M	2	FRU	7	0
19	S	1	GLC	1	0
19	V	1	GLC	3	0
19	Y	2	FRU	1	0
19	Y	1	GLC	1	0
19	O	2	FRU	14	0
19	U	2	FRU	9	0
19	W	1	GLC	13	0
19	U	1	GLC	6	0
19	V	2	FRU	3	0
19	Z	1	GLC	7	0
19	T	2	FRU	8	0
19	X	2	FRU	7	0
19	Q	1	GLC	10	0
19	O	1	GLC	5	0
19	Z	2	FRU	18	0
19	T	1	GLC	7	0
19	W	2	FRU	15	0
19	M	1	GLC	10	0
19	X	1	GLC	7	0
19	Q	2	FRU	9	0

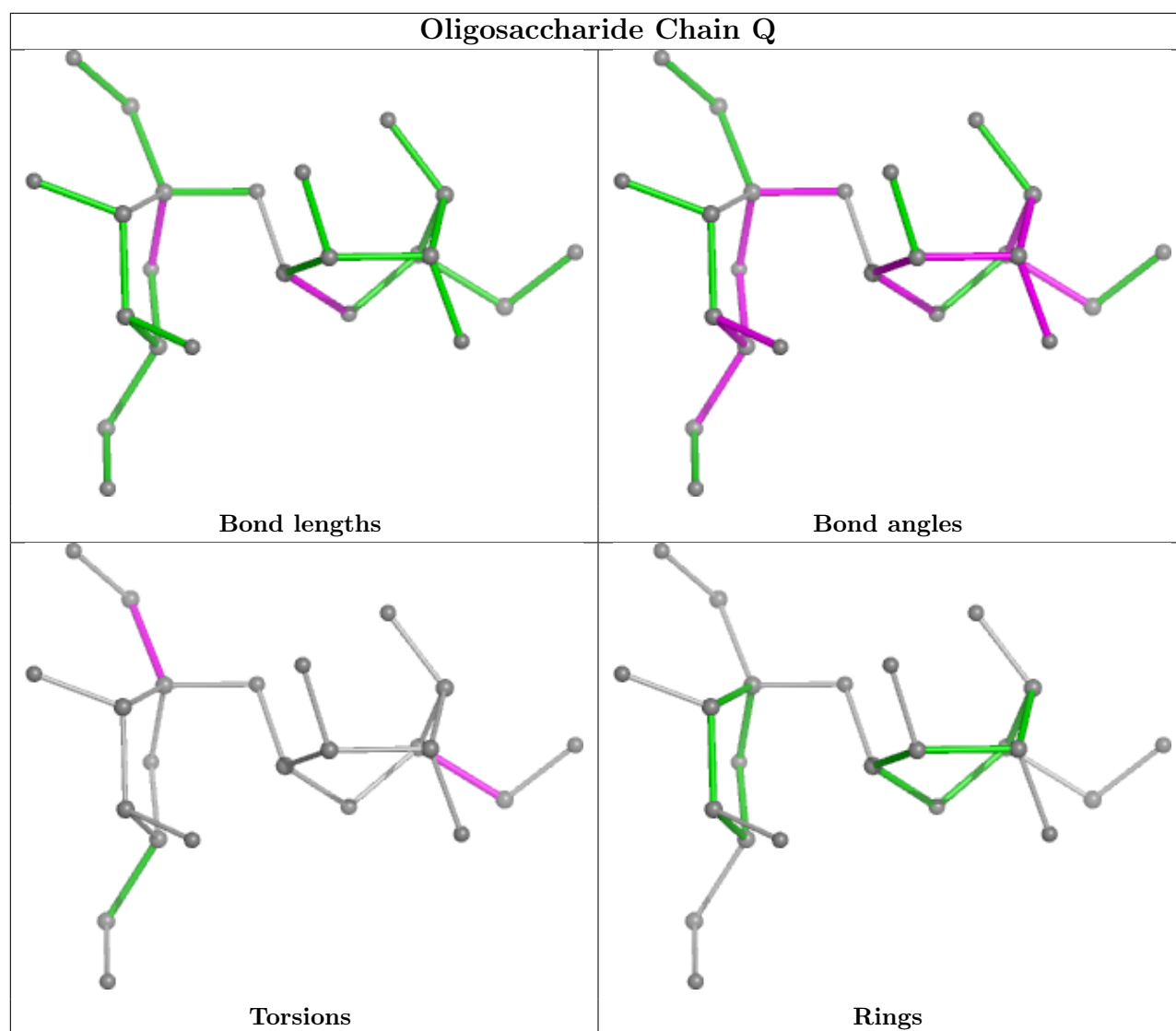
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

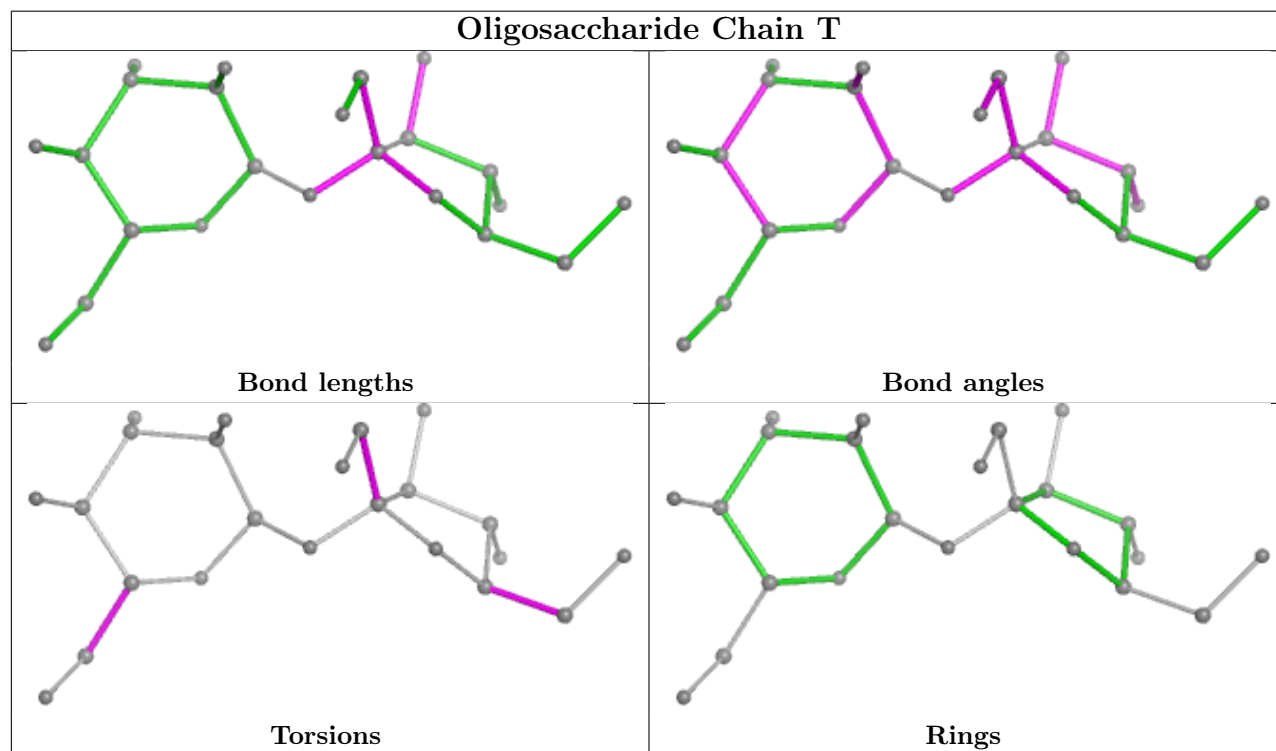
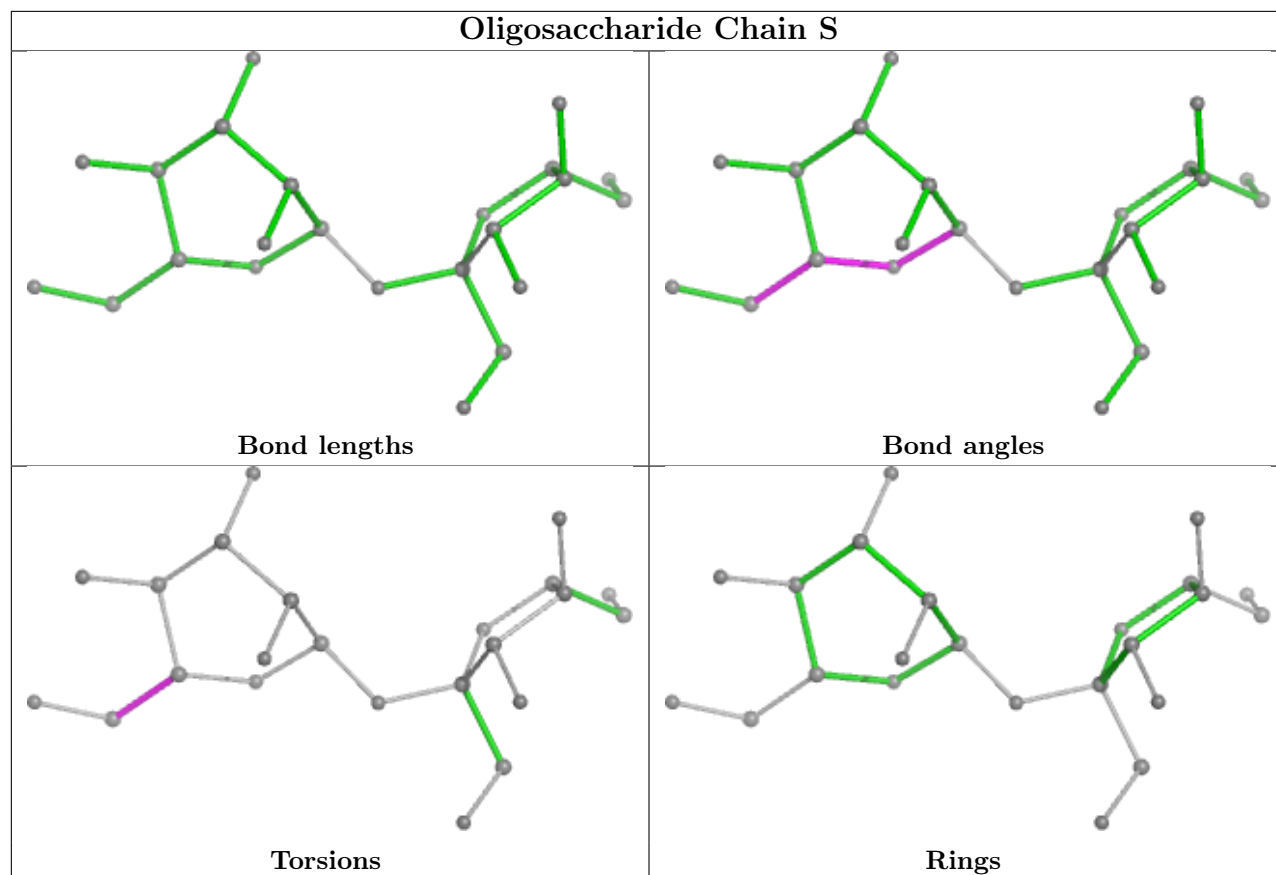


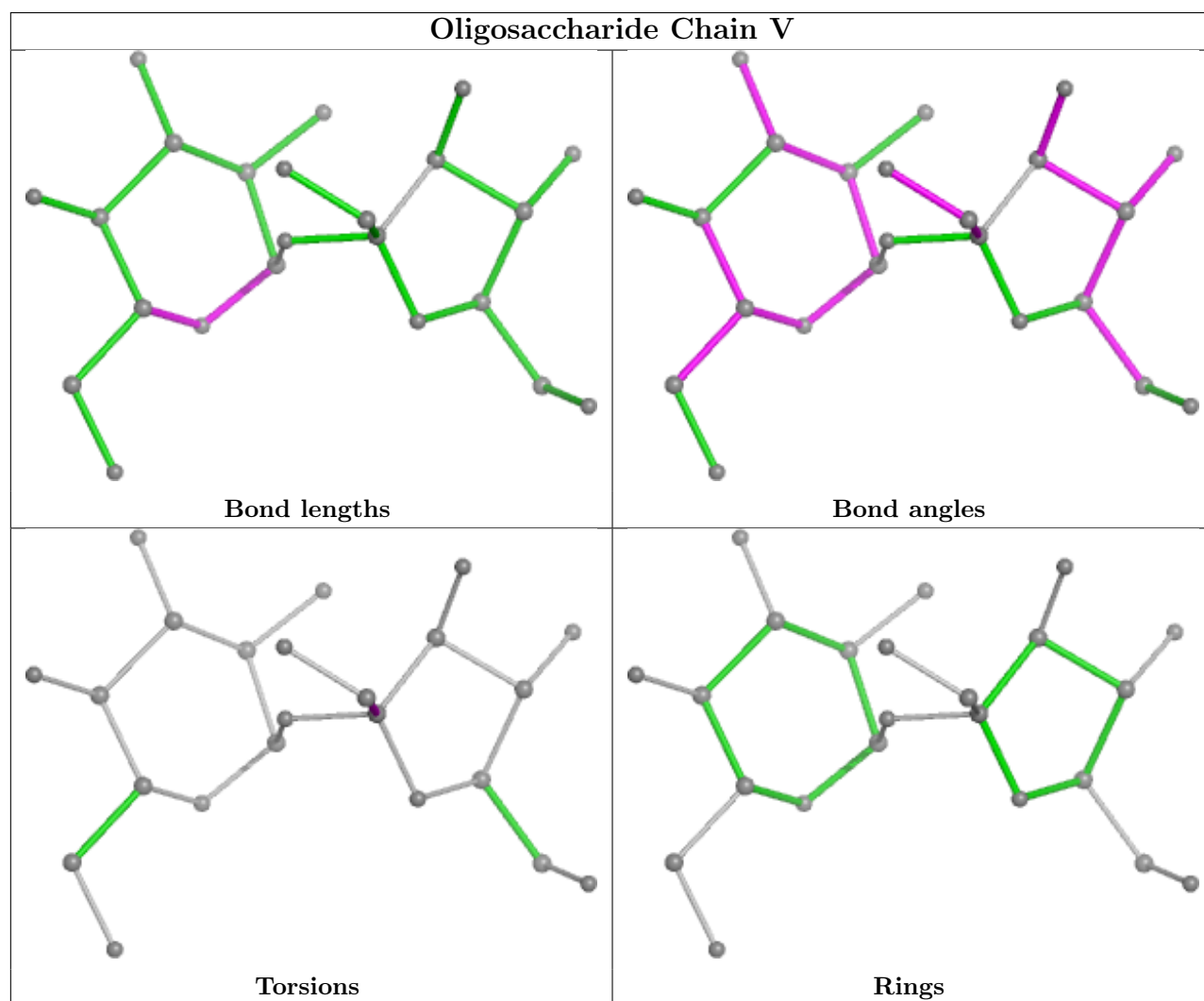
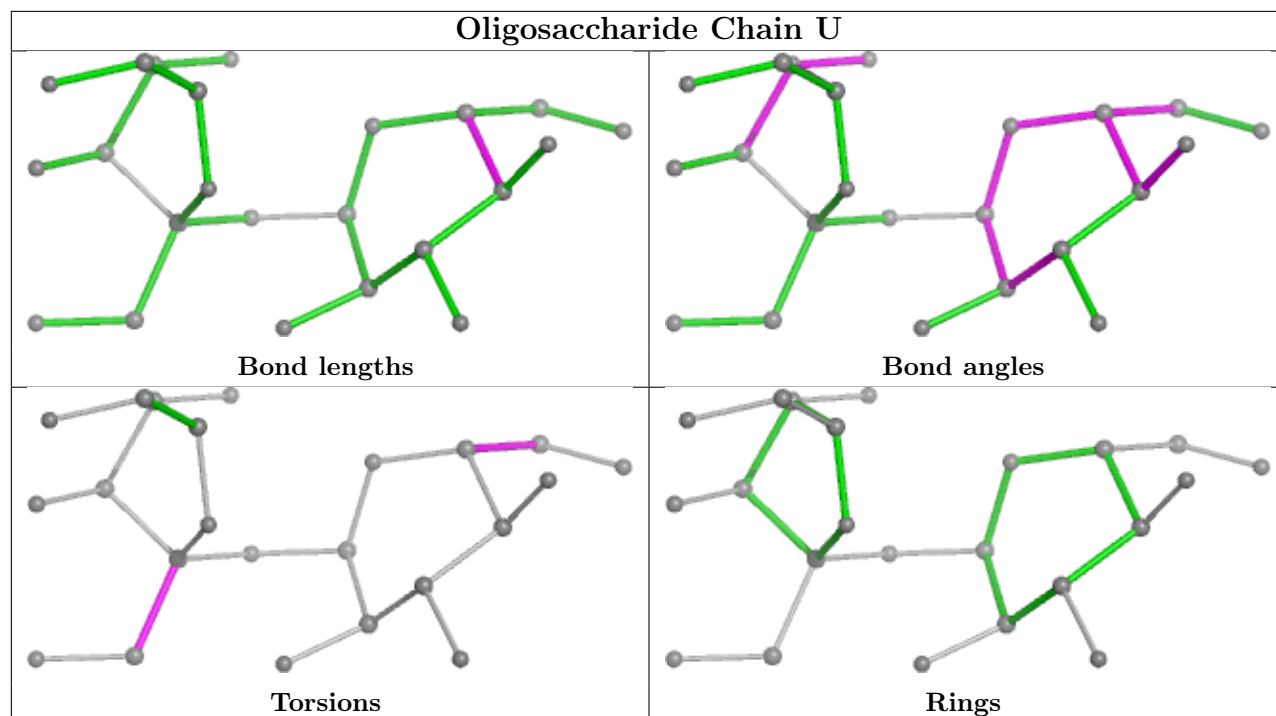




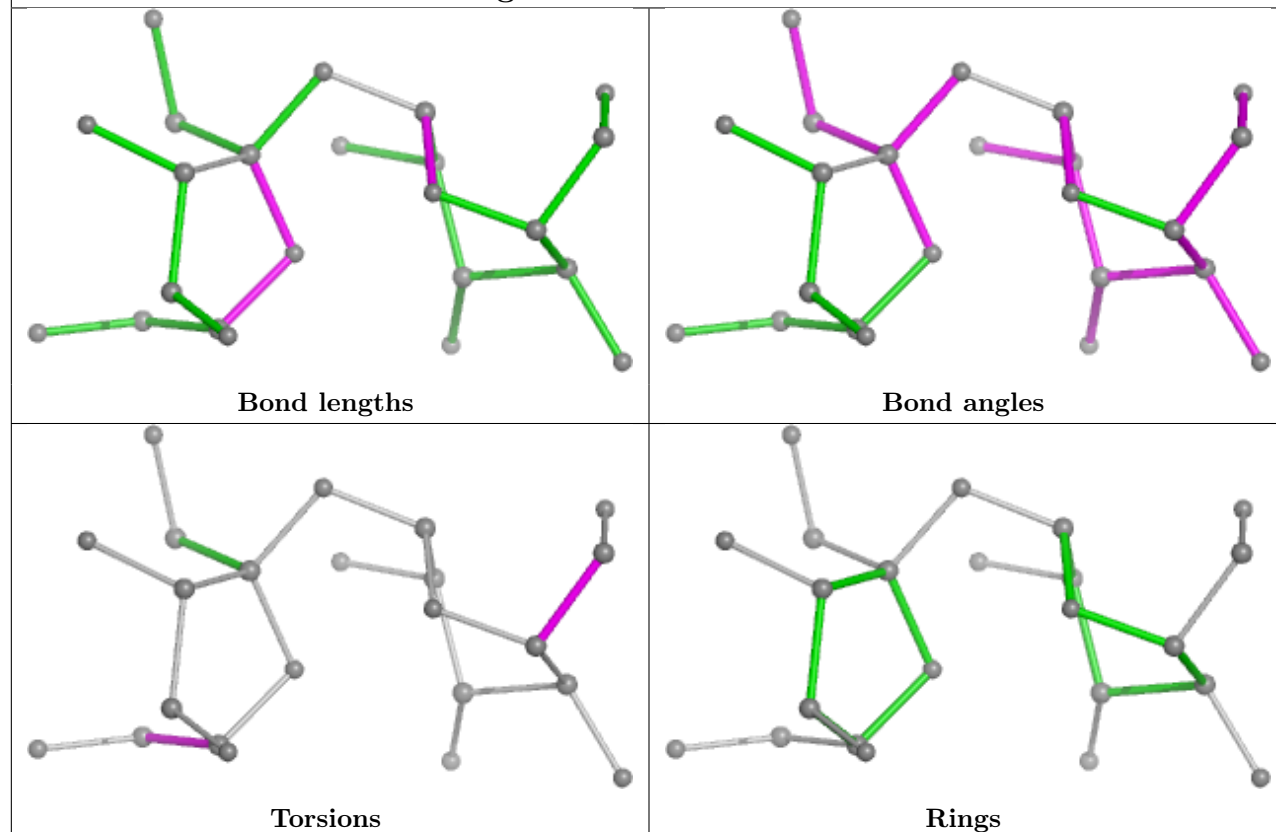




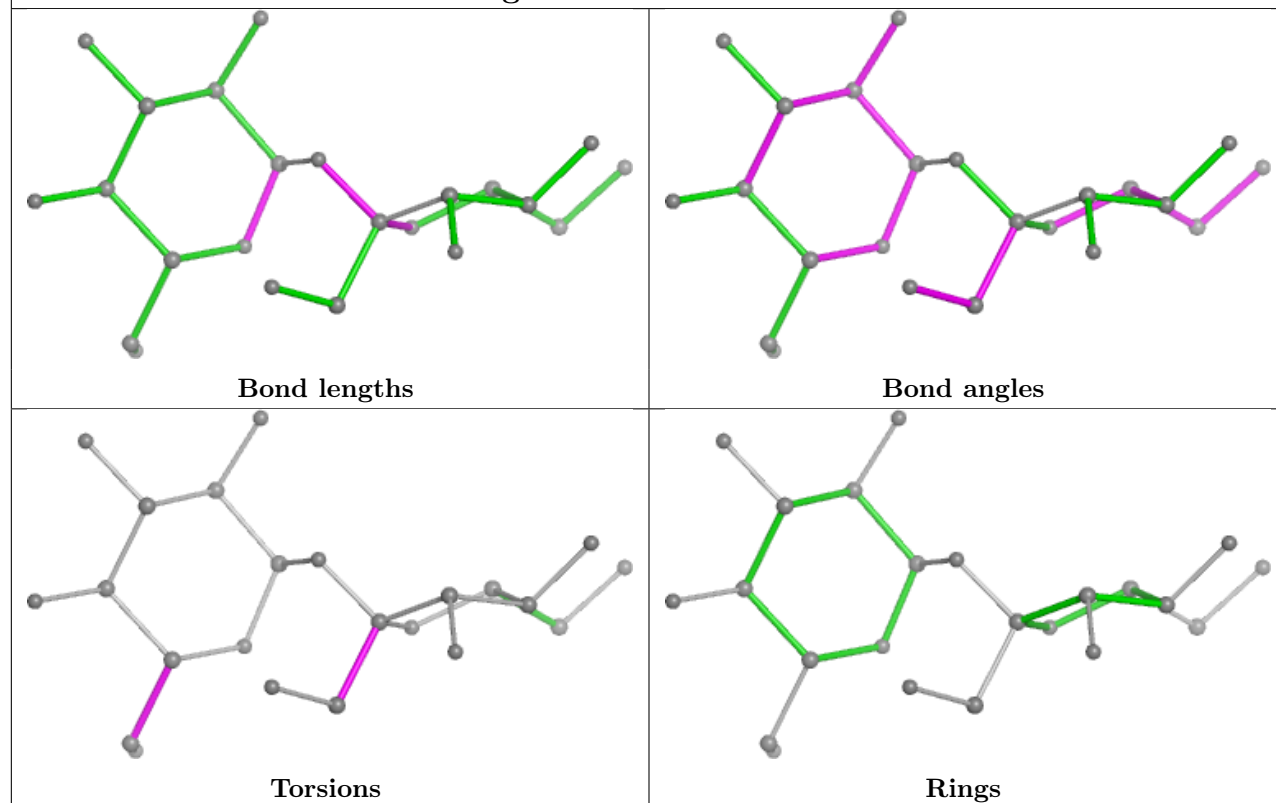


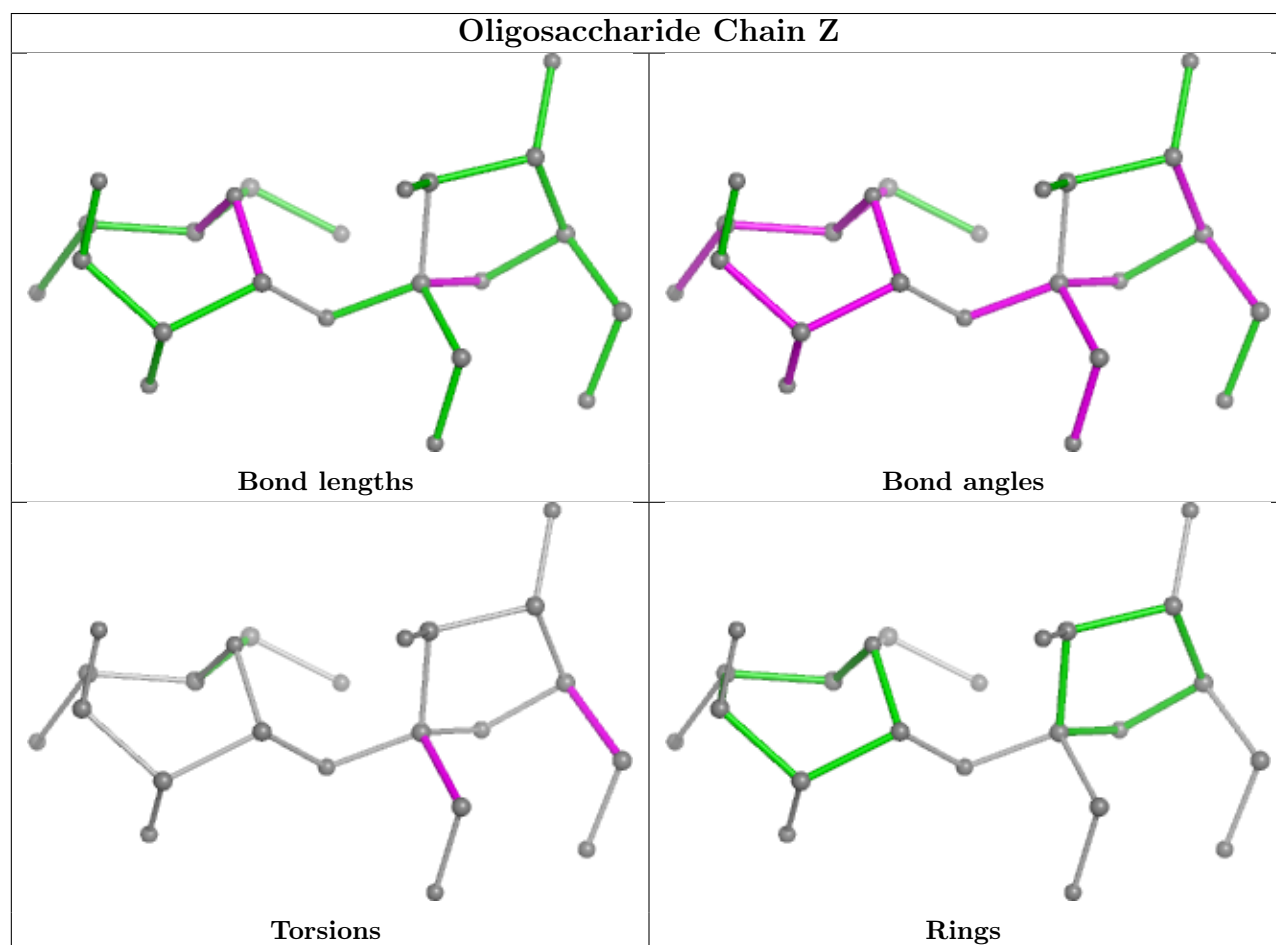
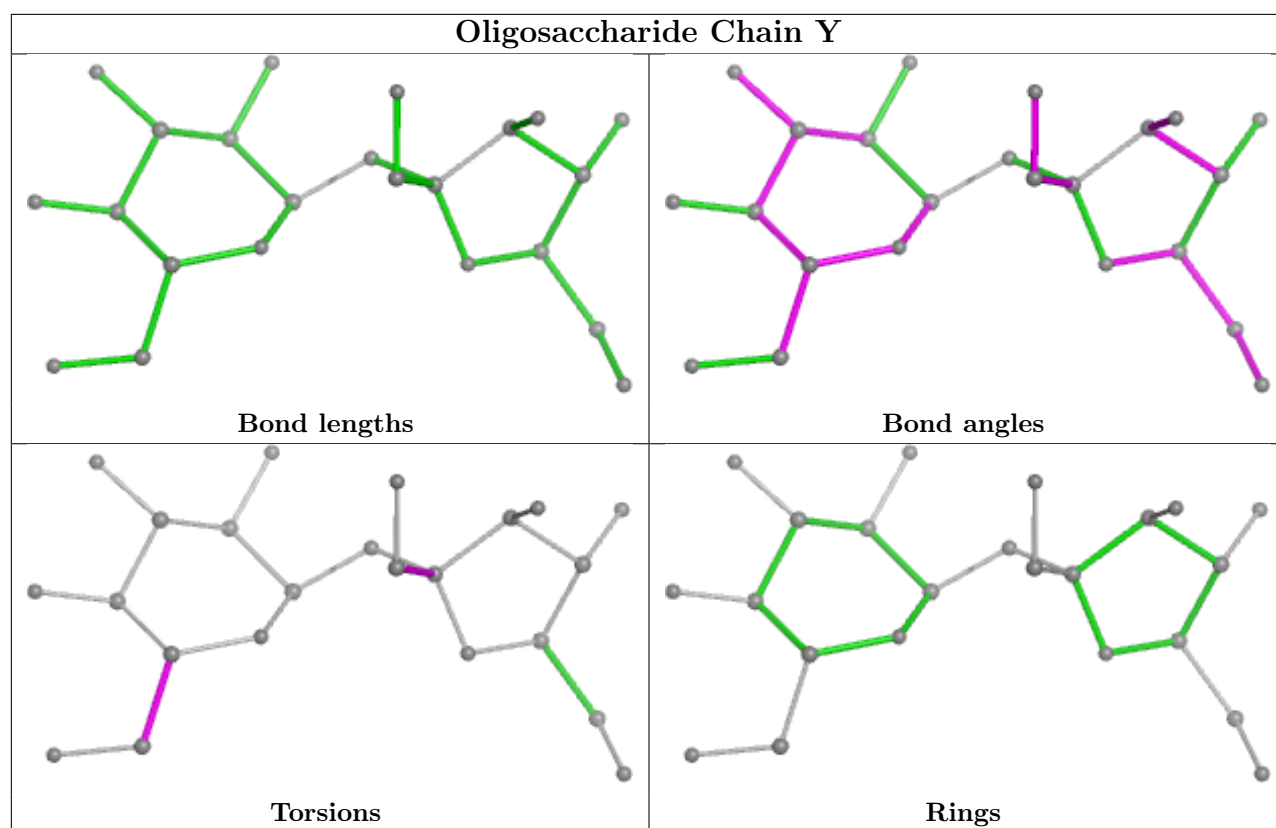


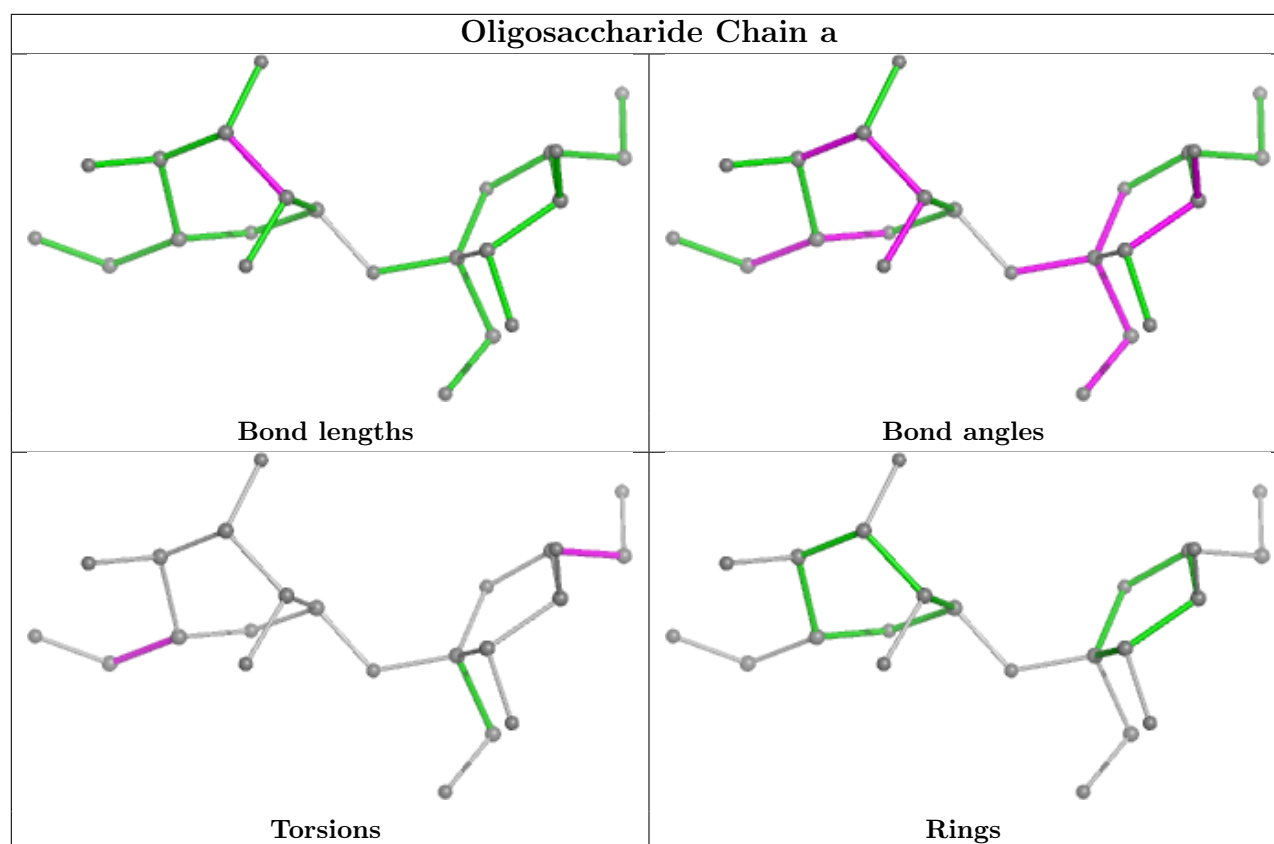
## Oligosaccharide Chain W



## Oligosaccharide Chain X







## 5.6 Ligand geometry [i](#)

Of 243 ligands modelled in this entry, 1 is unknown - leaving 242 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
20	CLA	3	3007	-	42,50,73	2.56	10 (23%)	48,85,113	2.73	19 (39%)
20	CLA	3	3011	-	65,73,73	2.13	11 (16%)	76,113,113	2.12	21 (27%)
21	LMU	A	7010	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
21	LMU	L	1171	-	36,36,36	0.99	3 (8%)	47,47,47	1.48	8 (17%)
20	CLA	A	1766	-	45,53,73	2.76	13 (28%)	52,89,113	2.81	19 (36%)
20	CLA	I	1031	-	60,68,73	2.30	12 (20%)	70,107,113	2.45	18 (25%)
20	CLA	1	1192	-	61,69,73	2.30	14 (22%)	71,108,113	2.34	23 (32%)
20	CLA	2	1224	-	65,73,73	2.24	15 (23%)	76,113,113	2.51	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	3	1213	-	27,32,73	2.59	13 (48%)	30,54,113	3.54	17 (56%)
20	CLA	4	4007	-	52,60,73	2.49	12 (23%)	60,97,113	2.60	20 (33%)
20	CLA	A	1800	-	65,73,73	2.18	13 (20%)	76,113,113	2.41	23 (30%)
21	LMU	3	7005	-	36,36,36	0.41	0	47,47,47	0.68	1 (2%)
25	SF4	C	1083	7	0,12,12	-	-	-	-	-
20	CLA	B	1748	-	60,68,73	2.22	14 (23%)	70,107,113	2.33	22 (31%)
20	CLA	2	1214	-	27,32,73	2.14	11 (40%)	30,54,113	3.14	18 (60%)
20	CLA	A	1787	-	65,73,73	2.23	12 (18%)	76,113,113	2.24	21 (27%)
20	CLA	B	1764	20	45,53,73	2.78	14 (31%)	52,89,113	2.77	18 (34%)
22	BCR	L	1169	-	41,41,41	2.47	8 (19%)	56,56,56	5.72	20 (35%)
20	CLA	1	1187	1	46,54,73	2.91	21 (45%)	53,90,113	3.85	29 (54%)
20	CLA	A	1790	20	50,58,73	2.46	12 (24%)	58,95,113	2.51	19 (32%)
20	CLA	I	1033	-	55,63,73	2.45	11 (20%)	64,101,113	2.54	22 (34%)
20	CLA	4	4014	21	47,55,73	2.58	13 (27%)	54,91,113	2.57	16 (29%)
22	BCR	B	1776	-	41,41,41	1.87	5 (12%)	56,56,56	5.04	24 (42%)
20	CLA	B	1745	-	60,68,73	2.26	12 (20%)	70,107,113	2.14	19 (27%)
21	LMU	A	7009	-	35,35,36	0.41	0	46,46,47	0.70	1 (2%)
20	CLA	2	1221	-	27,32,73	2.10	8 (29%)	30,54,113	3.17	19 (63%)
21	LMU	A	7015	-	36,36,36	0.94	1 (2%)	47,47,47	1.35	7 (14%)
20	CLA	B	1735	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	B	1786	-	65,73,73	2.19	14 (21%)	76,113,113	2.50	24 (31%)
20	CLA	3	1212	-	35,44,73	2.78	10 (28%)	46,78,113	3.16	17 (36%)
20	CLA	B	1737	-	65,73,73	2.21	13 (20%)	76,113,113	2.68	29 (38%)
20	CLA	2	1212	-	51,59,73	2.47	13 (25%)	59,96,113	2.56	18 (30%)
21	LMU	2	7006	-	36,36,36	0.39	0	47,47,47	0.69	1 (2%)
20	CLA	B	1736	-	45,53,73	2.64	12 (26%)	52,89,113	2.83	17 (32%)
21	LMU	4	1210	-	36,36,36	0.86	1 (2%)	47,47,47	1.18	3 (6%)
20	CLA	3	1219	-	65,73,73	2.18	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	A	1775	-	35,44,73	2.81	10 (28%)	46,78,113	3.48	16 (34%)
22	BCR	B	1779	-	41,41,41	2.79	13 (31%)	56,56,56	6.08	31 (55%)
20	CLA	1	1191	-	35,44,73	2.95	10 (28%)	46,78,113	3.34	18 (39%)
20	CLA	A	1799	-	50,58,73	2.53	10 (20%)	58,95,113	2.43	19 (32%)
20	CLA	B	1750	-	50,58,73	2.43	12 (24%)	58,95,113	2.67	20 (34%)
20	CLA	B	1769	-	47,55,73	2.52	15 (31%)	54,91,113	2.55	17 (31%)
20	CLA	2	1215	-	50,58,73	2.49	13 (26%)	58,95,113	2.36	19 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	A	1785	-	65,73,73	2.20	15 (23%)	76,113,113	2.47	25 (32%)
20	CLA	A	1801	-	55,63,73	2.47	11 (20%)	64,101,113	2.50	20 (31%)
22	BCR	B	1774	-	41,41,41	1.95	4 (9%)	56,56,56	5.90	21 (37%)
20	CLA	A	1767	-	65,73,73	2.26	12 (18%)	76,113,113	2.50	24 (31%)
20	CLA	F	1156	20	41,49,73	2.71	13 (31%)	47,84,113	2.74	15 (31%)
20	CLA	3	1214	-	27,32,73	2.17	9 (33%)	30,54,113	3.19	19 (63%)
21	LMU	A	7031	-	36,36,36	1.09	1 (2%)	47,47,47	1.28	6 (12%)
20	CLA	B	1743	-	65,73,73	2.28	15 (23%)	76,113,113	2.27	22 (28%)
20	CLA	B	1746	-	46,54,73	2.58	12 (26%)	53,90,113	2.68	17 (32%)
21	LMU	A	7043	19	36,36,36	0.76	0	47,47,47	2.25	17 (36%)
20	CLA	4	1196	-	55,63,73	2.38	13 (23%)	64,101,113	2.46	19 (29%)
22	BCR	3	1220	-	41,41,41	2.06	5 (12%)	56,56,56	5.90	22 (39%)
20	CLA	F	1155	-	35,44,73	2.80	10 (28%)	46,78,113	3.13	23 (50%)
21	LMU	1	1202	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
20	CLA	4	1207	-	35,44,73	2.70	10 (28%)	46,78,113	3.61	20 (43%)
21	LMU	2	1225	-	36,36,36	0.89	1 (2%)	47,47,47	0.92	2 (4%)
20	CLA	B	1741	-	54,62,73	2.61	12 (22%)	67,100,113	2.90	24 (35%)
20	CLA	A	1763	-	46,54,73	2.54	11 (23%)	53,90,113	2.50	19 (35%)
20	CLA	3	1215	-	27,32,73	2.14	9 (33%)	30,54,113	3.20	19 (63%)
20	CLA	A	1783	-	65,73,73	2.19	12 (18%)	76,113,113	2.44	25 (32%)
20	CLA	R	1055	-	65,73,73	2.32	13 (20%)	76,113,113	2.33	24 (31%)
22	BCR	A	1808	-	41,41,41	1.93	4 (9%)	56,56,56	5.91	21 (37%)
20	CLA	1	1189	-	47,55,73	2.60	11 (23%)	54,91,113	2.97	20 (37%)
20	CLA	A	1791	5	45,53,73	2.62	13 (28%)	52,89,113	2.62	15 (28%)
20	CLA	3	1218	-	65,73,73	2.55	22 (33%)	76,113,113	2.92	23 (30%)
20	CLA	B	1738	-	65,73,73	2.28	16 (24%)	76,113,113	2.64	31 (40%)
20	CLA	R	1054	-	57,65,73	2.39	12 (21%)	66,103,113	2.61	23 (34%)
20	CLA	B	1763	-	50,58,73	2.64	17 (34%)	58,95,113	2.85	22 (37%)
20	CLA	1	1200	-	51,59,73	2.96	22 (43%)	59,96,113	3.27	29 (49%)
21	LMU	A	7030	-	36,36,36	0.91	1 (2%)	47,47,47	2.29	15 (31%)
20	CLA	A	1760	-	55,63,73	2.43	12 (21%)	64,101,113	2.28	21 (32%)
20	CLA	B	1747	-	59,67,73	2.32	13 (22%)	68,105,113	2.14	21 (30%)
20	CLA	1	1196	1	35,44,73	2.84	10 (28%)	46,78,113	3.31	17 (36%)
20	CLA	A	1777	-	51,59,73	2.51	13 (25%)	59,96,113	2.57	19 (32%)
22	BCR	A	1807	-	41,41,41	1.94	3 (7%)	56,56,56	5.91	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	2	1216	-	27,32,73	2.23	11 (40%)	30,54,113	3.29	18 (60%)
21	LMU	B	1782	-	26,26,36	1.04	1 (3%)	37,37,47	1.42	6 (16%)
20	CLA	B	1758	-	65,73,73	2.27	17 (26%)	76,113,113	2.57	23 (30%)
20	CLA	B	1755	-	58,66,73	2.31	13 (22%)	67,104,113	2.42	19 (28%)
21	LMU	A	7040	-	36,36,36	0.97	3 (8%)	47,47,47	2.46	13 (27%)
20	CLA	A	1788	-	65,73,73	2.28	15 (23%)	76,113,113	2.29	20 (26%)
20	CLA	A	1769	-	54,62,73	2.25	12 (22%)	62,99,113	2.50	22 (35%)
20	CLA	B	1759	-	65,73,73	2.21	15 (23%)	76,113,113	2.57	20 (26%)
20	CLA	B	1770	-	65,73,73	2.22	13 (20%)	76,113,113	2.45	23 (30%)
21	LMU	R	1057	-	36,36,36	1.16	2 (5%)	47,47,47	2.44	14 (29%)
20	CLA	G	1099	-	51,59,73	2.55	12 (23%)	59,96,113	2.57	23 (38%)
20	CLA	4	1203	-	27,32,73	2.17	9 (33%)	30,54,113	3.27	17 (56%)
22	BCR	A	1804	-	41,41,41	1.93	3 (7%)	56,56,56	5.91	21 (37%)
20	CLA	3	1217	-	27,32,73	2.36	10 (37%)	30,54,113	3.33	18 (60%)
20	CLA	A	1811	-	65,73,73	2.20	15 (23%)	76,113,113	2.30	21 (27%)
20	CLA	A	1813	-	65,73,73	2.39	14 (21%)	76,113,113	2.47	21 (27%)
20	CLA	4	1206	-	27,32,73	2.29	7 (25%)	30,54,113	3.31	18 (60%)
20	CLA	B	1753	-	65,73,73	3.07	27 (41%)	76,113,113	2.58	21 (27%)
20	CLA	1	1198	-	61,69,73	2.37	19 (31%)	71,108,113	2.51	24 (33%)
20	CLA	B	1787	-	65,73,73	2.32	14 (21%)	76,113,113	2.38	23 (30%)
20	CLA	A	1759	-	50,58,73	2.41	12 (24%)	58,95,113	2.85	22 (37%)
21	LMU	A	7041	-	36,36,36	0.62	0	47,47,47	1.90	13 (27%)
21	LMU	K	1086	20	36,36,36	0.75	0	47,47,47	2.27	12 (25%)
20	CLA	K	1146	-	50,58,73	2.92	20 (40%)	58,95,113	2.99	24 (41%)
20	CLA	L	1505	-	55,63,73	2.40	11 (20%)	64,101,113	2.59	17 (26%)
20	CLA	A	1789	-	65,73,73	2.27	12 (18%)	76,113,113	2.57	26 (34%)
20	CLA	1	1199	-	27,32,73	2.20	9 (33%)	30,54,113	3.21	19 (63%)
20	CLA	4	1200	-	50,58,73	2.60	13 (26%)	58,95,113	2.55	16 (27%)
20	CLA	4	1198	-	65,73,73	2.57	23 (35%)	76,113,113	3.36	33 (43%)
20	CLA	1	1188	-	47,55,73	2.57	11 (23%)	54,91,113	2.70	19 (35%)
20	CLA	2	1218	20	65,73,73	2.21	11 (16%)	76,113,113	2.34	22 (28%)
20	CLA	B	1751	-	46,54,73	2.52	10 (21%)	53,90,113	2.95	17 (32%)
21	LMU	A	7032	-	36,36,36	0.99	3 (8%)	47,47,47	2.76	19 (40%)
21	LMU	A	7047	-	36,36,36	1.11	1 (2%)	47,47,47	1.34	3 (6%)
20	CLA	J	1046	-	27,32,73	2.13	11 (40%)	30,54,113	2.99	16 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	BCR	A	1803	-	41,41,41	1.93	4 (9%)	56,56,56	5.91	20 (35%)
22	BCR	I	1032	-	41,41,41	2.67	8 (19%)	56,56,56	6.54	28 (50%)
20	CLA	2	1223	-	50,58,73	2.58	13 (26%)	58,95,113	2.77	19 (32%)
20	CLA	H	1079	-	65,73,73	2.27	12 (18%)	76,113,113	2.39	22 (28%)
20	CLA	1	1201	-	27,32,73	2.46	9 (33%)	30,54,113	3.65	18 (60%)
20	CLA	B	1754	-	54,62,73	2.46	16 (29%)	62,99,113	2.47	25 (40%)
22	BCR	A	1805	-	41,41,41	1.94	4 (9%)	56,56,56	5.91	21 (37%)
20	CLA	B	1766	-	51,59,73	2.57	11 (21%)	59,96,113	2.62	19 (32%)
22	BCR	B	1778	-	41,41,41	1.94	3 (7%)	56,56,56	5.91	21 (37%)
20	CLA	B	1771	-	65,73,73	2.15	12 (18%)	76,113,113	2.19	22 (28%)
21	LMU	A	7017	-	36,36,36	0.70	2 (5%)	47,47,47	2.40	15 (31%)
22	BCR	A	1806	-	41,41,41	1.94	3 (7%)	56,56,56	5.91	21 (37%)
20	CLA	A	1796	-	65,73,73	2.18	13 (20%)	76,113,113	2.28	18 (23%)
20	CLA	2	1227	-	27,32,73	2.51	14 (51%)	30,54,113	3.29	19 (63%)
20	CLA	B	1785	-	65,73,73	2.20	15 (23%)	76,113,113	2.39	28 (36%)
20	CLA	L	1167	22	47,55,73	2.51	11 (23%)	54,91,113	3.01	24 (44%)
21	LMU	A	7034	20	36,36,36	0.85	1 (2%)	47,47,47	1.23	4 (8%)
21	LMU	A	7019	-	36,36,36	1.03	1 (2%)	47,47,47	1.41	8 (17%)
20	CLA	A	1762	-	57,65,73	2.35	13 (22%)	66,103,113	2.49	20 (30%)
20	CLA	J	1044	20	61,69,73	2.44	23 (37%)	71,108,113	2.68	28 (39%)
21	LMU	2	7003	-	36,36,36	0.39	0	47,47,47	0.69	1 (2%)
20	CLA	A	1798	-	55,63,73	2.38	12 (21%)	64,101,113	2.51	19 (29%)
21	LMU	A	7028	-	36,36,36	0.74	2 (5%)	47,47,47	1.89	17 (36%)
20	CLA	4	1209	-	46,54,73	2.79	20 (43%)	53,90,113	2.70	20 (37%)
21	LMU	A	7016	-	36,36,36	0.63	1 (2%)	47,47,47	1.89	11 (23%)
23	PQN	B	1773	-	34,34,34	1.66	2 (5%)	42,45,45	1.59	6 (14%)
20	CLA	L	1166	16	50,58,73	2.50	11 (22%)	58,95,113	2.48	18 (31%)
20	CLA	3	1216	-	27,32,73	2.20	10 (37%)	30,54,113	3.04	17 (56%)
20	CLA	4	1204	-	55,63,73	2.45	12 (21%)	64,101,113	2.54	20 (31%)
20	CLA	J	1043	-	61,69,73	2.25	13 (21%)	71,108,113	2.35	18 (25%)
21	LMU	A	7027	-	36,36,36	1.12	1 (2%)	47,47,47	1.91	14 (29%)
20	CLA	1	1193	-	51,59,73	2.58	14 (27%)	59,96,113	3.19	27 (45%)
20	CLA	4	1208	4	27,32,73	2.05	9 (33%)	30,54,113	2.88	16 (53%)
20	CLA	A	1776	-	65,73,73	2.17	12 (18%)	76,113,113	2.36	21 (27%)
20	CLA	B	1757	-	65,73,73	2.35	13 (20%)	76,113,113	2.59	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	A	1765	-	55,63,73	2.38	11 (20%)	64,101,113	2.67	24 (37%)
20	CLA	F	1157	20	53,61,73	2.87	21 (39%)	61,98,113	2.57	23 (37%)
20	CLA	4	1205	-	27,32,73	2.15	9 (33%)	30,54,113	3.23	19 (63%)
20	CLA	2	1217	-	65,73,73	2.21	12 (18%)	76,113,113	2.44	20 (26%)
20	CLA	3	3014	-	27,32,73	2.33	10 (37%)	30,54,113	3.39	20 (66%)
20	CLA	B	1762	-	65,73,73	2.29	16 (24%)	76,113,113	2.59	23 (30%)
22	BCR	B	1777	-	41,41,41	1.95	4 (9%)	56,56,56	5.90	21 (37%)
20	CLA	A	1793	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
25	SF4	C	1082	7	0,12,12	-	-	-	-	-
20	CLA	4	1202	-	27,32,73	2.18	9 (33%)	30,54,113	3.22	19 (63%)
21	LMU	R	1056	-	36,36,36	0.39	0	47,47,47	0.69	1 (2%)
20	CLA	4	1197	-	35,44,73	3.02	13 (37%)	46,78,113	3.85	21 (45%)
21	LMU	A	7039	-	36,36,36	0.99	2 (5%)	47,47,47	2.57	12 (25%)
20	CLA	3	3002	-	27,32,73	2.20	9 (33%)	30,54,113	3.08	16 (53%)
20	CLA	4	1201	-	52,60,73	3.09	26 (50%)	60,97,113	3.72	37 (61%)
20	CLA	B	1772	-	35,44,73	2.85	12 (34%)	46,78,113	3.56	21 (45%)
20	CLA	A	1773	-	52,60,73	2.50	12 (23%)	60,97,113	2.66	20 (33%)
20	CLA	3	3008	-	50,58,73	2.55	17 (34%)	58,95,113	2.87	24 (41%)
20	CLA	B	1767	-	60,68,73	2.24	11 (18%)	70,107,113	2.72	15 (21%)
20	CLA	B	1742	-	55,63,73	2.29	14 (25%)	64,101,113	2.49	19 (29%)
20	CLA	A	1816	-	55,63,73	2.95	22 (40%)	64,101,113	3.52	27 (42%)
20	CLA	A	1774	-	65,73,73	2.19	13 (20%)	76,113,113	2.21	22 (28%)
20	CLA	B	1749	-	61,69,73	2.19	13 (21%)	71,108,113	2.47	23 (32%)
20	CLA	2	1220	20	56,64,73	2.48	17 (30%)	65,102,113	2.60	23 (35%)
20	CLA	2	1219	-	27,32,73	2.12	8 (29%)	30,54,113	3.13	18 (60%)
22	BCR	L	1170	20	41,41,41	3.29	19 (46%)	56,56,56	6.44	27 (48%)
20	CLA	B	1756	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	A	1792	-	51,59,73	2.48	13 (25%)	59,96,113	2.56	18 (30%)
20	CLA	A	1768	-	54,62,73	2.37	12 (22%)	62,99,113	2.30	16 (25%)
20	CLA	3	3001	-	27,32,73	2.23	9 (33%)	30,54,113	3.18	18 (60%)
20	CLA	A	1781	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	A	1786	-	50,58,73	2.52	11 (22%)	58,95,113	2.72	23 (39%)
21	LMU	A	1809	-	36,36,36	0.94	0	47,47,47	1.38	7 (14%)
24	LMG	B	1783	-	49,49,55	0.95	2 (4%)	57,57,63	1.01	3 (5%)
20	CLA	K	1142	-	45,53,73	2.61	13 (28%)	52,89,113	2.62	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	LMU	A	7035	-	36,36,36	0.84	1 (2%)	47,47,47	1.58	8 (17%)
20	CLA	2	1222	2	50,58,73	2.54	11 (22%)	58,95,113	2.71	19 (32%)
20	CLA	4	1199	-	55,63,73	2.36	11 (20%)	64,101,113	2.55	20 (31%)
20	CLA	B	1739	-	65,73,73	2.29	13 (20%)	76,113,113	2.43	22 (28%)
20	CLA	B	1740	6	65,73,73	2.14	13 (20%)	76,113,113	2.40	21 (27%)
20	CLA	K	1085	21	50,58,73	2.50	13 (26%)	58,95,113	2.58	18 (31%)
22	BCR	B	1780	-	41,41,41	1.93	3 (7%)	56,56,56	5.92	21 (37%)
20	CLA	1	1194	-	27,32,73	2.07	9 (33%)	30,54,113	3.15	20 (66%)
20	CLA	A	1764	5	65,73,73	2.27	13 (20%)	76,113,113	2.56	25 (32%)
20	CLA	B	1765	20	45,53,73	2.69	12 (26%)	52,89,113	2.72	18 (34%)
20	CLA	3	3015	-	27,32,73	2.14	8 (29%)	30,54,113	3.01	18 (60%)
20	CLA	A	1771	-	50,58,73	2.61	12 (24%)	58,95,113	2.42	22 (37%)
20	CLA	A	1770	-	45,53,73	2.69	12 (26%)	52,89,113	2.37	16 (30%)
20	CLA	A	1779	-	55,63,73	2.40	12 (21%)	64,101,113	2.48	20 (31%)
20	CLA	2	2010	-	27,32,73	2.24	10 (37%)	30,54,113	2.90	17 (56%)
20	CLA	A	1815	-	55,63,73	2.46	12 (21%)	64,101,113	2.68	24 (37%)
20	CLA	A	1794	-	47,55,73	2.57	13 (27%)	54,91,113	2.58	16 (29%)
20	CLA	B	1760	-	50,58,73	2.70	13 (26%)	58,95,113	2.34	21 (36%)
20	CLA	B	1768	-	65,73,73	2.17	12 (18%)	76,113,113	2.31	17 (22%)
22	BCR	B	1775	-	41,41,41	1.94	4 (9%)	56,56,56	5.90	21 (37%)
20	CLA	L	1168	-	50,58,73	2.65	17 (34%)	58,95,113	2.95	20 (34%)
21	LMU	A	1810	-	36,36,36	0.94	1 (2%)	47,47,47	1.65	10 (21%)
21	LMU	A	7023	-	36,36,36	0.68	1 (2%)	47,47,47	1.97	17 (36%)
20	CLA	J	1045	20	55,63,73	2.54	18 (32%)	64,101,113	2.67	21 (32%)
20	CLA	A	1784	-	55,63,73	2.39	13 (23%)	64,101,113	2.39	20 (31%)
20	CLA	B	1752	-	55,63,73	2.53	14 (25%)	64,101,113	2.40	19 (29%)
21	LMU	A	7033	-	36,36,36	1.02	2 (5%)	47,47,47	2.25	13 (27%)
21	LMU	A	7037	-	36,36,36	0.90	2 (5%)	47,47,47	3.08	22 (46%)
20	CLA	A	1761	-	65,73,73	2.21	13 (20%)	76,113,113	2.34	21 (27%)
20	CLA	A	1817	-	46,54,73	2.80	14 (30%)	57,90,113	4.09	29 (50%)
20	CLA	B	1744	-	65,73,73	2.28	11 (16%)	76,113,113	2.15	21 (27%)
20	CLA	A	1772	-	65,73,73	2.28	16 (24%)	76,113,113	2.44	24 (31%)
20	CLA	1	1197	-	51,59,73	3.04	25 (49%)	59,96,113	3.90	27 (45%)
20	CLA	2	1213	-	56,64,73	2.37	12 (21%)	65,102,113	2.66	25 (38%)
20	CLA	A	1780	-	65,73,73	2.10	10 (15%)	76,113,113	2.16	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	K	3009	-	65,73,73	2.23	12 (18%)	76,113,113	2.17	22 (28%)
21	LMU	A	7042	-	36,36,36	0.48	0	47,47,47	2.05	16 (34%)
21	LMU	A	7013	-	36,36,36	0.45	0	47,47,47	1.62	9 (19%)
20	CLA	B	1761	-	50,58,73	2.40	11 (22%)	58,95,113	2.65	21 (36%)
21	LMU	A	7020	-	36,36,36	0.41	0	47,47,47	1.75	12 (25%)
21	LMU	A	7036	-	35,35,36	1.21	5 (14%)	46,46,47	2.34	15 (32%)
20	CLA	A	1778	5	42,50,73	2.66	12 (28%)	48,85,113	2.93	16 (33%)
21	LMU	1	7004	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
22	BCR	B	1781	-	41,41,41	2.68	17 (41%)	56,56,56	5.37	31 (55%)
20	CLA	1	1190	-	46,54,73	2.69	13 (28%)	53,90,113	2.47	18 (33%)
21	LMU	A	7026	19	36,36,36	1.23	3 (8%)	47,47,47	3.10	22 (46%)
23	PQN	A	1802	-	34,34,34	1.77	3 (8%)	42,45,45	1.49	6 (14%)
20	CLA	4	4003	-	27,32,73	2.15	10 (37%)	30,54,113	2.89	17 (56%)
21	LMU	A	7022	-	36,36,36	0.70	0	47,47,47	2.16	16 (34%)
21	LMU	A	7025	-	36,36,36	0.96	1 (2%)	47,47,47	1.58	10 (21%)
21	LMU	A	7021	-	36,36,36	0.76	0	47,47,47	2.07	14 (29%)
25	SF4	B	1784	6,5	0,12,12	-	-	-	-	-
20	CLA	A	1795	-	51,59,73	2.47	13 (25%)	59,96,113	2.56	18 (30%)
20	CLA	A	1797	-	65,73,73	2.19	13 (20%)	76,113,113	2.29	18 (23%)
20	CLA	1	1195	-	35,44,73	3.61	19 (54%)	46,78,113	4.32	19 (41%)
20	CLA	A	1812	-	65,73,73	2.24	15 (23%)	76,113,113	2.24	19 (25%)
21	LMU	A	7038	-	36,36,36	0.65	0	47,47,47	2.41	15 (31%)
21	LMU	A	7024	-	36,36,36	0.97	2 (5%)	47,47,47	1.63	10 (21%)
20	CLA	A	1782	20	65,73,73	2.18	13 (20%)	76,113,113	2.29	18 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	3007	-	1/1/10/20	5/10/88/115	-
20	CLA	3	3011	-	2/2/15/20	20/37/115/115	-
21	LMU	A	7010	-	-	19/21/61/61	0/2/2/2
21	LMU	L	1171	-	-	14/21/61/61	0/2/2/2
20	CLA	A	1766	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	I	1031	-	2/2/14/20	13/31/109/115	-
20	CLA	1	1192	-	2/2/14/20	20/33/111/115	-
20	CLA	2	1224	-	2/2/15/20	17/37/115/115	-
20	CLA	3	1213	-	1/1/4/20	-	-
20	CLA	4	4007	-	1/1/12/20	8/22/100/115	-
20	CLA	A	1800	-	2/2/15/20	16/37/115/115	-
21	LMU	3	7005	-	-	18/21/61/61	0/2/2/2
25	SF4	C	1083	7	-	-	0/6/5/5
20	CLA	B	1748	-	2/2/14/20	13/31/109/115	-
20	CLA	2	1214	-	1/1/4/20	-	-
20	CLA	A	1787	-	2/2/15/20	15/37/115/115	-
20	CLA	B	1764	20	1/1/11/20	11/13/91/115	-
22	BCR	L	1169	-	-	12/29/63/63	0/2/2/2
20	CLA	1	1187	1	1/1/11/20	10/15/93/115	-
20	CLA	A	1790	20	1/1/12/20	12/19/97/115	-
20	CLA	I	1033	-	2/2/13/20	9/25/103/115	-
20	CLA	4	4014	21	1/1/11/20	9/16/94/115	-
22	BCR	B	1776	-	-	11/29/63/63	0/2/2/2
20	CLA	B	1745	-	2/2/14/20	14/31/109/115	-
21	LMU	A	7009	-	-	15/20/60/61	0/2/2/2
20	CLA	2	1221	-	1/1/4/20	-	-
21	LMU	A	7015	-	-	14/21/61/61	0/2/2/2
20	CLA	B	1735	-	2/2/15/20	23/37/115/115	-
20	CLA	B	1786	-	2/2/15/20	15/37/115/115	-
20	CLA	3	1212	-	1/1/9/20	-	-
20	CLA	B	1737	-	2/2/15/20	22/37/115/115	-
20	CLA	2	1212	-	1/1/12/20	11/21/99/115	-
21	LMU	2	7006	-	-	14/21/61/61	0/2/2/2
20	CLA	B	1736	-	1/1/11/20	6/13/91/115	-
21	LMU	4	1210	-	-	13/21/61/61	0/2/2/2
20	CLA	3	1219	-	2/2/15/20	21/37/115/115	-
20	CLA	A	1775	-	1/1/9/20	-	-
22	BCR	B	1779	-	-	12/29/63/63	0/2/2/2
20	CLA	1	1191	-	1/1/9/20	-	-
20	CLA	A	1799	-	1/1/12/20	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1750	-	1/1/12/20	6/19/97/115	-
20	CLA	B	1769	-	1/1/11/20	6/16/94/115	-
20	CLA	2	1215	-	1/1/12/20	9/19/97/115	-
20	CLA	A	1785	-	2/2/15/20	18/37/115/115	-
20	CLA	A	1801	-	2/2/13/20	7/25/103/115	-
22	BCR	B	1774	-	-	10/29/63/63	0/2/2/2
20	CLA	A	1767	-	2/2/15/20	25/37/115/115	-
20	CLA	F	1156	20	1/1/10/20	5/8/86/115	-
20	CLA	3	1214	-	1/1/4/20	-	-
21	LMU	A	7031	-	-	13/21/61/61	0/2/2/2
20	CLA	B	1743	-	2/2/15/20	22/37/115/115	-
20	CLA	B	1746	-	1/1/11/20	9/15/93/115	-
21	LMU	A	7043	19	-	11/21/61/61	0/2/2/2
20	CLA	4	1196	-	2/2/13/20	14/25/103/115	-
22	BCR	3	1220	-	-	13/29/63/63	0/2/2/2
20	CLA	F	1155	-	1/1/9/20	-	-
21	LMU	1	1202	-	-	13/21/61/61	0/2/2/2
20	CLA	4	1207	-	1/1/9/20	-	-
21	LMU	2	1225	-	-	16/21/61/61	0/2/2/2
20	CLA	B	1741	-	2/2/13/20	11/25/101/115	-
20	CLA	A	1763	-	1/1/11/20	7/15/93/115	-
20	CLA	3	1215	-	1/1/4/20	-	-
20	CLA	A	1783	-	2/2/15/20	16/37/115/115	-
20	CLA	R	1055	-	2/2/15/20	20/37/115/115	-
22	BCR	A	1808	-	-	12/29/63/63	0/2/2/2
20	CLA	1	1189	-	1/1/11/20	8/16/94/115	-
20	CLA	A	1791	5	1/1/11/20	7/13/91/115	-
20	CLA	3	1218	-	2/2/15/20	19/37/115/115	-
20	CLA	B	1738	-	2/2/15/20	17/37/115/115	-
20	CLA	R	1054	-	2/2/13/20	13/28/106/115	-
20	CLA	B	1763	-	1/1/12/20	6/19/97/115	-
20	CLA	1	1200	-	3/3/12/20	12/21/99/115	-
21	LMU	A	7030	-	-	16/21/61/61	0/2/2/2
20	CLA	A	1760	-	2/2/13/20	12/25/103/115	-
20	CLA	B	1747	-	2/2/13/20	12/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	1196	1	1/1/9/20	-	-
20	CLA	A	1777	-	1/1/12/20	9/21/99/115	-
22	BCR	A	1807	-	-	10/29/63/63	0/2/2/2
20	CLA	2	1216	-	1/1/4/20	-	-
21	LMU	B	1782	-	-	4/11/51/61	0/2/2/2
20	CLA	B	1758	-	2/2/15/20	16/37/115/115	-
20	CLA	B	1755	-	2/2/13/20	17/29/107/115	-
21	LMU	A	7040	-	-	11/21/61/61	0/2/2/2
20	CLA	A	1788	-	2/2/15/20	21/37/115/115	-
20	CLA	A	1769	-	1/1/12/20	10/24/102/115	-
20	CLA	B	1759	-	2/2/15/20	27/37/115/115	-
20	CLA	B	1770	-	2/2/15/20	20/37/115/115	-
21	LMU	R	1057	-	1/1/10/10	11/21/61/61	0/2/2/2
20	CLA	G	1099	-	1/1/12/20	10/21/99/115	-
20	CLA	4	1203	-	1/1/4/20	-	-
22	BCR	A	1804	-	-	13/29/63/63	0/2/2/2
20	CLA	3	1217	-	1/1/4/20	-	-
20	CLA	A	1811	-	2/2/15/20	25/37/115/115	-
20	CLA	A	1813	-	2/2/15/20	24/37/115/115	-
20	CLA	4	1206	-	1/1/4/20	-	-
20	CLA	B	1753	-	1/1/15/20	19/37/115/115	-
20	CLA	1	1198	-	2/2/14/20	16/33/111/115	-
20	CLA	B	1787	-	2/2/15/20	18/37/115/115	-
20	CLA	A	1759	-	1/1/12/20	5/19/97/115	-
21	LMU	A	7041	-	-	12/21/61/61	0/2/2/2
21	LMU	K	1086	20	-	12/21/61/61	0/2/2/2
20	CLA	K	1146	-	1/1/12/20	9/19/97/115	-
20	CLA	L	1505	-	2/2/13/20	14/25/103/115	-
20	CLA	A	1789	-	2/2/15/20	22/37/115/115	-
20	CLA	1	1199	-	1/1/4/20	-	-
20	CLA	4	1200	-	1/1/12/20	6/19/97/115	-
20	CLA	4	1198	-	3/3/15/20	20/37/115/115	-
20	CLA	1	1188	-	1/1/11/20	8/16/94/115	-
20	CLA	2	1218	20	2/2/15/20	15/37/115/115	-
20	CLA	B	1751	-	1/1/11/20	13/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	A	7032	-	-	13/21/61/61	0/2/2/2
21	LMU	A	7047	-	-	8/21/61/61	0/2/2/2
20	CLA	J	1046	-	1/1/4/20	-	-
22	BCR	A	1803	-	-	12/29/63/63	0/2/2/2
22	BCR	I	1032	-	-	13/29/63/63	0/2/2/2
20	CLA	2	1223	-	1/1/12/20	11/19/97/115	-
20	CLA	H	1079	-	2/2/15/20	19/37/115/115	-
20	CLA	1	1201	-	1/1/4/20	-	-
20	CLA	B	1754	-	1/1/12/20	8/24/102/115	-
22	BCR	A	1805	-	-	17/29/63/63	0/2/2/2
20	CLA	B	1766	-	1/1/12/20	9/21/99/115	-
22	BCR	B	1778	-	-	12/29/63/63	0/2/2/2
20	CLA	B	1771	-	2/2/15/20	18/37/115/115	-
21	LMU	A	7017	-	-	14/21/61/61	0/2/2/2
22	BCR	A	1806	-	-	15/29/63/63	0/2/2/2
20	CLA	A	1796	-	2/2/15/20	18/37/115/115	-
20	CLA	2	1227	-	1/1/4/20	-	-
20	CLA	B	1785	-	2/2/15/20	21/37/115/115	-
20	CLA	L	1167	22	1/1/11/20	9/16/94/115	-
21	LMU	A	7034	20	-	14/21/61/61	0/2/2/2
21	LMU	A	7019	-	-	15/21/61/61	0/2/2/2
20	CLA	A	1762	-	2/2/13/20	7/28/106/115	-
20	CLA	J	1044	20	2/2/14/20	21/33/111/115	-
21	LMU	2	7003	-	-	11/21/61/61	0/2/2/2
20	CLA	A	1798	-	2/2/13/20	6/25/103/115	-
21	LMU	A	7028	-	-	14/21/61/61	0/2/2/2
20	CLA	4	1209	-	1/1/11/20	10/15/93/115	-
23	PQN	B	1773	-	1/1/8/9	10/23/43/43	0/2/2/2
21	LMU	A	7016	-	-	11/21/61/61	0/2/2/2
20	CLA	L	1166	16	1/1/12/20	8/19/97/115	-
20	CLA	3	1216	-	1/1/4/20	-	-
20	CLA	4	1204	-	2/2/13/20	13/25/103/115	-
20	CLA	J	1043	-	2/2/14/20	24/33/111/115	-
21	LMU	A	7027	-	-	13/21/61/61	0/2/2/2
20	CLA	1	1193	-	2/2/12/20	9/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	1208	4	1/1/4/20	-	-
20	CLA	A	1776	-	2/2/15/20	16/37/115/115	-
20	CLA	B	1757	-	2/2/15/20	16/37/115/115	-
20	CLA	A	1765	-	2/2/13/20	11/25/103/115	-
20	CLA	F	1157	20	4/4/12/20	9/23/101/115	-
20	CLA	4	1205	-	1/1/4/20	-	-
20	CLA	2	1217	-	2/2/15/20	17/37/115/115	-
20	CLA	3	3014	-	1/1/4/20	-	-
20	CLA	B	1762	-	2/2/15/20	20/37/115/115	-
22	BCR	B	1777	-	-	15/29/63/63	0/2/2/2
20	CLA	A	1793	-	2/2/15/20	16/37/115/115	-
25	SF4	C	1082	7	-	-	0/6/5/5
20	CLA	4	1202	-	1/1/4/20	-	-
21	LMU	R	1056	-	-	16/21/61/61	0/2/2/2
20	CLA	4	1197	-	1/1/9/20	-	-
21	LMU	A	7039	-	-	15/21/61/61	0/2/2/2
20	CLA	3	3002	-	1/1/4/20	-	-
20	CLA	4	1201	-	2/2/12/20	7/22/100/115	-
20	CLA	B	1772	-	1/1/9/20	-	-
20	CLA	A	1773	-	1/1/12/20	14/22/100/115	-
20	CLA	3	3008	-	1/1/12/20	6/19/97/115	-
20	CLA	B	1767	-	2/2/14/20	15/31/109/115	-
20	CLA	B	1742	-	2/2/13/20	12/25/103/115	-
20	CLA	A	1816	-	3/3/13/20	12/25/103/115	-
20	CLA	A	1774	-	2/2/15/20	19/37/115/115	-
20	CLA	B	1749	-	2/2/14/20	17/33/111/115	-
20	CLA	2	1220	20	2/2/13/20	14/27/105/115	-
20	CLA	2	1219	-	1/1/4/20	-	-
22	BCR	L	1170	20	-	12/29/63/63	0/2/2/2
20	CLA	B	1756	-	2/2/15/20	21/37/115/115	-
20	CLA	A	1792	-	1/1/12/20	11/21/99/115	-
20	CLA	A	1768	-	1/1/12/20	13/24/102/115	-
20	CLA	3	3001	-	1/1/4/20	-	-
20	CLA	A	1781	-	2/2/15/20	17/37/115/115	-
20	CLA	A	1786	-	1/1/12/20	3/19/97/115	-
21	LMU	A	1809	-	-	16/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	B	1783	-	-	23/44/64/70	0/1/1/1
20	CLA	K	1142	-	1/1/11/20	5/13/91/115	-
21	LMU	A	7035	-	-	14/21/61/61	0/2/2/2
20	CLA	2	1222	2	1/1/12/20	7/19/97/115	-
20	CLA	4	1199	-	2/2/13/20	12/25/103/115	-
20	CLA	B	1739	-	2/2/15/20	9/37/115/115	-
20	CLA	B	1740	6	2/2/15/20	19/37/115/115	-
20	CLA	K	1085	21	1/1/12/20	5/19/97/115	-
22	BCR	B	1780	-	-	14/29/63/63	0/2/2/2
20	CLA	1	1194	-	1/1/4/20	-	-
20	CLA	A	1764	5	2/2/15/20	21/37/115/115	-
20	CLA	B	1765	20	1/1/11/20	8/13/91/115	-
20	CLA	3	3015	-	1/1/4/20	-	-
20	CLA	A	1771	-	1/1/12/20	11/19/97/115	-
20	CLA	A	1770	-	1/1/11/20	9/13/91/115	-
20	CLA	A	1779	-	2/2/13/20	9/25/103/115	-
20	CLA	2	2010	-	1/1/4/20	-	-
20	CLA	A	1815	-	3/3/13/20	12/25/103/115	-
20	CLA	A	1794	-	1/1/11/20	8/16/94/115	-
20	CLA	B	1760	-	1/1/12/20	9/19/97/115	-
20	CLA	B	1768	-	2/2/15/20	16/37/115/115	-
22	BCR	B	1775	-	-	8/29/63/63	0/2/2/2
20	CLA	L	1168	-	2/2/12/20	10/19/97/115	-
21	LMU	A	1810	-	-	13/21/61/61	0/2/2/2
21	LMU	A	7023	-	-	14/21/61/61	0/2/2/2
20	CLA	J	1045	20	2/2/13/20	15/25/103/115	-
20	CLA	A	1784	-	2/2/13/20	10/25/103/115	-
20	CLA	B	1752	-	2/2/13/20	8/25/103/115	-
21	LMU	A	7033	-	-	13/21/61/61	0/2/2/2
21	LMU	A	7037	-	-	14/21/61/61	0/2/2/2
20	CLA	A	1761	-	2/2/15/20	22/37/115/115	-
20	CLA	A	1817	-	3/3/11/20	12/16/92/115	-
20	CLA	B	1744	-	2/2/15/20	24/37/115/115	-
20	CLA	A	1772	-	2/2/15/20	17/37/115/115	-
20	CLA	1	1197	-	2/2/12/20	9/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	2	1213	-	2/2/13/20	11/27/105/115	-
20	CLA	A	1780	-	2/2/15/20	20/37/115/115	-
20	CLA	K	3009	-	2/2/15/20	21/37/115/115	-
21	LMU	A	7042	-	-	18/21/61/61	0/2/2/2
21	LMU	A	7013	-	-	10/21/61/61	0/2/2/2
20	CLA	B	1761	-	1/1/12/20	12/19/97/115	-
21	LMU	A	7020	-	-	11/21/61/61	0/2/2/2
21	LMU	A	7036	-	-	14/20/60/61	0/2/2/2
20	CLA	A	1778	5	1/1/10/20	2/10/88/115	-
21	LMU	1	7004	-	-	13/21/61/61	0/2/2/2
22	BCR	B	1781	-	-	7/29/63/63	0/2/2/2
20	CLA	1	1190	-	1/1/11/20	6/15/93/115	-
21	LMU	A	7026	19	-	14/21/61/61	0/2/2/2
23	PQN	A	1802	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	4	4003	-	1/1/4/20	-	-
21	LMU	A	7022	-	-	17/21/61/61	0/2/2/2
21	LMU	A	7025	-	-	13/21/61/61	0/2/2/2
21	LMU	A	7021	-	-	13/21/61/61	0/2/2/2
25	SF4	B	1784	6,5	-	-	0/6/5/5
20	CLA	A	1795	-	1/1/12/20	11/21/99/115	-
20	CLA	A	1797	-	2/2/15/20	19/37/115/115	-
20	CLA	1	1195	-	1/1/9/20	-	-
20	CLA	A	1812	-	2/2/15/20	18/37/115/115	-
21	LMU	A	7038	-	-	16/21/61/61	0/2/2/2
21	LMU	A	7024	-	-	15/21/61/61	0/2/2/2
20	CLA	A	1782	20	2/2/15/20	23/37/115/115	-

All (2423) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	1170	BCR	C21-C22	-11.03	1.21	1.35
20	1	1195	CLA	CAB-C3B	-10.23	1.30	1.51
22	B	1781	BCR	C21-C22	-10.00	1.22	1.35
22	L	1170	BCR	C20-C21	-9.90	1.12	1.43
22	B	1779	BCR	C21-C22	-9.40	1.23	1.35
20	1	1197	CLA	C3B-CAB	-9.15	1.29	1.47
20	F	1157	CLA	C3B-CAB	-9.09	1.29	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	1032	BCR	C21-C22	-9.08	1.23	1.35
20	B	1753	CLA	C3B-CAB	-8.85	1.29	1.47
20	1	1191	CLA	CAB-C3B	-8.83	1.33	1.51
22	L	1169	BCR	C20-C21	-8.82	1.16	1.43
22	L	1169	BCR	C21-C22	-8.54	1.24	1.35
20	4	1197	CLA	CAB-C3B	-8.52	1.33	1.51
20	B	1753	CLA	C1B-NB	-8.49	1.27	1.35
22	B	1779	BCR	C20-C21	-8.41	1.17	1.43
20	4	1198	CLA	C3B-CAB	-8.41	1.30	1.47
22	3	1220	BCR	C20-C21	-8.21	1.18	1.43
20	B	1741	CLA	CAB-C3B	-8.20	1.34	1.51
20	2	1222	CLA	C3B-CAB	-8.19	1.31	1.47
22	A	1806	BCR	C20-C21	-8.14	1.18	1.43
22	B	1775	BCR	C20-C21	-8.11	1.18	1.43
22	B	1781	BCR	C20-C21	-8.11	1.18	1.43
22	B	1778	BCR	C20-C21	-8.09	1.18	1.43
22	B	1777	BCR	C20-C21	-8.08	1.18	1.43
20	B	1739	CLA	C3B-CAB	-8.08	1.31	1.47
22	A	1803	BCR	C20-C21	-8.07	1.18	1.43
20	B	1738	CLA	C3B-CAB	-8.07	1.31	1.47
20	1	1196	CLA	CAB-C3B	-8.07	1.34	1.51
22	A	1807	BCR	C20-C21	-8.06	1.18	1.43
22	A	1808	BCR	C20-C21	-8.05	1.18	1.43
22	A	1805	BCR	C20-C21	-8.03	1.18	1.43
22	B	1780	BCR	C20-C21	-8.03	1.18	1.43
20	B	1772	CLA	CAB-C3B	-8.02	1.34	1.51
22	B	1774	BCR	C20-C21	-8.02	1.18	1.43
22	A	1804	BCR	C20-C21	-8.01	1.18	1.43
20	A	1765	CLA	CHD-C1D	7.98	1.53	1.38
20	4	1207	CLA	CAB-C3B	-7.95	1.35	1.51
20	B	1743	CLA	C3B-CAB	-7.86	1.31	1.47
20	A	1775	CLA	CAB-C3B	-7.85	1.35	1.51
20	B	1753	CLA	C4C-C3C	-7.85	1.31	1.45
23	A	1802	PQN	C3-C2	7.83	1.49	1.35
22	3	1220	BCR	C21-C22	-7.82	1.25	1.35
20	A	1813	CLA	C3B-CAB	-7.77	1.32	1.47
22	L	1170	BCR	C17-C18	-7.72	1.25	1.35
20	A	1764	CLA	C3B-CAB	-7.69	1.32	1.47
22	I	1032	BCR	C20-C21	-7.69	1.19	1.43
20	A	1817	CLA	CAB-C3B	-7.68	1.35	1.51
20	4	1209	CLA	C3B-CAB	-7.66	1.32	1.47
20	B	1787	CLA	C3B-CAB	-7.65	1.32	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1776	BCR	C20-C21	-7.59	1.19	1.43
20	4	1201	CLA	C1B-NB	-7.56	1.28	1.35
22	B	1777	BCR	C21-C22	-7.55	1.25	1.35
20	B	1764	CLA	C3B-CAB	-7.54	1.32	1.47
20	J	1045	CLA	C3B-CAB	-7.53	1.32	1.47
23	B	1773	PQN	C3-C2	7.51	1.48	1.35
22	B	1774	BCR	C21-C22	-7.49	1.25	1.35
22	A	1807	BCR	C21-C22	-7.49	1.25	1.35
22	A	1805	BCR	C21-C22	-7.47	1.25	1.35
22	A	1804	BCR	C21-C22	-7.45	1.25	1.35
22	B	1778	BCR	C21-C22	-7.44	1.25	1.35
20	3	1212	CLA	CAB-C3B	-7.44	1.36	1.51
22	A	1803	BCR	C21-C22	-7.40	1.26	1.35
22	B	1775	BCR	C21-C22	-7.39	1.26	1.35
22	A	1808	BCR	C21-C22	-7.38	1.26	1.35
20	4	1201	CLA	C4C-C3C	-7.38	1.32	1.45
20	A	1799	CLA	CHD-C1D	7.38	1.52	1.38
22	A	1806	BCR	C21-C22	-7.36	1.26	1.35
22	B	1780	BCR	C21-C22	-7.36	1.26	1.35
20	F	1155	CLA	CAB-C3B	-7.34	1.36	1.51
20	A	1784	CLA	C3B-CAB	-7.31	1.33	1.47
20	A	1783	CLA	C3B-CAB	-7.29	1.33	1.47
20	A	1772	CLA	C3B-CAB	-7.28	1.33	1.47
20	2	1220	CLA	C3B-CAB	-7.27	1.33	1.47
20	4	1200	CLA	CHC-C1C	7.27	1.53	1.35
20	B	1768	CLA	C3B-CAB	-7.27	1.33	1.47
20	K	1146	CLA	C3B-CAB	-7.25	1.33	1.47
20	A	1788	CLA	CHD-C1D	7.23	1.52	1.38
20	A	1816	CLA	C3B-CAB	-7.23	1.33	1.47
20	A	1816	CLA	C3D-C4D	-7.17	1.28	1.44
20	B	1754	CLA	C3B-CAB	-7.17	1.33	1.47
20	B	1771	CLA	C3B-CAB	-7.14	1.33	1.47
20	1	1195	CLA	C1B-NB	-7.12	1.28	1.35
20	A	1771	CLA	CHD-C1D	7.11	1.52	1.38
20	B	1752	CLA	C3B-CAB	-7.10	1.33	1.47
20	1	1198	CLA	C3B-CAB	-7.10	1.33	1.47
20	A	1815	CLA	CHD-C1D	7.08	1.52	1.38
20	R	1055	CLA	C3B-CAB	-7.08	1.33	1.47
20	B	1753	CLA	C3D-C4D	-7.08	1.28	1.44
20	B	1762	CLA	C3B-CAB	-7.06	1.33	1.47
20	B	1743	CLA	CHC-C1C	7.06	1.53	1.35
20	A	1767	CLA	C3B-CAB	-7.06	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1215	CLA	CHC-C1C	7.04	1.53	1.35
20	A	1766	CLA	CHC-C1C	7.03	1.53	1.35
20	A	1789	CLA	CHD-C1D	7.03	1.52	1.38
20	A	1789	CLA	C3B-CAB	-7.03	1.33	1.47
20	B	1760	CLA	CHD-C1D	7.01	1.52	1.38
20	3	3008	CLA	C3B-CAB	-7.01	1.33	1.47
20	B	1767	CLA	C3B-CAB	-7.00	1.33	1.47
20	B	1745	CLA	CHC-C1C	6.96	1.52	1.35
20	A	1761	CLA	C3B-CAB	-6.96	1.33	1.47
20	B	1786	CLA	C3B-CAB	-6.93	1.33	1.47
20	B	1787	CLA	CHD-C1D	6.93	1.51	1.38
20	B	1760	CLA	C3B-CAB	-6.91	1.33	1.47
20	J	1044	CLA	C3B-CAB	-6.90	1.33	1.47
20	3	1218	CLA	C3B-CAB	-6.89	1.33	1.47
20	B	1760	CLA	CHC-C1C	6.89	1.52	1.35
20	B	1769	CLA	CHC-C1C	6.89	1.52	1.35
20	A	1792	CLA	C3B-CAB	-6.89	1.33	1.47
22	I	1032	BCR	C30-C25	-6.88	1.44	1.53
20	A	1776	CLA	CHC-C1C	6.88	1.52	1.35
20	A	1795	CLA	C3B-CAB	-6.88	1.33	1.47
20	3	1219	CLA	C3B-CAB	-6.87	1.33	1.47
20	A	1791	CLA	C3B-CAB	-6.87	1.33	1.47
20	B	1744	CLA	C3B-CAB	-6.87	1.33	1.47
20	A	1817	CLA	CHD-C1D	6.86	1.51	1.38
20	B	1753	CLA	C1D-ND	-6.86	1.29	1.37
20	1	1200	CLA	C3B-CAB	-6.86	1.34	1.47
20	A	1812	CLA	C3B-CAB	-6.86	1.34	1.47
20	A	1796	CLA	C3B-CAB	-6.85	1.34	1.47
20	I	1031	CLA	C3B-CAB	-6.85	1.34	1.47
20	F	1156	CLA	C3B-CAB	-6.85	1.34	1.47
20	B	1766	CLA	CHC-C1C	6.85	1.52	1.35
20	A	1794	CLA	C3B-CAB	-6.85	1.34	1.47
20	A	1788	CLA	C3B-CAB	-6.84	1.34	1.47
20	4	4014	CLA	C3B-CAB	-6.84	1.34	1.47
20	A	1781	CLA	C3B-CAB	-6.84	1.34	1.47
20	A	1793	CLA	C3B-CAB	-6.84	1.34	1.47
20	2	1215	CLA	CHD-C1D	6.84	1.51	1.38
20	4	1196	CLA	C3B-CAB	-6.84	1.34	1.47
20	B	1735	CLA	C3B-CAB	-6.84	1.34	1.47
20	A	1797	CLA	C3B-CAB	-6.83	1.34	1.47
20	A	1816	CLA	CHC-C1C	6.83	1.52	1.35
20	A	1786	CLA	CHC-C1C	6.83	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1212	CLA	C3B-CAB	-6.83	1.34	1.47
20	B	1756	CLA	C3B-CAB	-6.83	1.34	1.47
20	J	1043	CLA	C3B-CAB	-6.82	1.34	1.47
20	A	1801	CLA	CHC-C1C	6.82	1.52	1.35
20	K	1142	CLA	C3B-CAB	-6.82	1.34	1.47
20	I	1031	CLA	CHC-C1C	6.81	1.52	1.35
20	K	1085	CLA	C3B-CAB	-6.80	1.34	1.47
20	A	1766	CLA	CHD-C4C	6.79	1.54	1.39
20	B	1758	CLA	C3B-CAB	-6.79	1.34	1.47
20	B	1741	CLA	CHD-C1D	6.79	1.51	1.38
20	A	1813	CLA	CHD-C1D	6.77	1.51	1.38
20	A	1766	CLA	CHD-C1D	6.76	1.51	1.38
20	A	1782	CLA	C3B-CAB	-6.75	1.34	1.47
20	1	1196	CLA	CHC-C1C	6.75	1.52	1.35
20	3	1218	CLA	C4C-C3C	-6.75	1.33	1.45
20	B	1755	CLA	C3B-CAB	-6.75	1.34	1.47
20	B	1764	CLA	CHC-C1C	6.74	1.52	1.35
20	2	1222	CLA	CHD-C1D	6.74	1.51	1.38
20	B	1765	CLA	CHC-C1C	6.73	1.52	1.35
20	1	1193	CLA	CHC-C1C	6.73	1.52	1.35
20	A	1800	CLA	C3B-CAB	-6.73	1.34	1.47
20	B	1757	CLA	C3B-CAB	-6.72	1.34	1.47
20	B	1757	CLA	CHC-C1C	6.72	1.52	1.35
20	A	1765	CLA	C3B-CAB	-6.71	1.34	1.47
20	A	1813	CLA	CHD-C4C	6.71	1.54	1.39
20	B	1757	CLA	CHD-C4C	6.70	1.54	1.39
20	B	1765	CLA	C3B-CAB	-6.70	1.34	1.47
20	1	1191	CLA	CHD-C1D	6.70	1.51	1.38
20	B	1739	CLA	CHD-C1D	6.69	1.51	1.38
20	1	1191	CLA	CHC-C1C	6.69	1.52	1.35
20	B	1757	CLA	CHD-C1D	6.69	1.51	1.38
20	A	1786	CLA	CHD-C1D	6.69	1.51	1.38
20	4	1204	CLA	CHC-C1C	6.69	1.52	1.35
20	A	1759	CLA	C3B-CAB	-6.68	1.34	1.47
20	A	1778	CLA	CHD-C1D	6.67	1.51	1.38
20	B	1787	CLA	CHC-C1C	6.67	1.52	1.35
20	B	1736	CLA	CHD-C1D	6.67	1.51	1.38
20	A	1817	CLA	O2D-CGD	6.66	1.49	1.33
20	A	1763	CLA	CHD-C1D	6.66	1.51	1.38
20	L	1505	CLA	CHD-C1D	6.66	1.51	1.38
20	A	1783	CLA	CHD-C4C	6.65	1.54	1.39
20	4	1197	CLA	CHC-C1C	6.65	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1189	CLA	CHC-C1C	6.64	1.52	1.35
20	G	1099	CLA	CHD-C1D	6.64	1.51	1.38
20	L	1166	CLA	CHC-C1C	6.63	1.52	1.35
20	B	1763	CLA	C3B-CAB	-6.63	1.34	1.47
20	A	1777	CLA	CHC-C1C	6.63	1.52	1.35
20	4	1199	CLA	CHD-C1D	6.62	1.51	1.38
20	G	1099	CLA	CHC-C1C	6.62	1.51	1.35
20	R	1055	CLA	CHC-C1C	6.61	1.51	1.35
20	A	1764	CLA	CHC-C1C	6.61	1.51	1.35
20	B	1762	CLA	CHC-C1C	6.60	1.51	1.35
20	4	1206	CLA	CHD-C1D	6.60	1.52	1.38
20	A	1770	CLA	CHC-C1C	6.60	1.51	1.35
20	A	1815	CLA	CHD-C4C	6.60	1.54	1.39
20	A	1785	CLA	CHC-C1C	6.60	1.51	1.35
20	4	1199	CLA	C3B-CAB	-6.60	1.34	1.47
20	2	1223	CLA	CHC-C1C	6.60	1.51	1.35
20	L	1167	CLA	C3B-CAB	-6.59	1.34	1.47
20	B	1748	CLA	CHC-C1C	6.58	1.51	1.35
20	I	1033	CLA	CHD-C1D	6.58	1.51	1.38
20	A	1771	CLA	CHC-C1C	6.58	1.51	1.35
20	B	1766	CLA	C3B-CAB	-6.58	1.34	1.47
20	B	1770	CLA	CHC-C1C	6.57	1.51	1.35
20	B	1750	CLA	CHC-C1C	6.56	1.51	1.35
20	B	1752	CLA	CHD-C1D	6.55	1.51	1.38
20	B	1785	CLA	C3B-CAB	-6.54	1.34	1.47
20	B	1736	CLA	CHC-C1C	6.53	1.51	1.35
20	3	3007	CLA	CHD-C1D	6.53	1.51	1.38
20	H	1079	CLA	CHD-C1D	6.53	1.51	1.38
20	1	1189	CLA	CHD-C1D	6.53	1.51	1.38
20	A	1774	CLA	CHD-C1D	6.53	1.51	1.38
20	4	1207	CLA	CHC-C1C	6.53	1.51	1.35
20	A	1760	CLA	CHC-C1C	6.52	1.51	1.35
20	I	1031	CLA	CHD-C1D	6.52	1.51	1.38
20	K	3009	CLA	CHC-C1C	6.52	1.51	1.35
20	1	1193	CLA	C3B-CAB	-6.52	1.34	1.47
20	B	1747	CLA	CHC-C1C	6.51	1.51	1.35
20	A	1775	CLA	CHD-C1D	6.50	1.51	1.38
20	B	1768	CLA	CHD-C1D	6.50	1.51	1.38
20	A	1767	CLA	CHD-C1D	6.50	1.51	1.38
20	B	1744	CLA	CHC-C1C	6.50	1.51	1.35
20	A	1770	CLA	CHD-C1D	6.49	1.51	1.38
20	A	1777	CLA	CHD-C1D	6.48	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	1200	CLA	CHD-C1D	6.48	1.51	1.38
20	A	1787	CLA	C3B-CAB	-6.48	1.34	1.47
20	A	1771	CLA	CHD-C4C	6.48	1.54	1.39
20	2	1218	CLA	CHD-C1D	6.48	1.51	1.38
20	1	1197	CLA	C3D-C4D	-6.47	1.29	1.44
20	3	1212	CLA	CHD-C1D	6.47	1.51	1.38
20	A	1798	CLA	CHC-C1C	6.47	1.51	1.35
20	I	1033	CLA	CHC-C1C	6.47	1.51	1.35
20	1	1187	CLA	C3B-CAB	-6.47	1.34	1.47
20	A	1811	CLA	CHC-C1C	6.46	1.51	1.35
20	B	1785	CLA	CHC-C1C	6.46	1.51	1.35
20	A	1769	CLA	CHC-C1C	6.46	1.51	1.35
20	1	1200	CLA	C3D-C4D	-6.46	1.29	1.44
20	1	1193	CLA	CHD-C1D	6.46	1.50	1.38
20	A	1773	CLA	C3B-CAB	-6.46	1.34	1.47
20	2	1213	CLA	CHC-C1C	6.46	1.51	1.35
20	3	1218	CLA	C3D-C4D	-6.45	1.29	1.44
20	2	1222	CLA	CHC-C1C	6.45	1.51	1.35
20	2	1217	CLA	C3B-CAB	-6.45	1.34	1.47
20	L	1505	CLA	O2D-CGD	6.44	1.48	1.33
20	R	1054	CLA	CHD-C1D	6.44	1.50	1.38
20	R	1055	CLA	CHD-C1D	6.43	1.50	1.38
20	A	1799	CLA	CHD-C4C	6.43	1.53	1.39
20	1	1192	CLA	C3B-CAB	-6.42	1.34	1.47
20	1	1188	CLA	O2D-CGD	6.42	1.48	1.33
20	A	1784	CLA	CHC-C1C	6.42	1.51	1.35
20	B	1760	CLA	CHD-C4C	6.42	1.53	1.39
20	1	1196	CLA	CHD-C1D	6.42	1.50	1.38
20	B	1751	CLA	O2D-CGD	6.42	1.48	1.33
20	L	1168	CLA	C3B-CAB	-6.42	1.34	1.47
20	B	1741	CLA	CHC-C1C	6.41	1.51	1.35
20	4	4007	CLA	CHD-C1D	6.41	1.50	1.38
20	A	1780	CLA	CHC-C1C	6.41	1.51	1.35
20	L	1505	CLA	CHC-C1C	6.41	1.51	1.35
20	1	1190	CLA	CHD-C1D	6.41	1.50	1.38
20	A	1771	CLA	C3B-CAB	-6.40	1.34	1.47
20	4	4007	CLA	C3B-CAB	-6.39	1.34	1.47
20	B	1737	CLA	CHD-C1D	6.39	1.50	1.38
20	K	1146	CLA	C3D-C4D	-6.38	1.29	1.44
20	I	1033	CLA	C3B-CAB	-6.38	1.34	1.47
20	3	1218	CLA	O2D-CGD	6.38	1.48	1.33
20	B	1737	CLA	CHD-C4C	6.38	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1817	CLA	CHC-C1C	6.37	1.51	1.35
20	F	1155	CLA	CHC-C1C	6.37	1.51	1.35
20	R	1054	CLA	CHC-C1C	6.37	1.51	1.35
20	2	1217	CLA	O2D-CGD	6.37	1.48	1.33
20	B	1746	CLA	C3B-CAB	-6.37	1.35	1.47
20	B	1752	CLA	CHD-C4C	6.37	1.53	1.39
20	4	1200	CLA	O2D-CGD	6.37	1.48	1.33
20	1	1189	CLA	C3B-CAB	-6.37	1.35	1.47
20	B	1766	CLA	CHD-C1D	6.36	1.50	1.38
20	B	1740	CLA	C3B-CAB	-6.36	1.35	1.47
20	1	1188	CLA	CHD-C1D	6.36	1.50	1.38
20	2	1213	CLA	CHD-C1D	6.35	1.50	1.38
20	B	1739	CLA	CHC-C1C	6.35	1.51	1.35
20	B	1767	CLA	CHD-C1D	6.35	1.50	1.38
20	L	1167	CLA	CHC-C1C	6.34	1.51	1.35
20	A	1786	CLA	C3B-CAB	-6.34	1.35	1.47
20	A	1773	CLA	CHC-C1C	6.34	1.51	1.35
20	A	1817	CLA	CHD-C4C	6.34	1.53	1.39
20	B	1749	CLA	CHC-C1C	6.33	1.51	1.35
20	A	1779	CLA	CHC-C1C	6.33	1.51	1.35
20	B	1739	CLA	CHD-C4C	6.33	1.53	1.39
20	I	1033	CLA	CHD-C4C	6.33	1.53	1.39
20	2	1218	CLA	CHD-C4C	6.33	1.53	1.39
20	4	1201	CLA	C3D-C4D	-6.33	1.29	1.44
20	A	1783	CLA	CHC-C1C	6.32	1.51	1.35
20	A	1774	CLA	C3B-CAB	-6.32	1.35	1.47
20	2	1222	CLA	CHD-C4C	6.32	1.53	1.39
20	B	1770	CLA	CHD-C1D	6.31	1.50	1.38
20	A	1787	CLA	CHD-C4C	6.31	1.53	1.39
20	1	1190	CLA	C3B-CAB	-6.31	1.35	1.47
20	B	1759	CLA	CHC-C1C	6.31	1.51	1.35
20	A	1764	CLA	CHD-C1D	6.31	1.50	1.38
20	A	1798	CLA	C3B-CAB	-6.30	1.35	1.47
20	A	1787	CLA	CHC-C1C	6.30	1.51	1.35
20	1	1192	CLA	O2D-CGD	6.30	1.48	1.33
20	4	4007	CLA	O2D-CGD	6.29	1.48	1.33
20	B	1740	CLA	CHC-C1C	6.29	1.51	1.35
20	A	1774	CLA	CHC-C1C	6.29	1.51	1.35
20	A	1773	CLA	CHD-C1D	6.28	1.50	1.38
20	2	1218	CLA	CHC-C1C	6.28	1.51	1.35
20	A	1779	CLA	CHD-C1D	6.28	1.50	1.38
20	3	1212	CLA	CHC-C1C	6.28	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1765	CLA	CHD-C4C	6.27	1.53	1.39
20	G	1099	CLA	O2D-CGD	6.27	1.48	1.33
20	1	1187	CLA	C3D-C4D	-6.27	1.30	1.44
20	B	1770	CLA	CHD-C4C	6.26	1.53	1.39
20	A	1778	CLA	O2D-CGD	6.26	1.48	1.33
20	B	1786	CLA	CHC-C1C	6.26	1.51	1.35
20	A	1780	CLA	C3B-CAB	-6.26	1.35	1.47
20	L	1168	CLA	CHC-C1C	6.26	1.51	1.35
20	A	1815	CLA	O2D-CGD	6.25	1.48	1.33
20	A	1787	CLA	CHD-C1D	6.25	1.50	1.38
20	A	1790	CLA	CHC-C1C	6.25	1.51	1.35
20	A	1767	CLA	CHC-C1C	6.25	1.51	1.35
20	B	1742	CLA	CHC-C1C	6.25	1.51	1.35
20	B	1750	CLA	C3B-CAB	-6.25	1.35	1.47
20	B	1768	CLA	CHD-C4C	6.25	1.53	1.39
20	4	1196	CLA	CHC-C1C	6.24	1.51	1.35
20	K	1085	CLA	CHC-C1C	6.24	1.51	1.35
20	1	1197	CLA	C4C-C3C	-6.24	1.34	1.45
20	L	1166	CLA	O2D-CGD	6.24	1.48	1.33
20	F	1155	CLA	CHD-C4C	6.24	1.53	1.39
20	A	1775	CLA	CHC-C1C	6.23	1.50	1.35
20	B	1744	CLA	CHD-C1D	6.23	1.50	1.38
20	2	1212	CLA	CHC-C1C	6.23	1.50	1.35
20	B	1747	CLA	CHD-C4C	6.22	1.53	1.39
20	3	3007	CLA	CHC-C1C	6.22	1.50	1.35
20	B	1752	CLA	O2D-CGD	6.22	1.48	1.33
20	A	1778	CLA	C3B-CAB	-6.22	1.35	1.47
20	A	1798	CLA	CHD-C4C	6.22	1.53	1.39
20	A	1777	CLA	CHD-C4C	6.22	1.53	1.39
20	B	1767	CLA	CHD-C4C	6.21	1.53	1.39
20	B	1741	CLA	CHD-C4C	6.21	1.53	1.39
20	4	4014	CLA	CHC-C1C	6.21	1.50	1.35
20	A	1770	CLA	C3B-CAB	-6.21	1.35	1.47
20	2	1218	CLA	C3B-CAB	-6.20	1.35	1.47
20	3	1217	CLA	CHD-C1D	6.20	1.52	1.38
20	A	1792	CLA	CHC-C1C	6.20	1.50	1.35
20	2	1223	CLA	CHD-C1D	6.20	1.50	1.38
20	A	1771	CLA	O2D-CGD	6.20	1.48	1.33
20	B	1772	CLA	CHC-C1C	6.20	1.50	1.35
20	A	1783	CLA	CHD-C1D	6.20	1.50	1.38
20	B	1755	CLA	CHC-C1C	6.20	1.50	1.35
20	B	1759	CLA	CHD-C1D	6.20	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1213	CLA	CHD-C4C	6.19	1.53	1.39
20	H	1079	CLA	CHC-C1C	6.19	1.50	1.35
20	A	1762	CLA	CHC-C1C	6.19	1.50	1.35
20	A	1791	CLA	CHC-C1C	6.19	1.50	1.35
20	B	1735	CLA	CHC-C1C	6.18	1.50	1.35
20	A	1776	CLA	CHD-C1D	6.18	1.50	1.38
20	A	1780	CLA	CHD-C1D	6.18	1.50	1.38
20	A	1768	CLA	CHC-C1C	6.18	1.50	1.35
20	B	1756	CLA	CHC-C1C	6.18	1.50	1.35
20	A	1795	CLA	CHC-C1C	6.18	1.50	1.35
20	A	1794	CLA	CHC-C1C	6.18	1.50	1.35
20	A	1811	CLA	C3B-CAB	-6.18	1.35	1.47
20	A	1761	CLA	CHD-C4C	6.18	1.53	1.39
20	B	1763	CLA	O2D-CGD	6.18	1.48	1.33
20	J	1043	CLA	CHC-C1C	6.17	1.50	1.35
20	1	1199	CLA	CHD-C1D	6.17	1.52	1.38
20	K	1142	CLA	CHC-C1C	6.17	1.50	1.35
20	A	1782	CLA	CHC-C1C	6.17	1.50	1.35
20	B	1761	CLA	C3B-CAB	-6.17	1.35	1.47
20	A	1796	CLA	CHC-C1C	6.17	1.50	1.35
20	3	3011	CLA	CHC-C1C	6.17	1.50	1.35
20	I	1033	CLA	O2D-CGD	6.17	1.48	1.33
20	A	1770	CLA	CHD-C4C	6.17	1.53	1.39
20	A	1789	CLA	CHD-C4C	6.17	1.53	1.39
20	F	1156	CLA	CHC-C1C	6.16	1.50	1.35
20	4	1209	CLA	CHC-C1C	6.16	1.50	1.35
20	A	1797	CLA	CHC-C1C	6.16	1.50	1.35
20	B	1751	CLA	CHC-C1C	6.16	1.50	1.35
20	B	1786	CLA	CHD-C1D	6.16	1.50	1.38
20	1	1192	CLA	CHC-C1C	6.16	1.50	1.35
20	A	1793	CLA	CHC-C1C	6.16	1.50	1.35
20	A	1812	CLA	CHC-C1C	6.16	1.50	1.35
20	A	1778	CLA	CHD-C4C	6.16	1.53	1.39
20	B	1752	CLA	CHC-C1C	6.16	1.50	1.35
20	A	1801	CLA	C3B-CAB	-6.15	1.35	1.47
20	A	1781	CLA	CHC-C1C	6.15	1.50	1.35
20	4	1204	CLA	O2D-CGD	6.15	1.48	1.33
20	A	1760	CLA	C3B-CAB	-6.15	1.35	1.47
20	B	1770	CLA	C3B-CAB	-6.15	1.35	1.47
20	B	1744	CLA	CHD-C4C	6.15	1.53	1.39
20	L	1167	CLA	CHD-C4C	6.15	1.53	1.39
20	A	1762	CLA	CHD-C1D	6.15	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	1166	CLA	C3B-CAB	-6.15	1.35	1.47
20	3	1219	CLA	CHC-C1C	6.14	1.50	1.35
20	B	1765	CLA	CHD-C1D	6.14	1.50	1.38
20	4	1202	CLA	CHD-C1D	6.14	1.51	1.38
20	B	1760	CLA	O2D-CGD	6.13	1.48	1.33
20	B	1761	CLA	O2D-CGD	6.13	1.48	1.33
20	B	1772	CLA	CHD-C1D	6.12	1.50	1.38
20	B	1745	CLA	CHD-C1D	6.12	1.50	1.38
20	F	1156	CLA	CHD-C1D	6.12	1.50	1.38
20	A	1815	CLA	CHC-C1C	6.12	1.50	1.35
20	B	1746	CLA	CHC-C1C	6.11	1.50	1.35
20	A	1768	CLA	CHD-C4C	6.11	1.53	1.39
20	A	1763	CLA	CHC-C1C	6.11	1.50	1.35
20	A	1816	CLA	CHD-C1D	6.11	1.50	1.38
20	3	1212	CLA	CHD-C4C	6.11	1.53	1.39
20	A	1790	CLA	C3B-CAB	-6.10	1.35	1.47
20	R	1055	CLA	O2D-CGD	6.10	1.48	1.33
20	A	1801	CLA	O2D-CGD	6.10	1.48	1.33
20	3	3007	CLA	O2D-CGD	6.09	1.48	1.33
20	A	1811	CLA	O2D-CGD	6.09	1.48	1.33
20	A	1773	CLA	O2D-CGD	6.09	1.48	1.33
20	B	1759	CLA	C3B-CAB	-6.09	1.35	1.47
20	F	1155	CLA	CHD-C1D	6.09	1.50	1.38
20	A	1762	CLA	CHD-C4C	6.09	1.53	1.39
20	2	1224	CLA	CHC-C1C	6.09	1.50	1.35
20	1	1190	CLA	OBD-CAD	6.09	1.33	1.22
20	A	1788	CLA	CHC-C1C	6.09	1.50	1.35
20	2	1223	CLA	O2D-CGD	6.08	1.48	1.33
20	A	1790	CLA	CHD-C1D	6.07	1.50	1.38
20	B	1747	CLA	O2D-CGD	6.07	1.48	1.33
20	B	1767	CLA	CHC-C1C	6.07	1.50	1.35
20	3	3008	CLA	CHC-C1C	6.07	1.50	1.35
20	A	1800	CLA	CHC-C1C	6.07	1.50	1.35
20	2	1224	CLA	C3B-CAB	-6.07	1.35	1.47
20	4	1196	CLA	CHD-C1D	6.06	1.50	1.38
20	B	1786	CLA	CHD-C4C	6.06	1.53	1.39
20	4	1204	CLA	C3B-CAB	-6.06	1.35	1.47
20	R	1054	CLA	O2D-CGD	6.06	1.48	1.33
20	1	1200	CLA	C1B-NB	-6.06	1.29	1.35
20	B	1736	CLA	CHD-C4C	6.05	1.53	1.39
20	2	1217	CLA	CHC-C1C	6.05	1.50	1.35
20	K	1085	CLA	CHD-C1D	6.05	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	1776	BCR	C21-C22	-6.05	1.27	1.35
20	B	1758	CLA	CHC-C1C	6.05	1.50	1.35
20	A	1793	CLA	CHD-C1D	6.05	1.50	1.38
20	A	1791	CLA	CHD-C1D	6.04	1.50	1.38
20	4	1199	CLA	CHC-C1C	6.04	1.50	1.35
20	B	1735	CLA	CHD-C1D	6.04	1.50	1.38
20	A	1795	CLA	CHD-C1D	6.04	1.50	1.38
20	F	1157	CLA	C3D-C4D	-6.03	1.30	1.44
20	A	1798	CLA	CHD-C1D	6.03	1.50	1.38
20	L	1505	CLA	CHD-C4C	6.03	1.53	1.39
20	4	1198	CLA	CHD-C4C	6.03	1.53	1.39
20	A	1797	CLA	CHD-C1D	6.03	1.50	1.38
20	A	1779	CLA	C3B-CAB	-6.02	1.35	1.47
20	A	1792	CLA	CHD-C1D	6.02	1.50	1.38
20	A	1798	CLA	O2D-CGD	6.02	1.47	1.33
20	A	1794	CLA	CHD-C1D	6.02	1.50	1.38
20	A	1796	CLA	CHD-C1D	6.02	1.50	1.38
20	B	1771	CLA	CHD-C1D	6.01	1.50	1.38
20	B	1762	CLA	CHD-C1D	6.01	1.50	1.38
20	B	1763	CLA	CHD-C1D	6.01	1.50	1.38
20	2	1212	CLA	CHD-C1D	6.01	1.50	1.38
20	J	1043	CLA	CHD-C1D	6.01	1.50	1.38
20	G	1099	CLA	CHD-C4C	6.01	1.53	1.39
20	1	1190	CLA	O2D-CGD	6.01	1.47	1.33
20	B	1755	CLA	CHD-C1D	6.01	1.50	1.38
20	A	1768	CLA	CHD-C1D	6.01	1.50	1.38
20	R	1054	CLA	CHD-C4C	6.01	1.53	1.39
20	A	1759	CLA	CHC-C1C	6.00	1.50	1.35
20	A	1761	CLA	O2D-CGD	6.00	1.47	1.33
20	A	1764	CLA	CHD-C4C	6.00	1.52	1.39
20	B	1766	CLA	O2D-CGD	6.00	1.47	1.33
20	A	1766	CLA	O2D-CGD	5.99	1.47	1.33
20	3	3011	CLA	C3B-CAB	-5.99	1.35	1.47
20	B	1749	CLA	C3B-CAB	-5.99	1.35	1.47
20	A	1815	CLA	C3B-CAB	-5.98	1.35	1.47
20	A	1799	CLA	C3B-CAB	-5.98	1.35	1.47
20	K	1142	CLA	CHD-C1D	5.98	1.50	1.38
20	4	1201	CLA	CHC-C1C	5.98	1.50	1.35
20	1	1190	CLA	CHC-C1C	5.98	1.50	1.35
20	A	1781	CLA	CHD-C1D	5.97	1.50	1.38
20	A	1799	CLA	CHC-C1C	5.97	1.50	1.35
20	B	1756	CLA	CHD-C1D	5.97	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1223	CLA	C3B-CAB	-5.97	1.35	1.47
20	A	1778	CLA	CHC-C1C	5.97	1.50	1.35
20	A	1760	CLA	CHD-C4C	5.97	1.52	1.39
20	4	4014	CLA	CHD-C1D	5.97	1.50	1.38
20	2	1220	CLA	CHC-C1C	5.97	1.50	1.35
20	A	1770	CLA	O2D-CGD	5.97	1.47	1.33
20	4	4007	CLA	CHC-C1C	5.96	1.50	1.35
20	B	1785	CLA	CHD-C1D	5.96	1.50	1.38
20	B	1750	CLA	CHD-C1D	5.96	1.50	1.38
20	3	3011	CLA	CHD-C1D	5.96	1.50	1.38
20	3	1219	CLA	CHD-C1D	5.96	1.50	1.38
20	1	1196	CLA	CHD-C4C	5.95	1.52	1.39
20	A	1767	CLA	CHD-C4C	5.95	1.52	1.39
20	A	1763	CLA	CHD-C4C	5.95	1.52	1.39
20	L	1166	CLA	CHD-C1D	5.95	1.49	1.38
20	A	1785	CLA	CHD-C4C	5.95	1.52	1.39
20	A	1762	CLA	C3B-CAB	-5.94	1.35	1.47
20	A	1790	CLA	CHD-C4C	5.94	1.52	1.39
20	A	1790	CLA	O2D-CGD	5.94	1.47	1.33
20	J	1044	CLA	CHC-C1C	5.94	1.50	1.35
20	B	1748	CLA	C3B-CAB	-5.94	1.35	1.47
20	B	1746	CLA	CHD-C1D	5.93	1.49	1.38
20	L	1167	CLA	CHD-C1D	5.93	1.49	1.38
20	K	3009	CLA	CHD-C1D	5.93	1.49	1.38
20	A	1786	CLA	CHD-C4C	5.93	1.52	1.39
20	A	1780	CLA	CHD-C4C	5.92	1.52	1.39
20	A	1769	CLA	CHD-C1D	5.92	1.49	1.38
20	B	1757	CLA	C3D-C4D	-5.92	1.30	1.44
20	A	1760	CLA	CHD-C1D	5.91	1.49	1.38
20	2	2010	CLA	CHD-C1D	5.91	1.51	1.38
20	H	1079	CLA	CHD-C4C	5.91	1.52	1.39
20	B	1741	CLA	O2A-CGA	5.91	1.50	1.33
20	A	1782	CLA	CHD-C1D	5.91	1.49	1.38
20	L	1168	CLA	O2D-CGD	5.91	1.47	1.33
20	A	1776	CLA	O2D-CGD	5.91	1.47	1.33
20	B	1740	CLA	CHD-C4C	5.91	1.52	1.39
20	1	1188	CLA	C3B-CAB	-5.90	1.35	1.47
20	A	1785	CLA	C3B-CAB	-5.90	1.35	1.47
20	2	1224	CLA	CHD-C1D	5.90	1.49	1.38
20	A	1779	CLA	O2D-CGD	5.90	1.47	1.33
20	B	1744	CLA	O2D-CGD	5.90	1.47	1.33
20	A	1763	CLA	C3B-CAB	-5.90	1.35	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	1200	CLA	CHD-C4C	5.89	1.52	1.39
20	A	1801	CLA	OBD-CAD	5.89	1.32	1.22
20	B	1754	CLA	O2D-CGD	5.89	1.47	1.33
20	2	1215	CLA	CHD-C4C	5.89	1.52	1.39
20	1	1191	CLA	CHD-C4C	5.89	1.52	1.39
20	A	1772	CLA	CHC-C1C	5.89	1.50	1.35
20	A	1789	CLA	CHC-C1C	5.88	1.50	1.35
20	A	1789	CLA	O2D-CGD	5.88	1.47	1.33
20	B	1746	CLA	CHD-C4C	5.88	1.52	1.39
20	B	1766	CLA	CHD-C4C	5.88	1.52	1.39
20	B	1785	CLA	CHD-C4C	5.88	1.52	1.39
20	2	1218	CLA	O2D-CGD	5.88	1.47	1.33
20	B	1747	CLA	C3B-CAB	-5.87	1.36	1.47
20	G	1099	CLA	C3B-CAB	-5.87	1.36	1.47
20	A	1761	CLA	O2A-CGA	5.86	1.50	1.33
20	H	1079	CLA	O2D-CGD	5.86	1.47	1.33
20	A	1761	CLA	CHC-C1C	5.86	1.50	1.35
20	K	3009	CLA	C3B-CAB	-5.86	1.36	1.47
20	A	1759	CLA	CHD-C4C	5.86	1.52	1.39
20	B	1768	CLA	CHC-C1C	5.86	1.50	1.35
20	A	1762	CLA	O2D-CGD	5.86	1.47	1.33
20	B	1746	CLA	O2D-CGD	5.86	1.47	1.33
20	A	1788	CLA	CHD-C4C	5.86	1.52	1.39
20	A	1777	CLA	C3B-CAB	-5.85	1.36	1.47
20	B	1764	CLA	O2D-CGD	5.85	1.47	1.33
20	B	1738	CLA	CHD-C1D	5.85	1.49	1.38
20	3	3008	CLA	C3D-C4D	-5.85	1.31	1.44
20	3	3007	CLA	C3B-CAB	-5.85	1.36	1.47
20	B	1739	CLA	O2D-CGD	5.85	1.47	1.33
20	A	1787	CLA	O2D-CGD	5.84	1.47	1.33
20	B	1754	CLA	CHD-C4C	5.84	1.52	1.39
20	A	1776	CLA	CHD-C4C	5.84	1.52	1.39
20	1	1188	CLA	CHC-C1C	5.84	1.49	1.35
20	B	1740	CLA	CHD-C1D	5.84	1.49	1.38
20	L	1505	CLA	C3B-CAB	-5.84	1.36	1.47
20	L	1168	CLA	CHD-C4C	5.83	1.52	1.39
20	1	1188	CLA	O2A-CGA	5.82	1.50	1.33
20	B	1737	CLA	CHC-C1C	5.82	1.49	1.35
20	B	1745	CLA	C3B-CAB	-5.82	1.36	1.47
20	B	1765	CLA	CHD-C4C	5.81	1.52	1.39
20	A	1784	CLA	CHD-C1D	5.81	1.49	1.38
20	2	1220	CLA	C3D-C4D	-5.80	1.31	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1779	CLA	CHD-C4C	5.78	1.52	1.39
20	4	1199	CLA	CHD-C4C	5.78	1.52	1.39
20	B	1750	CLA	CHD-C4C	5.78	1.52	1.39
20	A	1816	CLA	C4B-NB	-5.78	1.30	1.35
20	2	1224	CLA	O2D-CGD	5.77	1.47	1.33
20	B	1754	CLA	CHC-C1C	5.77	1.49	1.35
20	B	1738	CLA	CHC-C1C	5.77	1.49	1.35
20	1	1198	CLA	C3D-C4D	-5.76	1.31	1.44
20	B	1737	CLA	C3B-CAB	-5.76	1.36	1.47
20	B	1765	CLA	O2D-CGD	5.76	1.47	1.33
20	B	1742	CLA	C3B-CAB	-5.75	1.36	1.47
20	B	1754	CLA	CHD-C1D	5.75	1.49	1.38
20	A	1813	CLA	CHC-C1C	5.75	1.49	1.35
20	B	1747	CLA	CHD-C1D	5.75	1.49	1.38
20	4	1203	CLA	CHD-C1D	5.75	1.51	1.38
20	B	1736	CLA	C3B-CAB	-5.75	1.36	1.47
20	2	1223	CLA	O2A-CGA	5.74	1.50	1.33
20	A	1769	CLA	CHD-C4C	5.74	1.52	1.39
20	A	1766	CLA	C3B-CAB	-5.74	1.36	1.47
20	3	3011	CLA	CHD-C4C	5.74	1.52	1.39
20	1	1189	CLA	CHD-C4C	5.74	1.52	1.39
20	A	1800	CLA	CHD-C4C	5.74	1.52	1.39
20	A	1774	CLA	CHD-C4C	5.73	1.52	1.39
20	1	1198	CLA	CHC-C1C	5.73	1.49	1.35
20	H	1079	CLA	C3D-C4D	-5.73	1.31	1.44
20	B	1761	CLA	CHC-C1C	5.73	1.49	1.35
20	A	1779	CLA	O2A-CGA	5.72	1.50	1.33
20	A	1785	CLA	O2D-CGD	5.72	1.47	1.33
20	3	3001	CLA	CHD-C1D	5.72	1.51	1.38
20	A	1801	CLA	CHD-C1D	5.72	1.49	1.38
20	A	1773	CLA	CHD-C4C	5.72	1.52	1.39
20	H	1079	CLA	C3B-CAB	-5.72	1.36	1.47
20	B	1787	CLA	CHD-C4C	5.72	1.52	1.39
20	B	1748	CLA	CHD-C1D	5.71	1.49	1.38
20	F	1157	CLA	CHC-C1C	5.71	1.49	1.35
20	B	1751	CLA	CHD-C4C	5.71	1.52	1.39
20	1	1187	CLA	O2D-CGD	5.71	1.47	1.33
20	3	3015	CLA	CHD-C1D	5.70	1.51	1.38
20	B	1738	CLA	CHD-C4C	5.70	1.52	1.39
20	4	1204	CLA	CHD-C4C	5.69	1.52	1.39
20	3	1213	CLA	C1B-NB	-5.69	1.30	1.35
20	A	1759	CLA	CHD-C1D	5.69	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1761	CLA	CHD-C1D	5.68	1.49	1.38
20	3	3007	CLA	CHD-C4C	5.68	1.52	1.39
20	B	1744	CLA	O2A-CGA	5.68	1.49	1.33
20	2	1215	CLA	C3B-CAB	-5.68	1.36	1.47
20	L	1167	CLA	O2D-CGD	5.67	1.47	1.33
20	2	1213	CLA	O2D-CGD	5.66	1.47	1.33
20	J	1044	CLA	O2D-CGD	5.66	1.47	1.33
20	A	1784	CLA	CHD-C4C	5.65	1.52	1.39
20	A	1775	CLA	CHD-C4C	5.65	1.52	1.39
20	K	3009	CLA	CHD-C4C	5.65	1.52	1.39
20	B	1760	CLA	C3D-C4D	-5.65	1.31	1.44
20	1	1190	CLA	CHD-C4C	5.65	1.52	1.39
20	A	1760	CLA	O2A-CGA	5.65	1.49	1.33
20	B	1743	CLA	CHD-C1D	5.64	1.49	1.38
20	4	1197	CLA	OBD-CAD	5.64	1.32	1.22
20	4	1204	CLA	CHD-C1D	5.64	1.49	1.38
20	J	1045	CLA	CHC-C1C	5.64	1.49	1.35
20	A	1812	CLA	CHD-C4C	5.63	1.52	1.39
20	4	4014	CLA	CHD-C4C	5.63	1.52	1.39
20	2	1227	CLA	CHD-C1D	5.63	1.50	1.38
20	3	3002	CLA	CHD-C1D	5.63	1.50	1.38
20	K	1146	CLA	CHD-C1D	5.63	1.49	1.38
20	4	4007	CLA	CHD-C4C	5.63	1.52	1.39
20	3	3008	CLA	CHD-C1D	5.63	1.49	1.38
20	B	1761	CLA	CHD-C4C	5.62	1.52	1.39
20	R	1054	CLA	C3B-CAB	-5.62	1.36	1.47
20	A	1777	CLA	O2D-CGD	5.62	1.46	1.33
20	B	1743	CLA	CHD-C4C	5.62	1.52	1.39
20	1	1195	CLA	C3D-C4D	-5.62	1.31	1.44
20	A	1772	CLA	C3D-C4D	-5.61	1.31	1.44
20	A	1763	CLA	O2D-CGD	5.60	1.46	1.33
20	B	1756	CLA	CHD-C4C	5.60	1.52	1.39
20	B	1742	CLA	CHD-C1D	5.60	1.49	1.38
20	B	1758	CLA	CHD-C1D	5.59	1.49	1.38
20	J	1045	CLA	C3D-C4D	-5.59	1.31	1.44
20	2	1212	CLA	CHD-C4C	5.58	1.52	1.39
20	R	1054	CLA	O2A-CGA	5.58	1.49	1.33
20	B	1737	CLA	O2D-CGD	5.57	1.46	1.33
20	A	1768	CLA	O2D-CGD	5.57	1.46	1.33
20	B	1745	CLA	O2D-CGD	5.57	1.46	1.33
20	4	1207	CLA	CHD-C1D	5.57	1.49	1.38
20	B	1763	CLA	CHD-C4C	5.57	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1188	CLA	CHD-C4C	5.57	1.51	1.39
20	B	1764	CLA	CHD-C4C	5.56	1.51	1.39
20	B	1769	CLA	C3B-CAB	-5.56	1.36	1.47
20	F	1157	CLA	CHD-C1D	5.56	1.49	1.38
20	A	1792	CLA	CHD-C4C	5.56	1.51	1.39
20	K	1085	CLA	CHD-C4C	5.56	1.51	1.39
20	3	3011	CLA	O2D-CGD	5.56	1.46	1.33
20	3	1219	CLA	CHD-C4C	5.56	1.51	1.39
20	4	1197	CLA	C3D-C4D	-5.56	1.31	1.44
20	A	1797	CLA	CHD-C4C	5.56	1.51	1.39
20	A	1800	CLA	CHD-C1D	5.55	1.49	1.38
20	B	1735	CLA	CHD-C4C	5.55	1.51	1.39
20	A	1772	CLA	CHD-C1D	5.55	1.49	1.38
20	I	1031	CLA	O2A-CGA	5.55	1.49	1.33
20	B	1757	CLA	O2D-CGD	5.55	1.46	1.33
20	L	1168	CLA	CHD-C1D	5.55	1.49	1.38
20	4	1196	CLA	CHD-C4C	5.54	1.51	1.39
20	4	1198	CLA	CHC-C1C	5.54	1.49	1.35
20	2	1217	CLA	OBD-CAD	5.54	1.32	1.22
20	2	1215	CLA	O2D-CGD	5.54	1.46	1.33
20	A	1784	CLA	O2D-CGD	5.54	1.46	1.33
20	A	1799	CLA	O2D-CGD	5.53	1.46	1.33
20	A	1795	CLA	CHD-C4C	5.53	1.51	1.39
20	B	1771	CLA	CHC-C1C	5.53	1.49	1.35
20	A	1793	CLA	CHD-C4C	5.53	1.51	1.39
20	I	1031	CLA	CHD-C4C	5.53	1.51	1.39
20	A	1796	CLA	CHD-C4C	5.53	1.51	1.39
20	A	1782	CLA	CHD-C4C	5.53	1.51	1.39
20	1	1195	CLA	C3A-C2A	-5.53	1.49	1.54
20	F	1156	CLA	CHD-C4C	5.53	1.51	1.39
20	A	1781	CLA	CHD-C4C	5.53	1.51	1.39
22	L	1170	BCR	C20-C19	-5.52	1.20	1.34
20	A	1811	CLA	CHD-C4C	5.52	1.51	1.39
20	A	1791	CLA	CHD-C4C	5.51	1.51	1.39
20	4	1200	CLA	C3B-CAB	-5.51	1.36	1.47
20	3	1215	CLA	CHD-C1D	5.51	1.50	1.38
20	K	1142	CLA	CHD-C4C	5.51	1.51	1.39
20	B	1748	CLA	O2D-CGD	5.51	1.46	1.33
20	B	1763	CLA	CHC-C1C	5.51	1.49	1.35
20	4	1201	CLA	C1C-C2C	-5.51	1.33	1.44
20	A	1794	CLA	CHD-C4C	5.51	1.51	1.39
20	B	1755	CLA	CHD-C4C	5.50	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1194	CLA	CHD-C1D	5.50	1.50	1.38
20	B	1745	CLA	CHD-C4C	5.50	1.51	1.39
20	2	1220	CLA	CHD-C1D	5.50	1.49	1.38
20	4	1198	CLA	C3D-C4D	-5.50	1.31	1.44
20	A	1812	CLA	CHD-C1D	5.50	1.49	1.38
20	F	1157	CLA	C3B-C2B	-5.49	1.32	1.40
20	1	1193	CLA	CHD-C4C	5.49	1.51	1.39
20	A	1785	CLA	CHD-C1D	5.49	1.49	1.38
20	2	1224	CLA	CHD-C4C	5.48	1.51	1.39
20	3	1214	CLA	CHD-C1D	5.48	1.50	1.38
20	A	1801	CLA	CHD-C4C	5.48	1.51	1.39
20	A	1769	CLA	C3B-CAB	-5.47	1.36	1.47
20	J	1043	CLA	CHD-C4C	5.47	1.51	1.39
20	R	1055	CLA	CHD-C4C	5.46	1.51	1.39
20	2	1213	CLA	O2A-CGA	5.46	1.49	1.33
22	B	1779	BCR	C30-C25	-5.45	1.46	1.53
20	A	1812	CLA	O2D-CGD	5.45	1.46	1.33
20	A	1815	CLA	O2A-CGA	5.45	1.49	1.33
20	3	3008	CLA	CHD-C4C	5.45	1.51	1.39
20	A	1768	CLA	O2A-CGA	5.44	1.49	1.33
20	4	1199	CLA	O2D-CGD	5.43	1.46	1.33
20	1	1193	CLA	O2D-CGD	5.42	1.46	1.33
20	1	1198	CLA	CHD-C1D	5.42	1.48	1.38
20	3	1216	CLA	CHD-C1D	5.42	1.50	1.38
20	1	1198	CLA	O2D-CGD	5.42	1.46	1.33
20	A	1786	CLA	O2A-CGA	5.42	1.49	1.33
20	K	1146	CLA	CHC-C1C	5.42	1.48	1.35
20	L	1166	CLA	CHD-C4C	5.41	1.51	1.39
20	A	1800	CLA	O2D-CGD	5.41	1.46	1.33
20	1	1197	CLA	CHC-C1C	5.41	1.48	1.35
20	B	1762	CLA	CHD-C4C	5.41	1.51	1.39
20	B	1764	CLA	OBD-CAD	5.41	1.31	1.22
20	B	1762	CLA	O2A-CGA	5.40	1.49	1.33
20	B	1787	CLA	O2D-CGD	5.39	1.46	1.33
20	4	1197	CLA	CHD-C1D	5.39	1.48	1.38
20	B	1772	CLA	CHD-C4C	5.39	1.51	1.39
20	4	4003	CLA	CHD-C1D	5.39	1.50	1.38
20	4	1197	CLA	CHD-C4C	5.39	1.51	1.39
20	2	1217	CLA	CHD-C4C	5.38	1.51	1.39
20	B	1742	CLA	CHD-C4C	5.37	1.51	1.39
20	A	1784	CLA	O2A-CGA	5.37	1.49	1.33
20	B	1751	CLA	O2A-CGA	5.37	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	1044	CLA	C3D-C4D	-5.37	1.32	1.44
20	K	3009	CLA	O2D-CGD	5.36	1.46	1.33
20	A	1762	CLA	OBD-CAD	5.36	1.31	1.22
20	B	1760	CLA	O2A-CGA	5.35	1.49	1.33
20	K	1146	CLA	C1C-C2C	-5.35	1.34	1.44
20	B	1742	CLA	O2D-CGD	5.34	1.46	1.33
20	B	1769	CLA	O2D-CGD	5.33	1.46	1.33
20	A	1816	CLA	C4D-ND	-5.33	1.30	1.37
20	A	1773	CLA	O2A-CGA	5.32	1.48	1.33
20	1	1197	CLA	C3B-C2B	-5.32	1.33	1.40
20	1	1189	CLA	C3D-C4D	-5.31	1.32	1.44
20	A	1776	CLA	C3B-CAB	-5.31	1.37	1.47
20	J	1045	CLA	CHD-C1D	5.31	1.48	1.38
20	4	1205	CLA	CHD-C1D	5.30	1.50	1.38
20	B	1747	CLA	O2A-CGA	5.30	1.48	1.33
20	B	1736	CLA	O2A-CGA	5.30	1.48	1.30
20	B	1738	CLA	O2D-CGD	5.30	1.46	1.33
20	B	1750	CLA	O2D-CGD	5.30	1.46	1.33
20	B	1769	CLA	C3D-C4D	-5.28	1.32	1.44
20	4	1207	CLA	CHD-C4C	5.28	1.51	1.39
20	B	1761	CLA	CHD-C1D	5.28	1.48	1.38
20	B	1769	CLA	CHD-C1D	5.27	1.48	1.38
20	R	1055	CLA	O2A-CGA	5.27	1.48	1.33
20	2	1217	CLA	CHD-C1D	5.27	1.48	1.38
20	B	1759	CLA	O2D-CGD	5.26	1.46	1.33
20	K	1146	CLA	O2D-CGD	5.26	1.46	1.33
20	A	1774	CLA	O2D-CGD	5.26	1.46	1.33
20	1	1189	CLA	O2D-CGD	5.26	1.46	1.33
20	J	1044	CLA	CHD-C1D	5.26	1.48	1.38
20	2	1223	CLA	CHD-C4C	5.26	1.51	1.39
20	B	1749	CLA	O2A-CGA	5.26	1.48	1.33
20	1	1192	CLA	OBD-CAD	5.26	1.31	1.22
20	B	1787	CLA	O2A-CGA	5.25	1.48	1.33
20	A	1789	CLA	C3D-C4D	-5.24	1.32	1.44
20	A	1782	CLA	O2D-CGD	5.24	1.46	1.33
20	2	1216	CLA	CHD-C1D	5.24	1.50	1.38
20	A	1812	CLA	O2A-CGA	5.24	1.48	1.33
20	K	1085	CLA	C3D-C4D	-5.24	1.32	1.44
20	4	1201	CLA	O2D-CGD	5.24	1.46	1.33
20	4	1206	CLA	CHC-C1C	5.23	1.52	1.39
20	B	1758	CLA	CHD-C4C	5.23	1.51	1.39
20	2	1223	CLA	C3D-C4D	-5.23	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	1196	CLA	O2D-CGD	5.23	1.46	1.33
20	B	1771	CLA	CHD-C4C	5.22	1.51	1.39
20	4	4014	CLA	O2D-CGD	5.22	1.45	1.33
20	A	1767	CLA	O2A-CGA	5.22	1.48	1.33
20	2	1220	CLA	O2D-CGD	5.22	1.45	1.33
20	B	1748	CLA	CHD-C4C	5.22	1.51	1.39
20	1	1187	CLA	C1B-NB	-5.22	1.30	1.35
20	F	1156	CLA	C3D-C4D	-5.21	1.32	1.44
20	B	1763	CLA	C3D-C4D	-5.21	1.32	1.44
20	A	1817	CLA	O2A-CGA	5.21	1.48	1.33
20	B	1741	CLA	O2D-CGD	5.21	1.45	1.33
20	A	1794	CLA	O2D-CGD	5.21	1.45	1.33
20	B	1737	CLA	O2A-CGA	5.21	1.48	1.33
20	A	1796	CLA	O2D-CGD	5.21	1.45	1.33
20	B	1756	CLA	C3D-C4D	-5.21	1.32	1.44
20	A	1767	CLA	O2D-CGD	5.20	1.45	1.33
20	A	1764	CLA	C3D-C4D	-5.20	1.32	1.44
20	B	1753	CLA	CHC-C1C	5.20	1.48	1.35
20	A	1797	CLA	O2D-CGD	5.19	1.45	1.33
20	B	1749	CLA	CHD-C4C	5.19	1.51	1.39
20	A	1795	CLA	O2D-CGD	5.19	1.45	1.33
20	A	1782	CLA	C3D-C4D	-5.19	1.32	1.44
20	A	1792	CLA	O2D-CGD	5.19	1.45	1.33
20	J	1043	CLA	O2D-CGD	5.19	1.45	1.33
20	1	1195	CLA	CHC-C1C	5.19	1.48	1.35
20	A	1759	CLA	O2D-CGD	5.19	1.45	1.33
20	K	1085	CLA	O2D-CGD	5.19	1.45	1.33
20	K	1146	CLA	C1B-NB	-5.19	1.30	1.35
20	3	3014	CLA	CHD-C1D	5.19	1.49	1.38
20	J	1046	CLA	CHD-C1D	5.18	1.49	1.38
20	4	1204	CLA	OBD-CAD	5.18	1.31	1.22
20	B	1735	CLA	O2D-CGD	5.18	1.45	1.33
20	B	1756	CLA	O2D-CGD	5.18	1.45	1.33
20	B	1740	CLA	O2D-CGD	5.18	1.45	1.33
20	B	1750	CLA	O2A-CGA	5.18	1.48	1.33
20	2	1224	CLA	O2A-CGA	5.18	1.48	1.33
20	F	1156	CLA	O2D-CGD	5.18	1.45	1.33
20	A	1794	CLA	C3D-C4D	-5.18	1.32	1.44
20	2	1213	CLA	C3B-CAB	-5.18	1.37	1.47
20	A	1793	CLA	O2D-CGD	5.17	1.45	1.33
20	4	1196	CLA	C3D-C4D	-5.17	1.32	1.44
20	2	1212	CLA	C3D-C4D	-5.17	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	3002	CLA	CHC-C1C	5.17	1.52	1.39
20	4	4014	CLA	C3D-C4D	-5.17	1.32	1.44
20	A	1791	CLA	O2D-CGD	5.17	1.45	1.33
20	J	1043	CLA	C3D-C4D	-5.17	1.32	1.44
20	B	1786	CLA	O2D-CGD	5.17	1.45	1.33
20	A	1792	CLA	C3D-C4D	-5.17	1.32	1.44
20	B	1735	CLA	C3D-C4D	-5.16	1.32	1.44
20	B	1755	CLA	C3D-C4D	-5.16	1.32	1.44
20	A	1781	CLA	C3D-C4D	-5.16	1.32	1.44
20	3	1219	CLA	C3D-C4D	-5.16	1.32	1.44
20	1	1192	CLA	CHD-C4C	5.16	1.51	1.39
20	3	3008	CLA	O2D-CGD	5.16	1.45	1.33
20	3	1219	CLA	O2D-CGD	5.16	1.45	1.33
20	B	1749	CLA	CHD-C1D	5.15	1.48	1.38
20	B	1764	CLA	CHD-C1D	5.15	1.48	1.38
20	A	1793	CLA	C3D-C4D	-5.15	1.32	1.44
20	A	1778	CLA	OBD-CAD	5.15	1.31	1.22
20	2	1218	CLA	OBD-CAD	5.15	1.31	1.22
20	A	1791	CLA	C3D-C4D	-5.14	1.32	1.44
20	A	1796	CLA	C3D-C4D	-5.14	1.32	1.44
20	2	1212	CLA	O2D-CGD	5.14	1.45	1.33
20	2	1224	CLA	C3D-C4D	-5.14	1.32	1.44
20	A	1797	CLA	C3D-C4D	-5.14	1.32	1.44
20	B	1769	CLA	CHD-C4C	5.13	1.51	1.39
20	B	1771	CLA	O2D-CGD	5.13	1.45	1.33
20	1	1190	CLA	C3D-C4D	-5.13	1.32	1.44
20	K	1146	CLA	CHD-C4C	5.13	1.50	1.39
20	H	1079	CLA	O2A-CGA	5.13	1.48	1.33
20	A	1795	CLA	C3D-C4D	-5.13	1.32	1.44
20	4	1208	CLA	CHC-C1C	5.12	1.52	1.39
20	2	1219	CLA	CHC-C1C	5.12	1.52	1.39
20	A	1786	CLA	C3D-C4D	-5.12	1.32	1.44
20	A	1781	CLA	O2D-CGD	5.12	1.45	1.33
20	B	1758	CLA	O2D-CGD	5.12	1.45	1.33
20	A	1813	CLA	O2D-CGD	5.12	1.45	1.33
20	K	1142	CLA	O2D-CGD	5.12	1.45	1.33
20	B	1755	CLA	O2D-CGD	5.11	1.45	1.33
20	B	1753	CLA	C3B-C2B	-5.11	1.33	1.40
20	L	1166	CLA	O2A-CGA	5.10	1.48	1.33
20	B	1764	CLA	C3D-C4D	-5.10	1.32	1.44
20	2	1220	CLA	CHD-C4C	5.09	1.50	1.39
20	1	1201	CLA	CHD-C1D	5.09	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1200	CLA	O2D-CGD	5.09	1.45	1.33
20	A	1813	CLA	OBD-CAD	5.09	1.31	1.22
20	B	1749	CLA	O2D-CGD	5.09	1.45	1.33
20	B	1772	CLA	OBD-CAD	5.08	1.31	1.22
20	B	1762	CLA	C3D-C4D	-5.08	1.32	1.44
20	B	1752	CLA	C3D-C4D	-5.08	1.32	1.44
20	B	1759	CLA	C3D-C4D	-5.07	1.32	1.44
20	A	1813	CLA	C3D-C4D	-5.07	1.32	1.44
20	B	1741	CLA	C3D-C4D	-5.07	1.32	1.44
20	A	1785	CLA	C3D-C4D	-5.07	1.32	1.44
20	A	1772	CLA	CHD-C4C	5.06	1.50	1.39
20	K	3009	CLA	O2A-CGA	5.06	1.48	1.33
20	1	1200	CLA	C1C-C2C	-5.06	1.34	1.44
20	4	1209	CLA	C3D-C4D	-5.06	1.32	1.44
20	B	1766	CLA	O2A-CGA	5.06	1.48	1.33
20	K	1142	CLA	C3D-C4D	-5.05	1.32	1.44
20	A	1768	CLA	C3B-CAB	-5.05	1.37	1.47
20	A	1766	CLA	C3D-C4D	-5.05	1.32	1.44
20	A	1766	CLA	O2A-CGA	5.05	1.47	1.30
20	A	1770	CLA	OBD-CAD	5.05	1.31	1.22
20	B	1786	CLA	O2A-CGA	5.05	1.48	1.33
20	3	1213	CLA	CHD-C1D	5.04	1.49	1.38
20	4	1201	CLA	C3B-CAB	-5.04	1.37	1.47
20	B	1766	CLA	C3D-C4D	-5.04	1.32	1.44
20	B	1743	CLA	O2D-CGD	5.03	1.45	1.33
20	B	1759	CLA	CHD-C4C	5.03	1.50	1.39
20	J	1045	CLA	O2D-CGD	5.03	1.45	1.33
20	A	1765	CLA	CHC-C1C	5.03	1.47	1.35
20	A	1816	CLA	CHD-C4C	5.03	1.50	1.39
20	B	1764	CLA	O2A-CGA	5.02	1.47	1.30
20	3	1218	CLA	CHD-C1D	5.02	1.48	1.38
20	B	1770	CLA	O2D-CGD	5.02	1.45	1.33
20	4	1198	CLA	C4D-ND	-5.01	1.30	1.37
20	A	1760	CLA	O2D-CGD	5.01	1.45	1.33
20	B	1767	CLA	O2A-CGA	5.00	1.48	1.33
20	I	1031	CLA	O2D-CGD	5.00	1.45	1.33
22	I	1032	BCR	C26-C25	-5.00	1.25	1.34
20	B	1751	CLA	CHD-C1D	5.00	1.48	1.38
20	K	3009	CLA	OBD-CAD	5.00	1.31	1.22
20	2	1217	CLA	C3D-C4D	-4.99	1.32	1.44
20	A	1771	CLA	O2A-CGA	4.99	1.47	1.33
20	A	1801	CLA	O2A-CGA	4.98	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1192	CLA	CHD-C1D	4.98	1.48	1.38
20	I	1031	CLA	C3D-C4D	-4.98	1.32	1.44
20	4	1199	CLA	O2A-CGA	4.98	1.47	1.33
20	4	1204	CLA	C3D-C4D	-4.98	1.32	1.44
20	1	1200	CLA	CHD-C4C	4.98	1.50	1.39
20	B	1753	CLA	CHD-C1D	4.97	1.48	1.38
20	A	1769	CLA	O2D-CGD	4.97	1.45	1.33
20	4	1201	CLA	CHD-C1D	4.96	1.48	1.38
20	A	1776	CLA	O2A-CGA	4.96	1.47	1.33
20	G	1099	CLA	C3D-C4D	-4.96	1.33	1.44
20	R	1055	CLA	OBD-CAD	4.96	1.31	1.22
20	A	1772	CLA	O2D-CGD	4.96	1.45	1.33
20	2	1222	CLA	O2D-CGD	4.95	1.45	1.33
20	B	1768	CLA	O2A-CGA	4.94	1.47	1.33
20	A	1790	CLA	O2A-CGA	4.94	1.47	1.33
20	B	1752	CLA	OBD-CAD	4.94	1.31	1.22
20	B	1761	CLA	O2A-CGA	4.94	1.47	1.33
20	K	3009	CLA	C3D-C4D	-4.92	1.33	1.44
20	B	1748	CLA	C3D-C4D	-4.92	1.33	1.44
20	B	1749	CLA	C3D-C4D	-4.92	1.33	1.44
20	A	1775	CLA	OBD-CAD	4.91	1.30	1.22
20	1	1193	CLA	O2A-CGA	4.90	1.47	1.33
20	A	1799	CLA	OBD-CAD	4.90	1.30	1.22
20	B	1736	CLA	O2D-CGD	4.90	1.45	1.33
20	2	1221	CLA	CHC-C1C	4.90	1.51	1.39
20	A	1811	CLA	CHD-C1D	4.90	1.47	1.38
20	4	1208	CLA	CHD-C1D	4.89	1.49	1.38
20	1	1200	CLA	C4C-C3C	-4.89	1.36	1.45
20	B	1785	CLA	O2D-CGD	4.89	1.45	1.33
20	1	1187	CLA	OBD-CAD	4.89	1.30	1.22
20	A	1774	CLA	O2A-CGA	4.89	1.47	1.33
20	2	1219	CLA	CHD-C1D	4.88	1.49	1.38
20	B	1738	CLA	C3D-C4D	-4.88	1.33	1.44
20	4	1200	CLA	OBD-CAD	4.88	1.30	1.22
20	B	1746	CLA	OBD-CAD	4.88	1.30	1.22
20	B	1751	CLA	C3B-CAB	-4.87	1.38	1.47
20	1	1201	CLA	MG-NA	-4.87	1.94	2.06
20	3	1216	CLA	CHC-C1C	4.86	1.51	1.39
20	B	1762	CLA	O2D-CGD	4.86	1.45	1.33
23	A	1802	PQN	C10-C5	4.85	1.48	1.40
20	3	3015	CLA	CHC-C1C	4.85	1.51	1.39
20	A	1798	CLA	O2A-CGA	4.85	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1765	CLA	O2A-CGA	4.85	1.47	1.30
20	J	1045	CLA	CHD-C4C	4.85	1.50	1.39
20	A	1788	CLA	O2A-CGA	4.84	1.47	1.33
20	3	3011	CLA	O2A-CGA	4.84	1.47	1.33
20	B	1770	CLA	O2A-CGA	4.84	1.47	1.33
20	1	1187	CLA	CHD-C1D	4.84	1.47	1.38
20	F	1155	CLA	C3D-C4D	-4.83	1.33	1.44
20	3	3001	CLA	CHC-C1C	4.82	1.51	1.39
20	1	1191	CLA	C3D-C4D	-4.82	1.33	1.44
20	K	1146	CLA	C4C-C3C	-4.82	1.36	1.45
20	1	1200	CLA	CHC-C1C	4.82	1.47	1.35
20	B	1767	CLA	O2D-CGD	4.82	1.45	1.33
20	B	1758	CLA	C3D-C4D	-4.81	1.33	1.44
20	A	1780	CLA	O2D-CGD	4.81	1.44	1.33
20	A	1777	CLA	C3D-C4D	-4.81	1.33	1.44
20	B	1737	CLA	C3D-C4D	-4.81	1.33	1.44
20	1	1198	CLA	CHD-C4C	4.81	1.50	1.39
20	1	1201	CLA	C1B-NB	-4.81	1.30	1.35
20	A	1769	CLA	O2A-CGA	4.80	1.47	1.33
20	B	1771	CLA	O2A-CGA	4.80	1.47	1.33
20	1	1195	CLA	CHD-C1D	4.80	1.47	1.38
20	B	1754	CLA	OBD-CAD	4.80	1.30	1.22
20	B	1743	CLA	O2A-CGA	4.79	1.47	1.33
20	2	1214	CLA	CHD-C1D	4.79	1.49	1.38
20	J	1045	CLA	C4C-C3C	-4.79	1.36	1.45
20	A	1787	CLA	OBD-CAD	4.79	1.30	1.22
20	1	1197	CLA	CHD-C1D	4.79	1.47	1.38
20	L	1168	CLA	CMA-C3A	4.79	1.63	1.53
20	B	1744	CLA	OBD-CAD	4.78	1.30	1.22
20	A	1786	CLA	O2D-CGD	4.77	1.44	1.33
20	G	1099	CLA	O2A-CGA	4.77	1.47	1.33
20	4	1202	CLA	CHC-C1C	4.76	1.51	1.39
20	2	1221	CLA	CHD-C1D	4.76	1.49	1.38
20	B	1753	CLA	C4D-ND	-4.75	1.31	1.37
20	B	1766	CLA	OBD-CAD	4.75	1.30	1.22
20	I	1033	CLA	O2A-CGA	4.75	1.47	1.33
20	1	1191	CLA	OBD-CAD	4.75	1.30	1.22
20	A	1777	CLA	O2A-CGA	4.75	1.47	1.33
20	3	1218	CLA	CHD-C4C	4.74	1.50	1.39
20	L	1166	CLA	C3D-C4D	-4.74	1.33	1.44
20	3	1213	CLA	MG-NA	-4.74	1.95	2.06
20	B	1769	CLA	O2A-CGA	4.74	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1754	CLA	C3D-C4D	-4.74	1.33	1.44
20	2	1222	CLA	O2A-CGA	4.73	1.47	1.33
20	L	1168	CLA	O2A-CGA	4.73	1.47	1.33
20	2	1218	CLA	O2A-CGA	4.73	1.47	1.33
20	A	1790	CLA	C3D-C4D	-4.73	1.33	1.44
20	4	1201	CLA	CHD-C4C	4.73	1.50	1.39
20	1	1187	CLA	CHD-C4C	4.72	1.50	1.39
20	1	1199	CLA	CHC-C1C	4.72	1.51	1.39
20	1	1197	CLA	C1B-NB	-4.72	1.31	1.35
20	A	1768	CLA	C3D-C4D	-4.72	1.33	1.44
20	A	1789	CLA	O2A-CGA	4.72	1.47	1.33
20	A	1799	CLA	C3D-C4D	-4.72	1.33	1.44
20	A	1765	CLA	O2A-CGA	4.71	1.47	1.33
20	B	1742	CLA	O2A-CGA	4.71	1.47	1.33
20	B	1754	CLA	O2A-CGA	4.70	1.47	1.33
20	B	1745	CLA	O2A-CGA	4.70	1.47	1.33
20	L	1167	CLA	O2A-CGA	4.70	1.47	1.33
20	2	2010	CLA	CHC-C1C	4.70	1.51	1.39
20	A	1763	CLA	C3D-C4D	-4.69	1.33	1.44
20	3	1212	CLA	C3D-C4D	-4.69	1.33	1.44
20	A	1780	CLA	C3D-C4D	-4.69	1.33	1.44
20	G	1099	CLA	OBD-CAD	4.69	1.30	1.22
20	R	1054	CLA	C3D-C4D	-4.69	1.33	1.44
20	B	1767	CLA	C3D-C4D	-4.68	1.33	1.44
20	A	1800	CLA	C3D-C4D	-4.68	1.33	1.44
20	B	1736	CLA	C3D-C4D	-4.68	1.33	1.44
20	2	1215	CLA	O2A-CGA	4.67	1.47	1.33
20	A	1787	CLA	O2A-CGA	4.67	1.47	1.33
20	3	3007	CLA	C3D-C4D	-4.67	1.33	1.44
20	4	1203	CLA	CHC-C1C	4.67	1.50	1.39
20	4	1198	CLA	C1C-C2C	-4.67	1.35	1.44
20	L	1505	CLA	O2A-CGA	4.67	1.47	1.33
20	1	1192	CLA	O2A-CGA	4.67	1.47	1.33
20	B	1736	CLA	OBD-CAD	4.67	1.30	1.22
20	B	1768	CLA	C3D-C4D	-4.67	1.33	1.44
22	B	1779	BCR	C1-C6	-4.67	1.47	1.53
20	4	4007	CLA	OBD-CAD	4.67	1.30	1.22
20	1	1192	CLA	C3D-C4D	-4.66	1.33	1.44
20	1	1195	CLA	C4C-C3C	-4.66	1.35	1.44
20	1	1195	CLA	C1C-C2C	-4.65	1.35	1.44
20	A	1771	CLA	C3D-C4D	-4.64	1.33	1.44
20	4	4007	CLA	O2A-CGA	4.64	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1227	CLA	C1B-NB	-4.64	1.31	1.35
20	L	1168	CLA	C3D-C4D	-4.64	1.33	1.44
20	1	1189	CLA	OBD-CAD	4.64	1.30	1.22
20	B	1742	CLA	C3D-C4D	-4.63	1.33	1.44
20	B	1785	CLA	C3D-C4D	-4.63	1.33	1.44
20	B	1751	CLA	OBD-CAD	4.63	1.30	1.22
20	B	1771	CLA	C3D-C4D	-4.63	1.33	1.44
20	1	1189	CLA	O2A-CGA	4.63	1.46	1.33
20	3	1218	CLA	C1C-C2C	-4.63	1.35	1.44
20	3	1214	CLA	CHC-C1C	4.62	1.50	1.39
20	4	1200	CLA	O2A-CGA	4.60	1.46	1.33
20	A	1760	CLA	OBD-CAD	4.60	1.30	1.22
20	F	1157	CLA	OBD-CAD	4.60	1.30	1.22
20	A	1775	CLA	C3D-C4D	-4.60	1.33	1.44
23	B	1773	PQN	C10-C5	4.60	1.48	1.40
20	3	3011	CLA	C3D-C4D	-4.60	1.33	1.44
20	B	1751	CLA	C3D-C4D	-4.59	1.33	1.44
20	A	1788	CLA	O2D-CGD	4.59	1.44	1.33
20	4	1200	CLA	C3D-C4D	-4.59	1.33	1.44
20	A	1773	CLA	C3D-C4D	-4.58	1.33	1.44
20	A	1763	CLA	OBD-CAD	4.58	1.30	1.22
20	I	1033	CLA	C3D-C4D	-4.57	1.33	1.44
20	A	1788	CLA	C3D-C4D	-4.57	1.33	1.44
20	4	1198	CLA	C1B-NB	-4.57	1.31	1.35
20	A	1760	CLA	C3D-C4D	-4.56	1.33	1.44
20	4	1209	CLA	C4C-C3C	-4.56	1.37	1.45
20	2	1214	CLA	CHC-C1C	4.56	1.50	1.39
20	1	1197	CLA	O2D-CGD	4.56	1.44	1.33
20	K	1146	CLA	C1D-ND	-4.56	1.32	1.37
20	A	1770	CLA	O2A-CGA	4.56	1.46	1.30
20	B	1758	CLA	OBD-CAD	4.56	1.30	1.22
20	B	1765	CLA	C3D-C4D	-4.55	1.33	1.44
20	B	1772	CLA	C3D-C4D	-4.55	1.33	1.44
20	F	1157	CLA	CHD-C4C	4.55	1.49	1.39
20	B	1768	CLA	O2D-CGD	4.55	1.44	1.33
20	1	1195	CLA	CHD-C4C	4.54	1.49	1.39
20	4	1198	CLA	C3B-C2B	-4.54	1.34	1.40
20	1	1195	CLA	MG-NA	-4.53	1.95	2.06
20	1	1198	CLA	C4C-C3C	-4.53	1.37	1.45
20	I	1033	CLA	OBD-CAD	4.53	1.30	1.22
20	2	1223	CLA	OBD-CAD	4.53	1.30	1.22
20	A	1816	CLA	O2D-CGD	4.52	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	1044	CLA	CHD-C4C	4.52	1.49	1.39
20	3	3007	CLA	OBD-CAD	4.52	1.30	1.22
20	1	1194	CLA	CHC-C1C	4.51	1.50	1.39
20	A	1791	CLA	O2A-CGA	4.51	1.45	1.30
20	F	1157	CLA	C4C-C3C	-4.50	1.37	1.45
20	L	1168	CLA	OBD-CAD	4.50	1.30	1.22
20	A	1779	CLA	C3D-C4D	-4.50	1.34	1.44
20	2	1215	CLA	C3D-C4D	-4.50	1.34	1.44
20	3	3014	CLA	CHC-C1C	4.50	1.50	1.39
20	1	1193	CLA	C3D-C4D	-4.49	1.34	1.44
20	B	1747	CLA	C3D-C4D	-4.49	1.34	1.44
20	A	1783	CLA	O2D-CGD	4.49	1.44	1.33
20	B	1744	CLA	C3D-C4D	-4.49	1.34	1.44
20	B	1746	CLA	C3D-C4D	-4.49	1.34	1.44
20	L	1505	CLA	C3D-C4D	-4.49	1.34	1.44
20	B	1752	CLA	O2A-CGA	4.48	1.46	1.33
20	1	1200	CLA	OBD-CAD	4.48	1.30	1.22
20	3	1215	CLA	CHC-C1C	4.48	1.50	1.39
20	K	1142	CLA	O2A-CGA	4.48	1.45	1.30
20	A	1774	CLA	C3D-C4D	-4.48	1.34	1.44
20	4	1199	CLA	OBD-CAD	4.48	1.30	1.22
20	3	1218	CLA	CHC-C1C	4.48	1.46	1.35
20	1	1201	CLA	CHC-C1C	4.48	1.50	1.39
20	A	1801	CLA	C3D-C4D	-4.47	1.34	1.44
20	L	1167	CLA	C3D-C4D	-4.47	1.34	1.44
20	1	1187	CLA	CHC-C1C	4.47	1.46	1.35
20	1	1193	CLA	OBD-CAD	4.47	1.30	1.22
20	A	1785	CLA	O2A-CGA	4.47	1.46	1.33
20	A	1762	CLA	O2A-CGA	4.46	1.46	1.33
20	B	1770	CLA	C3D-C4D	-4.45	1.34	1.44
20	A	1799	CLA	O2A-CGA	4.45	1.46	1.33
20	H	1079	CLA	OBD-CAD	4.45	1.30	1.22
20	4	1209	CLA	CHD-C1D	4.44	1.47	1.38
20	4	1207	CLA	OBD-CAD	4.44	1.30	1.22
20	3	1218	CLA	C1C-NC	-4.43	1.31	1.37
20	B	1741	CLA	OBD-CAD	4.43	1.30	1.22
20	2	1220	CLA	O2A-CGA	4.43	1.46	1.33
20	A	1798	CLA	OBD-CAD	4.42	1.30	1.22
22	L	1169	BCR	C20-C19	-4.42	1.23	1.34
20	A	1800	CLA	O2A-CGA	4.42	1.46	1.33
20	B	1786	CLA	C3D-C4D	-4.41	1.34	1.44
20	A	1769	CLA	C3D-C4D	-4.41	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1816	CLA	C1B-NB	-4.41	1.31	1.35
20	3	1212	CLA	OBD-CAD	4.41	1.30	1.22
20	A	1759	CLA	C3D-C4D	-4.41	1.34	1.44
20	1	1197	CLA	CHD-C4C	4.41	1.49	1.39
20	4	1205	CLA	CHC-C1C	4.40	1.50	1.39
20	4	1204	CLA	O2A-CGA	4.40	1.46	1.33
20	4	1197	CLA	C3A-C2A	-4.40	1.50	1.54
20	B	1739	CLA	O2A-CGA	4.40	1.46	1.33
20	A	1777	CLA	OBD-CAD	4.40	1.30	1.22
20	A	1765	CLA	O2D-CGD	4.39	1.43	1.33
20	B	1763	CLA	O2A-CGA	4.39	1.46	1.33
20	A	1764	CLA	O2A-CGA	4.39	1.46	1.33
20	4	4007	CLA	C3D-C4D	-4.38	1.34	1.44
20	B	1761	CLA	C3D-C4D	-4.38	1.34	1.44
20	A	1761	CLA	C3D-C4D	-4.38	1.34	1.44
20	A	1765	CLA	C3D-C4D	-4.38	1.34	1.44
20	1	1190	CLA	O2A-CGA	4.38	1.47	1.33
20	2	1217	CLA	O2A-CGA	4.38	1.46	1.33
20	A	1771	CLA	OBD-CAD	4.38	1.30	1.22
20	A	1770	CLA	C3D-C4D	-4.38	1.34	1.44
20	A	1759	CLA	O2A-CGA	4.37	1.46	1.33
20	2	1220	CLA	C4C-C3C	-4.37	1.37	1.45
20	F	1157	CLA	C1B-NB	-4.37	1.31	1.35
20	1	1197	CLA	C1C-C2C	-4.36	1.36	1.44
20	2	1213	CLA	OBD-CAD	4.36	1.30	1.22
20	4	4003	CLA	CHC-C1C	4.36	1.50	1.39
20	A	1776	CLA	C3D-C4D	-4.36	1.34	1.44
20	2	1213	CLA	C3D-C4D	-4.35	1.34	1.44
20	A	1762	CLA	C3D-C4D	-4.35	1.34	1.44
20	2	1224	CLA	OBD-CAD	4.35	1.30	1.22
20	A	1785	CLA	OBD-CAD	4.35	1.30	1.22
20	B	1745	CLA	C3D-C4D	-4.34	1.34	1.44
20	J	1046	CLA	CHC-C1C	4.34	1.50	1.39
20	4	1199	CLA	C3D-C4D	-4.33	1.34	1.44
20	A	1783	CLA	C3D-C4D	-4.32	1.34	1.44
20	A	1767	CLA	C3D-C4D	-4.32	1.34	1.44
20	A	1812	CLA	C3D-C4D	-4.31	1.34	1.44
20	1	1197	CLA	O2A-CGA	4.31	1.45	1.33
20	B	1755	CLA	O2A-CGA	4.31	1.45	1.33
20	R	1055	CLA	C3D-C4D	-4.31	1.34	1.44
20	1	1196	CLA	C3D-C4D	-4.31	1.34	1.44
20	4	4014	CLA	O2A-CGA	4.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1200	CLA	MG-ND	-4.31	1.97	2.05
20	B	1765	CLA	OBD-CAD	4.31	1.29	1.22
20	A	1765	CLA	C1C-C2C	-4.30	1.36	1.44
20	A	1797	CLA	O2A-CGA	4.30	1.45	1.33
20	A	1782	CLA	O2A-CGA	4.30	1.45	1.33
20	A	1766	CLA	OBD-CAD	4.30	1.29	1.22
20	A	1780	CLA	O2A-CGA	4.30	1.45	1.33
20	4	1201	CLA	MG-NA	-4.30	1.96	2.06
20	B	1756	CLA	O2A-CGA	4.29	1.45	1.33
20	B	1743	CLA	C3D-C4D	-4.29	1.34	1.44
20	B	1763	CLA	OBD-CAD	4.29	1.29	1.22
20	A	1796	CLA	O2A-CGA	4.29	1.45	1.33
20	A	1781	CLA	O2A-CGA	4.29	1.45	1.33
20	A	1795	CLA	O2A-CGA	4.29	1.45	1.33
20	A	1787	CLA	C3D-C4D	-4.29	1.34	1.44
20	A	1792	CLA	O2A-CGA	4.29	1.45	1.33
20	B	1740	CLA	C3D-C4D	-4.29	1.34	1.44
20	A	1778	CLA	C3D-C4D	-4.28	1.34	1.44
20	1	1189	CLA	C4B-CHC	4.28	1.52	1.41
20	A	1794	CLA	O2A-CGA	4.28	1.45	1.33
20	4	1198	CLA	CHD-C1D	4.28	1.46	1.38
20	A	1816	CLA	C4C-C3C	-4.28	1.37	1.45
20	A	1793	CLA	O2A-CGA	4.28	1.45	1.33
20	A	1763	CLA	O2A-CGA	4.27	1.46	1.33
20	B	1735	CLA	O2A-CGA	4.27	1.45	1.33
20	A	1811	CLA	C4B-CHC	4.27	1.52	1.41
20	A	1779	CLA	OBD-CAD	4.27	1.29	1.22
20	3	1219	CLA	O2A-CGA	4.27	1.45	1.33
20	2	1222	CLA	C3D-C4D	-4.27	1.34	1.44
20	2	1212	CLA	O2A-CGA	4.26	1.45	1.33
20	B	1738	CLA	O2A-CGA	4.26	1.45	1.33
20	A	1764	CLA	O2D-CGD	4.26	1.43	1.33
20	A	1811	CLA	O2A-CGA	4.26	1.45	1.33
20	J	1043	CLA	O2A-CGA	4.25	1.45	1.33
20	A	1800	CLA	OBD-CAD	4.25	1.29	1.22
20	1	1187	CLA	C4C-C3C	-4.25	1.37	1.45
20	4	1209	CLA	CHD-C4C	4.24	1.48	1.39
24	B	1783	LMG	O8-C28	4.24	1.45	1.33
20	1	1188	CLA	C3D-C4D	-4.24	1.34	1.44
22	L	1170	BCR	C10-C9	-4.24	1.30	1.35
20	F	1157	CLA	O2D-CGD	4.24	1.43	1.33
20	4	1196	CLA	O2A-CGA	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1200	CLA	O2A-CGA	4.24	1.45	1.33
20	B	1743	CLA	C4B-CHC	4.23	1.52	1.41
20	B	1753	CLA	MG-NA	-4.23	1.96	2.06
20	B	1747	CLA	OBD-CAD	4.22	1.29	1.22
20	A	1811	CLA	C3D-C4D	-4.22	1.34	1.44
20	K	1085	CLA	O2A-CGA	4.21	1.45	1.33
20	F	1155	CLA	OBD-CAD	4.21	1.29	1.22
20	B	1762	CLA	C4B-CHC	4.20	1.52	1.41
20	A	1816	CLA	O2A-CGA	4.18	1.45	1.33
20	4	1207	CLA	C3D-C4D	-4.18	1.34	1.44
20	B	1739	CLA	OBD-CAD	4.18	1.29	1.22
20	A	1817	CLA	C3D-C4D	-4.18	1.34	1.44
20	A	1811	CLA	C4C-C3C	-4.18	1.37	1.45
20	B	1759	CLA	O2A-CGA	4.17	1.45	1.33
20	K	3009	CLA	C4B-CHC	4.17	1.52	1.41
20	1	1200	CLA	C4B-NB	-4.16	1.31	1.35
20	F	1157	CLA	C1D-ND	-4.15	1.32	1.37
20	1	1187	CLA	C1D-C2D	-4.15	1.37	1.45
20	2	1218	CLA	C3D-C4D	-4.15	1.34	1.44
20	4	1198	CLA	C4C-C3C	-4.15	1.37	1.45
20	1	1198	CLA	O2A-CGA	4.15	1.45	1.33
24	B	1783	LMG	O7-C10	4.15	1.46	1.34
20	1	1196	CLA	OBD-CAD	4.14	1.29	1.22
20	4	1204	CLA	C4C-C3C	-4.14	1.37	1.45
20	B	1753	CLA	CHD-C4C	4.14	1.48	1.39
20	B	1786	CLA	OBD-CAD	4.13	1.29	1.22
20	A	1783	CLA	OBD-CAD	4.13	1.29	1.22
20	A	1798	CLA	C3D-C4D	-4.12	1.34	1.44
20	A	1759	CLA	OBD-CAD	4.12	1.29	1.22
20	2	1221	CLA	C4B-CHC	4.11	1.52	1.43
22	L	1169	BCR	C17-C18	-4.11	1.30	1.35
20	4	1209	CLA	C3B-C2B	-4.10	1.34	1.40
20	L	1505	CLA	OBD-CAD	4.10	1.29	1.22
22	I	1032	BCR	C1-C6	-4.09	1.48	1.53
20	1	1196	CLA	C4B-CHC	4.09	1.52	1.41
20	B	1757	CLA	O2A-CGA	4.09	1.45	1.33
20	B	1787	CLA	C3D-C4D	-4.05	1.35	1.44
20	1	1187	CLA	C1C-C2C	-4.05	1.36	1.44
20	2	1213	CLA	C4B-CHC	4.05	1.52	1.41
20	B	1758	CLA	O2A-CGA	4.04	1.45	1.33
20	A	1788	CLA	OBD-CAD	4.04	1.29	1.22
20	L	1167	CLA	OBD-CAD	4.04	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	1200	CLA	CHD-C1D	4.04	1.46	1.38
20	R	1055	CLA	C4B-CHC	4.02	1.52	1.41
20	1	1188	CLA	OBD-CAD	4.02	1.29	1.22
20	B	1738	CLA	C1C-C2C	-4.02	1.36	1.44
20	A	1773	CLA	OBD-CAD	4.02	1.29	1.22
20	B	1785	CLA	OBD-CAD	4.01	1.29	1.22
20	A	1801	CLA	C4C-C3C	-4.01	1.38	1.45
20	1	1200	CLA	C1D-C2D	-4.00	1.37	1.45
20	A	1816	CLA	C3B-C2B	-4.00	1.34	1.40
20	3	3011	CLA	OBD-CAD	3.99	1.29	1.22
20	2	1227	CLA	CHC-C1C	3.99	1.49	1.39
20	1	1191	CLA	C4B-CHC	3.99	1.52	1.41
20	A	1776	CLA	OBD-CAD	3.98	1.29	1.22
20	B	1745	CLA	C4B-CHC	3.98	1.52	1.41
20	4	1209	CLA	O2A-CGA	3.98	1.45	1.33
20	B	1785	CLA	O2A-CGA	3.97	1.45	1.33
20	3	1218	CLA	C4D-ND	-3.97	1.32	1.37
20	G	1099	CLA	C4B-CHC	3.97	1.52	1.41
20	A	1815	CLA	C3D-C4D	-3.97	1.35	1.44
20	B	1753	CLA	C1C-NC	-3.97	1.31	1.37
20	A	1772	CLA	C4C-C3C	-3.96	1.38	1.45
20	A	1815	CLA	OBD-CAD	3.95	1.29	1.22
20	A	1784	CLA	C3D-C4D	-3.94	1.35	1.44
20	1	1188	CLA	C1B-NB	-3.93	1.31	1.35
20	L	1166	CLA	OBD-CAD	3.93	1.29	1.22
20	J	1045	CLA	C1C-C2C	-3.93	1.37	1.44
20	A	1767	CLA	OBD-CAD	3.92	1.29	1.22
20	3	3014	CLA	MG-NA	-3.92	1.97	2.06
20	A	1813	CLA	O2A-CGA	3.92	1.44	1.33
20	B	1737	CLA	OBD-CAD	3.92	1.29	1.22
20	B	1759	CLA	C4C-C3C	-3.92	1.38	1.45
20	4	1200	CLA	C4B-CHC	3.92	1.51	1.41
20	I	1031	CLA	C4B-CHC	3.92	1.51	1.41
20	A	1784	CLA	OBD-CAD	3.91	1.29	1.22
20	1	1200	CLA	C1C-NC	-3.91	1.32	1.37
20	B	1757	CLA	C4B-CHC	3.90	1.51	1.41
20	B	1766	CLA	C4B-CHC	3.90	1.51	1.41
20	B	1746	CLA	O2A-CGA	3.90	1.45	1.33
20	3	3008	CLA	O2A-CGA	3.89	1.44	1.33
20	3	1213	CLA	CHB-C4A	-3.89	1.31	1.34
20	A	1777	CLA	C4B-CHC	3.89	1.51	1.41
20	B	1750	CLA	C3D-C4D	-3.88	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1753	CLA	C1C-C2C	-3.87	1.37	1.44
20	2	1216	CLA	CHC-C1C	3.87	1.49	1.39
20	B	1748	CLA	O2A-CGA	3.87	1.44	1.33
20	B	1743	CLA	C4C-C3C	-3.87	1.38	1.45
20	L	1166	CLA	C4B-CHC	3.86	1.51	1.41
20	B	1763	CLA	C1C-C2C	-3.86	1.37	1.44
20	4	1198	CLA	O2D-CGD	3.86	1.42	1.33
20	A	1770	CLA	C4B-CHC	3.86	1.51	1.41
20	1	1197	CLA	C3D-CAD	-3.86	1.32	1.45
20	1	1200	CLA	C1D-ND	-3.84	1.33	1.37
20	A	1781	CLA	OBD-CAD	3.84	1.29	1.22
20	3	3002	CLA	C4B-CHC	3.83	1.51	1.43
20	A	1768	CLA	OBD-CAD	3.83	1.29	1.22
20	3	3001	CLA	C4B-CHC	3.83	1.51	1.43
20	B	1741	CLA	C4B-CHC	3.83	1.51	1.41
20	A	1774	CLA	C4C-C3C	-3.82	1.38	1.45
20	A	1816	CLA	C1C-NC	-3.81	1.32	1.37
20	J	1044	CLA	C1B-NB	-3.81	1.31	1.35
20	A	1816	CLA	C4B-CHC	3.81	1.51	1.41
20	A	1776	CLA	C4B-CHC	3.81	1.51	1.41
22	B	1779	BCR	C20-C19	-3.81	1.24	1.34
20	A	1768	CLA	C4B-CHC	3.81	1.51	1.41
20	B	1769	CLA	C4B-CHC	3.80	1.51	1.41
20	4	1205	CLA	C4B-CHC	3.80	1.51	1.43
20	B	1770	CLA	C4B-CHC	3.80	1.51	1.41
20	A	1794	CLA	OBD-CAD	3.80	1.29	1.22
21	A	7031	LMU	O1'-C1'	3.79	1.46	1.40
20	B	1739	CLA	C3D-C4D	-3.79	1.35	1.44
20	A	1793	CLA	OBD-CAD	3.79	1.29	1.22
20	B	1750	CLA	C4B-CHC	3.79	1.51	1.41
20	2	1227	CLA	MG-NA	-3.79	1.97	2.06
20	1	1195	CLA	C1C-NC	-3.79	1.32	1.37
20	B	1757	CLA	OBD-CAD	3.78	1.29	1.22
20	J	1043	CLA	OBD-CAD	3.78	1.29	1.22
20	B	1746	CLA	C4B-CHC	3.78	1.51	1.41
20	B	1786	CLA	C4B-CHC	3.78	1.51	1.41
20	A	1792	CLA	OBD-CAD	3.78	1.29	1.22
20	4	1203	CLA	CHD-C4C	3.78	1.53	1.40
20	K	1085	CLA	OBD-CAD	3.77	1.29	1.22
20	4	1196	CLA	OBD-CAD	3.77	1.29	1.22
20	B	1735	CLA	OBD-CAD	3.77	1.29	1.22
20	K	1146	CLA	MG-NA	-3.77	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1783	CLA	O2A-CGA	3.77	1.44	1.33
20	A	1765	CLA	OBD-CAD	3.76	1.29	1.22
20	J	1045	CLA	O2A-CGA	3.75	1.44	1.33
20	A	1797	CLA	OBD-CAD	3.75	1.28	1.22
20	B	1755	CLA	OBD-CAD	3.75	1.28	1.22
20	4	4014	CLA	OBD-CAD	3.75	1.28	1.22
20	A	1779	CLA	C4B-CHC	3.75	1.51	1.41
20	B	1756	CLA	OBD-CAD	3.75	1.28	1.22
20	B	1760	CLA	C4B-CHC	3.75	1.51	1.41
20	A	1795	CLA	OBD-CAD	3.75	1.28	1.22
20	B	1787	CLA	C4C-C3C	-3.75	1.38	1.45
20	L	1168	CLA	C4B-CHC	3.74	1.51	1.41
20	I	1033	CLA	C4B-CHC	3.74	1.51	1.41
20	2	1216	CLA	C3D-C4D	-3.74	1.36	1.44
20	3	3014	CLA	CHB-C4A	-3.74	1.31	1.34
20	3	1219	CLA	OBD-CAD	3.73	1.28	1.22
20	J	1044	CLA	C1D-ND	-3.73	1.33	1.37
20	A	1760	CLA	C4B-CHC	3.73	1.51	1.41
20	B	1745	CLA	OBD-CAD	3.73	1.28	1.22
20	F	1156	CLA	OBD-CAD	3.73	1.28	1.22
20	A	1796	CLA	OBD-CAD	3.73	1.28	1.22
20	B	1764	CLA	C4B-CHC	3.72	1.51	1.41
20	B	1770	CLA	C4B-NB	3.72	1.38	1.35
20	3	1218	CLA	C1D-ND	-3.72	1.33	1.37
20	A	1766	CLA	C4B-CHC	3.72	1.51	1.41
20	B	1761	CLA	OBD-CAD	3.72	1.28	1.22
20	2	1214	CLA	MG-NA	-3.72	1.97	2.06
20	A	1791	CLA	OBD-CAD	3.72	1.28	1.22
20	L	1505	CLA	C4B-CHC	3.71	1.51	1.41
20	A	1790	CLA	OBD-CAD	3.71	1.28	1.22
20	J	1044	CLA	OBD-CAD	3.71	1.28	1.22
21	A	7047	LMU	O1'-C1'	3.71	1.46	1.40
20	A	1812	CLA	OBD-CAD	3.70	1.28	1.22
20	K	1146	CLA	MG-ND	-3.69	1.98	2.05
20	B	1756	CLA	C4C-C3C	-3.69	1.38	1.45
20	4	1209	CLA	C1C-C2C	-3.69	1.37	1.44
20	K	1142	CLA	OBD-CAD	3.69	1.28	1.22
20	B	1765	CLA	C4B-CHC	3.69	1.51	1.41
20	A	1771	CLA	C4B-CHC	3.69	1.51	1.41
20	1	1187	CLA	O2A-CGA	3.69	1.44	1.33
20	J	1044	CLA	O2A-CGA	3.68	1.44	1.33
22	B	1781	BCR	C20-C19	-3.68	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1782	CLA	OBD-CAD	3.68	1.28	1.22
20	B	1770	CLA	OBD-CAD	3.68	1.28	1.22
20	3	3008	CLA	C4C-C3C	-3.68	1.38	1.45
20	1	1198	CLA	OBD-CAD	3.68	1.28	1.22
20	A	1772	CLA	O2A-CGA	3.67	1.44	1.33
20	1	1193	CLA	C4B-CHC	3.67	1.51	1.41
20	B	1742	CLA	OBD-CAD	3.67	1.28	1.22
20	B	1772	CLA	C4B-CHC	3.67	1.51	1.41
20	J	1044	CLA	C4B-NB	-3.66	1.31	1.35
20	A	1773	CLA	C4B-CHC	3.66	1.51	1.41
22	B	1779	BCR	C14-C13	-3.65	1.30	1.35
20	2	1212	CLA	OBD-CAD	3.65	1.28	1.22
20	3	1218	CLA	O2A-CGA	3.65	1.44	1.33
20	2	1222	CLA	OBD-CAD	3.65	1.28	1.22
20	F	1156	CLA	C4C-C3C	-3.65	1.38	1.45
20	2	1215	CLA	C4B-CHC	3.65	1.51	1.41
20	B	1759	CLA	OBD-CAD	3.64	1.28	1.22
20	B	1764	CLA	C4C-C3C	-3.64	1.38	1.45
20	A	1781	CLA	C4C-C3C	-3.63	1.38	1.45
20	4	1207	CLA	C4B-CHC	3.63	1.51	1.41
20	3	3001	CLA	CHD-C4C	3.63	1.52	1.40
20	1	1194	CLA	C4B-CHC	3.63	1.51	1.43
20	A	1770	CLA	C3B-C2B	-3.62	1.35	1.40
20	4	1203	CLA	C4B-CHC	3.62	1.51	1.43
20	1	1192	CLA	C4B-CHC	3.62	1.51	1.41
20	1	1187	CLA	C1D-ND	-3.62	1.33	1.37
20	A	1782	CLA	C4C-C3C	-3.62	1.38	1.45
20	4	4007	CLA	C4C-C3C	-3.61	1.38	1.45
20	A	1792	CLA	C4C-C3C	-3.61	1.38	1.45
20	2	1215	CLA	OBD-CAD	3.61	1.28	1.22
20	2	1212	CLA	C4C-C3C	-3.61	1.38	1.45
20	4	4014	CLA	C4C-C3C	-3.61	1.38	1.45
20	A	1817	CLA	OBD-CAD	3.60	1.28	1.22
20	R	1054	CLA	OBD-CAD	3.60	1.28	1.22
20	3	1217	CLA	CHD-C4C	3.60	1.52	1.40
20	B	1758	CLA	C4B-CHC	3.60	1.51	1.41
20	B	1753	CLA	C4B-NB	-3.59	1.32	1.35
20	F	1156	CLA	C3A-C2A	-3.58	1.51	1.54
20	B	1748	CLA	C4C-C3C	-3.58	1.38	1.45
20	J	1043	CLA	C4C-C3C	-3.58	1.38	1.45
20	A	1796	CLA	C4C-C3C	-3.58	1.38	1.45
20	A	1764	CLA	OBD-CAD	3.58	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1813	CLA	C4B-CHC	3.57	1.50	1.41
20	A	1783	CLA	C4B-CHC	3.57	1.50	1.41
20	4	1209	CLA	O2D-CGD	3.57	1.41	1.33
20	A	1788	CLA	C4C-C3C	-3.57	1.38	1.45
20	K	1142	CLA	C4C-C3C	-3.56	1.38	1.45
20	A	1793	CLA	C4C-C3C	-3.56	1.38	1.45
20	B	1769	CLA	C4C-C3C	-3.55	1.38	1.45
20	B	1735	CLA	C4C-C3C	-3.55	1.38	1.45
20	2	2010	CLA	CHD-C4C	3.55	1.52	1.40
20	B	1755	CLA	C4C-C3C	-3.55	1.38	1.45
20	A	1795	CLA	C4C-C3C	-3.55	1.38	1.45
20	B	1772	CLA	C3A-C2A	-3.55	1.51	1.54
21	A	7026	LMU	O3B-C3B	3.54	1.51	1.43
20	A	1797	CLA	C4C-C3C	-3.54	1.38	1.45
20	J	1044	CLA	C4C-C3C	-3.54	1.38	1.45
20	1	1197	CLA	C4D-ND	-3.54	1.32	1.37
22	3	1220	BCR	C20-C19	-3.54	1.25	1.34
20	3	1212	CLA	C4B-CHC	3.54	1.50	1.41
20	K	1085	CLA	C4C-C3C	-3.53	1.38	1.45
20	B	1740	CLA	C4B-CHC	3.53	1.50	1.41
20	B	1740	CLA	OBD-CAD	3.53	1.28	1.22
20	1	1195	CLA	OBD-CAD	3.53	1.28	1.22
20	A	1767	CLA	C1C-C2C	-3.52	1.37	1.44
20	B	1760	CLA	OBD-CAD	3.52	1.28	1.22
20	4	1204	CLA	C4B-CHC	3.52	1.50	1.41
21	A	7036	LMU	O1B-C4'	-3.52	1.34	1.43
20	2	1223	CLA	C4B-CHC	3.52	1.50	1.41
20	B	1787	CLA	OBD-CAD	3.52	1.28	1.22
20	A	1775	CLA	C4B-CHC	3.52	1.50	1.41
20	A	1816	CLA	MG-NA	-3.52	1.97	2.06
20	A	1774	CLA	OBD-CAD	3.52	1.28	1.22
20	L	1167	CLA	C4B-CHC	3.51	1.50	1.41
20	3	1219	CLA	C4C-C3C	-3.51	1.39	1.45
20	A	1794	CLA	C4C-C3C	-3.51	1.39	1.45
20	B	1785	CLA	C4B-CHC	3.51	1.50	1.41
20	1	1201	CLA	CHD-C4C	3.51	1.52	1.40
20	B	1753	CLA	O2A-CGA	3.51	1.43	1.33
20	A	1791	CLA	C4C-C3C	-3.51	1.39	1.45
20	2	1217	CLA	C4B-CHC	3.50	1.50	1.41
20	B	1751	CLA	C4B-CHC	3.50	1.50	1.41
20	1	1199	CLA	CHD-C4C	3.50	1.52	1.40
20	2	1219	CLA	MG-NA	-3.50	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	1201	CLA	C1C-NC	-3.50	1.32	1.37
20	B	1747	CLA	C4B-CHC	3.50	1.50	1.41
20	3	3011	CLA	C4B-CHC	3.49	1.50	1.41
20	B	1737	CLA	C1C-C2C	-3.49	1.37	1.44
20	4	1196	CLA	C4C-C3C	-3.49	1.39	1.45
20	3	1217	CLA	MG-NA	-3.49	1.98	2.06
20	F	1157	CLA	O2A-CGA	3.48	1.43	1.33
20	B	1762	CLA	OBD-CAD	3.48	1.28	1.22
20	4	1206	CLA	C4B-CHC	3.48	1.50	1.43
22	A	1804	BCR	C20-C19	-3.48	1.25	1.34
20	3	3014	CLA	C4B-CHC	3.48	1.50	1.43
20	F	1157	CLA	C4B-NB	-3.48	1.32	1.35
20	B	1744	CLA	C4B-CHC	3.48	1.50	1.41
20	A	1767	CLA	C4B-CHC	3.47	1.50	1.41
20	4	1202	CLA	CHD-C4C	3.47	1.52	1.40
20	A	1763	CLA	C4B-CHC	3.47	1.50	1.41
20	3	1218	CLA	C4B-NB	-3.47	1.32	1.35
20	B	1758	CLA	C4C-C3C	-3.46	1.39	1.45
20	A	1789	CLA	OBD-CAD	3.46	1.28	1.22
20	A	1772	CLA	C1C-C2C	-3.46	1.37	1.44
20	B	1763	CLA	C4B-CHC	3.46	1.50	1.41
20	4	1208	CLA	C4B-CHC	3.46	1.50	1.43
20	A	1781	CLA	C4B-CHC	3.45	1.50	1.41
22	B	1781	BCR	C5-C6	-3.45	1.28	1.34
20	A	1793	CLA	C4B-CHC	3.45	1.50	1.41
20	3	1218	CLA	C1B-NB	-3.44	1.32	1.35
20	3	1214	CLA	CHA-C1A	3.44	1.50	1.40
20	A	1797	CLA	C4B-CHC	3.44	1.50	1.41
20	B	1767	CLA	OBD-CAD	3.43	1.28	1.22
20	1	1190	CLA	C4B-CHC	3.43	1.50	1.41
20	B	1749	CLA	C4B-CHC	3.43	1.50	1.41
20	A	1780	CLA	C4B-CHC	3.43	1.50	1.41
20	A	1791	CLA	C4B-CHC	3.43	1.50	1.41
20	A	1792	CLA	C4B-CHC	3.43	1.50	1.41
20	1	1187	CLA	MG-NA	-3.43	1.98	2.06
20	4	1196	CLA	C4B-CHC	3.42	1.50	1.41
20	A	1801	CLA	C4B-CHC	3.42	1.50	1.41
22	B	1780	BCR	C20-C19	-3.42	1.25	1.34
20	A	1795	CLA	C4B-CHC	3.42	1.50	1.41
20	A	1812	CLA	C4B-CHC	3.42	1.50	1.41
20	A	1794	CLA	C4B-CHC	3.42	1.50	1.41
20	B	1755	CLA	C4B-CHC	3.42	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1227	CLA	C4B-NB	-3.42	1.32	1.35
20	B	1756	CLA	C4B-CHC	3.42	1.50	1.41
20	3	1217	CLA	CHA-C1A	3.42	1.50	1.40
20	A	1799	CLA	C4B-CHC	3.42	1.50	1.41
20	A	1796	CLA	C4B-CHC	3.41	1.50	1.41
22	B	1774	BCR	C20-C19	-3.41	1.25	1.34
20	K	1142	CLA	C4B-CHC	3.41	1.50	1.41
20	3	1215	CLA	C4B-CHC	3.41	1.50	1.43
20	K	1146	CLA	O2A-CGA	3.41	1.43	1.33
20	A	1782	CLA	C4B-CHC	3.41	1.50	1.41
20	B	1771	CLA	OBD-CAD	3.41	1.28	1.22
20	3	1219	CLA	C4B-CHC	3.41	1.50	1.41
20	B	1735	CLA	C4B-CHC	3.41	1.50	1.41
20	F	1156	CLA	C4B-CHC	3.41	1.50	1.41
20	B	1763	CLA	C4C-C3C	-3.40	1.39	1.45
20	4	1201	CLA	C3A-C2A	-3.40	1.45	1.54
20	B	1739	CLA	C1C-C2C	-3.40	1.38	1.44
20	2	1219	CLA	CHA-C1A	3.40	1.50	1.40
20	3	3014	CLA	C3D-C4D	-3.40	1.36	1.44
20	2	1227	CLA	C3D-C4D	-3.40	1.36	1.44
20	F	1155	CLA	C4B-CHC	3.40	1.50	1.41
20	3	3015	CLA	C4B-CHC	3.39	1.50	1.43
20	K	1085	CLA	C4B-CHC	3.39	1.50	1.41
20	4	4014	CLA	C4B-CHC	3.39	1.50	1.41
22	B	1778	BCR	C20-C19	-3.39	1.25	1.34
20	A	1813	CLA	C4C-C3C	-3.39	1.39	1.45
20	3	1213	CLA	CHC-C1C	3.39	1.47	1.39
20	1	1197	CLA	C1C-NC	-3.39	1.32	1.37
20	A	1798	CLA	C4B-CHC	3.39	1.50	1.41
20	A	1785	CLA	C4B-CHC	3.39	1.50	1.41
20	A	1787	CLA	C4B-CHC	3.39	1.50	1.41
20	B	1785	CLA	C1D-ND	-3.38	1.33	1.37
20	3	1215	CLA	CHA-C1A	3.38	1.50	1.40
20	1	1198	CLA	C1C-C2C	-3.38	1.38	1.44
20	R	1055	CLA	C1B-CHB	3.38	1.50	1.41
20	1	1195	CLA	C4B-NB	-3.38	1.32	1.35
20	A	1764	CLA	C4B-CHC	3.37	1.50	1.41
20	2	1212	CLA	C4B-CHC	3.37	1.50	1.41
20	3	1217	CLA	C1B-NB	-3.37	1.32	1.35
21	A	7019	LMU	O1'-C1'	3.37	1.45	1.40
22	A	1807	BCR	C20-C19	-3.37	1.25	1.34
20	3	1217	CLA	C3D-C4D	-3.37	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1786	CLA	C4B-CHC	3.36	1.50	1.41
22	A	1808	BCR	C20-C19	-3.36	1.25	1.34
22	B	1775	BCR	C20-C19	-3.36	1.25	1.34
22	B	1777	BCR	C20-C19	-3.36	1.25	1.34
22	A	1805	BCR	C20-C19	-3.36	1.25	1.34
20	I	1031	CLA	C4C-C3C	-3.35	1.39	1.45
20	2	2010	CLA	C4B-CHC	3.35	1.50	1.43
20	3	1214	CLA	CHD-C4C	3.35	1.51	1.40
20	3	1215	CLA	CHD-C4C	3.35	1.51	1.40
20	J	1045	CLA	MG-NA	-3.35	1.98	2.06
20	F	1157	CLA	C4B-CHC	3.34	1.50	1.41
20	J	1043	CLA	C4B-CHC	3.34	1.50	1.41
20	3	1214	CLA	C4B-CHC	3.34	1.50	1.43
20	4	1201	CLA	O2A-CGA	3.34	1.43	1.33
20	B	1738	CLA	MG-NA	-3.34	1.98	2.06
22	B	1779	BCR	C17-C18	-3.34	1.31	1.35
20	K	1146	CLA	C4B-CHC	3.34	1.50	1.41
22	A	1803	BCR	C20-C19	-3.34	1.26	1.34
20	J	1046	CLA	MG-NA	-3.34	1.98	2.06
22	A	1806	BCR	C20-C19	-3.33	1.26	1.34
20	B	1736	CLA	C4B-CHC	3.33	1.50	1.41
20	4	1201	CLA	C2A-C1A	-3.33	1.44	1.52
20	2	1222	CLA	C4B-CHC	3.32	1.50	1.41
20	R	1054	CLA	C4B-CHC	3.32	1.50	1.41
20	3	3001	CLA	CHA-C1A	3.32	1.50	1.40
20	1	1194	CLA	CHD-C4C	3.32	1.51	1.40
20	4	1197	CLA	C4B-CHC	3.32	1.50	1.41
20	4	4007	CLA	C4B-CHC	3.32	1.50	1.41
20	A	1789	CLA	C1C-C2C	-3.32	1.38	1.44
20	B	1752	CLA	C4B-CHC	3.32	1.50	1.41
20	3	3002	CLA	CHD-C4C	3.32	1.51	1.40
20	B	1753	CLA	C1D-C2D	-3.31	1.38	1.45
20	4	1206	CLA	C3D-C4D	-3.31	1.37	1.44
20	B	1761	CLA	C4B-CHC	3.30	1.50	1.41
20	4	1205	CLA	CHD-C4C	3.30	1.51	1.40
20	B	1753	CLA	C4B-CHC	3.30	1.50	1.41
20	1	1199	CLA	C4B-CHC	3.30	1.50	1.43
20	A	1772	CLA	C1B-NB	-3.30	1.32	1.35
20	2	1224	CLA	C4B-CHC	3.28	1.50	1.41
20	A	1762	CLA	C4B-CHC	3.27	1.50	1.41
20	A	1800	CLA	C4B-CHC	3.27	1.50	1.41
20	A	1788	CLA	C1C-C2C	-3.27	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1220	CLA	C4B-CHC	3.27	1.50	1.41
20	B	1738	CLA	C3B-C2B	-3.27	1.35	1.40
20	2	1216	CLA	MG-NA	-3.27	1.98	2.06
20	4	1202	CLA	C4B-CHC	3.27	1.50	1.43
20	4	1201	CLA	C1D-ND	-3.26	1.33	1.37
20	A	1784	CLA	C4B-CHC	3.26	1.50	1.41
20	B	1771	CLA	C4B-CHC	3.26	1.50	1.41
20	4	1206	CLA	MG-NA	-3.26	1.98	2.06
20	4	1198	CLA	MG-NA	-3.25	1.98	2.06
20	4	1198	CLA	OBD-CAD	3.25	1.28	1.22
20	3	3015	CLA	CHD-C4C	3.25	1.51	1.40
20	B	1787	CLA	C1C-C2C	-3.24	1.38	1.44
20	B	1751	CLA	C4C-C3C	-3.24	1.39	1.45
20	B	1748	CLA	C4B-CHC	3.23	1.50	1.41
22	B	1781	BCR	C26-C25	-3.23	1.28	1.34
20	A	1812	CLA	C4C-C3C	-3.23	1.39	1.45
20	B	1749	CLA	C4C-C3C	-3.23	1.39	1.45
20	B	1787	CLA	C4B-CHC	3.23	1.50	1.41
20	A	1769	CLA	C4B-CHC	3.22	1.50	1.41
20	B	1742	CLA	C4B-CHC	3.22	1.50	1.41
20	3	1213	CLA	C3D-C4D	-3.22	1.37	1.44
20	B	1754	CLA	C4B-CHC	3.22	1.49	1.41
20	3	1213	CLA	CHD-C4C	3.22	1.51	1.40
20	2	1218	CLA	C4B-CHC	3.21	1.49	1.41
20	H	1079	CLA	C4B-CHC	3.21	1.49	1.41
20	3	1216	CLA	CHD-C4C	3.21	1.51	1.40
20	2	1220	CLA	C1C-C2C	-3.21	1.38	1.44
20	1	1195	CLA	C1D-ND	-3.21	1.33	1.37
20	J	1045	CLA	C1B-NB	-3.20	1.32	1.35
20	L	1168	CLA	C4C-C3C	-3.20	1.39	1.45
20	J	1044	CLA	C1C-C2C	-3.20	1.38	1.44
20	B	1768	CLA	C1C-C2C	-3.20	1.38	1.44
20	4	1205	CLA	MG-NA	-3.20	1.98	2.06
20	A	1788	CLA	C4B-CHC	3.19	1.49	1.41
20	4	1201	CLA	CAA-C2A	-3.19	1.48	1.54
22	I	1032	BCR	C20-C19	-3.19	1.26	1.34
20	H	1079	CLA	C4C-C3C	-3.19	1.39	1.45
20	J	1044	CLA	MG-ND	-3.19	1.99	2.05
20	A	1811	CLA	OBD-CAD	3.19	1.28	1.22
20	3	3007	CLA	C4B-CHC	3.18	1.49	1.41
20	B	1753	CLA	C4D-CHA	-3.18	1.27	1.38
20	4	1208	CLA	CHA-C1A	3.18	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1749	CLA	OBD-CAD	3.18	1.28	1.22
20	F	1157	CLA	C1D-C2D	-3.18	1.39	1.45
20	1	1193	CLA	C2A-C1A	-3.18	1.45	1.52
20	1	1193	CLA	C4C-C3C	-3.17	1.39	1.45
20	A	1769	CLA	OBD-CAD	3.17	1.27	1.22
20	B	1739	CLA	C4B-CHC	3.17	1.49	1.41
20	B	1746	CLA	C1C-C2C	-3.16	1.38	1.44
20	B	1768	CLA	C4C-C3C	-3.16	1.39	1.45
20	1	1198	CLA	C4B-CHC	3.16	1.49	1.41
20	J	1044	CLA	C4B-CHC	3.16	1.49	1.41
22	L	1170	BCR	C39-C30	-3.16	1.47	1.53
20	1	1192	CLA	C4C-C3C	-3.16	1.39	1.45
20	1	1194	CLA	CHA-C1A	3.15	1.49	1.40
20	A	1780	CLA	OBD-CAD	3.15	1.27	1.22
20	A	1813	CLA	C1C-C2C	-3.15	1.38	1.44
20	B	1740	CLA	O2A-CGA	3.15	1.42	1.33
20	A	1815	CLA	C4B-CHC	3.15	1.49	1.41
21	R	1057	LMU	O2B-C2B	3.14	1.50	1.43
20	3	1217	CLA	CHC-C1C	3.14	1.47	1.39
20	1	1197	CLA	C1B-CHB	3.14	1.49	1.41
20	3	3008	CLA	C4B-CHC	3.14	1.49	1.41
20	1	1201	CLA	C3D-C4D	-3.13	1.37	1.44
20	A	1783	CLA	C1C-C2C	-3.13	1.38	1.44
22	L	1170	BCR	C40-C30	-3.13	1.47	1.53
20	1	1195	CLA	C4D-ND	-3.12	1.33	1.37
20	A	1790	CLA	C4B-CHC	3.12	1.49	1.41
20	A	1772	CLA	OBD-CAD	3.12	1.27	1.22
20	A	1774	CLA	C4B-CHC	3.12	1.49	1.41
20	4	1209	CLA	C4B-CHC	3.11	1.49	1.41
20	A	1759	CLA	C4B-CHC	3.11	1.49	1.41
20	A	1772	CLA	C4B-CHC	3.11	1.49	1.41
20	A	1811	CLA	C1D-C2D	-3.11	1.39	1.45
20	A	1786	CLA	OBD-CAD	3.11	1.27	1.22
20	4	4003	CLA	C3D-C4D	-3.10	1.37	1.44
20	4	1201	CLA	C4D-ND	-3.10	1.33	1.37
20	4	4003	CLA	CHD-C4C	3.10	1.50	1.40
20	2	1221	CLA	CHA-C1A	3.10	1.49	1.40
20	4	1209	CLA	MG-NA	-3.10	1.98	2.06
22	B	1779	BCR	C29-C30	-3.10	1.46	1.54
20	B	1761	CLA	C4C-C3C	-3.09	1.39	1.45
21	B	1782	LMU	O1'-C1'	3.09	1.45	1.40
20	1	1195	CLA	C4B-CHC	3.09	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	1216	CLA	CHA-C1A	3.09	1.49	1.40
20	A	1816	CLA	C1D-ND	-3.08	1.34	1.37
20	B	1765	CLA	C4C-C3C	-3.08	1.39	1.45
20	J	1046	CLA	CHD-C4C	3.08	1.50	1.40
20	A	1762	CLA	C1C-C2C	-3.08	1.38	1.44
20	3	3014	CLA	CHD-C4C	3.08	1.50	1.40
20	G	1099	CLA	C4C-C3C	-3.08	1.39	1.45
20	4	1206	CLA	CHD-C4C	3.08	1.50	1.40
20	K	3009	CLA	C4C-C3C	-3.08	1.39	1.45
20	B	1785	CLA	C4C-C3C	-3.07	1.39	1.45
22	L	1170	BCR	C14-C13	-3.07	1.31	1.35
20	4	1209	CLA	C1D-C2D	-3.07	1.39	1.45
20	4	1196	CLA	C1C-C2C	-3.07	1.38	1.44
20	2	1214	CLA	C3D-C4D	-3.07	1.37	1.44
20	L	1166	CLA	C1B-CHB	3.07	1.49	1.41
20	L	1166	CLA	C4C-C3C	-3.07	1.39	1.45
20	4	4014	CLA	C1C-C2C	-3.06	1.38	1.44
20	4	1209	CLA	CBD-CGD	-3.06	1.42	1.52
20	4	1198	CLA	C1D-C2D	-3.06	1.39	1.45
20	A	1764	CLA	C4C-C3C	-3.06	1.39	1.45
20	4	1198	CLA	O2A-CGA	3.06	1.42	1.33
20	2	1216	CLA	C4B-CHC	3.06	1.50	1.43
20	2	1219	CLA	CHD-C4C	3.06	1.50	1.40
20	1	1199	CLA	CHA-C1A	3.06	1.49	1.40
20	3	3015	CLA	CHA-C1A	3.06	1.49	1.40
20	1	1200	CLA	C3B-C2B	-3.05	1.36	1.40
20	J	1045	CLA	C4B-CHC	3.05	1.49	1.41
20	4	1202	CLA	CHA-C1A	3.05	1.49	1.40
20	A	1816	CLA	MG-ND	-3.05	1.99	2.05
20	J	1045	CLA	OBD-CAD	3.05	1.27	1.22
20	4	1208	CLA	CHD-C4C	3.05	1.50	1.40
20	B	1756	CLA	C1C-C2C	-3.04	1.38	1.44
20	B	1746	CLA	C4C-C3C	-3.04	1.39	1.45
20	2	2010	CLA	MG-NA	-3.04	1.99	2.06
20	4	1209	CLA	C1D-ND	-3.04	1.34	1.37
20	B	1769	CLA	OBD-CAD	3.04	1.27	1.22
20	B	1750	CLA	OBD-CAD	3.04	1.27	1.22
20	B	1738	CLA	C4C-C3C	-3.04	1.39	1.45
20	B	1740	CLA	C1C-C2C	-3.03	1.38	1.44
20	J	1046	CLA	C3D-C4D	-3.03	1.37	1.44
20	A	1817	CLA	C1C-C2C	-3.03	1.38	1.44
20	K	1146	CLA	C4D-ND	-3.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1778	CLA	C4B-CHC	3.03	1.49	1.41
20	4	1201	CLA	MG-NC	-3.03	1.99	2.06
20	B	1740	CLA	C4C-C3C	-3.03	1.39	1.45
20	4	4007	CLA	C1B-CHB	3.02	1.49	1.41
20	3	3002	CLA	CHA-C1A	3.02	1.49	1.40
20	A	1789	CLA	C4B-CHC	3.02	1.49	1.41
20	2	1221	CLA	CHD-C4C	3.02	1.50	1.40
20	A	1761	CLA	C1C-C2C	-3.01	1.38	1.44
20	K	1085	CLA	C1C-C2C	-3.01	1.38	1.44
21	A	7024	LMU	O1'-C1'	3.01	1.45	1.40
20	3	1216	CLA	CHB-C4A	-3.01	1.32	1.34
20	4	4007	CLA	C1C-C2C	-3.00	1.38	1.44
20	A	1817	CLA	C4B-CHC	3.00	1.49	1.41
20	2	1214	CLA	C4B-CHC	3.00	1.49	1.43
20	2	1220	CLA	OBD-CAD	3.00	1.27	1.22
20	A	1768	CLA	C4C-C3C	-3.00	1.39	1.45
20	A	1800	CLA	C1B-CHB	3.00	1.49	1.41
20	A	1801	CLA	C1B-CHB	3.00	1.49	1.41
20	A	1784	CLA	C3B-C2B	-2.99	1.36	1.40
20	B	1737	CLA	C4B-CHC	2.99	1.49	1.41
20	A	1759	CLA	C4C-C3C	-2.99	1.39	1.45
20	J	1043	CLA	C1C-C2C	-2.99	1.38	1.44
20	3	1216	CLA	MG-NA	-2.99	1.99	2.06
20	A	1816	CLA	OBD-CAD	2.98	1.27	1.22
20	2	1212	CLA	C1C-C2C	-2.98	1.38	1.44
20	A	1769	CLA	C1C-C2C	-2.98	1.38	1.44
20	1	1187	CLA	C4B-NB	-2.98	1.32	1.35
20	3	3008	CLA	C1C-C2C	-2.98	1.38	1.44
20	B	1758	CLA	C1B-CHB	2.98	1.49	1.41
21	A	1810	LMU	O1'-C1'	2.97	1.45	1.40
20	A	1772	CLA	MG-NA	-2.97	1.99	2.06
20	A	1797	CLA	C1C-C2C	-2.97	1.38	1.44
20	A	1792	CLA	C1C-C2C	-2.97	1.38	1.44
20	B	1767	CLA	C1B-CHB	2.97	1.49	1.41
20	B	1735	CLA	C1C-C2C	-2.97	1.38	1.44
20	A	1796	CLA	C1C-C2C	-2.97	1.38	1.44
20	B	1755	CLA	C1C-C2C	-2.97	1.38	1.44
20	A	1793	CLA	C1C-C2C	-2.97	1.38	1.44
20	4	1198	CLA	C1D-ND	-2.96	1.34	1.37
20	A	1813	CLA	MG-NA	-2.96	1.99	2.06
22	B	1779	BCR	C39-C30	-2.96	1.47	1.53
21	A	7036	LMU	C4'-C5'	-2.96	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1791	CLA	C1C-C2C	-2.96	1.38	1.44
20	A	1794	CLA	C1C-C2C	-2.96	1.38	1.44
20	A	1795	CLA	C1C-C2C	-2.96	1.38	1.44
20	B	1762	CLA	C4C-C3C	-2.95	1.39	1.45
20	3	1214	CLA	MG-NA	-2.95	1.99	2.06
22	B	1781	BCR	C1-C6	-2.95	1.49	1.53
20	A	1781	CLA	C1C-C2C	-2.95	1.38	1.44
20	4	1205	CLA	C3D-C4D	-2.95	1.37	1.44
20	A	1782	CLA	C1C-C2C	-2.95	1.38	1.44
20	B	1747	CLA	C1C-C2C	-2.95	1.38	1.44
20	4	1200	CLA	C4C-C3C	-2.94	1.40	1.45
20	A	1817	CLA	CMA-C3A	2.94	1.59	1.53
20	3	1216	CLA	C4B-CHC	2.94	1.49	1.43
20	4	1199	CLA	C1C-C2C	-2.94	1.38	1.44
20	1	1198	CLA	MG-NA	-2.93	1.99	2.06
20	A	1815	CLA	C1C-C2C	-2.93	1.38	1.44
20	J	1046	CLA	C4B-CHC	2.93	1.49	1.43
20	4	4003	CLA	MG-NA	-2.93	1.99	2.06
20	1	1192	CLA	C1B-CHB	2.93	1.49	1.41
20	3	1215	CLA	MG-NA	-2.93	1.99	2.06
22	B	1779	BCR	C40-C30	-2.92	1.48	1.53
20	2	1220	CLA	C1D-ND	-2.92	1.34	1.37
20	3	1219	CLA	C1C-C2C	-2.92	1.38	1.44
20	K	1142	CLA	C1C-C2C	-2.92	1.38	1.44
20	B	1752	CLA	C1C-C2C	-2.92	1.38	1.44
20	4	1204	CLA	C1B-CHB	2.92	1.49	1.41
20	A	1778	CLA	C1C-C2C	-2.91	1.38	1.44
20	B	1743	CLA	OBD-CAD	2.91	1.27	1.22
20	A	1778	CLA	C1B-CHB	2.91	1.49	1.41
20	2	1224	CLA	C1C-C2C	-2.91	1.38	1.44
20	B	1758	CLA	C1B-NB	2.91	1.37	1.35
20	2	1227	CLA	CHD-C4C	2.91	1.50	1.40
20	B	1759	CLA	C1C-C2C	-2.91	1.38	1.44
20	A	1775	CLA	C4C-C3C	-2.91	1.38	1.44
20	2	1224	CLA	C4C-C3C	-2.91	1.40	1.45
20	A	1777	CLA	C4C-C3C	-2.90	1.40	1.45
20	A	1776	CLA	C1C-C2C	-2.90	1.39	1.44
22	L	1170	BCR	C29-C30	-2.90	1.47	1.54
20	2	1220	CLA	MG-NA	-2.90	1.99	2.06
20	B	1757	CLA	C4C-C3C	-2.90	1.40	1.45
20	4	1199	CLA	C4B-CHC	2.90	1.49	1.41
20	2	2010	CLA	CHA-C1A	2.89	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1772	CLA	C3B-C2B	-2.89	1.36	1.40
20	B	1757	CLA	C1C-C2C	-2.89	1.39	1.44
20	B	1768	CLA	OBD-CAD	2.89	1.27	1.22
20	A	1768	CLA	C1C-C2C	-2.89	1.39	1.44
20	4	1200	CLA	C1B-CHB	2.89	1.49	1.41
20	3	1213	CLA	C2C-C1C	-2.89	1.36	1.43
20	B	1737	CLA	C4C-C3C	-2.89	1.40	1.45
20	B	1743	CLA	C4B-NB	2.89	1.37	1.35
20	B	1763	CLA	C1C-NC	-2.88	1.33	1.37
20	4	1198	CLA	C1C-NC	-2.88	1.33	1.37
20	4	4003	CLA	C4B-CHC	2.88	1.49	1.43
20	1	1199	CLA	MG-NA	-2.88	1.99	2.06
20	2	1219	CLA	C4B-CHC	2.88	1.49	1.43
20	B	1753	CLA	O2D-CGD	2.87	1.40	1.33
20	A	1761	CLA	C4B-CHC	2.87	1.49	1.41
21	A	7026	LMU	O5'-C1'	2.87	1.49	1.41
20	3	3007	CLA	C1B-CHB	2.87	1.49	1.41
20	3	3001	CLA	MG-NA	-2.87	1.99	2.06
20	A	1774	CLA	C3B-C2B	-2.87	1.36	1.40
20	2	1214	CLA	CHD-C4C	2.87	1.50	1.40
20	F	1156	CLA	C1C-C2C	-2.86	1.39	1.44
20	B	1759	CLA	C4B-CHC	2.86	1.48	1.41
20	4	1202	CLA	MG-NA	-2.86	1.99	2.06
20	2	1223	CLA	C4C-C3C	-2.86	1.40	1.45
20	F	1155	CLA	C1C-C2C	-2.86	1.39	1.44
20	A	1767	CLA	C4C-C3C	-2.85	1.40	1.45
20	1	1200	CLA	C4D-ND	-2.85	1.33	1.37
21	A	7040	LMU	C4B-C5B	-2.83	1.47	1.53
20	2	1215	CLA	C4C-C3C	-2.83	1.40	1.45
20	1	1190	CLA	C1C-C2C	-2.83	1.39	1.44
21	A	7026	LMU	O1'-C1'	2.82	1.45	1.40
20	B	1770	CLA	C4C-C3C	-2.82	1.40	1.45
21	A	7027	LMU	O1'-C1'	2.82	1.45	1.40
20	B	1768	CLA	C1B-CHB	2.82	1.48	1.41
20	A	1760	CLA	C4C-C3C	-2.82	1.40	1.45
20	A	1783	CLA	C4C-C3C	-2.81	1.40	1.45
22	B	1781	BCR	C4-C5	-2.81	1.45	1.51
22	L	1170	BCR	C30-C25	-2.81	1.49	1.53
20	3	1217	CLA	C2C-C1C	-2.80	1.36	1.43
21	A	7036	LMU	C3'-C4'	-2.80	1.44	1.52
20	3	3002	CLA	C3D-C4D	-2.80	1.38	1.44
20	A	1775	CLA	C1C-C2C	-2.80	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1811	CLA	C1D-ND	-2.80	1.34	1.37
20	A	1765	CLA	C1B-CHB	2.80	1.48	1.41
20	2	1227	CLA	CHB-C4A	-2.80	1.32	1.34
20	B	1770	CLA	C1C-C2C	-2.79	1.39	1.44
20	4	1209	CLA	C4B-NB	-2.79	1.32	1.35
20	3	3008	CLA	MG-NA	-2.79	1.99	2.06
20	B	1738	CLA	C4B-CHC	2.79	1.48	1.41
20	3	3008	CLA	OBD-CAD	2.79	1.27	1.22
20	2	1217	CLA	C1B-CHB	2.79	1.48	1.41
21	A	7039	LMU	O5B-C5B	-2.78	1.37	1.44
22	3	1220	BCR	C1-C6	-2.78	1.49	1.53
20	F	1157	CLA	C1C-C2C	-2.78	1.39	1.44
20	F	1155	CLA	C3A-C2A	-2.78	1.51	1.54
20	A	1773	CLA	C4C-C3C	-2.78	1.40	1.45
20	1	1200	CLA	MG-NA	-2.78	1.99	2.06
20	J	1044	CLA	C1D-C2D	-2.77	1.39	1.45
20	F	1157	CLA	C1C-NC	-2.77	1.33	1.37
20	B	1741	CLA	C4C-C3C	-2.77	1.40	1.45
20	K	1146	CLA	C1D-C2D	-2.77	1.39	1.45
20	1	1198	CLA	C4D-ND	-2.77	1.33	1.37
20	B	1759	CLA	MG-NA	-2.77	1.99	2.06
20	1	1201	CLA	C4B-CHC	2.76	1.49	1.43
20	B	1749	CLA	C1B-CHB	2.76	1.48	1.41
20	3	1216	CLA	C1B-NB	-2.76	1.32	1.35
20	J	1045	CLA	C3B-C2B	-2.76	1.36	1.40
22	L	1170	BCR	C31-C1	-2.75	1.48	1.53
20	2	1213	CLA	C1C-C2C	-2.75	1.39	1.44
20	1	1197	CLA	C3D-C2D	-2.75	1.31	1.39
20	B	1769	CLA	C1B-CHB	2.75	1.48	1.41
20	2	1218	CLA	C1C-C2C	-2.74	1.39	1.44
22	L	1169	BCR	C30-C25	-2.74	1.50	1.53
20	3	1218	CLA	OBD-CAD	2.74	1.27	1.22
20	B	1748	CLA	OBD-CAD	2.73	1.27	1.22
20	A	1766	CLA	C1C-C2C	-2.73	1.39	1.44
20	B	1758	CLA	C1D-C2D	-2.73	1.39	1.45
20	B	1742	CLA	C4C-C3C	-2.73	1.40	1.45
20	2	1221	CLA	MG-NA	-2.73	1.99	2.06
20	A	1816	CLA	C1C-C2C	-2.73	1.39	1.44
20	A	1817	CLA	C1B-CHB	2.73	1.48	1.41
20	2	2010	CLA	C1B-CHB	2.73	1.49	1.43
20	2	1222	CLA	C1C-C2C	-2.72	1.39	1.44
20	3	1216	CLA	C3D-C4D	-2.72	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1800	CLA	C4C-C3C	-2.72	1.40	1.45
20	2	1224	CLA	C1B-CHB	2.72	1.48	1.41
20	2	1216	CLA	C2C-C1C	-2.72	1.36	1.43
21	R	1057	LMU	O1'-C1'	2.72	1.44	1.40
20	B	1767	CLA	C4B-CHC	2.71	1.48	1.41
20	B	1768	CLA	C4B-CHC	2.71	1.48	1.41
20	4	1205	CLA	CHA-C1A	2.71	1.48	1.40
20	B	1753	CLA	MG-ND	-2.71	2.00	2.05
21	2	1225	LMU	O1'-C1'	2.71	1.44	1.40
20	A	1762	CLA	C4C-C3C	-2.71	1.40	1.45
20	2	1216	CLA	C3C-C4C	-2.70	1.36	1.43
20	B	1760	CLA	C1D-ND	-2.70	1.34	1.37
20	B	1766	CLA	C1B-CHB	2.70	1.48	1.41
22	L	1170	BCR	C2-C1	-2.70	1.47	1.54
20	1	1195	CLA	C3B-C2B	-2.70	1.32	1.41
20	B	1741	CLA	C1C-C2C	-2.70	1.39	1.44
20	K	3009	CLA	C1B-CHB	2.69	1.48	1.41
20	A	1816	CLA	C3D-CAD	-2.69	1.36	1.45
20	B	1769	CLA	C1C-C2C	-2.69	1.39	1.44
20	A	1816	CLA	C4D-CHA	-2.69	1.28	1.38
20	1	1198	CLA	C1D-ND	-2.69	1.34	1.37
20	2	1216	CLA	CHD-C4C	2.68	1.49	1.40
20	A	1759	CLA	C1B-CHB	2.68	1.48	1.41
20	A	1766	CLA	C4C-C3C	-2.68	1.40	1.45
20	4	4003	CLA	CHA-C1A	2.67	1.48	1.40
20	4	1203	CLA	CHA-C1A	2.67	1.48	1.40
20	A	1813	CLA	C1C-NC	-2.67	1.33	1.37
20	4	1209	CLA	C1B-NB	-2.67	1.32	1.35
20	A	1763	CLA	C1B-CHB	2.67	1.48	1.41
20	1	1188	CLA	C4B-CHC	2.67	1.48	1.41
20	2	1220	CLA	C1B-NB	-2.66	1.32	1.35
20	B	1760	CLA	C1C-C2C	-2.66	1.39	1.44
20	B	1738	CLA	OBD-CAD	2.66	1.27	1.22
20	B	1750	CLA	C1B-CHB	2.66	1.48	1.41
22	3	1220	BCR	C30-C25	-2.66	1.50	1.53
20	4	1203	CLA	MG-NA	-2.66	2.00	2.06
20	A	1759	CLA	C1C-C2C	-2.65	1.39	1.44
20	3	1218	CLA	C1D-C2D	-2.65	1.40	1.45
22	I	1032	BCR	C38-C26	-2.65	1.46	1.50
20	1	1196	CLA	C4C-C3C	-2.65	1.39	1.44
20	3	3015	CLA	MG-NA	-2.65	2.00	2.06
20	B	1740	CLA	C1B-NB	-2.64	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	1212	CLA	C4C-C3C	-2.64	1.39	1.44
20	2	1227	CLA	CHA-C1A	2.64	1.48	1.40
20	A	1811	CLA	C3B-C2B	-2.64	1.36	1.40
20	R	1054	CLA	C1B-CHB	2.64	1.48	1.41
21	A	7025	LMU	O1'-C1'	2.63	1.44	1.40
20	3	3015	CLA	C1B-CHB	2.63	1.49	1.43
21	4	1210	LMU	O1'-C1'	2.63	1.44	1.40
20	B	1750	CLA	C4C-C3C	-2.63	1.40	1.45
20	A	1799	CLA	C1C-C2C	-2.63	1.39	1.44
20	3	1218	CLA	MG-NA	-2.62	2.00	2.06
20	A	1785	CLA	C3B-C2B	-2.62	1.36	1.40
20	3	1213	CLA	C3C-C4C	-2.62	1.37	1.43
20	4	1198	CLA	CBD-CHA	-2.62	1.39	1.52
20	3	3002	CLA	MG-NA	-2.62	2.00	2.06
20	B	1753	CLA	CAC-C3C	-2.61	1.44	1.51
20	3	1218	CLA	C1B-CHB	2.61	1.48	1.41
20	2	1217	CLA	C4C-C3C	-2.61	1.40	1.45
20	B	1736	CLA	C4C-C3C	-2.61	1.40	1.45
20	3	3001	CLA	C3D-C4D	-2.61	1.38	1.44
20	B	1758	CLA	C1D-ND	-2.61	1.34	1.37
22	L	1170	BCR	C37-C22	-2.61	1.45	1.50
20	B	1786	CLA	C4C-C3C	-2.60	1.40	1.45
20	B	1739	CLA	C4C-C3C	-2.60	1.40	1.45
20	B	1787	CLA	MG-NA	-2.60	2.00	2.06
20	2	1221	CLA	C3D-C4D	-2.60	1.38	1.44
20	B	1763	CLA	C1B-NB	-2.60	1.32	1.35
20	2	1219	CLA	C3D-C4D	-2.60	1.38	1.44
20	4	1201	CLA	C1D-C2D	-2.59	1.40	1.45
20	4	4003	CLA	C1B-NB	-2.59	1.32	1.35
20	A	1774	CLA	C1C-C2C	-2.59	1.39	1.44
20	B	1766	CLA	C4C-C3C	-2.59	1.40	1.45
20	A	1813	CLA	C1B-NB	-2.59	1.32	1.35
20	4	1207	CLA	C3A-C2A	-2.59	1.52	1.54
20	B	1748	CLA	C1C-C2C	-2.59	1.39	1.44
22	B	1779	BCR	C32-C1	-2.59	1.48	1.53
20	K	1146	CLA	OBD-CAD	2.59	1.26	1.22
20	J	1045	CLA	C1D-ND	-2.58	1.34	1.37
20	1	1191	CLA	C1B-CHB	2.58	1.48	1.41
20	A	1775	CLA	C1B-CHB	2.58	1.48	1.41
20	3	1218	CLA	C4B-CHC	2.57	1.48	1.41
20	A	1773	CLA	C1B-CHB	2.57	1.48	1.41
20	A	1786	CLA	C1C-C2C	-2.57	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	1200	CLA	C4B-NB	2.57	1.37	1.35
20	3	3014	CLA	CHA-C1A	2.57	1.48	1.40
20	B	1748	CLA	C1B-CHB	2.57	1.48	1.41
21	L	1171	LMU	O1'-C1'	2.57	1.44	1.40
20	A	1761	CLA	C1B-CHB	2.57	1.48	1.41
20	J	1046	CLA	CHA-C1A	2.57	1.47	1.40
20	4	1208	CLA	C1B-CHB	2.57	1.49	1.43
20	4	1197	CLA	C4C-C3C	-2.57	1.39	1.44
21	A	7015	LMU	O1'-C1'	2.57	1.44	1.40
20	2	1215	CLA	C1B-CHB	2.56	1.48	1.41
21	A	7032	LMU	O5'-C5'	-2.56	1.38	1.44
20	3	3008	CLA	C1D-ND	-2.56	1.34	1.37
20	1	1187	CLA	C3D-CAD	-2.56	1.36	1.45
20	4	1208	CLA	C3D-C4D	-2.56	1.38	1.44
20	B	1785	CLA	C1C-C2C	-2.56	1.39	1.44
20	2	1222	CLA	C1B-CHB	2.55	1.48	1.41
20	A	1788	CLA	MG-NA	-2.55	2.00	2.06
20	A	1786	CLA	C1B-CHB	2.55	1.48	1.41
20	B	1746	CLA	C1B-CHB	2.55	1.48	1.41
20	B	1754	CLA	C3B-C2B	-2.55	1.36	1.40
21	A	7039	LMU	C4B-C3B	2.54	1.58	1.52
20	L	1505	CLA	C1B-CHB	2.54	1.48	1.41
20	A	1812	CLA	C1C-C2C	-2.54	1.39	1.44
20	B	1772	CLA	C1B-CHB	2.54	1.48	1.41
20	A	1812	CLA	MG-NA	-2.54	2.00	2.06
20	A	1763	CLA	C4C-C3C	-2.54	1.40	1.45
20	1	1196	CLA	C1B-CHB	2.54	1.48	1.41
20	A	1773	CLA	C1C-C2C	-2.54	1.39	1.44
20	R	1055	CLA	C3B-C2B	-2.53	1.36	1.40
20	1	1189	CLA	C1B-CHB	2.53	1.48	1.41
20	A	1770	CLA	C1C-C2C	-2.53	1.39	1.44
21	A	7037	LMU	C4'-C5'	-2.52	1.46	1.52
20	B	1745	CLA	C4C-C3C	-2.52	1.40	1.45
20	A	1761	CLA	OBD-CAD	2.52	1.26	1.22
20	R	1054	CLA	C4C-C3C	-2.52	1.40	1.45
20	B	1738	CLA	C4B-NB	-2.52	1.33	1.35
20	B	1737	CLA	MG-NA	-2.52	2.00	2.06
22	B	1776	BCR	C20-C19	-2.52	1.28	1.34
20	A	1771	CLA	C1B-CHB	2.52	1.48	1.41
20	1	1197	CLA	MG-NA	-2.52	2.00	2.06
20	4	1209	CLA	C1B-CHB	2.51	1.48	1.41
20	B	1763	CLA	MG-NA	-2.50	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1772	CLA	C1D-ND	-2.50	1.34	1.37
20	A	1785	CLA	C4C-C3C	-2.50	1.40	1.45
20	2	1224	CLA	C1B-NB	-2.50	1.33	1.35
20	1	1190	CLA	MG-NA	-2.50	2.00	2.06
20	1	1193	CLA	C1B-CHB	2.50	1.47	1.41
20	A	1765	CLA	C4B-CHC	2.50	1.47	1.41
20	1	1187	CLA	C1C-NC	-2.49	1.34	1.37
20	1	1201	CLA	C4B-NB	-2.49	1.33	1.35
20	B	1770	CLA	MG-NA	-2.49	2.00	2.06
20	K	1142	CLA	MG-NA	-2.49	2.00	2.06
20	3	1213	CLA	C1C-NC	-2.49	1.33	1.38
20	A	1769	CLA	C4C-C3C	-2.49	1.40	1.45
20	2	1214	CLA	CHA-C1A	2.49	1.47	1.40
20	B	1753	CLA	C2A-C1A	-2.49	1.46	1.52
20	3	3008	CLA	C1B-NB	-2.49	1.33	1.35
20	4	1207	CLA	C1C-C2C	-2.48	1.39	1.44
20	1	1189	CLA	C4C-C3C	-2.48	1.40	1.45
20	J	1045	CLA	C4D-ND	-2.48	1.34	1.37
20	1	1197	CLA	C4B-NB	-2.48	1.33	1.35
20	1	1191	CLA	C4C-C3C	-2.48	1.39	1.44
20	3	1212	CLA	C1B-CHB	2.48	1.47	1.41
20	1	1190	CLA	C4C-C3C	-2.48	1.40	1.45
20	4	1203	CLA	C3D-C2D	2.48	1.40	1.35
20	4	1209	CLA	MG-ND	-2.48	2.00	2.05
20	B	1754	CLA	C1C-C2C	-2.47	1.39	1.44
20	B	1762	CLA	C1C-C2C	-2.47	1.39	1.44
20	B	1753	CLA	C3C-C2C	-2.47	1.31	1.36
20	J	1044	CLA	C3B-C2B	-2.47	1.36	1.40
20	2	1216	CLA	C4C-NC	-2.46	1.33	1.37
22	L	1170	BCR	C36-C18	-2.46	1.45	1.50
20	3	1219	CLA	MG-NA	-2.46	2.00	2.06
20	4	1196	CLA	MG-NA	-2.46	2.00	2.06
22	L	1169	BCR	C1-C6	-2.46	1.50	1.53
20	B	1749	CLA	C1D-ND	-2.46	1.34	1.37
20	B	1736	CLA	MG-NA	-2.46	2.00	2.06
20	B	1763	CLA	C1D-C2D	-2.46	1.40	1.45
20	K	1085	CLA	MG-NA	-2.46	2.00	2.06
20	A	1761	CLA	C3B-C2B	-2.46	1.37	1.40
20	K	1146	CLA	C1C-NC	-2.46	1.34	1.37
20	A	1795	CLA	MG-NA	-2.45	2.00	2.06
20	B	1765	CLA	C1B-CHB	2.45	1.47	1.41
20	A	1787	CLA	C4C-C3C	-2.45	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1771	CLA	C1C-C2C	-2.45	1.39	1.44
20	1	1197	CLA	C4B-CHC	2.45	1.47	1.41
20	A	1817	CLA	C2A-C1A	-2.45	1.46	1.52
20	3	1215	CLA	C3D-C2D	2.44	1.40	1.35
20	A	1764	CLA	C1D-ND	-2.44	1.34	1.37
20	2	1227	CLA	C2C-C1C	-2.44	1.37	1.43
20	A	1815	CLA	C4C-C3C	-2.44	1.40	1.45
21	A	7034	LMU	O1'-C1'	2.44	1.44	1.40
20	B	1749	CLA	C1D-C2D	-2.44	1.40	1.45
20	1	1191	CLA	C3A-C2A	-2.44	1.52	1.54
21	A	7033	LMU	C4B-C5B	2.44	1.58	1.53
20	B	1759	CLA	C1B-CHB	2.44	1.47	1.41
20	A	1816	CLA	C1D-C2D	-2.43	1.40	1.45
20	B	1764	CLA	C1D-C2D	-2.43	1.40	1.45
20	B	1755	CLA	MG-NA	-2.43	2.00	2.06
20	4	1199	CLA	C1B-CHB	2.43	1.47	1.41
20	B	1771	CLA	C1B-CHB	2.43	1.47	1.41
20	1	1200	CLA	C3A-C2A	-2.43	1.47	1.54
20	2	2010	CLA	C4B-NB	2.43	1.37	1.35
20	2	1212	CLA	MG-NA	-2.43	2.00	2.06
20	3	3014	CLA	C1B-NB	-2.43	1.33	1.35
21	L	1171	LMU	O5B-C1B	2.43	1.48	1.41
20	4	4014	CLA	MG-NA	-2.42	2.00	2.06
20	1	1190	CLA	C1B-CHB	2.42	1.47	1.41
20	B	1743	CLA	C1C-C2C	-2.42	1.39	1.44
20	B	1758	CLA	C4B-NB	2.42	1.37	1.35
20	B	1764	CLA	C1C-C2C	-2.42	1.39	1.44
20	B	1762	CLA	C1B-CHB	2.42	1.47	1.41
20	F	1157	CLA	C1B-CHB	2.42	1.47	1.41
20	2	1223	CLA	C1B-NB	-2.42	1.33	1.35
20	A	1781	CLA	MG-NA	-2.42	2.00	2.06
20	A	1793	CLA	MG-NA	-2.42	2.00	2.06
20	A	1774	CLA	C1B-CHB	2.41	1.47	1.41
21	A	7016	LMU	O5'-C5'	-2.41	1.38	1.44
20	B	1736	CLA	C3B-C2B	-2.41	1.37	1.40
20	A	1794	CLA	MG-NA	-2.41	2.00	2.06
20	3	3001	CLA	C3D-C2D	2.41	1.40	1.35
20	J	1043	CLA	MG-NA	-2.41	2.00	2.06
22	B	1781	BCR	C29-C30	-2.41	1.48	1.54
20	F	1157	CLA	MG-ND	-2.41	2.01	2.05
20	A	1771	CLA	C4C-C3C	-2.41	1.40	1.45
20	I	1031	CLA	OBD-CAD	2.41	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1753	CLA	C3D-CAD	-2.40	1.37	1.45
20	A	1767	CLA	C3B-C2B	-2.40	1.37	1.40
20	A	1796	CLA	MG-NA	-2.40	2.00	2.06
20	B	1764	CLA	C1D-ND	-2.40	1.34	1.37
20	B	1742	CLA	C1B-CHB	2.40	1.47	1.41
20	B	1742	CLA	C1C-C2C	-2.40	1.39	1.44
20	F	1155	CLA	C4C-C3C	-2.40	1.39	1.44
20	B	1764	CLA	C1B-CHB	2.40	1.47	1.41
20	2	1218	CLA	C1B-CHB	2.40	1.47	1.41
20	A	1762	CLA	MG-NA	-2.40	2.00	2.06
20	A	1785	CLA	C1B-CHB	2.40	1.47	1.41
20	A	1787	CLA	C1B-CHB	2.40	1.47	1.41
20	A	1791	CLA	MG-NA	-2.40	2.00	2.06
20	B	1735	CLA	MG-NA	-2.40	2.00	2.06
21	A	7032	LMU	C1B-C2B	-2.39	1.45	1.52
20	J	1044	CLA	C3A-C2A	-2.39	1.47	1.54
20	3	1214	CLA	C3D-C2D	2.39	1.40	1.35
20	B	1763	CLA	C1B-CHB	2.39	1.47	1.41
20	2	1227	CLA	C4B-CHC	2.39	1.48	1.43
20	A	1777	CLA	C1B-CHB	2.39	1.47	1.41
20	A	1792	CLA	MG-NA	-2.39	2.00	2.06
20	F	1156	CLA	MG-NA	-2.39	2.00	2.06
20	J	1044	CLA	MG-NA	-2.39	2.00	2.06
20	B	1756	CLA	MG-NA	-2.38	2.00	2.06
21	A	7040	LMU	O1'-C1'	2.38	1.44	1.40
20	A	1782	CLA	MG-NA	-2.38	2.00	2.06
20	2	1216	CLA	CHA-C1A	2.38	1.47	1.40
21	A	7023	LMU	C4B-C5B	-2.38	1.48	1.53
20	A	1797	CLA	MG-NA	-2.38	2.00	2.06
20	B	1747	CLA	C1B-CHB	2.38	1.47	1.41
20	A	1784	CLA	C4C-C3C	-2.38	1.40	1.45
20	G	1099	CLA	C1B-CHB	2.38	1.47	1.41
20	1	1198	CLA	C1B-NB	-2.38	1.33	1.35
20	B	1742	CLA	C1D-ND	-2.38	1.34	1.37
20	A	1779	CLA	C4C-C3C	-2.37	1.40	1.45
21	A	7030	LMU	C4B-C5B	-2.37	1.48	1.53
20	1	1197	CLA	CBD-CGD	-2.37	1.45	1.52
20	B	1769	CLA	C4B-NB	2.37	1.37	1.35
22	L	1170	BCR	C5-C6	-2.37	1.30	1.34
20	3	3007	CLA	C1C-C2C	-2.36	1.40	1.44
20	B	1741	CLA	C1B-CHB	2.36	1.47	1.41
20	A	1783	CLA	C1B-CHB	2.36	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1790	CLA	MG-NA	-2.36	2.00	2.06
22	B	1781	BCR	C40-C30	-2.36	1.49	1.53
22	B	1776	BCR	C12-C13	2.36	1.51	1.45
20	4	1203	CLA	C1B-CHB	2.36	1.48	1.43
20	4	1201	CLA	C4D-CHA	-2.36	1.30	1.38
20	B	1763	CLA	C1D-ND	-2.35	1.34	1.37
20	R	1055	CLA	C4C-C3C	-2.35	1.41	1.45
20	J	1045	CLA	C1C-NC	-2.35	1.34	1.37
20	4	1205	CLA	C2D-C1D	-2.35	1.39	1.44
20	B	1743	CLA	MG-NA	-2.35	2.00	2.06
20	A	1766	CLA	C4B-NB	2.35	1.37	1.35
20	B	1743	CLA	C1B-NB	-2.35	1.33	1.35
20	A	1784	CLA	C1C-C2C	-2.35	1.40	1.44
20	4	1197	CLA	C1C-C2C	-2.34	1.40	1.44
20	A	1789	CLA	C1B-CHB	2.34	1.47	1.41
20	B	1752	CLA	C1B-NB	-2.34	1.33	1.35
20	B	1772	CLA	C1C-C2C	-2.34	1.40	1.44
21	A	7028	LMU	C4B-C5B	-2.34	1.48	1.53
20	4	1201	CLA	CAC-C3C	-2.34	1.45	1.51
20	A	1784	CLA	C1B-CHB	2.34	1.47	1.41
20	A	1766	CLA	C1B-CHB	2.34	1.47	1.41
20	B	1745	CLA	C1B-CHB	2.33	1.47	1.41
20	B	1744	CLA	C4C-C3C	-2.33	1.41	1.45
20	A	1760	CLA	C1C-C2C	-2.33	1.40	1.44
20	B	1771	CLA	C1D-ND	-2.33	1.34	1.37
20	3	1217	CLA	C4B-NB	-2.33	1.33	1.35
20	2	1217	CLA	C1C-C2C	-2.33	1.40	1.44
22	L	1169	BCR	C40-C30	-2.33	1.49	1.53
20	1	1187	CLA	C4D-ND	-2.33	1.34	1.37
20	3	1213	CLA	CHA-C1A	2.33	1.47	1.40
20	F	1157	CLA	CAA-C2A	-2.33	1.49	1.54
20	4	1209	CLA	C3D-CAD	-2.33	1.37	1.45
20	4	1201	CLA	C4B-CHC	2.32	1.47	1.41
21	A	7040	LMU	O5B-C5B	-2.32	1.38	1.44
20	B	1785	CLA	C3B-C2B	-2.32	1.37	1.40
20	B	1738	CLA	C1C-NC	-2.32	1.34	1.37
20	4	1198	CLA	C3A-C2A	-2.32	1.48	1.54
20	1	1192	CLA	C1C-C2C	-2.32	1.40	1.44
20	3	1218	CLA	MG-ND	-2.32	2.01	2.05
20	4	1203	CLA	C3D-C4D	-2.32	1.39	1.44
20	3	3011	CLA	C4C-C3C	-2.31	1.41	1.45
20	4	1204	CLA	C1D-ND	-2.31	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	3015	CLA	C3D-C4D	-2.31	1.39	1.44
20	2	1212	CLA	C1B-CHB	2.31	1.47	1.41
20	3	1212	CLA	C1C-C2C	-2.31	1.40	1.44
20	L	1168	CLA	C4D-ND	-2.31	1.34	1.37
20	2	1213	CLA	MG-NA	-2.30	2.00	2.06
20	4	1201	CLA	C3D-CAD	-2.30	1.37	1.45
20	2	1227	CLA	C3C-C4C	-2.30	1.37	1.43
20	A	1792	CLA	C1B-CHB	2.30	1.47	1.41
20	A	1777	CLA	C1C-C2C	-2.30	1.40	1.44
20	A	1782	CLA	C1B-CHB	2.29	1.47	1.41
20	B	1767	CLA	C4C-C3C	-2.29	1.41	1.45
20	R	1055	CLA	C4B-NB	2.29	1.37	1.35
20	A	1793	CLA	C1B-CHB	2.29	1.47	1.41
20	B	1735	CLA	C1B-CHB	2.28	1.47	1.41
20	A	1760	CLA	C1B-CHB	2.28	1.47	1.41
20	B	1756	CLA	C1B-CHB	2.28	1.47	1.41
22	L	1170	BCR	C32-C1	-2.28	1.49	1.53
20	B	1754	CLA	C1B-NB	-2.28	1.33	1.35
22	B	1781	BCR	C32-C1	-2.28	1.49	1.53
22	L	1170	BCR	C16-C15	-2.28	1.30	1.36
20	1	1198	CLA	C1B-CHB	2.28	1.47	1.41
20	A	1797	CLA	C1B-CHB	2.28	1.47	1.41
20	2	1213	CLA	C4C-C3C	-2.28	1.41	1.45
20	A	1798	CLA	C1B-CHB	2.28	1.47	1.41
20	A	1795	CLA	C1B-CHB	2.27	1.47	1.41
20	B	1785	CLA	C1B-CHB	2.27	1.47	1.41
20	K	1142	CLA	C1B-CHB	2.27	1.47	1.41
20	B	1760	CLA	C1B-NB	-2.27	1.33	1.35
20	B	1761	CLA	C1B-CHB	2.27	1.47	1.41
20	2	1227	CLA	C1C-NC	-2.27	1.33	1.38
20	1	1194	CLA	C3D-C2D	2.27	1.40	1.35
22	I	1032	BCR	C10-C9	-2.27	1.32	1.35
20	F	1156	CLA	C1B-CHB	2.26	1.47	1.41
20	A	1796	CLA	C1B-CHB	2.26	1.47	1.41
20	3	1219	CLA	C1B-CHB	2.26	1.47	1.41
20	A	1778	CLA	C4C-C3C	-2.26	1.41	1.45
20	K	1085	CLA	C1B-CHB	2.26	1.47	1.41
20	A	1798	CLA	C3B-C2B	-2.26	1.37	1.40
20	H	1079	CLA	C1C-C2C	-2.26	1.40	1.44
22	B	1781	BCR	C34-C9	-2.26	1.46	1.50
20	1	1188	CLA	C1C-C2C	-2.26	1.40	1.44
20	B	1786	CLA	C3B-C2B	-2.26	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1781	CLA	C1B-CHB	2.26	1.47	1.41
20	B	1744	CLA	C1B-CHB	2.26	1.47	1.41
20	I	1033	CLA	C1B-CHB	2.25	1.47	1.41
22	L	1170	BCR	C34-C9	-2.25	1.46	1.50
20	1	1198	CLA	C1D-C2D	-2.25	1.40	1.45
22	B	1776	BCR	C19-C18	2.25	1.50	1.45
20	3	1218	CLA	C3D-CAD	-2.25	1.37	1.45
20	B	1759	CLA	C3D-CAD	-2.25	1.37	1.45
20	4	4014	CLA	C1B-CHB	2.25	1.47	1.41
20	L	1168	CLA	C1B-CHB	2.25	1.47	1.41
20	B	1765	CLA	C1C-C2C	-2.25	1.40	1.44
20	4	1198	CLA	C4B-CHC	2.25	1.47	1.41
20	A	1791	CLA	C1B-CHB	2.25	1.47	1.41
20	B	1755	CLA	C1B-CHB	2.25	1.47	1.41
20	B	1757	CLA	C1B-CHB	2.24	1.47	1.41
20	A	1812	CLA	C3B-C2B	-2.24	1.37	1.40
20	A	1794	CLA	C1B-CHB	2.24	1.47	1.41
20	2	1220	CLA	C3B-C2B	-2.24	1.37	1.40
20	4	1196	CLA	C1B-CHB	2.24	1.47	1.41
20	1	1193	CLA	C3A-C2A	-2.24	1.48	1.54
20	J	1044	CLA	C1C-NC	-2.24	1.34	1.37
20	J	1043	CLA	C1B-CHB	2.24	1.47	1.41
20	R	1054	CLA	C1C-C2C	-2.24	1.40	1.44
20	B	1740	CLA	C4D-ND	-2.23	1.34	1.37
20	A	1798	CLA	C4C-C3C	-2.23	1.41	1.45
20	L	1505	CLA	C4C-C3C	-2.23	1.41	1.45
20	L	1168	CLA	C3B-C2B	-2.23	1.37	1.40
20	3	1216	CLA	C3D-C2D	2.23	1.40	1.35
20	A	1764	CLA	C3B-C2B	-2.22	1.37	1.40
20	3	3014	CLA	C2C-C1C	-2.22	1.38	1.43
22	B	1781	BCR	C37-C22	-2.22	1.46	1.50
20	1	1197	CLA	OBD-CAD	2.22	1.26	1.22
20	4	1197	CLA	C1D-ND	-2.22	1.35	1.37
20	B	1758	CLA	C1C-C2C	-2.22	1.40	1.44
20	B	1758	CLA	C3B-C2B	-2.21	1.37	1.40
20	A	1790	CLA	C1C-C2C	-2.21	1.40	1.44
22	B	1781	BCR	C16-C17	2.21	1.50	1.43
20	L	1168	CLA	CBD-CGD	-2.21	1.45	1.52
20	2	1214	CLA	CHB-C4A	-2.21	1.33	1.34
20	4	1208	CLA	C3D-C2D	2.21	1.40	1.35
20	1	1199	CLA	C3D-C2D	2.21	1.40	1.35
22	B	1779	BCR	C37-C22	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1747	CLA	C4C-C3C	-2.21	1.41	1.45
20	B	1785	CLA	MG-NA	-2.20	2.01	2.06
21	L	1171	LMU	C4B-C5B	2.20	1.57	1.53
20	1	1196	CLA	C1C-C2C	-2.20	1.40	1.44
22	L	1170	BCR	C4-C5	-2.20	1.46	1.51
20	A	1776	CLA	C1B-CHB	2.20	1.47	1.41
20	B	1753	CLA	CBD-CHA	-2.20	1.41	1.52
20	I	1031	CLA	C1C-C2C	-2.19	1.40	1.44
20	1	1198	CLA	MG-ND	-2.19	2.01	2.05
20	B	1750	CLA	C1C-C2C	-2.19	1.40	1.44
20	4	1202	CLA	C3D-C2D	2.19	1.40	1.35
20	3	1213	CLA	C2D-C1D	-2.19	1.39	1.44
20	1	1192	CLA	C1D-ND	-2.19	1.35	1.37
20	B	1748	CLA	C1D-C2D	-2.19	1.41	1.45
20	A	1812	CLA	C1B-NB	-2.19	1.33	1.35
20	A	1769	CLA	C1B-CHB	2.19	1.47	1.41
20	1	1195	CLA	C3D-CAD	-2.19	1.37	1.45
20	A	1800	CLA	C1D-C2D	-2.19	1.41	1.45
20	B	1769	CLA	C1D-ND	-2.18	1.35	1.37
20	1	1199	CLA	C1B-CHB	2.18	1.48	1.43
20	B	1739	CLA	C1B-CHB	2.18	1.47	1.41
20	A	1800	CLA	C1C-C2C	-2.18	1.40	1.44
21	A	7037	LMU	C4B-C3B	-2.18	1.46	1.52
20	J	1045	CLA	C3D-CAD	-2.18	1.37	1.45
20	B	1752	CLA	MG-NA	-2.18	2.01	2.06
21	A	7017	LMU	O1'-C1'	2.18	1.43	1.40
20	2	1214	CLA	C2D-C1D	-2.18	1.39	1.44
20	A	1779	CLA	C1C-C2C	-2.18	1.40	1.44
20	B	1754	CLA	C2-C3	2.17	1.38	1.33
21	A	7035	LMU	O1'-C1'	2.17	1.43	1.40
22	B	1781	BCR	C10-C9	-2.17	1.32	1.35
21	A	7024	LMU	O5B-C1B	2.17	1.47	1.41
20	1	1199	CLA	C3D-C4D	-2.17	1.39	1.44
21	A	7017	LMU	C4B-C5B	-2.16	1.48	1.53
20	K	1146	CLA	O2A-C1	-2.16	1.40	1.46
20	1	1197	CLA	CBA-CGA	2.16	1.57	1.50
20	2	1227	CLA	C4C-NC	-2.16	1.33	1.37
20	B	1747	CLA	C1B-NB	-2.16	1.33	1.35
20	3	3008	CLA	C1B-CHB	2.16	1.47	1.41
23	A	1802	PQN	O1-C1	2.16	1.27	1.23
20	L	1168	CLA	C3A-C2A	-2.16	1.48	1.54
20	3	1214	CLA	C1B-CHB	2.16	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1757	CLA	MG-NA	-2.16	2.01	2.06
20	4	1202	CLA	C1B-CHB	2.16	1.48	1.43
20	B	1752	CLA	C1B-CHB	2.15	1.47	1.41
20	2	1220	CLA	C4D-ND	-2.15	1.34	1.37
20	A	1815	CLA	MG-NA	-2.15	2.01	2.06
20	A	1789	CLA	C3A-C2A	-2.15	1.48	1.54
20	I	1033	CLA	C1C-C2C	-2.15	1.40	1.44
20	2	2010	CLA	C3D-C2D	2.15	1.40	1.35
20	A	1779	CLA	C1B-CHB	2.15	1.47	1.41
20	2	1216	CLA	C1C-NC	-2.15	1.33	1.38
20	1	1187	CLA	C3D-C2D	-2.15	1.33	1.39
20	J	1044	CLA	C3A-C4A	-2.14	1.44	1.51
20	2	1220	CLA	C3D-CAD	-2.14	1.37	1.45
20	B	1739	CLA	C3B-C2B	-2.14	1.37	1.40
20	J	1046	CLA	C2C-C1C	-2.14	1.38	1.43
21	A	7032	LMU	C3B-C2B	-2.14	1.46	1.52
20	H	1079	CLA	C1B-CHB	2.14	1.46	1.41
20	B	1769	CLA	C1D-C2D	-2.14	1.41	1.45
20	3	3001	CLA	C1B-CHB	2.14	1.48	1.43
20	A	1785	CLA	C1D-C2D	-2.14	1.41	1.45
20	3	1215	CLA	C1B-CHB	2.14	1.48	1.43
20	2	1214	CLA	C1B-NB	-2.14	1.33	1.35
20	A	1778	CLA	C3B-C2B	-2.14	1.37	1.40
20	1	1200	CLA	MG-NC	-2.13	2.01	2.06
20	J	1046	CLA	C3C-C4C	-2.13	1.38	1.43
20	B	1760	CLA	C1D-C2D	-2.13	1.41	1.45
20	J	1044	CLA	C4D-ND	-2.13	1.34	1.37
20	1	1192	CLA	MG-NA	-2.13	2.01	2.06
20	4	1201	CLA	C4B-NB	-2.13	1.33	1.35
20	L	1167	CLA	C1C-C2C	-2.13	1.40	1.44
20	G	1099	CLA	MG-NA	-2.13	2.01	2.06
20	3	3002	CLA	C3D-C2D	2.12	1.40	1.35
20	4	1201	CLA	C3C-C2C	-2.12	1.32	1.36
20	B	1762	CLA	C1A-CHA	2.12	1.51	1.43
20	4	1197	CLA	C4B-NB	-2.12	1.33	1.35
20	4	1202	CLA	C3D-C4D	-2.12	1.39	1.44
20	B	1787	CLA	C1B-CHB	2.12	1.46	1.41
20	B	1754	CLA	C1D-C2D	-2.12	1.41	1.45
20	A	1788	CLA	C1B-NB	-2.12	1.33	1.35
20	1	1200	CLA	C4B-CHC	2.12	1.46	1.41
20	K	3009	CLA	C4B-NB	2.12	1.37	1.35
20	F	1157	CLA	C4D-ND	-2.12	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1761	CLA	C1A-CHA	2.12	1.51	1.43
20	1	1187	CLA	MG-ND	-2.12	2.01	2.05
20	B	1737	CLA	C1B-CHB	2.11	1.46	1.41
20	4	1198	CLA	O2A-C1	-2.11	1.40	1.46
20	A	1772	CLA	C1C-NC	-2.11	1.34	1.37
20	4	1200	CLA	C1C-C2C	-2.11	1.40	1.44
20	K	1146	CLA	C3B-C2B	-2.11	1.37	1.40
20	A	1770	CLA	C1B-CHB	2.11	1.46	1.41
20	A	1817	CLA	C3A-C2A	-2.11	1.48	1.54
20	B	1787	CLA	C1C-NC	-2.11	1.34	1.37
20	3	1214	CLA	C3C-C4C	-2.11	1.38	1.43
20	1	1198	CLA	C1C-NC	-2.10	1.34	1.37
22	B	1774	BCR	C30-C25	-2.10	1.50	1.53
20	4	1197	CLA	C1B-CHB	2.10	1.46	1.41
20	A	1762	CLA	C1B-CHB	2.10	1.46	1.41
20	2	1214	CLA	C3C-C4C	-2.10	1.38	1.43
20	B	1742	CLA	C1-C2	2.10	1.55	1.49
20	4	1198	CLA	CBD-CGD	-2.10	1.45	1.52
20	2	1219	CLA	C1B-NB	-2.10	1.33	1.35
20	B	1754	CLA	C4C-C3C	-2.10	1.41	1.45
20	B	1752	CLA	C4C-C3C	-2.10	1.41	1.45
20	3	3011	CLA	C1C-C2C	-2.10	1.40	1.44
20	4	1206	CLA	CHA-C1A	2.10	1.46	1.40
20	I	1031	CLA	C1B-CHB	2.10	1.46	1.41
20	2	1224	CLA	C1D-C2D	-2.09	1.41	1.45
20	4	1207	CLA	MG-NA	-2.09	2.01	2.06
20	A	1768	CLA	C1B-CHB	2.09	1.46	1.41
20	B	1772	CLA	C4C-C3C	-2.09	1.40	1.44
20	3	1213	CLA	C4B-NB	-2.09	1.33	1.35
20	A	1790	CLA	C1B-NB	-2.09	1.33	1.35
20	B	1745	CLA	C1C-C2C	-2.09	1.40	1.44
20	1	1187	CLA	C3B-C2B	-2.09	1.37	1.40
20	B	1754	CLA	C1A-CHA	2.09	1.51	1.43
22	L	1169	BCR	C26-C25	-2.09	1.30	1.34
20	1	1197	CLA	C1D-C2D	-2.08	1.41	1.45
20	A	1785	CLA	C1D-ND	-2.08	1.35	1.37
20	B	1743	CLA	C1B-CHB	2.08	1.46	1.41
20	2	1221	CLA	C2D-C1D	-2.08	1.39	1.44
20	3	1215	CLA	C3C-C4C	-2.08	1.38	1.43
20	1	1193	CLA	CAA-C2A	-2.08	1.50	1.54
20	3	3002	CLA	C1B-CHB	2.08	1.48	1.43
22	B	1779	BCR	C26-C25	-2.08	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1215	CLA	C1C-C2C	-2.08	1.40	1.44
22	B	1781	BCR	C30-C25	-2.08	1.50	1.53
20	J	1046	CLA	C2D-C1D	-2.08	1.39	1.44
22	B	1775	BCR	C1-C6	-2.07	1.50	1.53
20	A	1811	CLA	C1C-C2C	-2.07	1.40	1.44
20	B	1786	CLA	C1A-CHA	2.07	1.51	1.43
21	A	7036	LMU	C4B-C5B	-2.07	1.48	1.53
20	A	1776	CLA	C4C-C3C	-2.07	1.41	1.45
20	2	1223	CLA	C3D-CAD	-2.07	1.38	1.45
21	A	7028	LMU	O5'-C5'	-2.07	1.39	1.44
20	1	1195	CLA	C1D-C2D	-2.07	1.41	1.45
20	B	1753	CLA	CMB-C2B	-2.07	1.47	1.51
20	J	1046	CLA	C1B-CHB	2.07	1.48	1.43
20	A	1811	CLA	C1B-CHB	2.06	1.46	1.41
20	3	3008	CLA	C3D-CAD	-2.06	1.38	1.45
20	A	1812	CLA	CBD-CGD	-2.06	1.46	1.52
20	2	1224	CLA	C1D-ND	-2.06	1.35	1.37
20	B	1786	CLA	C1C-C2C	-2.06	1.40	1.44
20	4	1208	CLA	C2D-C1D	-2.06	1.39	1.44
20	2	1223	CLA	C1D-C2D	-2.06	1.41	1.45
22	B	1781	BCR	C2-C1	-2.06	1.49	1.54
21	A	7033	LMU	O1'-C1'	2.06	1.43	1.40
20	B	1759	CLA	C1D-ND	-2.06	1.35	1.37
20	A	1788	CLA	C1B-CHB	2.06	1.46	1.41
20	4	1201	CLA	C3A-C4A	-2.06	1.45	1.51
20	4	4003	CLA	C2C-C1C	-2.05	1.38	1.43
22	B	1781	BCR	C33-C5	-2.05	1.47	1.50
20	1	1194	CLA	MG-NA	-2.04	2.01	2.06
20	A	1777	CLA	MG-NA	-2.04	2.01	2.06
22	A	1808	BCR	C1-C6	-2.04	1.51	1.53
20	A	1785	CLA	C1C-C2C	-2.04	1.40	1.44
20	3	1217	CLA	C4B-CHC	2.04	1.48	1.43
20	B	1738	CLA	C1B-CHB	2.04	1.46	1.41
20	A	1780	CLA	C1C-C2C	-2.04	1.40	1.44
20	B	1772	CLA	MG-NA	-2.04	2.01	2.06
20	1	1197	CLA	C1D-ND	-2.04	1.35	1.37
20	A	1787	CLA	C1C-C2C	-2.04	1.40	1.44
20	B	1786	CLA	MG-NA	-2.03	2.01	2.06
20	L	1168	CLA	C1B-NB	-2.03	1.33	1.35
20	L	1167	CLA	C1B-CHB	2.03	1.46	1.41
20	B	1762	CLA	C3B-C2B	-2.03	1.37	1.40
20	B	1748	CLA	MG-NA	-2.03	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1215	CLA	C1A-CHA	2.03	1.51	1.43
20	A	1764	CLA	MG-NA	-2.03	2.01	2.06
21	A	7036	LMU	C4B-C3B	-2.02	1.47	1.52
20	1	1197	CLA	CMB-C2B	-2.02	1.47	1.51
22	A	1803	BCR	C1-C6	-2.02	1.51	1.53
20	3	1218	CLA	C4D-CHA	-2.02	1.31	1.38
20	B	1762	CLA	C3D-CAD	-2.02	1.38	1.45
20	1	1194	CLA	C3D-C4D	-2.02	1.39	1.44
20	J	1044	CLA	C1A-CHA	2.02	1.51	1.43
20	4	1205	CLA	C1B-CHB	2.02	1.47	1.43
20	B	1753	CLA	O2D-CED	-2.02	1.40	1.45
20	1	1194	CLA	C1B-CHB	2.02	1.47	1.43
22	B	1777	BCR	C1-C6	-2.02	1.51	1.53
22	A	1805	BCR	C1-C6	-2.02	1.51	1.53
20	4	4003	CLA	C1B-CHB	2.02	1.47	1.43
20	4	1198	CLA	C4D-CHA	-2.02	1.31	1.38
20	3	3008	CLA	C4D-ND	-2.01	1.34	1.37
20	1	1201	CLA	CHB-C4A	-2.01	1.33	1.34
20	B	1771	CLA	MG-NA	-2.01	2.01	2.06
20	A	1788	CLA	C5-C3	2.01	1.55	1.51
20	B	1762	CLA	C4D-ND	-2.00	1.34	1.37
20	2	2010	CLA	C3D-C4D	-2.00	1.40	1.44

All (4431) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1780	BCR	C20-C21-C22	36.92	179.99	127.31
22	A	1808	BCR	C20-C21-C22	36.90	179.97	127.31
22	A	1805	BCR	C20-C21-C22	36.89	179.95	127.31
22	A	1806	BCR	C20-C21-C22	36.88	179.95	127.31
22	A	1804	BCR	C20-C21-C22	36.87	179.93	127.31
22	A	1807	BCR	C20-C21-C22	36.86	179.91	127.31
22	B	1778	BCR	C20-C21-C22	36.84	179.89	127.31
22	A	1803	BCR	C20-C21-C22	36.84	179.88	127.31
22	B	1774	BCR	C20-C21-C22	36.83	179.88	127.31
22	B	1775	BCR	C20-C21-C22	36.81	179.84	127.31
22	B	1777	BCR	C20-C21-C22	36.80	179.84	127.31
22	3	1220	BCR	C20-C21-C22	35.66	178.21	127.31
22	L	1170	BCR	C20-C21-C22	35.16	177.48	127.31
22	L	1169	BCR	C20-C21-C22	35.03	177.30	127.31
22	B	1779	BCR	C20-C21-C22	34.73	176.88	127.31
22	I	1032	BCR	C20-C21-C22	34.15	176.05	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1776	BCR	C20-C21-C22	30.08	170.25	127.31
22	B	1781	BCR	C20-C21-C22	24.91	162.87	127.31
22	A	1805	BCR	C21-C20-C19	18.19	179.98	123.22
22	A	1803	BCR	C21-C20-C19	18.19	179.97	123.22
22	A	1807	BCR	C21-C20-C19	18.18	179.97	123.22
22	A	1806	BCR	C21-C20-C19	18.18	179.95	123.22
22	B	1780	BCR	C21-C20-C19	18.18	179.94	123.22
22	B	1777	BCR	C21-C20-C19	18.18	179.94	123.22
22	A	1808	BCR	C21-C20-C19	18.17	179.93	123.22
22	B	1778	BCR	C21-C20-C19	18.17	179.93	123.22
22	B	1774	BCR	C21-C20-C19	18.16	179.90	123.22
22	A	1804	BCR	C21-C20-C19	18.16	179.90	123.22
22	B	1775	BCR	C21-C20-C19	18.16	179.89	123.22
22	3	1220	BCR	C21-C20-C19	17.67	178.35	123.22
22	L	1169	BCR	C21-C20-C19	17.59	178.12	123.22
22	B	1779	BCR	C21-C20-C19	17.30	177.20	123.22
22	I	1032	BCR	C21-C20-C19	17.08	176.51	123.22
22	L	1170	BCR	C21-C20-C19	16.89	175.92	123.22
20	1	1195	CLA	CAB-C3B-C4B	-16.07	103.76	128.46
20	4	1197	CLA	CAB-C3B-C4B	-14.83	105.67	128.46
22	B	1776	BCR	C21-C20-C19	14.82	169.48	123.22
22	B	1781	BCR	C24-C23-C22	-13.78	105.41	126.23
20	B	1772	CLA	CAB-C3B-C4B	-13.78	107.28	128.46
22	B	1781	BCR	C21-C20-C19	13.44	165.16	123.22
20	A	1817	CLA	CAB-C3B-C4B	-13.35	107.94	128.46
20	4	1207	CLA	CAB-C3B-C4B	-13.28	108.05	128.46
20	2	1224	CLA	OBD-CAD-C3D	-13.21	96.73	128.52
20	1	1197	CLA	OBD-CAD-C3D	-13.21	96.73	128.52
22	L	1170	BCR	C7-C8-C9	-13.07	106.49	126.23
20	1	1195	CLA	CAB-C3B-C2B	-12.91	99.40	124.69
22	I	1032	BCR	C30-C25-C26	-12.80	104.59	122.61
20	1	1196	CLA	CAB-C3B-C4B	-12.41	109.39	128.46
20	3	1218	CLA	OBD-CAD-C3D	-12.12	99.36	128.52
22	L	1170	BCR	C15-C16-C17	-11.76	99.38	123.47
20	2	1217	CLA	OBD-CAD-C3D	-11.65	100.48	128.52
20	A	1775	CLA	CAB-C3B-C4B	-11.51	110.78	128.46
20	1	1200	CLA	OBD-CAD-C3D	-11.48	100.88	128.52
20	B	1767	CLA	OBD-CAD-C3D	-11.44	100.99	128.52
20	A	1817	CLA	OBD-CAD-C3D	-11.42	101.03	128.52
20	B	1740	CLA	OBD-CAD-C3D	-11.30	101.33	128.52
20	1	1187	CLA	C4A-NA-C1A	11.25	111.76	106.71
20	B	1757	CLA	OBD-CAD-C3D	-11.17	101.63	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	1197	CLA	CMD-C2D-C1D	11.09	144.26	124.71
20	H	1079	CLA	OBD-CAD-C3D	-11.00	102.06	128.52
20	A	1764	CLA	OBD-CAD-C3D	-10.85	102.42	128.52
20	I	1031	CLA	OBD-CAD-C3D	-10.80	102.53	128.52
22	B	1781	BCR	C7-C8-C9	-10.78	109.94	126.23
20	B	1751	CLA	OBD-CAD-C3D	-10.73	102.69	128.52
20	L	1168	CLA	OBD-CAD-C3D	-10.72	102.72	128.52
20	A	1816	CLA	OBD-CAD-C3D	-10.71	102.75	128.52
20	2	1223	CLA	OBD-CAD-C3D	-10.62	102.96	128.52
20	A	1800	CLA	OBD-CAD-C3D	-10.49	103.27	128.52
20	4	1201	CLA	OBD-CAD-C3D	-10.48	103.31	128.52
20	B	1741	CLA	CAB-C3B-C4B	-10.47	112.37	128.46
22	I	1032	BCR	C24-C23-C22	-10.45	110.45	126.23
20	A	1815	CLA	OBD-CAD-C3D	-10.30	103.72	128.52
20	1	1191	CLA	OBD-CAD-C3D	-10.29	103.76	128.52
20	B	1766	CLA	OBD-CAD-C3D	-10.26	103.82	128.52
20	1	1187	CLA	OBD-CAD-C3D	-10.24	103.89	128.52
20	A	1816	CLA	C1-C2-C3	-10.20	108.40	126.04
20	A	1786	CLA	OBD-CAD-C3D	-10.17	104.04	128.52
20	B	1753	CLA	OBD-CAD-C3D	-10.17	104.05	128.52
20	A	1783	CLA	OBD-CAD-C3D	-10.13	104.13	128.52
20	A	1779	CLA	OBD-CAD-C3D	-10.11	104.18	128.52
20	A	1813	CLA	OBD-CAD-C3D	-10.00	104.46	128.52
20	A	1775	CLA	OBD-CAD-C3D	-9.99	104.47	128.52
20	1	1191	CLA	CAB-C3B-C4B	-9.97	113.14	128.46
20	B	1785	CLA	OBD-CAD-C3D	-9.81	104.91	128.52
20	A	1776	CLA	OBD-CAD-C3D	-9.79	104.96	128.52
20	4	1198	CLA	OBD-CAD-C3D	-9.78	105.00	128.52
20	B	1763	CLA	OBD-CAD-C3D	-9.69	105.19	128.52
20	A	1785	CLA	OBD-CAD-C3D	-9.68	105.23	128.52
20	B	1764	CLA	OBD-CAD-C3D	-9.64	105.32	128.52
20	B	1765	CLA	OBD-CAD-C3D	-9.63	105.34	128.52
20	1	1189	CLA	OBD-CAD-C3D	-9.60	105.41	128.52
20	A	1788	CLA	OBD-CAD-C3D	-9.51	105.62	128.52
22	B	1779	BCR	C15-C14-C13	-9.51	113.74	127.31
20	1	1196	CLA	CAB-C3B-C2B	-9.51	106.06	124.69
20	4	1200	CLA	OBD-CAD-C3D	-9.51	105.64	128.52
22	B	1781	BCR	C23-C22-C21	9.50	133.51	118.94
20	A	1762	CLA	OBD-CAD-C3D	-9.47	105.73	128.52
20	3	1212	CLA	CAB-C3B-C4B	-9.44	113.96	128.46
20	A	1766	CLA	OBD-CAD-C3D	-9.43	105.83	128.52
22	I	1032	BCR	C1-C6-C5	-9.41	109.35	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1773	CLA	OBD-CAD-C3D	-9.37	105.97	128.52
20	L	1168	CLA	O2D-CGD-CBD	9.36	127.90	111.27
20	A	1772	CLA	OBD-CAD-C3D	-9.33	106.06	128.52
20	I	1033	CLA	OBD-CAD-C3D	-9.30	106.14	128.52
20	2	1220	CLA	OBD-CAD-C3D	-9.27	106.22	128.52
20	A	1761	CLA	OBD-CAD-C3D	-9.25	106.26	128.52
20	B	1762	CLA	CAA-C2A-C3A	-9.17	87.67	112.78
20	4	1198	CLA	CGD-CBD-CAD	9.13	140.30	110.73
20	B	1742	CLA	OBD-CAD-C3D	-9.10	106.63	128.52
22	3	1220	BCR	C16-C17-C18	-9.08	114.35	127.31
20	3	3008	CLA	OBD-CAD-C3D	-9.03	106.78	128.52
20	A	1777	CLA	OBD-CAD-C3D	-9.01	106.83	128.52
20	A	1817	CLA	CAB-C3B-C2B	-9.01	107.05	124.69
20	2	1222	CLA	OBD-CAD-C3D	-9.00	106.85	128.52
20	A	1759	CLA	OBD-CAD-C3D	-8.98	106.91	128.52
20	B	1749	CLA	OBD-CAD-C3D	-8.96	106.96	128.52
20	R	1054	CLA	OBD-CAD-C3D	-8.94	107.01	128.52
20	A	1759	CLA	O2D-CGD-CBD	8.92	127.12	111.27
20	A	1817	CLA	C4D-C3D-CAD	8.83	118.51	108.10
20	1	1198	CLA	OBD-CAD-C3D	-8.83	107.27	128.52
20	L	1167	CLA	OBD-CAD-C3D	-8.80	107.34	128.52
20	4	1207	CLA	OBD-CAD-C3D	-8.75	107.47	128.52
20	K	1146	CLA	OBD-CAD-C3D	-8.70	107.59	128.52
20	1	1195	CLA	OBD-CAD-C3D	-8.65	107.71	128.52
21	A	7017	LMU	C1B-O1B-C4'	-8.61	96.66	117.96
20	4	4014	CLA	OBD-CAD-C3D	-8.56	107.93	128.52
20	3	1219	CLA	OBD-CAD-C3D	-8.55	107.95	128.52
20	B	1762	CLA	OBD-CAD-C3D	-8.55	107.95	128.52
20	2	1212	CLA	OBD-CAD-C3D	-8.55	107.95	128.52
20	J	1043	CLA	OBD-CAD-C3D	-8.54	107.96	128.52
20	A	1793	CLA	OBD-CAD-C3D	-8.54	107.96	128.52
20	A	1792	CLA	OBD-CAD-C3D	-8.54	107.96	128.52
20	B	1755	CLA	OBD-CAD-C3D	-8.54	107.98	128.52
20	A	1797	CLA	OBD-CAD-C3D	-8.54	107.98	128.52
20	B	1756	CLA	OBD-CAD-C3D	-8.53	107.99	128.52
20	K	1142	CLA	OBD-CAD-C3D	-8.53	107.99	128.52
20	A	1794	CLA	OBD-CAD-C3D	-8.53	107.99	128.52
20	A	1791	CLA	OBD-CAD-C3D	-8.53	108.00	128.52
20	A	1796	CLA	OBD-CAD-C3D	-8.52	108.02	128.52
20	A	1781	CLA	OBD-CAD-C3D	-8.52	108.03	128.52
20	B	1735	CLA	OBD-CAD-C3D	-8.52	108.03	128.52
20	4	1196	CLA	OBD-CAD-C3D	-8.51	108.03	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1782	CLA	OBD-CAD-C3D	-8.51	108.04	128.52
20	A	1795	CLA	OBD-CAD-C3D	-8.51	108.04	128.52
20	K	1085	CLA	OBD-CAD-C3D	-8.50	108.07	128.52
21	A	7030	LMU	C3B-C4B-C5B	-8.49	95.09	110.24
20	F	1156	CLA	OBD-CAD-C3D	-8.49	108.08	128.52
20	3	1212	CLA	OBD-CAD-C3D	-8.46	108.15	128.52
20	4	1197	CLA	OBD-CAD-C3D	-8.44	108.21	128.52
20	B	1748	CLA	OBD-CAD-C3D	-8.42	108.27	128.52
21	A	7033	LMU	C1B-O1B-C4'	-8.40	97.17	117.96
20	B	1737	CLA	OBD-CAD-C3D	-8.39	108.34	128.52
20	B	1786	CLA	OBD-CAD-C3D	-8.35	108.42	128.52
20	F	1157	CLA	OBD-CAD-C3D	-8.31	108.53	128.52
20	4	1198	CLA	CMD-C2D-C1D	8.28	139.31	124.71
20	B	1750	CLA	OBD-CAD-C3D	-8.28	108.60	128.52
20	1	1193	CLA	C3A-C2A-C1A	8.26	113.71	101.34
20	B	1772	CLA	CAB-C3B-C2B	-8.24	108.55	124.69
20	4	4007	CLA	OBD-CAD-C3D	-8.24	108.70	128.52
20	3	1213	CLA	C4A-NA-C1A	8.23	110.41	106.71
21	A	7032	LMU	C1B-C2B-C3B	-8.22	92.88	110.00
20	4	1198	CLA	C4D-CHA-C1A	8.21	131.24	121.25
20	A	1816	CLA	CMD-C2D-C1D	8.20	139.16	124.71
20	B	1761	CLA	OBD-CAD-C3D	-8.14	108.92	128.52
22	B	1779	BCR	C30-C25-C26	-8.14	111.15	122.61
20	L	1505	CLA	OBD-CAD-C3D	-8.14	108.94	128.52
20	A	1771	CLA	OBD-CAD-C3D	-8.08	109.06	128.52
20	B	1745	CLA	OBD-CAD-C3D	-8.08	109.08	128.52
20	B	1767	CLA	CMD-C2D-C1D	8.08	138.95	124.71
20	A	1816	CLA	C1D-CHD-C4C	-8.06	108.66	126.06
20	1	1195	CLA	CMD-C2D-C1D	8.05	138.90	124.71
22	B	1781	BCR	C3-C4-C5	-8.04	99.73	114.08
20	B	1738	CLA	OBD-CAD-C3D	-8.02	109.22	128.52
20	3	3007	CLA	OBD-CAD-C3D	-8.02	109.22	128.52
20	A	1812	CLA	OBD-CAD-C3D	-8.00	109.27	128.52
20	A	1817	CLA	CMD-C2D-C1D	7.97	138.76	124.71
20	J	1044	CLA	OBD-CAD-C3D	-7.97	109.35	128.52
20	J	1045	CLA	OBD-CAD-C3D	-7.97	109.35	128.52
20	B	1739	CLA	O2D-CGD-CBD	7.94	125.38	111.27
20	A	1767	CLA	CMD-C2D-C1D	7.92	138.67	124.71
20	B	1770	CLA	CMD-C2D-C1D	7.92	138.67	124.71
20	B	1758	CLA	O2D-CGD-CBD	7.88	125.27	111.27
20	B	1752	CLA	OBD-CAD-C3D	-7.85	109.63	128.52
22	I	1032	BCR	C16-C15-C14	-7.84	107.42	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	1201	CLA	CHD-C4C-NC	7.79	136.48	124.20
20	A	1790	CLA	OBD-CAD-C3D	-7.79	109.77	128.52
20	2	1218	CLA	OBD-CAD-C3D	-7.78	109.81	128.52
21	A	7037	LMU	C1B-O5B-C5B	-7.77	98.43	113.69
20	A	1784	CLA	O2D-CGD-CBD	7.77	125.07	111.27
20	L	1505	CLA	CMD-C2D-C1D	7.76	138.39	124.71
20	1	1189	CLA	CMD-C2D-C1D	7.74	138.35	124.71
21	A	7037	LMU	C4B-C3B-C2B	-7.72	97.34	110.82
20	1	1201	CLA	C2B-C1B-NB	7.71	116.86	110.11
20	1	1200	CLA	C1D-CHD-C4C	-7.69	109.46	126.06
20	3	3008	CLA	CMD-C2D-C1D	7.66	138.21	124.71
20	A	1763	CLA	OBD-CAD-C3D	-7.64	110.13	128.52
20	2	1213	CLA	CMD-C2D-C1D	7.64	138.17	124.71
20	A	1786	CLA	O2D-CGD-CBD	7.64	124.84	111.27
20	R	1055	CLA	CMD-C2D-C1D	7.64	138.17	124.71
20	A	1775	CLA	CAB-C3B-C2B	-7.62	109.75	124.69
20	B	1759	CLA	O2D-CGD-CBD	7.62	124.80	111.27
21	A	7026	LMU	C3B-C4B-C5B	-7.58	96.72	110.24
20	4	1209	CLA	O2D-CGD-CBD	7.57	124.71	111.27
22	L	1170	BCR	C15-C14-C13	-7.54	116.54	127.31
20	R	1054	CLA	CMD-C2D-C1D	7.52	137.96	124.71
20	A	1789	CLA	CMD-C2D-C1D	7.51	137.95	124.71
20	B	1759	CLA	CMD-C2D-C1D	7.50	137.94	124.71
20	A	1799	CLA	CMD-C2D-C1D	7.50	137.93	124.71
20	1	1193	CLA	CMD-C2D-C1D	7.46	137.87	124.71
20	A	1798	CLA	OBD-CAD-C3D	-7.46	110.56	128.52
20	A	1768	CLA	OBD-CAD-C3D	-7.46	110.58	128.52
20	B	1746	CLA	OBD-CAD-C3D	-7.45	110.58	128.52
20	2	1218	CLA	O2D-CGD-CBD	7.45	124.50	111.27
22	I	1032	BCR	C34-C9-C10	-7.45	112.49	122.92
20	F	1155	CLA	C1B-C2B-C3B	-7.44	100.00	106.92
20	B	1736	CLA	O2D-CGD-CBD	7.42	124.46	111.27
20	A	1784	CLA	OBD-CAD-C3D	-7.41	110.69	128.52
20	L	1167	CLA	CAA-C2A-C3A	-7.39	92.53	112.78
20	B	1759	CLA	OBD-CAD-C3D	-7.38	110.77	128.52
20	B	1769	CLA	OBD-CAD-C3D	-7.38	110.77	128.52
20	G	1099	CLA	OBD-CAD-C3D	-7.36	110.82	128.52
21	A	7039	LMU	C1B-O5B-C5B	-7.35	99.26	113.69
20	A	1789	CLA	OBD-CAD-C3D	-7.35	110.83	128.52
20	3	1218	CLA	CHD-C4C-C3C	-7.32	114.08	124.84
20	B	1744	CLA	CMD-C2D-C1D	7.32	137.61	124.71
20	L	1166	CLA	OBD-CAD-C3D	-7.32	110.91	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	1215	CLA	OBD-CAD-C3D	-7.31	110.92	128.52
20	B	1749	CLA	O2D-CGD-CBD	7.31	124.26	111.27
20	B	1758	CLA	OBD-CAD-C3D	-7.31	110.93	128.52
21	A	7040	LMU	O5B-C5B-C4B	-7.30	96.43	109.69
20	B	1768	CLA	O2D-CGD-CBD	7.29	124.23	111.27
22	L	1170	BCR	C3-C4-C5	-7.29	101.06	114.08
20	4	1198	CLA	C1D-CHD-C4C	-7.27	110.36	126.06
20	B	1760	CLA	OBD-CAD-C3D	-7.27	111.03	128.52
20	1	1197	CLA	CHD-C4C-NC	7.27	135.65	124.20
20	A	1778	CLA	OBD-CAD-C3D	-7.26	111.05	128.52
20	4	1199	CLA	OBD-CAD-C3D	-7.26	111.05	128.52
20	1	1187	CLA	CMD-C2D-C1D	7.24	137.47	124.71
20	4	1197	CLA	C1D-CHD-C4C	-7.22	110.49	126.06
20	B	1787	CLA	OBD-CAD-C3D	-7.21	111.16	128.52
20	4	1201	CLA	C1D-CHD-C4C	-7.20	110.53	126.06
20	A	1799	CLA	OBD-CAD-C3D	-7.19	111.22	128.52
20	A	1790	CLA	CMD-C2D-C1D	7.18	137.37	124.71
20	3	1217	CLA	C2B-C1B-NB	7.17	116.39	110.11
20	3	1218	CLA	CHD-C4C-NC	7.17	135.50	124.20
20	4	1203	CLA	CHA-C4D-ND	7.13	131.40	124.52
20	B	1750	CLA	CMD-C2D-C1D	7.09	137.21	124.71
20	2	1213	CLA	OBD-CAD-C3D	-7.08	111.48	128.52
20	F	1155	CLA	CMD-C2D-C1D	7.08	137.19	124.71
20	1	1197	CLA	CHD-C4C-C3C	-7.07	114.45	124.84
20	1	1190	CLA	O2D-CGD-CBD	7.06	123.81	111.27
20	4	1206	CLA	CHA-C4D-ND	7.06	131.33	124.52
20	A	1777	CLA	CMD-C2D-C1D	7.05	137.15	124.71
20	1	1189	CLA	C4D-C3D-CAD	7.03	116.38	108.10
20	4	1199	CLA	O2D-CGD-CBD	7.03	123.76	111.27
20	1	1197	CLA	C4D-C3D-CAD	7.02	116.37	108.10
20	1	1193	CLA	O2D-CGD-CBD	7.01	123.72	111.27
20	B	1772	CLA	OBD-CAD-C3D	-7.01	111.65	128.52
21	A	7036	LMU	C2'-C3'-C4'	-7.00	93.70	109.68
20	4	1198	CLA	CHD-C4C-NC	7.00	135.23	124.20
20	1	1187	CLA	C4D-C3D-CAD	6.99	116.33	108.10
20	B	1767	CLA	O2D-CGD-CBD	6.98	123.67	111.27
20	B	1766	CLA	CMD-C2D-C1D	6.98	137.01	124.71
20	B	1741	CLA	CMD-C2D-C1D	6.98	137.01	124.71
21	A	7026	LMU	C1B-C2B-C3B	-6.98	95.47	110.00
20	B	1758	CLA	C4A-NA-C1A	6.98	109.84	106.71
20	3	1218	CLA	O2D-CGD-CBD	6.97	123.66	111.27
20	B	1737	CLA	CAA-C2A-C3A	-6.97	93.69	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	7038	LMU	C3'-C4'-C5'	-6.97	94.96	110.93
20	A	1811	CLA	OBD-CAD-C3D	-6.97	111.76	128.52
20	B	1751	CLA	CMD-C2D-C1D	6.96	136.98	124.71
20	1	1190	CLA	CMD-C2D-C1D	6.96	136.97	124.71
20	1	1193	CLA	OBD-CAD-C3D	-6.96	111.78	128.52
20	B	1741	CLA	CAB-C3B-C2B	-6.93	111.11	124.69
20	A	1765	CLA	OBD-CAD-C3D	-6.92	111.86	128.52
20	A	1817	CLA	O2D-CGD-CBD	6.88	123.50	111.27
20	1	1197	CLA	O2A-CGA-O1A	-6.88	106.22	123.59
22	3	1220	BCR	C11-C10-C9	-6.88	117.50	127.31
20	4	1204	CLA	OBD-CAD-C3D	-6.87	111.98	128.52
21	A	7037	LMU	O2'-C2'-C1'	-6.87	93.37	110.05
20	B	1736	CLA	CMD-C2D-C1D	6.86	136.81	124.71
20	1	1197	CLA	C4A-NA-C1A	6.86	109.79	106.71
20	B	1754	CLA	O2D-CGD-CBD	6.86	123.46	111.27
20	L	1166	CLA	O2D-CGD-CBD	6.86	123.45	111.27
20	3	1218	CLA	C1D-CHD-C4C	-6.85	111.28	126.06
22	L	1170	BCR	C8-C9-C10	6.85	129.45	118.94
20	1	1197	CLA	C1D-CHD-C4C	-6.84	111.29	126.06
20	A	1785	CLA	O2D-CGD-CBD	6.84	123.42	111.27
20	I	1033	CLA	O2D-CGD-CBD	6.84	123.42	111.27
20	4	1201	CLA	CMB-C2B-C1B	-6.83	117.96	128.46
20	2	1227	CLA	C2B-C1B-NB	6.83	116.09	110.11
20	3	3011	CLA	OBD-CAD-C3D	-6.82	112.10	128.52
21	K	1086	LMU	C3B-C4B-C5B	-6.82	98.07	110.24
20	B	1759	CLA	C4D-C3D-CAD	6.82	116.13	108.10
20	3	3014	CLA	C2B-C1B-NB	6.81	116.08	110.11
20	K	1146	CLA	O2D-CGD-CBD	6.81	123.37	111.27
20	B	1737	CLA	CMD-C2D-C1D	6.80	136.70	124.71
21	A	7032	LMU	C1B-O5B-C5B	6.80	127.03	113.69
20	4	1197	CLA	CAB-C3B-C2B	-6.79	111.39	124.69
20	A	1766	CLA	CMD-C2D-C1D	6.76	136.63	124.71
20	A	1789	CLA	O2D-CGD-CBD	6.76	123.27	111.27
20	A	1778	CLA	O2D-CGD-CBD	6.75	123.26	111.27
21	R	1057	LMU	C4B-C3B-C2B	-6.74	99.05	110.82
20	B	1757	CLA	O2D-CGD-CBD	6.74	123.25	111.27
20	B	1736	CLA	OBD-CAD-C3D	-6.74	112.30	128.52
20	1	1192	CLA	OBD-CAD-C3D	-6.74	112.31	128.52
20	1	1195	CLA	C4D-C3D-CAD	6.72	116.02	108.10
20	4	1208	CLA	CHA-C4D-ND	6.71	131.00	124.52
20	A	1764	CLA	CMD-C2D-C1D	6.71	136.54	124.71
20	J	1045	CLA	CMD-C2D-C1D	6.71	136.53	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1768	CLA	CMD-C2D-C1D	6.70	136.52	124.71
20	A	1813	CLA	CMD-C2D-C1D	6.69	136.50	124.71
20	J	1044	CLA	C1D-CHD-C4C	-6.68	111.64	126.06
20	1	1188	CLA	CMD-C2D-C1D	6.68	136.49	124.71
21	A	7026	LMU	C3'-C4'-C5'	-6.68	95.61	110.93
20	A	1765	CLA	CMD-C2D-C1D	6.68	136.48	124.71
20	A	1787	CLA	OBD-CAD-C3D	-6.67	112.46	128.52
20	2	1222	CLA	CMD-C2D-C1D	6.67	136.47	124.71
20	B	1769	CLA	O2D-CGD-CBD	6.67	123.12	111.27
21	R	1057	LMU	O2B-C2B-C3B	6.66	125.75	110.35
22	L	1170	BCR	C4-C5-C6	-6.64	113.09	122.73
20	A	1773	CLA	CMD-C2D-C1D	6.64	136.41	124.71
20	B	1750	CLA	C4D-C3D-CAD	6.63	115.91	108.10
20	4	1198	CLA	CHC-C1C-NC	6.63	134.27	124.20
20	B	1787	CLA	CMD-C2D-C1D	6.63	136.39	124.71
20	R	1054	CLA	C4D-C3D-CAD	6.63	115.91	108.10
20	A	1783	CLA	CMD-C2D-C1D	6.62	136.39	124.71
20	J	1044	CLA	O2D-CGD-CBD	6.60	122.99	111.27
20	L	1168	CLA	C1D-CHD-C4C	-6.59	111.84	126.06
20	A	1816	CLA	O2D-CGD-CBD	6.59	122.97	111.27
20	L	1167	CLA	CMD-C2D-C1D	6.58	136.30	124.71
20	1	1198	CLA	C1D-CHD-C4C	-6.56	111.90	126.06
20	3	3007	CLA	CMD-C2D-C1D	6.56	136.28	124.71
20	2	1221	CLA	C2B-C1B-NB	6.55	115.85	110.11
21	R	1057	LMU	O1B-C1B-C2B	6.54	125.04	108.10
20	B	1738	CLA	O2D-CGD-CBD	6.53	122.88	111.27
20	4	1201	CLA	CHC-C1C-NC	6.52	134.10	124.20
20	A	1775	CLA	CMD-C2D-C1D	6.52	136.21	124.71
20	K	1146	CLA	CMD-C2D-C1D	6.52	136.21	124.71
20	B	1752	CLA	CMD-C2D-C1D	6.52	136.21	124.71
20	B	1770	CLA	OBD-CAD-C3D	-6.51	112.84	128.52
20	A	1778	CLA	CMD-C2D-C1D	6.51	136.18	124.71
22	B	1779	BCR	C3-C4-C5	-6.49	102.49	114.08
20	2	1220	CLA	CMD-C2D-C1D	6.49	136.15	124.71
20	A	1769	CLA	OBD-CAD-C3D	-6.47	112.94	128.52
20	B	1771	CLA	OBD-CAD-C3D	-6.47	112.94	128.52
20	B	1757	CLA	CMD-C2D-C1D	6.47	136.12	124.71
20	B	1739	CLA	O1D-CGD-CBD	-6.45	111.28	124.48
20	B	1743	CLA	OBD-CAD-C3D	-6.45	112.99	128.52
20	B	1741	CLA	O2D-CGD-CBD	6.45	122.73	111.27
20	4	1196	CLA	CMD-C2D-C1D	6.45	136.08	124.71
20	A	1780	CLA	OBD-CAD-C3D	-6.44	113.01	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1746	CLA	CMD-C2D-C1D	6.44	136.07	124.71
20	A	1792	CLA	CMD-C2D-C1D	6.43	136.05	124.71
20	A	1801	CLA	O2D-CGD-CBD	6.43	122.69	111.27
20	J	1045	CLA	C1D-CHD-C4C	-6.43	112.19	126.06
20	B	1786	CLA	C4-C3-C5	6.43	126.08	115.27
20	4	1209	CLA	C1D-CHD-C4C	-6.42	112.21	126.06
20	3	1219	CLA	CMD-C2D-C1D	6.42	136.03	124.71
20	A	1796	CLA	CMD-C2D-C1D	6.42	136.02	124.71
20	F	1156	CLA	CMD-C2D-C1D	6.41	136.01	124.71
20	A	1782	CLA	CMD-C2D-C1D	6.41	136.01	124.71
20	B	1764	CLA	C4D-C3D-CAD	6.41	115.65	108.10
20	J	1043	CLA	CMD-C2D-C1D	6.41	136.01	124.71
20	K	1085	CLA	CMD-C2D-C1D	6.41	136.01	124.71
20	B	1735	CLA	CMD-C2D-C1D	6.41	136.01	124.71
20	1	1200	CLA	O2D-CGD-CBD	6.41	122.65	111.27
20	B	1751	CLA	C1D-CHD-C4C	-6.41	112.24	126.06
20	A	1766	CLA	O2D-CGD-CBD	6.41	122.65	111.27
20	K	1142	CLA	CMD-C2D-C1D	6.41	136.00	124.71
20	A	1797	CLA	CMD-C2D-C1D	6.40	136.00	124.71
20	A	1791	CLA	CMD-C2D-C1D	6.40	136.00	124.71
20	B	1755	CLA	CMD-C2D-C1D	6.40	136.00	124.71
20	A	1795	CLA	CMD-C2D-C1D	6.40	135.99	124.71
20	A	1794	CLA	CMD-C2D-C1D	6.39	135.98	124.71
20	2	1212	CLA	CMD-C2D-C1D	6.39	135.98	124.71
20	A	1760	CLA	CMD-C2D-C1D	6.39	135.97	124.71
20	A	1793	CLA	CMD-C2D-C1D	6.39	135.97	124.71
20	B	1756	CLA	CMD-C2D-C1D	6.38	135.95	124.71
20	4	4014	CLA	CMD-C2D-C1D	6.38	135.95	124.71
20	1	1193	CLA	C4D-C3D-CAD	6.38	115.61	108.10
20	A	1774	CLA	OBD-CAD-C3D	-6.37	113.18	128.52
20	B	1762	CLA	CMD-C2D-C1D	6.37	135.94	124.71
20	A	1781	CLA	CMD-C2D-C1D	6.37	135.94	124.71
20	B	1768	CLA	OBD-CAD-C3D	-6.37	113.20	128.52
20	J	1044	CLA	CAA-C2A-C3A	-6.36	95.37	112.78
20	B	1751	CLA	CHD-C4C-NC	6.35	134.21	124.20
20	A	1811	CLA	C4D-C3D-CAD	6.35	115.58	108.10
20	F	1157	CLA	C1-C2-C3	-6.35	115.06	126.04
20	4	1198	CLA	CAA-C2A-C3A	-6.34	95.41	112.78
20	B	1751	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
20	B	1742	CLA	CMD-C2D-C1D	6.34	135.88	124.71
20	B	1753	CLA	CHD-C4C-C3C	-6.34	115.53	124.84
20	A	1787	CLA	CMD-C2D-C1D	6.33	135.87	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1763	CLA	O2D-CGD-CBD	6.32	122.51	111.27
20	B	1765	CLA	CMD-C2D-C1D	6.31	135.84	124.71
20	3	1213	CLA	C2B-C1B-NB	6.31	115.64	110.11
20	1	1189	CLA	O2D-CGD-CBD	6.31	122.48	111.27
20	B	1743	CLA	C1D-CHD-C4C	-6.30	112.46	126.06
20	A	1801	CLA	OBD-CAD-C3D	-6.30	113.36	128.52
20	A	1817	CLA	CAA-C2A-C3A	6.29	130.01	112.78
20	A	1778	CLA	C4D-C3D-CAD	6.29	115.51	108.10
20	4	1199	CLA	CMD-C2D-C1D	6.29	135.80	124.71
20	3	1212	CLA	CMD-C2D-C1D	6.29	135.79	124.71
20	2	1215	CLA	CMD-C2D-C1D	6.28	135.79	124.71
20	4	1204	CLA	CMD-C2D-C1D	6.28	135.78	124.71
20	A	1801	CLA	CMD-C2D-C1D	6.27	135.77	124.71
20	A	1763	CLA	O2D-CGD-CBD	6.27	122.41	111.27
22	B	1779	BCR	C24-C23-C22	-6.27	116.77	126.23
20	I	1031	CLA	C1D-CHD-C4C	-6.25	112.57	126.06
22	I	1032	BCR	C8-C9-C10	6.25	128.53	118.94
20	A	1770	CLA	OBD-CAD-C3D	-6.25	113.48	128.52
20	A	1762	CLA	CMD-C2D-C1D	6.24	135.72	124.71
20	A	1779	CLA	C4D-C3D-CAD	6.24	115.45	108.10
20	K	3009	CLA	OBD-CAD-C3D	-6.24	113.50	128.52
20	A	1759	CLA	CMD-C2D-C1D	6.23	135.69	124.71
20	1	1197	CLA	CMD-C2D-C3D	-6.23	113.29	127.61
20	H	1079	CLA	CMD-C2D-C1D	6.23	135.69	124.71
20	1	1191	CLA	CMD-C2D-C1D	6.23	135.68	124.71
20	B	1761	CLA	O2D-CGD-CBD	6.22	122.32	111.27
20	1	1194	CLA	C2B-C1B-NB	6.22	115.55	110.11
20	G	1099	CLA	CMD-C2D-C1D	6.21	135.66	124.71
20	4	1201	CLA	CMD-C2D-C1D	6.21	135.66	124.71
20	1	1198	CLA	O2D-CGD-CBD	6.21	122.30	111.27
20	3	1218	CLA	O1D-CGD-CBD	-6.21	111.79	124.48
20	3	3002	CLA	CHA-C4D-ND	6.20	130.50	124.52
20	1	1195	CLA	C1D-CHD-C4C	-6.20	112.69	126.06
20	1	1199	CLA	C2B-C1B-NB	6.19	115.53	110.11
20	4	1202	CLA	C2B-C1B-NB	6.19	115.53	110.11
20	A	1811	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
20	4	1204	CLA	C4D-C3D-CAD	6.18	115.38	108.10
20	B	1740	CLA	C1D-CHD-C4C	-6.17	112.74	126.06
20	A	1780	CLA	CMD-C2D-C1D	6.17	135.59	124.71
20	1	1201	CLA	C4A-NA-C1A	6.16	109.48	106.71
20	2	1223	CLA	C4A-NA-C1A	6.16	109.47	106.71
20	A	1798	CLA	O2D-CGD-CBD	6.16	122.21	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	1212	CLA	CAB-C3B-C2B	-6.15	112.63	124.69
20	B	1759	CLA	C1D-CHD-C4C	-6.15	112.78	126.06
20	4	1204	CLA	C1D-CHD-C4C	-6.15	112.79	126.06
20	2	1222	CLA	C4D-C3D-CAD	6.14	115.33	108.10
20	4	1205	CLA	C2B-C1B-NB	6.13	115.48	110.11
20	I	1031	CLA	O2D-CGD-CBD	6.13	122.16	111.27
20	B	1786	CLA	O2D-CGD-CBD	6.12	122.14	111.27
20	4	1207	CLA	CAB-C3B-C2B	-6.10	112.73	124.69
20	1	1196	CLA	CMD-C2D-C1D	6.10	135.47	124.71
20	B	1764	CLA	C1D-CHD-C4C	-6.10	112.91	126.06
20	3	3008	CLA	C4D-C3D-CAD	6.09	115.27	108.10
20	3	1213	CLA	CHC-C1C-NC	6.09	133.22	124.23
20	1	1192	CLA	C1D-CHD-C4C	-6.08	112.95	126.06
20	4	1201	CLA	CAA-C2A-C1A	6.08	131.89	111.97
20	2	1217	CLA	C1D-CHD-C4C	-6.07	112.96	126.06
20	A	1767	CLA	C1D-CHD-C4C	-6.07	112.96	126.06
20	B	1763	CLA	C4D-C3D-CAD	6.07	115.25	108.10
22	I	1032	BCR	C38-C26-C27	6.06	125.26	113.62
20	B	1770	CLA	O2D-CGD-CBD	6.06	122.04	111.27
20	B	1767	CLA	C4D-C3D-CAD	6.06	115.23	108.10
20	2	1217	CLA	CMD-C2D-C1D	6.05	135.38	124.71
21	A	7026	LMU	C1'-C2'-C3'	-6.05	97.40	110.00
20	4	1202	CLA	C3A-C4A-CHB	-6.05	116.51	123.91
21	A	7039	LMU	O5B-C5B-C6B	-6.04	91.41	106.44
20	1	1199	CLA	C3A-C4A-CHB	-6.04	116.52	123.91
22	I	1032	BCR	C11-C10-C9	-6.03	118.70	127.31
20	A	1779	CLA	CMD-C2D-C1D	6.03	135.34	124.71
20	B	1743	CLA	CHD-C4C-NC	6.03	133.71	124.20
20	A	1776	CLA	CMD-C2D-C1D	6.02	135.33	124.71
20	B	1758	CLA	C4D-C3D-CAD	6.02	115.19	108.10
20	1	1191	CLA	C4D-C3D-CAD	6.02	115.19	108.10
20	2	1223	CLA	C1D-CHD-C4C	-6.01	113.09	126.06
20	B	1736	CLA	C4D-C3D-CAD	6.01	115.18	108.10
20	2	1220	CLA	C1D-CHD-C4C	-6.01	113.10	126.06
20	4	1204	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
20	A	1812	CLA	C1D-CHD-C4C	-6.00	113.12	126.06
20	A	1816	CLA	C4-C3-C5	6.00	125.36	115.27
20	4	4003	CLA	CHA-C4D-ND	6.00	130.31	124.52
20	4	1206	CLA	C2B-C1B-NB	5.99	115.36	110.11
20	B	1763	CLA	CMD-C2D-C1D	5.99	135.27	124.71
20	1	1193	CLA	CBA-CAA-C2A	-5.99	96.19	113.86
20	1	1187	CLA	C1D-CHD-C4C	-5.99	113.14	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1770	CLA	CMD-C2D-C1D	5.99	135.26	124.71
20	A	1772	CLA	CMD-C2D-C1D	5.98	135.26	124.71
20	A	1787	CLA	O2D-CGD-CBD	5.98	121.90	111.27
20	4	1207	CLA	C4D-C3D-CAD	5.98	115.14	108.10
20	1	1195	CLA	CHD-C4C-NC	5.97	133.62	124.20
20	4	1209	CLA	OBD-CAD-C3D	-5.97	114.14	128.52
20	2	1214	CLA	C2B-C1B-NB	5.97	115.34	110.11
20	B	1743	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
20	F	1157	CLA	C1D-CHD-C4C	-5.97	113.18	126.06
20	A	1772	CLA	C1D-CHD-C4C	-5.97	113.18	126.06
20	J	1045	CLA	CHD-C4C-NC	5.97	133.60	124.20
20	A	1768	CLA	CMD-C2D-C1D	5.97	135.23	124.71
20	L	1167	CLA	O2D-CGD-CBD	5.96	121.86	111.27
20	4	1204	CLA	CHD-C4C-NC	5.96	133.59	124.20
20	B	1771	CLA	C4D-C3D-CAD	5.96	115.12	108.10
20	A	1765	CLA	CHC-C1C-NC	5.95	133.23	124.20
20	B	1763	CLA	C1D-CHD-C4C	-5.95	113.23	126.06
20	B	1754	CLA	C1D-CHD-C4C	-5.94	113.25	126.06
20	A	1773	CLA	C4D-C3D-CAD	5.93	115.08	108.10
20	4	4007	CLA	CMD-C2D-C1D	5.93	135.16	124.71
22	L	1170	BCR	C34-C9-C10	-5.93	114.62	122.92
20	B	1738	CLA	C4A-NA-C1A	5.92	109.37	106.71
22	I	1032	BCR	C38-C26-C25	-5.92	117.88	124.53
20	3	1216	CLA	C2B-C1B-NB	5.92	115.29	110.11
20	B	1764	CLA	CMD-C2D-C1D	5.91	135.13	124.71
20	B	1762	CLA	O2D-CGD-CBD	5.90	121.76	111.27
20	2	1213	CLA	O2D-CGD-CBD	5.90	121.76	111.27
20	2	1220	CLA	C4D-C3D-CAD	5.90	115.05	108.10
20	1	1200	CLA	CHD-C4C-NC	5.90	133.50	124.20
20	3	3014	CLA	C3A-C4A-CHB	-5.89	116.70	123.91
20	3	1217	CLA	C4A-NA-C1A	5.89	109.35	106.71
20	A	1788	CLA	CMD-C2D-C1D	5.89	135.09	124.71
20	4	1197	CLA	C4D-C3D-CAD	5.89	115.03	108.10
20	A	1767	CLA	C4D-C3D-CAD	5.88	115.03	108.10
20	A	1813	CLA	O2D-CGD-CBD	5.88	121.72	111.27
20	J	1046	CLA	CHA-C4D-ND	5.88	130.20	124.52
22	L	1169	BCR	C27-C26-C25	-5.88	114.19	122.73
20	4	1200	CLA	CMD-C2D-C1D	5.88	135.07	124.71
20	A	1816	CLA	C4D-C3D-CAD	5.87	115.02	108.10
20	1	1200	CLA	C4-C3-C5	5.87	122.70	115.98
20	3	3001	CLA	C2B-C1B-NB	5.87	115.25	110.11
20	B	1738	CLA	C1D-CHD-C4C	-5.87	113.39	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	3011	CLA	CMD-C2D-C1D	5.87	135.05	124.71
20	J	1044	CLA	C4D-C3D-CAD	5.86	115.01	108.10
20	B	1737	CLA	O2D-CGD-CBD	5.86	121.69	111.27
20	A	1775	CLA	C1D-CHD-C4C	-5.86	113.41	126.06
20	B	1769	CLA	C1D-CHD-C4C	-5.86	113.41	126.06
20	B	1761	CLA	CHD-C4C-NC	5.86	133.44	124.20
20	4	1199	CLA	C4D-C3D-CAD	5.86	115.00	108.10
20	B	1767	CLA	O2D-CGD-O1D	-5.86	112.39	123.84
20	L	1505	CLA	C4D-C3D-CAD	5.86	115.00	108.10
20	1	1198	CLA	CMD-C2D-C1D	5.85	135.03	124.71
20	B	1746	CLA	O2D-CGD-CBD	5.85	121.66	111.27
20	4	1197	CLA	CMD-C2D-C1D	5.84	135.00	124.71
20	1	1191	CLA	CAB-C3B-C2B	-5.84	113.26	124.69
21	A	7040	LMU	C1B-O1B-C4'	-5.83	103.52	117.96
20	A	1817	CLA	CMD-C2D-C3D	-5.83	114.19	127.61
20	3	1216	CLA	CHA-C4D-ND	5.83	130.15	124.52
20	B	1748	CLA	C1D-CHD-C4C	-5.82	113.49	126.06
20	3	1214	CLA	C3A-C4A-CHB	-5.82	116.78	123.91
20	A	1767	CLA	OBD-CAD-C3D	-5.82	114.51	128.52
20	K	1085	CLA	C1D-CHD-C4C	-5.82	113.50	126.06
20	K	1142	CLA	C1D-CHD-C4C	-5.82	113.50	126.06
20	B	1787	CLA	C4D-C3D-CAD	5.82	114.95	108.10
20	B	1737	CLA	C4D-C3D-CAD	5.82	114.95	108.10
20	4	1196	CLA	C1D-CHD-C4C	-5.81	113.53	126.06
21	A	7040	LMU	C3B-C4B-C5B	-5.80	99.88	110.24
20	2	1212	CLA	C1D-CHD-C4C	-5.80	113.54	126.06
20	3	1212	CLA	C1D-CHD-C4C	-5.80	113.54	126.06
20	A	1797	CLA	C1D-CHD-C4C	-5.80	113.55	126.06
20	3	1215	CLA	C3A-C4A-CHB	-5.80	116.81	123.91
20	3	3008	CLA	C1D-CHD-C4C	-5.80	113.55	126.06
20	4	4014	CLA	C1D-CHD-C4C	-5.80	113.55	126.06
20	B	1762	CLA	C4D-C3D-CAD	5.80	114.93	108.10
20	J	1043	CLA	C1D-CHD-C4C	-5.80	113.55	126.06
20	B	1735	CLA	C1D-CHD-C4C	-5.80	113.56	126.06
20	A	1791	CLA	C1D-CHD-C4C	-5.79	113.56	126.06
20	A	1788	CLA	C4D-C3D-CAD	5.79	114.92	108.10
20	A	1815	CLA	CMD-C2D-C1D	5.79	134.92	124.71
20	F	1156	CLA	C1D-CHD-C4C	-5.79	113.56	126.06
20	B	1755	CLA	C1D-CHD-C4C	-5.79	113.56	126.06
20	B	1753	CLA	CBC-CAC-C3C	-5.79	96.47	112.43
20	3	1219	CLA	C1D-CHD-C4C	-5.79	113.57	126.06
20	1	1201	CLA	C2A-C1A-CHA	-5.79	112.76	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1795	CLA	C1D-CHD-C4C	-5.79	113.58	126.06
20	A	1794	CLA	C1D-CHD-C4C	-5.78	113.58	126.06
20	B	1751	CLA	C4D-C3D-CAD	5.78	114.91	108.10
20	3	1218	CLA	CMD-C2D-C1D	5.78	134.91	124.71
20	1	1197	CLA	CGD-CBD-CAD	-5.78	92.03	110.73
20	B	1756	CLA	C1D-CHD-C4C	-5.78	113.60	126.06
20	B	1752	CLA	C4D-C3D-CAD	5.77	114.90	108.10
20	A	1792	CLA	C1D-CHD-C4C	-5.77	113.60	126.06
20	4	1205	CLA	CHA-C4D-ND	5.77	130.09	124.52
20	A	1793	CLA	C1D-CHD-C4C	-5.77	113.60	126.06
20	B	1761	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
20	A	1782	CLA	C1D-CHD-C4C	-5.77	113.61	126.06
20	A	1781	CLA	C1D-CHD-C4C	-5.77	113.61	126.06
20	A	1796	CLA	C1D-CHD-C4C	-5.76	113.62	126.06
20	2	1224	CLA	O2D-CGD-CBD	5.76	121.50	111.27
20	3	3015	CLA	CHA-C4D-ND	5.76	130.08	124.52
20	4	1209	CLA	O1D-CGD-CBD	-5.76	112.70	124.48
20	B	1765	CLA	C4D-C3D-CAD	5.76	114.88	108.10
20	A	1798	CLA	CMD-C2D-C1D	5.75	134.85	124.71
20	B	1758	CLA	C1D-CHD-C4C	-5.75	113.66	126.06
20	4	1201	CLA	C3A-C2A-C1A	5.74	109.94	101.34
20	B	1741	CLA	OBD-CAD-C3D	-5.74	114.71	128.52
20	K	3009	CLA	O2D-CGD-CBD	5.73	121.44	111.27
20	2	1222	CLA	O2D-CGD-CBD	5.72	121.44	111.27
20	4	1201	CLA	CBA-CAA-C2A	-5.71	97.00	113.86
20	B	1739	CLA	C4A-NA-C1A	5.71	109.27	106.71
20	4	1200	CLA	C1D-CHD-C4C	-5.71	113.74	126.06
20	B	1765	CLA	O2D-CGD-CBD	5.71	121.41	111.27
22	B	1779	BCR	C35-C13-C14	-5.70	114.93	122.92
20	1	1196	CLA	C1D-CHD-C4C	-5.70	113.75	126.06
20	4	1207	CLA	C1D-CHD-C4C	-5.70	113.76	126.06
20	F	1155	CLA	C1D-CHD-C4C	-5.70	113.77	126.06
20	1	1187	CLA	O2D-CGD-CBD	5.69	121.39	111.27
20	4	4007	CLA	C4D-C3D-CAD	5.69	114.81	108.10
20	B	1739	CLA	C4D-C3D-CAD	5.69	114.81	108.10
20	A	1798	CLA	C1D-CHD-C4C	-5.69	113.78	126.06
22	B	1781	BCR	C30-C25-C24	5.69	131.87	115.78
20	1	1193	CLA	CGD-CBD-CAD	-5.69	92.32	110.73
20	B	1738	CLA	CMD-C2D-C1D	5.68	134.73	124.71
20	A	1761	CLA	C1D-CHD-C4C	-5.68	113.80	126.06
21	A	7026	LMU	C1'-O5'-C5'	5.68	124.84	113.69
20	L	1166	CLA	C1D-CHD-C4C	-5.68	113.81	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1770	CLA	O2D-CGD-CBD	5.67	121.35	111.27
20	2	1216	CLA	C2D-C3D-C4D	-5.67	101.00	107.28
21	A	7039	LMU	O4'-C4B-C3B	5.67	123.47	110.35
21	A	7032	LMU	C3B-C4B-C5B	-5.67	100.12	110.24
20	B	1767	CLA	C1D-CHD-C4C	-5.67	113.83	126.06
20	2	1216	CLA	CHA-C4D-ND	5.67	129.99	124.52
20	A	1769	CLA	C1D-CHD-C4C	-5.66	113.84	126.06
20	A	1768	CLA	C1D-CHD-C4C	-5.66	113.84	126.06
22	I	1032	BCR	C15-C16-C17	5.66	135.07	123.47
20	A	1761	CLA	CMD-C2D-C1D	5.66	134.69	124.71
20	B	1736	CLA	C1D-CHD-C4C	-5.66	113.86	126.06
20	1	1200	CLA	CHC-C1C-NC	5.65	132.78	124.20
20	A	1789	CLA	C1D-CHD-C4C	-5.65	113.87	126.06
21	A	7016	LMU	C1'-O5'-C5'	-5.65	102.60	113.69
20	1	1192	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
20	B	1750	CLA	C1D-CHD-C4C	-5.64	113.90	126.06
20	L	1168	CLA	CHD-C4C-NC	5.63	133.07	124.20
22	I	1032	BCR	C29-C30-C25	-5.63	101.82	110.48
20	3	1213	CLA	CHD-C4C-NC	5.62	132.88	124.21
20	A	1813	CLA	C4D-C3D-CAD	5.62	114.72	108.10
20	A	1783	CLA	C1D-CHD-C4C	-5.62	113.93	126.06
20	I	1031	CLA	CMD-C2D-C1D	5.62	134.62	124.71
20	G	1099	CLA	O2D-CGD-CBD	5.62	121.26	111.27
20	B	1762	CLA	C1D-CHD-C4C	-5.62	113.93	126.06
20	L	1505	CLA	C1D-CHD-C4C	-5.62	113.93	126.06
20	G	1099	CLA	C1D-CHD-C4C	-5.62	113.93	126.06
20	A	1800	CLA	O2D-CGD-CBD	5.62	121.25	111.27
20	1	1191	CLA	C1D-CHD-C4C	-5.62	113.94	126.06
20	A	1811	CLA	CHD-C4C-NC	5.61	133.04	124.20
22	I	1032	BCR	C16-C17-C18	-5.61	119.31	127.31
20	B	1769	CLA	CMD-C2D-C1D	5.61	134.60	124.71
20	1	1187	CLA	CAC-C3C-C4C	5.61	132.08	124.81
20	3	3001	CLA	C3A-C4A-CHB	-5.61	117.05	123.91
20	1	1192	CLA	C4D-C3D-CAD	5.60	114.70	108.10
20	A	1801	CLA	C1D-CHD-C4C	-5.60	113.97	126.06
20	3	1214	CLA	CHD-C4C-NC	5.60	132.85	124.21
20	B	1742	CLA	C4D-C3D-CAD	5.60	114.70	108.10
20	1	1188	CLA	C4A-NA-C1A	5.60	109.22	106.71
20	A	1816	CLA	CMD-C2D-C3D	-5.59	114.75	127.61
20	3	1215	CLA	CHD-C4C-NC	5.59	132.83	124.21
20	K	1146	CLA	C4D-C3D-CAD	5.59	114.68	108.10
20	F	1155	CLA	C4D-C3D-CAD	5.58	114.67	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	3002	CLA	C2B-C1B-NB	5.58	115.00	110.11
20	A	1773	CLA	C1D-CHD-C4C	-5.58	114.02	126.06
20	B	1753	CLA	CHD-C4C-NC	5.58	132.99	124.20
20	I	1033	CLA	C1D-CHD-C4C	-5.58	114.02	126.06
20	B	1752	CLA	C1D-CHD-C4C	-5.58	114.03	126.06
20	A	1798	CLA	C4D-C3D-CAD	5.57	114.66	108.10
20	4	1203	CLA	C2B-C1B-NB	5.57	114.98	110.11
20	B	1743	CLA	CMD-C2D-C1D	5.55	134.50	124.71
20	A	1785	CLA	C1D-CHD-C4C	-5.55	114.08	126.06
20	4	1197	CLA	CHD-C4C-NC	5.55	132.95	124.20
21	K	1086	LMU	O1'-C1'-C2'	5.55	116.97	108.30
20	A	1774	CLA	C1D-CHD-C4C	-5.54	114.10	126.06
20	1	1198	CLA	CHD-C4C-NC	5.54	132.94	124.20
20	A	1783	CLA	C4D-C3D-CAD	5.54	114.63	108.10
20	B	1757	CLA	C1D-CHD-C4C	-5.54	114.10	126.06
20	2	1213	CLA	C4D-C3D-CAD	5.54	114.62	108.10
20	2	1219	CLA	C2B-C1B-NB	5.54	114.96	110.11
22	B	1779	BCR	C10-C11-C12	-5.54	105.93	123.22
20	3	3014	CLA	CHA-C4D-ND	5.54	129.86	124.52
20	1	1188	CLA	C4D-C3D-CAD	5.53	114.62	108.10
20	B	1787	CLA	C1D-CHD-C4C	-5.53	114.13	126.06
20	A	1780	CLA	C1D-CHD-C4C	-5.53	114.13	126.06
21	A	7040	LMU	O3B-C3B-C2B	-5.53	97.57	110.35
20	4	1209	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
20	1	1197	CLA	O2A-CGA-CBA	5.52	129.24	111.91
21	A	7043	LMU	O5B-C5B-C4B	5.52	119.72	109.69
20	L	1168	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
20	A	1788	CLA	C1D-CHD-C4C	-5.51	114.18	126.06
20	B	1785	CLA	C4D-C3D-CAD	5.50	114.58	108.10
20	1	1201	CLA	C3B-C2B-C1B	-5.50	101.58	106.29
20	A	1765	CLA	O2D-CGD-CBD	5.50	121.03	111.27
20	A	1761	CLA	CHC-C1C-NC	5.49	132.53	124.20
20	1	1194	CLA	CHA-C4D-ND	5.49	129.82	124.52
20	R	1055	CLA	C4D-C3D-CAD	5.49	114.56	108.10
20	B	1749	CLA	C1D-CHD-C4C	-5.49	114.22	126.06
20	B	1741	CLA	C1D-CHD-C4C	-5.49	114.22	126.06
20	2	1220	CLA	CHD-C4C-NC	5.49	132.85	124.20
20	2	1215	CLA	C4D-C3D-CAD	5.49	114.56	108.10
21	A	7017	LMU	O4'-C4B-C5B	-5.49	95.68	109.30
20	B	1772	CLA	CMD-C2D-C1D	5.48	134.37	124.71
20	L	1168	CLA	CMD-C2D-C1D	5.48	134.37	124.71
20	B	1750	CLA	CHD-C4C-NC	5.48	132.84	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	1212	CLA	CHD-C4C-NC	5.48	132.83	124.20
20	A	1769	CLA	CMD-C2D-C1D	5.47	134.36	124.71
22	I	1032	BCR	C7-C8-C9	5.47	134.50	126.23
20	2	1224	CLA	C1D-CHD-C4C	-5.47	114.26	126.06
22	L	1170	BCR	C36-C18-C19	5.46	126.68	118.08
20	B	1747	CLA	CMD-C2D-C1D	5.46	134.33	124.71
20	A	1816	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
20	A	1777	CLA	C4D-C3D-CAD	5.45	114.52	108.10
21	A	7041	LMU	C6B-C5B-C4B	-5.45	100.24	113.00
20	B	1753	CLA	C6-C5-C3	-5.45	99.16	113.45
20	2	1223	CLA	O2D-CGD-CBD	5.45	120.95	111.27
20	3	1215	CLA	C2B-C1B-NB	5.45	114.88	110.11
20	B	1738	CLA	CHC-C1C-NC	5.45	132.47	124.20
22	B	1781	BCR	C4-C5-C6	-5.45	114.82	122.73
20	A	1790	CLA	C4D-C3D-CAD	5.44	114.51	108.10
20	2	1216	CLA	C2A-C1A-CHA	-5.44	113.35	122.63
20	B	1749	CLA	C4D-C3D-CAD	5.44	114.51	108.10
20	2	1216	CLA	C2B-C1B-NB	5.44	114.88	110.11
20	2	2010	CLA	CHA-C4D-ND	5.44	129.77	124.52
20	A	1775	CLA	C4D-C3D-CAD	5.44	114.50	108.10
20	B	1737	CLA	CHC-C1C-NC	5.43	132.45	124.20
20	B	1759	CLA	C4A-NA-C1A	5.43	109.15	106.71
20	3	3007	CLA	C4D-C3D-CAD	5.43	114.50	108.10
20	4	1198	CLA	C4D-C3D-CAD	5.43	114.49	108.10
20	B	1771	CLA	C4A-NA-C1A	5.42	109.14	106.71
20	K	3009	CLA	C1D-CHD-C4C	-5.42	114.37	126.06
20	B	1770	CLA	C4D-C3D-CAD	5.42	114.48	108.10
20	1	1187	CLA	CMD-C2D-C3D	-5.42	115.15	127.61
20	3	1214	CLA	C2B-C1B-NB	5.42	114.85	110.11
20	A	1776	CLA	C1D-CHD-C4C	-5.42	114.37	126.06
20	B	1737	CLA	C1D-CHD-C4C	-5.41	114.38	126.06
20	1	1190	CLA	C1D-CHD-C4C	-5.41	114.38	126.06
20	A	1773	CLA	O2D-CGD-CBD	5.41	120.88	111.27
20	B	1745	CLA	C1D-CHD-C4C	-5.41	114.39	126.06
20	A	1769	CLA	CHC-C1C-NC	5.41	132.41	124.20
20	L	1166	CLA	C4D-C3D-CAD	5.41	114.47	108.10
20	B	1754	CLA	CMD-C2D-C1D	5.41	134.24	124.71
20	F	1155	CLA	CHD-C4C-NC	5.41	132.72	124.20
20	A	1767	CLA	CMD-C2D-C3D	-5.40	115.18	127.61
20	4	1198	CLA	CMD-C2D-C3D	-5.40	115.19	127.61
20	4	1205	CLA	C4C-CHD-C1D	-5.40	112.75	126.11
20	3	1213	CLA	C2A-C1A-CHA	-5.40	113.42	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	3009	CLA	CMD-C2D-C1D	5.40	134.23	124.71
20	2	2010	CLA	C2B-C1B-NB	5.40	114.84	110.11
20	A	1759	CLA	C1D-CHD-C4C	-5.39	114.43	126.06
20	B	1747	CLA	OBD-CAD-C3D	-5.39	115.55	128.52
21	A	7041	LMU	C4B-C3B-C2B	-5.39	101.41	110.82
20	3	1218	CLA	CED-O2D-CGD	5.39	128.13	115.94
20	A	1789	CLA	C4D-C3D-CAD	5.39	114.45	108.10
20	2	1221	CLA	CHA-C4D-ND	5.38	129.72	124.52
20	4	1201	CLA	CMB-C2B-C3B	5.38	134.75	124.68
20	1	1198	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
20	3	1215	CLA	C4C-CHD-C1D	-5.37	112.82	126.11
21	A	7021	LMU	O3B-C3B-C4B	-5.37	97.93	110.35
20	B	1744	CLA	C4D-C3D-CAD	5.37	114.42	108.10
20	1	1195	CLA	CHD-C4C-C3C	-5.37	116.59	124.98
20	3	1214	CLA	C4C-CHD-C1D	-5.37	112.83	126.11
20	A	1774	CLA	CMD-C2D-C1D	5.37	134.17	124.71
20	1	1192	CLA	CMD-C2D-C1D	5.36	134.17	124.71
20	3	3008	CLA	CHD-C4C-NC	5.36	132.66	124.20
20	A	1760	CLA	C1D-CHD-C4C	-5.36	114.50	126.06
20	B	1786	CLA	C1D-CHD-C4C	-5.36	114.50	126.06
20	A	1815	CLA	C4D-C3D-CAD	5.36	114.41	108.10
20	A	1764	CLA	C4D-C3D-CAD	5.36	114.41	108.10
20	1	1196	CLA	C4D-C3D-CAD	5.35	114.41	108.10
20	H	1079	CLA	C1D-CHD-C4C	-5.35	114.52	126.06
20	A	1774	CLA	C4D-C3D-CAD	5.35	114.40	108.10
20	A	1772	CLA	O2D-CGD-CBD	5.35	120.78	111.27
20	B	1746	CLA	C1D-CHD-C4C	-5.35	114.52	126.06
20	H	1079	CLA	C4D-C3D-CAD	5.34	114.39	108.10
20	A	1816	CLA	O2D-CGD-O1D	-5.34	113.40	123.84
20	2	1212	CLA	C4D-C3D-CAD	5.34	114.39	108.10
21	A	7036	LMU	C1B-O1B-C4'	-5.34	104.76	117.96
20	A	1761	CLA	CHD-C4C-NC	5.34	132.61	124.20
20	A	1781	CLA	C4D-C3D-CAD	5.33	114.38	108.10
20	B	1747	CLA	O2D-CGD-CBD	5.33	120.74	111.27
20	A	1767	CLA	CHC-C1C-NC	5.33	132.29	124.20
20	4	4007	CLA	C4A-NA-C1A	5.33	109.10	106.71
20	A	1786	CLA	CMD-C2D-C1D	5.33	134.10	124.71
20	2	1216	CLA	CHC-C1C-NC	5.33	132.09	124.23
20	A	1785	CLA	CMD-C2D-C1D	5.33	134.10	124.71
20	B	1749	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
20	B	1746	CLA	C4D-C3D-CAD	5.32	114.37	108.10
20	F	1156	CLA	C4D-C3D-CAD	5.32	114.37	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1760	CLA	CHD-C4C-NC	5.32	132.58	124.20
20	A	1779	CLA	C1D-CHD-C4C	-5.32	114.59	126.06
22	L	1169	BCR	C30-C25-C26	-5.32	115.12	122.61
20	B	1740	CLA	C4D-C3D-CAD	5.32	114.36	108.10
20	B	1735	CLA	C4D-C3D-CAD	5.31	114.36	108.10
20	A	1796	CLA	C4D-C3D-CAD	5.31	114.36	108.10
20	1	1201	CLA	C3A-C4A-CHB	-5.31	117.41	123.91
20	A	1764	CLA	O2D-CGD-CBD	5.31	120.70	111.27
20	4	1196	CLA	C4D-C3D-CAD	5.31	114.35	108.10
20	2	1224	CLA	CMD-C2D-C1D	5.31	134.06	124.71
20	L	1167	CLA	C1D-CHD-C4C	-5.30	114.61	126.06
20	B	1756	CLA	C4D-C3D-CAD	5.30	114.34	108.10
21	A	7022	LMU	O3B-C3B-C4B	-5.30	98.09	110.35
20	A	1791	CLA	C4D-C3D-CAD	5.30	114.34	108.10
20	K	1085	CLA	C4D-C3D-CAD	5.30	114.34	108.10
20	A	1793	CLA	C4D-C3D-CAD	5.30	114.34	108.10
20	J	1046	CLA	C2B-C1B-NB	5.30	114.75	110.11
20	A	1762	CLA	C4D-C3D-CAD	5.30	114.34	108.10
20	A	1792	CLA	C4D-C3D-CAD	5.29	114.34	108.10
20	B	1755	CLA	C4D-C3D-CAD	5.29	114.33	108.10
20	A	1794	CLA	C4D-C3D-CAD	5.29	114.33	108.10
20	A	1797	CLA	C4D-C3D-CAD	5.29	114.33	108.10
20	2	1218	CLA	CMD-C2D-C1D	5.29	134.03	124.71
20	2	1217	CLA	C4D-C3D-CAD	5.29	114.33	108.10
20	3	1219	CLA	C4D-C3D-CAD	5.28	114.32	108.10
20	A	1784	CLA	C1D-CHD-C4C	-5.28	114.67	126.06
20	A	1795	CLA	C4D-C3D-CAD	5.28	114.32	108.10
20	A	1799	CLA	C1D-CHD-C4C	-5.28	114.67	126.06
20	J	1043	CLA	C4D-C3D-CAD	5.28	114.32	108.10
20	1	1188	CLA	OBD-CAD-C3D	-5.28	115.82	128.52
20	A	1765	CLA	C1D-CHD-C4C	-5.27	114.68	126.06
20	A	1776	CLA	O2D-CGD-CBD	5.27	120.63	111.27
20	A	1777	CLA	O2D-CGD-CBD	5.27	120.63	111.27
20	A	1790	CLA	C1D-CHD-C4C	-5.27	114.69	126.06
20	2	1227	CLA	C2D-C3D-C4D	-5.27	101.45	107.28
20	B	1771	CLA	CMD-C2D-C1D	5.27	133.99	124.71
20	1	1189	CLA	CMD-C2D-C3D	-5.26	115.50	127.61
20	A	1775	CLA	CHD-C4C-NC	5.25	132.48	124.20
20	1	1195	CLA	CMD-C2D-C3D	-5.25	115.53	127.61
20	4	1205	CLA	C3A-C4A-CHB	-5.25	117.48	123.91
20	B	1786	CLA	CMD-C2D-C1D	5.25	133.96	124.71
20	A	1777	CLA	C1D-CHD-C4C	-5.25	114.74	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	7039	LMU	C1B-C2B-C3B	-5.24	99.08	110.00
20	B	1766	CLA	C4D-C3D-CAD	5.24	114.27	108.10
20	A	1778	CLA	C4A-NA-C1A	5.24	109.06	106.71
20	1	1196	CLA	OBD-CAD-C3D	-5.23	115.92	128.52
20	3	3014	CLA	C3B-C2B-C1B	-5.23	101.81	106.29
20	A	1801	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
20	A	1811	CLA	CMD-C2D-C1D	5.23	133.93	124.71
21	A	7037	LMU	C3B-C4B-C5B	-5.23	100.92	110.24
20	1	1200	CLA	CAA-C2A-C3A	-5.23	98.47	112.78
22	B	1778	BCR	C11-C10-C9	-5.22	119.86	127.31
20	A	1782	CLA	C4D-C3D-CAD	5.22	114.25	108.10
20	F	1155	CLA	OBD-CAD-C3D	-5.22	115.97	128.52
20	B	1741	CLA	C4D-C3D-CAD	5.22	114.24	108.10
20	3	1217	CLA	C3B-C2B-C1B	-5.22	101.83	106.29
20	2	1213	CLA	C1D-CHD-C4C	-5.21	114.81	126.06
22	B	1778	BCR	C15-C14-C13	-5.21	119.88	127.31
20	A	1815	CLA	C1D-CHD-C4C	-5.21	114.83	126.06
20	1	1188	CLA	C1D-CHD-C4C	-5.20	114.84	126.06
20	A	1800	CLA	CMD-C2D-C1D	5.20	133.88	124.71
20	3	3008	CLA	CMD-C2D-C3D	-5.20	115.65	127.61
21	A	7039	LMU	O5B-C1B-C2B	-5.20	99.34	110.35
20	4	1209	CLA	CHD-C4C-NC	5.20	132.39	124.20
22	B	1775	BCR	C11-C10-C9	-5.19	119.90	127.31
20	1	1187	CLA	CHB-C4A-NA	5.19	131.69	124.51
20	3	3007	CLA	O2D-CGD-CBD	5.19	120.50	111.27
20	K	3009	CLA	C4D-C3D-CAD	5.19	114.22	108.10
22	A	1807	BCR	C16-C17-C18	-5.19	119.91	127.31
20	K	1142	CLA	CHD-C4C-NC	5.19	132.38	124.20
20	4	1207	CLA	C4A-NA-C1A	5.19	109.04	106.71
20	3	3011	CLA	C1D-CHD-C4C	-5.19	114.87	126.06
20	A	1778	CLA	O1D-CGD-CBD	-5.19	113.87	124.48
20	K	1085	CLA	CHD-C4C-NC	5.19	132.37	124.20
20	4	1196	CLA	CHD-C4C-NC	5.18	132.37	124.20
20	A	1791	CLA	CHD-C4C-NC	5.18	132.37	124.20
20	1	1189	CLA	C1D-CHD-C4C	-5.18	114.88	126.06
21	A	7039	LMU	O1B-C1B-C2B	5.18	121.53	108.10
20	B	1765	CLA	C1D-CHD-C4C	-5.18	114.88	126.06
22	B	1781	BCR	C37-C22-C21	-5.18	115.67	122.92
20	A	1797	CLA	CHD-C4C-NC	5.17	132.35	124.20
22	A	1806	BCR	C15-C14-C13	-5.17	119.93	127.31
20	R	1055	CLA	C1D-CHD-C4C	-5.17	114.90	126.06
20	A	1774	CLA	CHD-C4C-NC	5.17	132.35	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1758	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
20	F	1156	CLA	CHD-C4C-NC	5.17	132.34	124.20
20	J	1043	CLA	CHD-C4C-NC	5.16	132.34	124.20
20	K	1142	CLA	C4D-C3D-CAD	5.16	114.18	108.10
20	2	1221	CLA	C3B-C2B-C1B	-5.16	101.87	106.29
20	1	1200	CLA	C4A-NA-C1A	-5.16	104.39	106.71
20	4	1200	CLA	C4D-C3D-CAD	5.16	114.18	108.10
20	A	1759	CLA	C4D-C3D-CAD	5.16	114.18	108.10
20	B	1735	CLA	CHD-C4C-NC	5.16	132.33	124.20
20	B	1755	CLA	CHD-C4C-NC	5.16	132.33	124.20
20	A	1817	CLA	C4A-NA-C1A	5.16	109.03	106.71
20	3	1219	CLA	CHD-C4C-NC	5.16	132.33	124.20
20	A	1795	CLA	CHD-C4C-NC	5.16	132.33	124.20
20	R	1054	CLA	C1D-CHD-C4C	-5.16	114.93	126.06
20	A	1794	CLA	CHD-C4C-NC	5.15	132.32	124.20
22	A	1808	BCR	C15-C14-C13	-5.15	119.95	127.31
22	B	1780	BCR	C16-C17-C18	-5.15	119.95	127.31
20	3	3015	CLA	C2B-C1B-NB	5.15	114.62	110.11
22	A	1806	BCR	C11-C10-C9	-5.15	119.96	127.31
20	B	1736	CLA	O2D-CGD-O1D	-5.15	113.78	123.84
20	I	1033	CLA	CMD-C2D-C1D	5.15	133.78	124.71
20	2	1221	CLA	C3A-C4A-CHB	-5.14	117.61	123.91
20	1	1193	CLA	C1D-CHD-C4C	-5.14	114.97	126.06
20	A	1793	CLA	CHD-C4C-NC	5.14	132.30	124.20
20	A	1796	CLA	CHD-C4C-NC	5.14	132.30	124.20
20	2	1219	CLA	C4A-NA-C1A	5.14	109.02	106.71
22	A	1803	BCR	C16-C17-C18	-5.13	119.98	127.31
20	B	1748	CLA	CHD-C4C-C3C	-5.13	117.29	124.84
22	B	1775	BCR	C15-C14-C13	-5.13	119.98	127.31
22	A	1803	BCR	C15-C14-C13	-5.13	119.98	127.31
23	B	1773	PQN	C11-C12-C13	-5.13	118.25	126.79
20	A	1781	CLA	CHD-C4C-NC	5.13	132.29	124.20
20	B	1768	CLA	C4D-C3D-CAD	5.13	114.14	108.10
20	A	1765	CLA	CAC-C3C-C4C	5.13	131.47	124.81
20	A	1792	CLA	CHD-C4C-NC	5.13	132.28	124.20
22	A	1805	BCR	C11-C10-C9	-5.13	119.99	127.31
22	B	1778	BCR	C16-C17-C18	-5.13	119.99	127.31
20	A	1782	CLA	CHD-C4C-NC	5.13	132.28	124.20
20	A	1771	CLA	CMD-C2D-C1D	5.13	133.75	124.71
20	B	1756	CLA	CHD-C4C-NC	5.12	132.28	124.20
22	A	1808	BCR	C16-C17-C18	-5.12	120.00	127.31
22	B	1777	BCR	C15-C14-C13	-5.12	120.00	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	7035	LMU	O1B-C4'-C3'	5.12	120.90	107.28
20	4	4014	CLA	CHD-C4C-NC	5.12	132.27	124.20
20	4	1203	CLA	C4C-CHD-C1D	-5.12	113.45	126.11
22	A	1804	BCR	C11-C10-C9	-5.12	120.01	127.31
22	B	1777	BCR	C11-C10-C9	-5.12	120.01	127.31
20	B	1746	CLA	C4A-NA-C1A	5.12	109.01	106.71
22	A	1807	BCR	C11-C10-C9	-5.12	120.01	127.31
22	A	1804	BCR	C15-C14-C13	-5.12	120.01	127.31
20	F	1157	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
20	B	1761	CLA	C1D-CHD-C4C	-5.11	115.03	126.06
22	B	1776	BCR	C24-C23-C22	-5.11	118.51	126.23
22	A	1806	BCR	C16-C17-C18	-5.11	120.01	127.31
20	A	1759	CLA	CHD-C4C-NC	5.11	132.25	124.20
22	A	1804	BCR	C16-C17-C18	-5.11	120.02	127.31
22	A	1805	BCR	C16-C17-C18	-5.11	120.02	127.31
20	3	1213	CLA	CHA-C4D-ND	5.11	129.45	124.52
20	2	1212	CLA	CHD-C4C-NC	5.11	132.25	124.20
20	1	1197	CLA	CHC-C1C-NC	5.10	131.95	124.20
22	B	1780	BCR	C15-C14-C13	-5.10	120.03	127.31
20	A	1786	CLA	C1D-CHD-C4C	-5.10	115.05	126.06
22	B	1780	BCR	C11-C10-C9	-5.10	120.03	127.31
20	2	1222	CLA	C4A-NA-C1A	5.10	109.00	106.71
20	4	4014	CLA	C4D-C3D-CAD	5.10	114.10	108.10
21	A	7037	LMU	O4'-C4B-C5B	5.09	121.95	109.30
20	A	1778	CLA	C1D-CHD-C4C	-5.09	115.07	126.06
20	B	1761	CLA	CMD-C2D-C1D	5.09	133.69	124.71
22	B	1777	BCR	C16-C17-C18	-5.09	120.05	127.31
22	L	1170	BCR	C10-C11-C12	-5.09	107.34	123.22
20	A	1787	CLA	C4-C3-C5	5.09	123.83	115.27
22	B	1775	BCR	C16-C17-C18	-5.09	120.05	127.31
20	A	1769	CLA	C4D-C3D-CAD	5.09	114.09	108.10
20	A	1771	CLA	C1D-CHD-C4C	-5.08	115.09	126.06
20	A	1772	CLA	C1-C2-C3	-5.08	117.25	126.04
20	B	1772	CLA	C1D-CHD-C4C	-5.08	115.09	126.06
22	A	1808	BCR	C11-C10-C9	-5.08	120.06	127.31
20	A	1812	CLA	CMD-C2D-C1D	5.08	133.67	124.71
20	3	1216	CLA	C3A-C4A-CHB	-5.08	117.69	123.91
20	I	1033	CLA	C4D-C3D-CAD	5.08	114.08	108.10
20	A	1787	CLA	C1D-CHD-C4C	-5.08	115.10	126.06
21	R	1057	LMU	C1'-C2'-C3'	-5.08	99.42	110.00
20	1	1201	CLA	CHA-C4D-ND	5.08	129.42	124.52
20	4	1201	CLA	CBC-CAC-C3C	-5.08	98.43	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1805	BCR	C15-C14-C13	-5.08	120.06	127.31
20	G	1099	CLA	CHD-C4C-NC	5.08	132.20	124.20
22	A	1807	BCR	C15-C14-C13	-5.07	120.07	127.31
20	3	3011	CLA	O2D-CGD-CBD	5.07	120.28	111.27
20	2	1220	CLA	O2D-CGD-CBD	5.07	120.28	111.27
20	B	1739	CLA	C1D-CHD-C4C	-5.07	115.12	126.06
20	A	1815	CLA	O2D-CGD-CBD	5.07	120.28	111.27
20	B	1766	CLA	O2D-CGD-CBD	5.07	120.28	111.27
22	B	1774	BCR	C16-C17-C18	-5.07	120.08	127.31
22	B	1774	BCR	C15-C14-C13	-5.06	120.08	127.31
20	A	1789	CLA	CMD-C2D-C3D	-5.06	115.96	127.61
20	L	1167	CLA	C4D-C3D-CAD	5.06	114.06	108.10
20	4	1206	CLA	C2A-C1A-CHA	-5.06	114.00	122.63
22	B	1774	BCR	C11-C10-C9	-5.06	120.09	127.31
20	A	1782	CLA	O2D-CGD-CBD	5.06	120.25	111.27
20	4	1198	CLA	O2A-CGA-O1A	-5.06	110.83	123.59
20	A	1786	CLA	O2D-CGD-O1D	-5.06	113.95	123.84
20	K	1146	CLA	C1D-CHD-C4C	-5.05	115.16	126.06
21	A	7030	LMU	C4B-C3B-C2B	-5.05	102.01	110.82
20	4	1199	CLA	CHC-C1C-NC	5.05	131.86	124.20
20	B	1745	CLA	CMD-C2D-C1D	5.05	133.61	124.71
22	A	1803	BCR	C11-C10-C9	-5.05	120.11	127.31
20	4	1201	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
20	A	1764	CLA	C1D-CHD-C4C	-5.05	115.17	126.06
20	A	1801	CLA	CHD-C4C-NC	5.04	132.15	124.20
20	2	1217	CLA	CHD-C4C-NC	5.04	132.15	124.20
20	4	1200	CLA	O2D-CGD-CBD	5.04	120.23	111.27
20	2	1227	CLA	C3B-C2B-C1B	-5.04	101.97	106.29
20	4	1197	CLA	C1B-C2B-C3B	-5.04	102.23	106.92
20	B	1770	CLA	CMD-C2D-C3D	-5.04	116.02	127.61
20	A	1801	CLA	C4D-C3D-CAD	5.04	114.03	108.10
20	B	1766	CLA	C1D-CHD-C4C	-5.04	115.19	126.06
20	A	1785	CLA	C4D-C3D-CAD	5.04	114.03	108.10
20	R	1055	CLA	CMD-C2D-C3D	-5.03	116.03	127.61
20	1	1187	CLA	CAC-C3C-C2C	-5.03	118.92	127.53
20	A	1812	CLA	CHD-C4C-NC	5.03	132.13	124.20
20	A	1765	CLA	C4D-C3D-CAD	5.03	114.02	108.10
20	1	1188	CLA	CAA-C2A-C1A	5.03	128.45	111.97
20	A	1781	CLA	O2D-CGD-CBD	5.02	120.19	111.27
20	A	1795	CLA	O2D-CGD-CBD	5.02	120.19	111.27
20	B	1772	CLA	C4D-C3D-CAD	5.02	114.01	108.10
20	3	3002	CLA	C4C-CHD-C1D	-5.02	113.70	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	1212	CLA	O2D-CGD-CBD	5.02	120.18	111.27
20	A	1792	CLA	O2D-CGD-CBD	5.02	120.18	111.27
20	K	1085	CLA	O2D-CGD-CBD	5.02	120.18	111.27
20	K	1142	CLA	O2D-CGD-CBD	5.02	120.18	111.27
20	A	1817	CLA	C1D-CHD-C4C	-5.02	115.24	126.06
20	A	1791	CLA	O2D-CGD-CBD	5.02	120.18	111.27
20	A	1793	CLA	O2D-CGD-CBD	5.01	120.18	111.27
20	J	1043	CLA	O2D-CGD-CBD	5.01	120.18	111.27
20	B	1753	CLA	C2A-C1A-CHA	-5.01	115.09	123.86
20	2	1220	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
20	2	1219	CLA	CHD-C4C-NC	5.01	131.94	124.21
20	B	1769	CLA	CHD-C4C-NC	5.01	132.10	124.20
20	B	1761	CLA	C4A-NA-C1A	5.01	108.96	106.71
20	4	4014	CLA	O2D-CGD-CBD	5.01	120.17	111.27
20	B	1770	CLA	CHC-C1C-NC	5.01	131.80	124.20
21	A	7022	LMU	O1B-C1B-C2B	5.01	121.07	108.10
20	B	1767	CLA	CMD-C2D-C3D	-5.00	116.10	127.61
20	B	1736	CLA	CHD-C4C-NC	5.00	132.09	124.20
20	B	1735	CLA	O2D-CGD-CBD	5.00	120.16	111.27
20	J	1045	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
20	A	1799	CLA	CMD-C2D-C3D	-5.00	116.11	127.61
20	B	1756	CLA	O2D-CGD-CBD	5.00	120.16	111.27
20	4	4007	CLA	CHD-C4C-NC	5.00	132.08	124.20
20	3	1219	CLA	O2D-CGD-CBD	5.00	120.15	111.27
20	A	1799	CLA	C4D-C3D-CAD	5.00	113.99	108.10
20	A	1794	CLA	O2D-CGD-CBD	5.00	120.15	111.27
21	A	7043	LMU	C1B-C2B-C3B	5.00	120.40	110.00
20	B	1763	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
20	A	1762	CLA	O2D-CGD-CBD	4.99	120.14	111.27
20	A	1763	CLA	CMD-C2D-C1D	4.99	133.51	124.71
20	B	1765	CLA	CHD-C4C-NC	4.99	132.07	124.20
20	A	1796	CLA	O2D-CGD-CBD	4.99	120.14	111.27
21	A	7017	LMU	O5B-C5B-C4B	-4.99	100.63	109.69
20	A	1797	CLA	O2D-CGD-CBD	4.99	120.14	111.27
20	4	1205	CLA	CHD-C4C-NC	4.99	131.91	124.21
20	1	1201	CLA	C2D-C3D-C4D	-4.99	101.75	107.28
20	A	1812	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
21	A	7043	LMU	C4B-C3B-C2B	-4.99	102.11	110.82
22	I	1032	BCR	C15-C14-C13	4.99	134.43	127.31
20	4	1196	CLA	O2D-CGD-CBD	4.98	120.13	111.27
20	1	1194	CLA	C3A-C4A-CHB	-4.98	117.81	123.91
20	B	1743	CLA	C4D-C3D-CAD	4.98	113.97	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1816	CLA	C4-C3-C2	-4.98	110.89	123.68
20	B	1755	CLA	O2D-CGD-CBD	4.98	120.12	111.27
20	F	1156	CLA	O2D-CGD-CBD	4.98	120.12	111.27
20	A	1785	CLA	C4A-NA-C1A	4.98	108.94	106.71
20	4	1202	CLA	C3B-C2B-C1B	-4.97	102.03	106.29
20	4	4007	CLA	C1D-CHD-C4C	-4.97	115.33	126.06
20	B	1744	CLA	OBD-CAD-C3D	-4.97	116.55	128.52
20	1	1199	CLA	C3B-C2B-C1B	-4.97	102.03	106.29
20	1	1198	CLA	C4D-C3D-CAD	4.97	113.95	108.10
20	A	1817	CLA	CHC-C1C-NC	4.97	131.74	124.20
20	A	1762	CLA	C1D-CHD-C4C	-4.97	115.34	126.06
20	B	1737	CLA	CHD-C4C-NC	4.97	132.03	124.20
20	B	1749	CLA	CMD-C2D-C1D	4.96	133.46	124.71
20	K	1146	CLA	CHC-C1C-NC	4.96	131.73	124.20
20	1	1193	CLA	C2A-C3A-C4A	-4.96	93.86	101.87
20	B	1742	CLA	C1D-CHD-C4C	-4.96	115.36	126.06
21	A	7021	LMU	O1B-C4'-C3'	4.96	120.47	107.28
20	J	1044	CLA	CMD-C2D-C1D	4.95	133.44	124.71
20	B	1766	CLA	C4-C3-C5	4.95	121.64	115.98
20	B	1771	CLA	C1D-CHD-C4C	-4.95	115.38	126.06
20	A	1772	CLA	CHD-C4C-NC	4.95	132.00	124.20
20	1	1192	CLA	CHD-C4C-NC	4.95	132.00	124.20
20	4	1202	CLA	CHA-C4D-ND	4.94	129.29	124.52
22	B	1779	BCR	C16-C17-C18	-4.94	120.26	127.31
21	A	7026	LMU	O5B-C5B-C4B	-4.93	100.73	109.69
20	A	1772	CLA	C4D-C3D-CAD	4.93	113.91	108.10
20	4	1201	CLA	C4D-C3D-CAD	4.93	113.91	108.10
20	2	1222	CLA	C1D-CHD-C4C	-4.93	115.42	126.06
20	A	1770	CLA	C1D-CHD-C4C	-4.93	115.42	126.06
20	3	1215	CLA	CHC-C1C-NC	4.93	131.51	124.23
20	A	1800	CLA	C1D-CHD-C4C	-4.93	115.42	126.06
20	3	3001	CLA	CHA-C4D-ND	4.93	129.28	124.52
20	A	1800	CLA	C4D-C3D-CAD	4.93	113.90	108.10
20	2	1218	CLA	C4D-C3D-CAD	4.92	113.90	108.10
20	4	1203	CLA	C2A-C1A-CHA	-4.92	114.24	122.63
20	A	1776	CLA	C4D-C3D-CAD	4.92	113.90	108.10
20	A	1768	CLA	C4D-C3D-CAD	4.92	113.89	108.10
20	A	1769	CLA	CHD-C4C-NC	4.92	131.95	124.20
20	4	1206	CLA	C3B-C2B-C1B	-4.91	102.08	106.29
20	A	1811	CLA	C1D-CHD-C4C	-4.91	115.46	126.06
20	4	1198	CLA	CHD-C4C-C3C	-4.91	117.62	124.84
20	B	1770	CLA	CHD-C4C-NC	4.91	131.94	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	1198	CLA	O2D-CGD-CBD	4.91	119.99	111.27
20	A	1763	CLA	C4D-C3D-CAD	4.91	113.88	108.10
20	G	1099	CLA	C4D-C3D-CAD	4.90	113.88	108.10
20	B	1740	CLA	CHD-C4C-NC	4.90	131.93	124.20
20	B	1768	CLA	C1D-CHD-C4C	-4.90	115.49	126.06
20	B	1787	CLA	CHC-C1C-NC	4.90	131.63	124.20
20	B	1759	CLA	CMD-C2D-C3D	-4.90	116.35	127.61
20	A	1761	CLA	C4D-C3D-CAD	4.90	113.87	108.10
20	A	1771	CLA	C4D-C3D-CAD	4.90	113.87	108.10
20	3	1214	CLA	CHC-C1C-NC	4.90	131.46	124.23
21	K	1086	LMU	O5B-C5B-C4B	-4.89	100.81	109.69
20	1	1199	CLA	C4C-CHD-C1D	-4.89	114.01	126.11
20	R	1054	CLA	CMD-C2D-C3D	-4.89	116.36	127.61
20	2	1215	CLA	C1D-CHD-C4C	-4.89	115.50	126.06
20	1	1199	CLA	CHA-C4D-ND	4.89	129.24	124.52
20	2	1223	CLA	C4D-C3D-CAD	4.89	113.86	108.10
20	B	1744	CLA	CMD-C2D-C3D	-4.89	116.36	127.61
20	2	1219	CLA	CHC-C1C-NC	4.89	131.45	124.23
20	B	1749	CLA	CHD-C4C-NC	4.89	131.90	124.20
20	B	1760	CLA	C4D-C3D-CAD	4.89	113.85	108.10
20	B	1753	CLA	O2D-CGD-O1D	-4.88	114.29	123.84
20	1	1194	CLA	C3B-C2B-C1B	-4.88	102.11	106.29
22	3	1220	BCR	C33-C5-C6	-4.88	119.05	124.53
20	2	1214	CLA	C4C-CHD-C1D	-4.88	114.05	126.11
20	A	1768	CLA	CHD-C4C-NC	4.88	131.89	124.20
20	4	1202	CLA	C4C-CHD-C1D	-4.87	114.06	126.11
20	2	1227	CLA	C2A-C1A-CHA	-4.87	114.32	122.63
20	B	1741	CLA	CMD-C2D-C3D	-4.87	116.41	127.61
20	B	1786	CLA	C4A-NA-C1A	4.87	108.90	106.71
20	B	1739	CLA	CMD-C2D-C1D	4.87	133.29	124.71
20	L	1505	CLA	CMD-C2D-C3D	-4.87	116.42	127.61
20	2	1219	CLA	C4C-CHD-C1D	-4.87	114.08	126.11
20	J	1045	CLA	C4D-C3D-CAD	4.86	113.83	108.10
20	A	1769	CLA	O2D-CGD-CBD	4.86	119.91	111.27
20	B	1765	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
20	B	1748	CLA	C4D-C3D-CAD	4.86	113.83	108.10
20	A	1789	CLA	O1D-CGD-CBD	-4.86	114.55	124.48
20	1	1197	CLA	CBA-CAA-C2A	4.85	128.19	113.86
20	L	1505	CLA	C4-C3-C5	4.85	123.44	115.27
20	4	1199	CLA	C4A-NA-C1A	4.85	108.89	106.71
20	4	1207	CLA	CMD-C2D-C1D	4.85	133.26	124.71
20	1	1194	CLA	C4C-CHD-C1D	-4.85	114.12	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1770	CLA	C4D-C3D-CAD	4.85	113.81	108.10
20	3	3001	CLA	C4C-CHD-C1D	-4.85	114.13	126.11
20	4	4003	CLA	C2B-C1B-NB	4.84	114.35	110.11
20	A	1813	CLA	C1D-CHD-C4C	-4.84	115.61	126.06
20	3	3007	CLA	C1D-CHD-C4C	-4.84	115.62	126.06
20	3	3014	CLA	C2D-C3D-C4D	-4.84	101.92	107.28
20	B	1746	CLA	CHD-C4C-NC	4.84	131.82	124.20
20	3	3008	CLA	O2D-CGD-CBD	4.83	119.86	111.27
22	B	1776	BCR	C27-C26-C25	-4.83	115.71	122.73
20	2	1224	CLA	C4D-C3D-CAD	4.83	113.79	108.10
20	J	1045	CLA	C4A-NA-C1A	4.83	108.88	106.71
20	2	1214	CLA	CHD-C4C-NC	4.83	131.66	124.21
20	1	1191	CLA	CHD-C4C-NC	4.83	131.81	124.20
20	A	1813	CLA	CHD-C4C-NC	4.83	131.81	124.20
22	3	1220	BCR	C7-C8-C9	-4.82	118.95	126.23
20	2	1221	CLA	C4C-CHD-C1D	-4.82	114.19	126.11
20	2	1213	CLA	CMD-C2D-C3D	-4.82	116.52	127.61
22	L	1169	BCR	C7-C8-C9	-4.82	118.95	126.23
20	B	1757	CLA	C4D-C3D-CAD	4.82	113.78	108.10
20	L	1166	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
20	1	1193	CLA	CAA-C2A-C3A	4.82	125.97	112.78
20	I	1031	CLA	CHD-C4C-NC	4.82	131.79	124.20
20	B	1750	CLA	O2D-CGD-CBD	4.81	119.82	111.27
20	2	1227	CLA	CHA-C4D-ND	4.81	129.16	124.52
20	L	1166	CLA	CHD-C4C-NC	4.81	131.78	124.20
20	3	1217	CLA	CHC-C1C-NC	4.81	131.33	124.23
20	2	1218	CLA	C1D-CHD-C4C	-4.81	115.69	126.06
20	4	1201	CLA	C4A-NA-C1A	4.81	108.87	106.71
20	B	1736	CLA	CMD-C2D-C3D	-4.81	116.56	127.61
21	A	7026	LMU	O3B-C3B-C4B	4.80	121.46	110.35
20	A	1816	CLA	C2D-C1D-ND	-4.80	106.57	110.10
22	L	1169	BCR	C33-C5-C6	-4.80	119.14	124.53
20	2	1227	CLA	C4A-NA-C1A	4.80	108.86	106.71
21	A	7021	LMU	C1B-O1B-C4'	4.80	129.83	117.96
20	A	1785	CLA	CHD-C4C-NC	4.79	131.75	124.20
20	B	1757	CLA	CHD-C4C-NC	4.79	131.75	124.20
20	3	1212	CLA	CHD-C4C-C3C	-4.79	117.50	124.98
23	B	1773	PQN	C2M-C2-C3	-4.79	116.59	124.40
20	B	1748	CLA	CHD-C4C-NC	4.79	131.75	124.20
21	A	7038	LMU	C6B-C5B-C4B	-4.79	101.79	113.00
20	A	1816	CLA	C4D-CHA-C1A	4.79	127.08	121.25
20	B	1737	CLA	CMD-C2D-C3D	-4.79	116.61	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	1216	CLA	CHD-C4C-NC	4.79	131.59	124.21
20	B	1744	CLA	C1D-CHD-C4C	-4.79	115.73	126.06
20	1	1192	CLA	O2D-CGD-CBD	4.79	119.77	111.27
20	A	1783	CLA	CHD-C4C-NC	4.78	131.74	124.20
20	B	1764	CLA	CHD-C4C-NC	4.78	131.74	124.20
20	B	1786	CLA	CHD-C4C-NC	4.78	131.74	124.20
20	K	1146	CLA	CMA-C3A-C4A	-4.78	98.92	111.77
21	A	7043	LMU	O3'-C3'-C4'	-4.78	97.27	109.94
22	L	1169	BCR	C36-C18-C19	4.78	125.61	118.08
20	B	1764	CLA	C4A-NA-C1A	4.78	108.86	106.71
20	K	1146	CLA	CMB-C2B-C3B	4.78	133.61	124.68
22	B	1781	BCR	C28-C27-C26	-4.77	105.55	114.08
20	B	1767	CLA	CHD-C4C-NC	4.77	131.73	124.20
20	B	1747	CLA	C1D-CHD-C4C	-4.77	115.76	126.06
20	B	1764	CLA	CHD-C4C-C3C	-4.77	117.82	124.84
20	1	1201	CLA	CHC-C1C-NC	4.77	131.27	124.23
20	B	1768	CLA	O2D-CGD-O1D	-4.77	114.51	123.84
20	1	1187	CLA	CHD-C4C-NC	4.76	131.71	124.20
21	A	7039	LMU	O3B-C3B-C4B	4.76	121.36	110.35
20	L	1166	CLA	CMD-C2D-C1D	4.76	133.11	124.71
20	2	2010	CLA	C4C-CHD-C1D	-4.76	114.34	126.11
20	A	1789	CLA	CHC-C1C-NC	4.76	131.43	124.20
20	A	1780	CLA	C4D-C3D-CAD	4.76	113.70	108.10
20	3	3001	CLA	C4A-NA-C1A	4.76	108.84	106.71
20	A	1763	CLA	C1D-CHD-C4C	-4.74	115.82	126.06
22	L	1170	BCR	C33-C5-C4	4.74	122.72	113.62
20	2	1213	CLA	CHD-C4C-NC	4.74	131.67	124.20
20	2	1214	CLA	CHA-C4D-ND	4.74	129.09	124.52
20	A	1787	CLA	CHD-C4C-NC	4.74	131.66	124.20
20	3	1217	CLA	C2D-C3D-C4D	-4.73	102.03	107.28
20	3	3014	CLA	C2A-C1A-CHA	-4.73	114.56	122.63
20	F	1157	CLA	C4-C3-C5	4.73	123.23	115.27
22	B	1776	BCR	C16-C17-C18	-4.73	120.56	127.31
20	B	1740	CLA	CMD-C2D-C1D	4.73	133.04	124.71
20	3	3002	CLA	C2A-C1A-CHA	-4.73	114.57	122.63
20	A	1766	CLA	CMD-C2D-C3D	-4.72	116.75	127.61
20	J	1046	CLA	C2A-C1A-CHA	-4.72	114.58	122.63
21	A	7026	LMU	O4'-C4B-C5B	4.72	121.02	109.30
21	A	7038	LMU	O2'-C2'-C3'	4.72	121.26	110.35
20	4	1206	CLA	C3D-C4D-CHA	-4.72	115.04	124.98
20	B	1750	CLA	CHD-C4C-C3C	-4.72	117.91	124.84
20	A	1760	CLA	C1-O2A-CGA	4.71	128.81	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1738	CLA	CHD-C4C-NC	4.71	131.63	124.20
20	A	1816	CLA	CHD-C4C-NC	4.71	131.63	124.20
20	K	3009	CLA	CHD-C4C-C3C	-4.71	117.92	124.84
20	B	1763	CLA	CHD-C4C-NC	4.71	131.62	124.20
20	3	1217	CLA	C2A-C1A-CHA	-4.71	114.61	122.63
20	A	1759	CLA	CHD-C4C-C3C	-4.70	117.93	124.84
20	B	1772	CLA	C4A-NA-C1A	4.70	108.82	106.71
20	3	3015	CLA	C4C-CHD-C1D	-4.70	114.50	126.11
20	A	1766	CLA	C4D-C3D-CAD	4.70	113.63	108.10
20	A	1817	CLA	CAC-C3C-C4C	4.69	130.90	124.81
21	A	7026	LMU	O3B-C3B-C2B	4.69	121.19	110.35
20	B	1787	CLA	CHB-C4A-NA	4.69	131.00	124.51
20	2	1216	CLA	C3D-C4D-CHA	-4.69	115.11	124.98
20	K	3009	CLA	CHD-C4C-NC	4.69	131.59	124.20
20	B	1738	CLA	C6-C5-C3	-4.68	101.17	113.45
21	A	7036	LMU	C6B-C5B-C4B	-4.68	102.03	113.00
21	R	1057	LMU	O1'-C1'-C2'	4.68	115.62	108.30
20	4	1207	CLA	C1B-C2B-C3B	-4.68	102.57	106.92
20	B	1748	CLA	CHC-C1C-NC	4.68	131.30	124.20
20	A	1790	CLA	O2D-CGD-CBD	4.68	119.58	111.27
20	2	1218	CLA	CHC-C1C-NC	4.68	131.30	124.20
21	A	7027	LMU	C1B-O1B-C4'	-4.68	106.39	117.96
20	A	1767	CLA	CHD-C4C-NC	4.67	131.56	124.20
20	2	1214	CLA	C3A-C4A-CHB	-4.67	118.19	123.91
20	R	1055	CLA	CHD-C4C-NC	4.67	131.55	124.20
20	B	1770	CLA	C1D-CHD-C4C	-4.66	116.00	126.06
20	1	1193	CLA	CMD-C2D-C3D	-4.66	116.90	127.61
21	A	7027	LMU	O1'-C1'-C2'	4.66	115.58	108.30
22	L	1169	BCR	C38-C26-C27	4.66	122.56	113.62
21	A	7030	LMU	O5'-C1'-C2'	-4.65	100.50	110.35
20	B	1737	CLA	C4A-NA-C1A	4.65	108.80	106.71
20	F	1155	CLA	CHC-C1C-NC	4.65	131.26	124.20
20	3	3015	CLA	CHC-C1C-NC	4.65	131.09	124.23
21	A	7017	LMU	C1'-O5'-C5'	4.64	122.81	113.69
20	3	3002	CLA	CHD-C4C-NC	4.64	131.37	124.21
20	A	1765	CLA	CMD-C2D-C3D	-4.64	116.93	127.61
20	2	1218	CLA	O2D-CGD-O1D	-4.64	114.76	123.84
20	4	1197	CLA	CHD-C4C-C3C	-4.64	117.73	124.98
20	A	1788	CLA	CHD-C4C-NC	4.64	131.51	124.20
22	B	1781	BCR	C37-C22-C23	-4.64	110.77	118.08
20	B	1738	CLA	C4D-C3D-CAD	4.64	113.56	108.10
20	F	1155	CLA	CMD-C2D-C3D	-4.64	116.95	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1779	BCR	C34-C9-C8	4.64	125.38	118.08
20	B	1759	CLA	CHD-C4C-NC	4.63	131.50	124.20
21	A	7042	LMU	O1B-C4'-C5'	4.63	122.14	109.45
22	B	1781	BCR	C30-C25-C26	-4.63	116.09	122.61
20	L	1167	CLA	CHD-C4C-NC	4.63	131.50	124.20
20	2	1223	CLA	CMD-C2D-C1D	4.63	132.87	124.71
20	B	1768	CLA	CHD-C4C-NC	4.62	131.49	124.20
20	1	1187	CLA	CBC-CAC-C3C	-4.62	99.68	112.43
20	A	1798	CLA	CHD-C4C-NC	4.62	131.49	124.20
20	A	1764	CLA	CHD-C4C-NC	4.62	131.49	124.20
20	A	1767	CLA	C1-C2-C3	-4.62	118.05	126.04
20	K	1146	CLA	C1-C2-C3	-4.62	119.28	126.75
20	A	1798	CLA	CHD-C4C-C3C	-4.62	118.05	124.84
20	4	1201	CLA	O2A-CGA-O1A	-4.62	111.94	123.59
20	1	1188	CLA	CED-O2D-CGD	4.62	126.38	115.94
21	K	1086	LMU	C1B-C2B-C3B	4.61	119.60	110.00
20	A	1766	CLA	C1D-CHD-C4C	-4.61	116.11	126.06
20	4	4007	CLA	CHD-C4C-C3C	-4.61	118.06	124.84
20	B	1787	CLA	CHD-C4C-NC	4.61	131.47	124.20
20	L	1168	CLA	C4D-C3D-CAD	4.61	113.53	108.10
20	B	1762	CLA	CHD-C4C-NC	4.61	131.46	124.20
20	F	1155	CLA	CAB-C3B-C4B	-4.61	121.39	128.46
20	1	1196	CLA	CHD-C4C-NC	4.60	131.46	124.20
20	G	1099	CLA	CHD-C4C-C3C	-4.60	118.07	124.84
22	3	1220	BCR	C16-C15-C14	-4.60	114.05	123.47
20	B	1760	CLA	C1D-CHD-C4C	-4.60	116.13	126.06
20	2	1227	CLA	C3A-C4A-CHB	-4.60	118.28	123.91
20	B	1762	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
20	1	1200	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
20	A	1800	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
20	1	1193	CLA	C4A-NA-C1A	4.59	108.77	106.71
20	J	1045	CLA	O2D-CGD-CBD	4.59	119.42	111.27
20	A	1775	CLA	CHD-C4C-C3C	-4.58	117.82	124.98
20	3	1215	CLA	C4A-NA-C1A	4.58	108.76	106.71
22	L	1169	BCR	C3-C4-C5	-4.58	105.91	114.08
20	A	1786	CLA	CHC-C1C-NC	4.58	131.15	124.20
20	L	1505	CLA	CHD-C4C-NC	4.57	131.41	124.20
20	2	1221	CLA	CHD-C4C-NC	4.57	131.26	124.21
20	A	1760	CLA	O2A-CGA-CBA	4.57	126.25	111.91
20	1	1189	CLA	O2D-CGD-O1D	-4.57	114.91	123.84
20	1	1187	CLA	CHC-C1C-NC	4.57	131.13	124.20
20	1	1188	CLA	CHC-C1C-NC	4.57	131.13	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1745	CLA	C4D-C3D-CAD	4.57	113.48	108.10
20	1	1201	CLA	C4C-CHD-C1D	-4.56	114.82	126.11
20	3	3015	CLA	CHD-C4C-NC	4.56	131.25	124.21
20	B	1738	CLA	CHB-C4A-NA	4.56	130.82	124.51
20	A	1813	CLA	C1-C2-C3	4.56	133.93	126.04
20	B	1769	CLA	CHD-C4C-C3C	-4.56	118.14	124.84
22	B	1779	BCR	C8-C7-C6	-4.56	114.40	127.20
20	A	1801	CLA	C4A-NA-C1A	4.56	108.75	106.71
20	B	1769	CLA	CHC-C1C-NC	4.56	131.11	124.20
20	3	3001	CLA	CHD-C4C-NC	4.56	131.24	124.21
20	B	1762	CLA	O2D-CGD-O1D	-4.55	114.93	123.84
20	H	1079	CLA	CHD-C4C-NC	4.55	131.38	124.20
20	J	1046	CLA	CHC-C1C-NC	4.55	130.95	124.23
21	A	7038	LMU	O5'-C5'-C6'	4.55	117.75	106.44
20	2	1223	CLA	CHD-C4C-C3C	-4.55	118.16	124.84
20	I	1031	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
20	A	1783	CLA	C1-C2-C3	-4.54	118.19	126.04
20	4	4007	CLA	CHC-C1C-NC	4.54	131.09	124.20
20	A	1773	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
20	A	1790	CLA	CMD-C2D-C3D	-4.54	117.17	127.61
20	B	1739	CLA	OBD-CAD-C3D	-4.54	117.59	128.52
20	4	4007	CLA	O2D-CGD-CBD	4.54	119.33	111.27
20	A	1812	CLA	C4D-C3D-CAD	4.54	113.45	108.10
20	3	3015	CLA	C3A-C4A-CHB	-4.53	118.36	123.91
20	4	1205	CLA	C3B-C2B-C1B	-4.53	102.41	106.29
20	2	1219	CLA	CHA-C4D-ND	4.53	128.89	124.52
20	3	1213	CLA	C3A-C4A-CHB	-4.53	118.36	123.91
20	B	1785	CLA	C1D-CHD-C4C	-4.52	116.30	126.06
22	L	1170	BCR	C16-C17-C18	-4.52	120.86	127.31
20	3	1212	CLA	C4D-C3D-CAD	4.52	113.42	108.10
20	B	1747	CLA	CHC-C1C-NC	4.52	131.06	124.20
20	B	1768	CLA	CHC-C1C-NC	4.52	131.06	124.20
20	A	1817	CLA	O2D-CGD-O1D	-4.52	115.01	123.84
20	F	1155	CLA	C4B-C3B-C2B	4.51	111.12	106.92
21	A	7032	LMU	O5B-C5B-C4B	-4.51	101.50	109.69
20	2	1219	CLA	C3A-C4A-CHB	-4.51	118.39	123.91
20	R	1055	CLA	O2A-C1-C2	4.51	120.48	108.64
20	A	1784	CLA	CHD-C4C-NC	4.51	131.30	124.20
20	A	1813	CLA	CMD-C2D-C3D	-4.51	117.25	127.61
20	R	1055	CLA	CHD-C4C-C3C	-4.51	118.22	124.84
20	B	1753	CLA	CAA-C2A-C1A	-4.50	97.22	111.97
20	A	1768	CLA	O2D-CGD-CBD	4.50	119.27	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1785	CLA	CHC-C1C-NC	4.50	131.03	124.20
20	H	1079	CLA	O2D-CGD-CBD	4.50	119.26	111.27
20	2	1222	CLA	CMD-C2D-C3D	-4.50	117.27	127.61
20	A	1762	CLA	CHD-C4C-NC	4.50	131.29	124.20
20	B	1744	CLA	CHD-C4C-NC	4.49	131.28	124.20
20	4	1203	CLA	CHD-C4C-NC	4.49	131.14	124.21
20	B	1755	CLA	CHD-C4C-C3C	-4.49	118.24	124.84
20	4	1208	CLA	C4C-CHD-C1D	-4.49	115.01	126.11
20	B	1758	CLA	CHD-C4C-NC	4.49	131.28	124.20
20	4	1196	CLA	CHD-C4C-C3C	-4.49	118.25	124.84
20	F	1156	CLA	CHD-C4C-C3C	-4.49	118.25	124.84
20	1	1201	CLA	CHD-C4C-NC	4.48	131.12	124.21
20	B	1768	CLA	CMD-C2D-C3D	-4.48	117.31	127.61
20	K	1146	CLA	CMD-C2D-C3D	-4.48	117.31	127.61
20	4	1203	CLA	CHD-C1D-ND	4.48	128.84	124.52
20	4	1206	CLA	C4C-CHD-C1D	-4.48	115.04	126.11
20	2	1214	CLA	CHC-C1C-NC	4.48	130.84	124.23
20	A	1816	CLA	C1B-CHB-C4A	-4.47	121.26	130.12
20	3	3002	CLA	CHC-C1C-NC	4.47	130.84	124.23
20	1	1201	CLA	C3D-C4D-CHA	-4.47	115.56	124.98
20	B	1741	CLA	CHD-C4C-NC	4.47	131.25	124.20
20	3	1214	CLA	C4A-NA-C1A	4.47	108.72	106.71
20	4	1203	CLA	C4A-NA-C1A	4.47	108.72	106.71
20	B	1754	CLA	C4D-C3D-CAD	4.47	113.36	108.10
20	B	1756	CLA	CHD-C4C-C3C	-4.47	118.27	124.84
20	A	1765	CLA	CHC-C1C-C2C	-4.47	114.36	126.72
20	A	1761	CLA	C4A-NA-C1A	4.47	108.71	106.71
20	K	1085	CLA	CHD-C4C-C3C	-4.47	118.28	124.84
20	B	1763	CLA	O1D-CGD-CBD	-4.47	115.35	124.48
20	1	1193	CLA	CHD-C4C-C3C	-4.46	118.28	124.84
20	B	1752	CLA	CMD-C2D-C3D	-4.46	117.35	127.61
20	B	1772	CLA	CAA-C2A-C3A	-4.46	105.69	116.10
20	A	1791	CLA	CHD-C4C-C3C	-4.46	118.29	124.84
21	A	7042	LMU	C4B-C3B-C2B	-4.46	103.04	110.82
20	A	1797	CLA	CHD-C4C-C3C	-4.46	118.29	124.84
20	A	1760	CLA	CMD-C2D-C3D	-4.45	117.37	127.61
20	1	1189	CLA	CGD-CBD-CAD	-4.45	96.31	110.73
20	A	1760	CLA	CHC-C1C-NC	4.45	130.96	124.20
20	A	1789	CLA	C4-C3-C5	4.45	122.76	115.27
20	B	1753	CLA	CMD-C2D-C1D	4.45	132.55	124.71
20	A	1793	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
20	3	1217	CLA	C3A-C4A-CHB	-4.45	118.46	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1783	CLA	CMD-C2D-C3D	-4.45	117.38	127.61
20	R	1054	CLA	O2D-CGD-CBD	4.45	119.17	111.27
20	1	1193	CLA	CHD-C4C-NC	4.44	131.21	124.20
20	3	1219	CLA	CHD-C4C-C3C	-4.44	118.31	124.84
21	A	7040	LMU	O3'-C3'-C2'	-4.44	100.08	110.35
20	3	1216	CLA	C4C-CHD-C1D	-4.44	115.13	126.11
22	L	1170	BCR	C37-C22-C21	-4.44	116.70	122.92
20	A	1794	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
20	4	4014	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
20	J	1043	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
20	B	1735	CLA	CHD-C4C-C3C	-4.43	118.32	124.84
20	A	1795	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
20	B	1743	CLA	CHC-C1C-NC	4.43	130.92	124.20
20	B	1739	CLA	CHC-C1C-NC	4.43	130.92	124.20
20	4	1207	CLA	CBD-CHA-C1A	4.43	134.52	127.43
21	A	7038	LMU	O1B-C4'-C3'	4.42	119.05	107.28
20	B	1736	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
20	K	1142	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
20	B	1736	CLA	CHC-C1C-NC	4.42	130.91	124.20
20	3	3015	CLA	C2A-C1A-CHA	-4.42	115.10	122.63
20	2	1215	CLA	O2D-CGD-CBD	4.42	119.12	111.27
21	A	7037	LMU	O1'-C1'-C2'	-4.42	101.41	108.30
20	A	1781	CLA	CHD-C4C-C3C	-4.42	118.35	124.84
20	B	1747	CLA	C4D-C3D-CAD	4.42	113.30	108.10
20	A	1796	CLA	CHD-C4C-C3C	-4.42	118.35	124.84
20	A	1760	CLA	CHD-C4C-C3C	-4.41	118.35	124.84
20	B	1759	CLA	CHD-C4C-C3C	-4.41	118.35	124.84
20	A	1792	CLA	CHD-C4C-C3C	-4.41	118.35	124.84
20	A	1800	CLA	C4A-NA-C1A	4.41	108.69	106.71
20	A	1778	CLA	CHC-C1C-NC	4.41	130.90	124.20
20	A	1782	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
20	B	1737	CLA	CHB-C4A-NA	4.41	130.61	124.51
20	A	1777	CLA	CHD-C4C-NC	4.41	131.15	124.20
20	3	3008	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
20	2	1212	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
20	A	1764	CLA	O2D-CGD-O1D	-4.40	115.24	123.84
20	A	1787	CLA	CMB-C2B-C3B	4.40	132.91	124.68
20	2	1214	CLA	C2A-C1A-CHA	-4.39	115.14	122.63
20	B	1757	CLA	O1D-CGD-CBD	-4.39	115.50	124.48
20	4	1204	CLA	C4A-NA-C1A	4.39	108.68	106.71
20	A	1800	CLA	C1-C2-C3	-4.39	118.45	126.04
20	B	1753	CLA	C1D-CHD-C4C	-4.39	116.59	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	3001	CLA	C2A-C1A-CHA	-4.39	115.15	122.63
20	2	1217	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
20	B	1770	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
20	2	2010	CLA	CHD-C4C-NC	4.39	130.98	124.21
20	I	1031	CLA	C4D-C3D-CAD	4.38	113.26	108.10
20	1	1189	CLA	CHD-C4C-NC	4.38	131.11	124.20
20	2	1222	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
20	A	1774	CLA	CHD-C4C-C3C	-4.38	118.40	124.84
21	L	1171	LMU	C3B-C4B-C5B	4.38	118.05	110.24
20	1	1200	CLA	O2A-CGA-O1A	-4.38	112.54	123.59
20	4	1203	CLA	CHC-C1C-NC	4.38	130.69	124.23
20	A	1769	CLA	C4A-NA-C1A	4.38	108.67	106.71
20	A	1773	CLA	CHD-C4C-NC	4.38	131.10	124.20
20	A	1815	CLA	CED-O2D-CGD	4.38	125.84	115.94
20	B	1772	CLA	CHD-C4C-NC	4.38	131.10	124.20
20	G	1099	CLA	C4-C3-C5	4.38	120.98	115.98
20	3	1215	CLA	C3B-C2B-C1B	-4.38	102.54	106.29
21	A	7024	LMU	O5B-C1B-C2B	4.37	119.61	110.35
20	B	1771	CLA	O2A-CGA-CBA	4.37	125.62	111.91
20	A	1764	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
20	A	1786	CLA	C4D-C3D-CAD	4.37	113.25	108.10
20	B	1752	CLA	CHC-C1C-NC	4.36	130.82	124.20
20	4	1206	CLA	CHD-C1D-ND	4.36	128.73	124.52
20	B	1745	CLA	CHD-C4C-NC	4.36	131.08	124.20
20	2	2010	CLA	C3A-C4A-CHB	-4.36	118.57	123.91
20	A	1777	CLA	CMD-C2D-C3D	-4.36	117.58	127.61
20	B	1746	CLA	CHD-C4C-C3C	-4.36	118.43	124.84
20	2	1219	CLA	C2A-C1A-CHA	-4.36	115.20	122.63
20	1	1189	CLA	CHD-C4C-C3C	-4.36	118.43	124.84
20	R	1054	CLA	O2A-CGA-CBA	4.36	125.58	111.91
20	B	1742	CLA	C4A-NA-C1A	4.36	108.66	106.71
21	A	1810	LMU	C3B-C4B-C5B	-4.35	102.47	110.24
21	A	7033	LMU	O1B-C4'-C5'	-4.35	97.52	109.45
20	J	1046	CLA	CHD-C4C-NC	4.35	130.92	124.21
22	I	1032	BCR	C7-C6-C5	4.35	132.00	121.46
20	J	1046	CLA	C4C-CHD-C1D	-4.35	115.36	126.11
20	B	1754	CLA	O2D-CGD-O1D	-4.35	115.34	123.84
20	B	1787	CLA	CGD-CBD-CAD	4.35	124.81	110.73
20	B	1769	CLA	C4D-C3D-CAD	4.34	113.21	108.10
20	1	1196	CLA	CMD-C2D-C3D	-4.34	117.63	127.61
20	A	1766	CLA	CHC-C1C-NC	4.34	130.79	124.20
20	A	1771	CLA	CHD-C4C-NC	4.34	131.04	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	1209	CLA	CGD-CBD-CAD	-4.34	96.69	110.73
20	B	1785	CLA	C4A-NA-C1A	4.34	108.66	106.71
20	3	3008	CLA	CHC-C1C-NC	4.33	130.78	124.20
21	A	7042	LMU	C1'-O5'-C5'	-4.33	105.19	113.69
21	A	7015	LMU	O1'-C1'-C2'	4.33	115.06	108.30
20	4	1205	CLA	CHC-C1C-NC	4.33	130.62	124.23
20	B	1750	CLA	CMD-C2D-C3D	-4.32	117.67	127.61
20	2	1220	CLA	CMD-C2D-C3D	-4.32	117.67	127.61
20	4	1203	CLA	C3D-C4D-CHA	-4.32	115.88	124.98
20	A	1759	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
20	B	1786	CLA	C4D-C3D-CAD	4.32	113.19	108.10
20	A	1779	CLA	CHD-C4C-NC	4.32	131.01	124.20
20	1	1196	CLA	CHD-C4C-C3C	-4.32	118.23	124.98
20	B	1760	CLA	C1-O2A-CGA	4.32	127.77	116.44
20	1	1187	CLA	CED-O2D-CGD	4.32	125.70	115.94
21	A	7013	LMU	C4B-C3B-C2B	-4.32	103.29	110.82
21	A	7035	LMU	C3'-C4'-C5'	-4.31	101.03	110.93
22	B	1776	BCR	C30-C25-C26	-4.31	116.54	122.61
20	B	1743	CLA	O2D-CGD-CBD	4.31	118.93	111.27
20	3	3007	CLA	CHC-C1C-NC	4.31	130.75	124.20
21	A	7032	LMU	C2'-C3'-C4'	4.31	119.53	109.68
20	A	1780	CLA	C4-C3-C5	4.31	122.52	115.27
22	B	1776	BCR	C37-C22-C21	-4.30	116.89	122.92
20	B	1766	CLA	CHD-C4C-NC	4.30	130.98	124.20
20	1	1194	CLA	CHD-C4C-NC	4.30	130.85	124.21
20	4	1202	CLA	C4A-NA-C1A	4.30	108.64	106.71
20	B	1757	CLA	CMD-C2D-C3D	-4.30	117.72	127.61
20	A	1812	CLA	CAA-C2A-C1A	4.30	126.06	111.97
20	F	1156	CLA	CHC-C1C-NC	4.30	130.72	124.20
22	B	1776	BCR	C8-C9-C10	4.30	125.53	118.94
20	A	1766	CLA	CHD-C4C-NC	4.29	130.96	124.20
20	J	1045	CLA	CHC-C1C-NC	4.29	130.71	124.20
21	A	7034	LMU	O1'-C1'-C2'	4.28	114.99	108.30
20	B	1740	CLA	CHD-C4C-C3C	-4.28	118.55	124.84
20	3	1217	CLA	CHA-C4D-ND	4.28	128.65	124.52
20	4	1199	CLA	CMD-C2D-C3D	-4.28	117.77	127.61
20	3	3014	CLA	C4A-NA-C1A	4.28	108.63	106.71
20	B	1742	CLA	O2D-CGD-CBD	4.27	118.86	111.27
20	B	1757	CLA	O2A-CGA-CBA	4.27	125.32	111.91
20	4	1199	CLA	CAC-C3C-C4C	4.27	130.35	124.81
20	R	1054	CLA	CHD-C4C-NC	4.27	130.93	124.20
20	3	1219	CLA	CHC-C1C-NC	4.27	130.68	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	7037	LMU	O3B-C3B-C2B	4.27	120.21	110.35
20	B	1752	CLA	CHD-C4C-NC	4.27	130.92	124.20
20	A	1817	CLA	O2A-CGA-CBA	4.26	125.29	111.91
20	L	1168	CLA	O2D-CGD-O1D	-4.26	115.50	123.84
20	2	1220	CLA	CHC-C1C-NC	4.26	130.67	124.20
20	L	1505	CLA	CHD-C4C-C3C	-4.26	118.58	124.84
20	4	1206	CLA	C2D-C3D-C4D	-4.26	102.56	107.28
21	A	7038	LMU	C2'-C3'-C4'	-4.26	99.96	109.68
21	A	7016	LMU	O1'-C1'-C2'	4.26	114.95	108.30
20	4	1201	CLA	CMD-C2D-C3D	-4.26	117.83	127.61
20	A	1798	CLA	C4-C3-C5	4.26	122.43	115.27
21	A	7040	LMU	O1'-C1'-C2'	4.25	114.94	108.30
20	1	1191	CLA	CHD-C4C-C3C	-4.25	118.34	124.98
20	B	1771	CLA	CHD-C4C-C3C	-4.25	118.60	124.84
20	F	1157	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
22	3	1220	BCR	C38-C26-C25	-4.25	119.76	124.53
20	3	1216	CLA	CHD-C4C-NC	4.25	130.76	124.21
21	A	7042	LMU	O1'-C1'-C2'	4.24	114.93	108.30
20	3	1218	CLA	C4D-C3D-CAD	4.24	113.10	108.10
20	R	1055	CLA	O2A-CGA-CBA	4.24	125.23	111.91
20	A	1767	CLA	C4A-NA-C1A	4.24	108.61	106.71
20	1	1190	CLA	CHD-C4C-C3C	-4.24	118.61	124.84
20	3	1216	CLA	CHC-C1C-NC	4.24	130.49	124.23
20	F	1155	CLA	CMB-C2B-C3B	4.24	132.99	124.69
20	B	1759	CLA	CHC-C1C-NC	4.24	130.63	124.20
20	3	3014	CLA	C4C-CHD-C1D	-4.24	115.63	126.11
20	B	1756	CLA	CHC-C1C-NC	4.24	130.63	124.20
22	I	1032	BCR	C27-C26-C25	-4.24	116.58	122.73
20	J	1046	CLA	C3A-C4A-CHB	-4.24	118.72	123.91
20	2	2010	CLA	CHC-C1C-NC	4.24	130.49	124.23
20	K	1142	CLA	CHC-C1C-NC	4.23	130.62	124.20
20	B	1755	CLA	CHC-C1C-NC	4.23	130.62	124.20
20	4	1205	CLA	C2A-C1A-CHA	-4.23	115.42	122.63
20	1	1200	CLA	CGD-CBD-CAD	-4.23	97.03	110.73
20	2	1227	CLA	C3D-C4D-CHA	-4.23	116.07	124.98
20	A	1782	CLA	CHC-C1C-NC	4.22	130.61	124.20
20	4	1201	CLA	C2A-C3A-C4A	-4.22	95.05	101.87
20	B	1786	CLA	CHB-C4A-NA	4.22	130.35	124.51
20	4	4003	CLA	C2A-C1A-CHA	-4.22	115.44	122.63
20	A	1769	CLA	C1-C2-C3	-4.22	118.75	126.04
20	A	1764	CLA	CAA-C2A-C1A	-4.22	98.15	111.97
20	1	1187	CLA	CGD-CBD-CAD	-4.22	97.08	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	1212	CLA	CHC-C1C-NC	4.22	130.60	124.20
20	B	1735	CLA	CHC-C1C-NC	4.21	130.59	124.20
20	3	1218	CLA	C4A-NA-C1A	4.21	108.60	106.71
20	1	1190	CLA	CMD-C2D-C3D	-4.21	117.93	127.61
20	B	1745	CLA	CHD-C4C-C3C	-4.21	118.65	124.84
20	4	1202	CLA	CHD-C4C-NC	4.21	130.70	124.21
20	B	1742	CLA	CHD-C4C-NC	4.21	130.83	124.20
20	B	1755	CLA	CMD-C2D-C3D	-4.21	117.93	127.61
20	1	1190	CLA	O2D-CGD-O1D	-4.21	115.61	123.84
20	3	3002	CLA	C3A-C4A-CHB	-4.21	118.76	123.91
20	3	3008	CLA	C1-C2-C3	-4.21	119.94	126.75
20	B	1758	CLA	CMD-C2D-C1D	4.21	132.13	124.71
20	A	1815	CLA	CHC-C1C-NC	4.21	130.59	124.20
20	A	1796	CLA	CHC-C1C-NC	4.21	130.58	124.20
20	A	1794	CLA	CHC-C1C-NC	4.21	130.58	124.20
20	A	1795	CLA	CHC-C1C-NC	4.21	130.58	124.20
20	A	1771	CLA	CHC-C1C-NC	4.20	130.58	124.20
20	A	1781	CLA	CMD-C2D-C3D	-4.20	117.94	127.61
20	3	1217	CLA	CHD-C4C-NC	4.20	130.69	124.21
21	A	7016	LMU	C1-O1'-C1'	-4.20	106.88	113.84
20	A	1775	CLA	CMD-C2D-C3D	-4.20	117.95	127.61
20	2	1213	CLA	CHC-C1C-NC	4.20	130.57	124.20
20	B	1756	CLA	CMD-C2D-C3D	-4.20	117.96	127.61
20	A	1784	CLA	CHC-C1C-NC	4.20	130.57	124.20
20	3	3011	CLA	C4D-C3D-CAD	4.20	113.04	108.10
20	A	1797	CLA	CMD-C2D-C3D	-4.20	117.96	127.61
20	A	1791	CLA	CHC-C1C-NC	4.20	130.57	124.20
20	3	3014	CLA	C3D-C4D-CHA	-4.19	116.15	124.98
20	A	1793	CLA	CHC-C1C-NC	4.19	130.57	124.20
20	K	1142	CLA	CMD-C2D-C3D	-4.19	117.97	127.61
20	K	1146	CLA	O2D-CGD-O1D	-4.19	115.64	123.84
21	A	7047	LMU	O1'-C1'-C2'	4.19	114.85	108.30
20	A	1791	CLA	CMD-C2D-C3D	-4.19	117.97	127.61
22	A	1805	BCR	C7-C8-C9	-4.19	119.90	126.23
20	1	1199	CLA	CHD-C4C-NC	4.19	130.68	124.21
20	A	1792	CLA	CHC-C1C-NC	4.19	130.56	124.20
20	A	1797	CLA	CHC-C1C-NC	4.19	130.56	124.20
20	2	2010	CLA	C2A-C1A-CHA	-4.19	115.48	122.63
20	B	1766	CLA	CMD-C2D-C3D	-4.19	117.97	127.61
20	2	1222	CLA	CAC-C3C-C4C	4.19	130.25	124.81
22	A	1803	BCR	C24-C23-C22	-4.19	119.90	126.23
20	4	1206	CLA	C3A-C4A-CHB	-4.19	118.78	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1808	BCR	C7-C8-C9	-4.19	119.91	126.23
20	A	1796	CLA	CMD-C2D-C3D	-4.19	117.98	127.61
20	A	1778	CLA	CHD-C4C-NC	4.19	130.80	124.20
20	4	1201	CLA	O2A-CGA-CBA	4.19	125.05	111.91
20	3	1214	CLA	CHA-C4D-ND	4.19	128.56	124.52
20	K	1085	CLA	CHC-C1C-NC	4.19	130.55	124.20
20	A	1765	CLA	O2D-CGD-O1D	-4.19	115.66	123.84
20	4	1207	CLA	CAC-C3C-C4C	4.18	131.41	125.04
22	A	1804	BCR	C7-C8-C9	-4.18	119.91	126.23
20	A	1793	CLA	CMD-C2D-C3D	-4.18	117.99	127.61
20	3	1213	CLA	C4C-CHD-C1D	-4.18	115.77	126.11
20	B	1735	CLA	CMD-C2D-C3D	-4.18	118.00	127.61
20	A	1792	CLA	CMD-C2D-C3D	-4.18	118.00	127.61
20	A	1794	CLA	CMD-C2D-C3D	-4.18	118.00	127.61
20	2	1214	CLA	C2D-C3D-C4D	-4.18	102.65	107.28
20	4	1196	CLA	CMD-C2D-C3D	-4.18	118.00	127.61
20	A	1795	CLA	CMD-C2D-C3D	-4.18	118.00	127.61
20	A	1776	CLA	CHD-C4C-NC	4.18	130.78	124.20
20	F	1157	CLA	CHD-C4C-NC	4.17	130.78	124.20
20	2	1212	CLA	CMD-C2D-C3D	-4.17	118.01	127.61
20	A	1781	CLA	CHC-C1C-NC	4.17	130.53	124.20
20	4	1198	CLA	C1-O2A-CGA	-4.17	105.51	116.44
20	1	1190	CLA	CHD-C4C-NC	4.17	130.77	124.20
20	4	4014	CLA	CMD-C2D-C3D	-4.17	118.03	127.61
20	A	1815	CLA	CHB-C4A-NA	4.16	130.27	124.51
22	B	1780	BCR	C38-C26-C25	-4.16	119.86	124.53
20	B	1746	CLA	CHC-C1C-NC	4.16	130.52	124.20
20	A	1784	CLA	CMD-C2D-C1D	4.16	132.05	124.71
20	4	1200	CLA	CHD-C4C-NC	4.16	130.76	124.20
20	4	1207	CLA	CHD-C4C-NC	4.16	130.76	124.20
20	3	3007	CLA	CMD-C2D-C3D	-4.16	118.04	127.61
21	A	7019	LMU	C2'-C3'-C4'	4.16	119.17	109.68
20	4	4014	CLA	CHC-C1C-NC	4.16	130.51	124.20
20	A	1782	CLA	CMD-C2D-C3D	-4.16	118.05	127.61
20	J	1043	CLA	CMD-C2D-C3D	-4.16	118.05	127.61
20	3	1219	CLA	CMD-C2D-C3D	-4.16	118.05	127.61
20	3	3001	CLA	C3B-C2B-C1B	-4.15	102.73	106.29
22	B	1774	BCR	C7-C8-C9	-4.15	119.96	126.23
20	4	1206	CLA	C4A-NA-C1A	4.15	108.57	106.71
20	A	1768	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
23	A	1802	PQN	C14-C13-C15	4.15	122.25	115.27
20	B	1785	CLA	CHD-C4C-NC	4.15	130.74	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1780	BCR	C24-C23-C22	-4.15	119.96	126.23
22	B	1778	BCR	C24-C23-C22	-4.15	119.97	126.23
22	B	1781	BCR	C38-C26-C27	4.15	121.59	113.62
20	A	1815	CLA	CAA-C2A-C3A	-4.15	101.42	112.78
22	B	1775	BCR	C24-C23-C22	-4.15	119.97	126.23
20	K	1085	CLA	CMD-C2D-C3D	-4.15	118.07	127.61
22	B	1777	BCR	C7-C8-C9	-4.15	119.97	126.23
20	F	1156	CLA	CMD-C2D-C3D	-4.15	118.08	127.61
22	A	1806	BCR	C24-C23-C22	-4.14	119.97	126.23
22	A	1803	BCR	C7-C8-C9	-4.14	119.97	126.23
20	2	1214	CLA	C4A-NA-C1A	4.14	108.57	106.71
20	4	1196	CLA	CHC-C1C-NC	4.14	130.48	124.20
22	A	1805	BCR	C24-C23-C22	-4.14	119.98	126.23
22	B	1780	BCR	C7-C8-C9	-4.14	119.98	126.23
22	3	1220	BCR	C11-C12-C13	-4.14	114.80	126.42
20	J	1043	CLA	CHC-C1C-NC	4.13	130.48	124.20
21	A	7023	LMU	O3'-C3'-C2'	-4.13	100.79	110.35
20	A	1774	CLA	CHC-C1C-NC	4.13	130.47	124.20
20	4	1197	CLA	CMD-C2D-C3D	-4.13	118.10	127.61
20	1	1188	CLA	CMD-C2D-C3D	-4.13	118.11	127.61
20	2	1217	CLA	C4A-NA-C1A	4.13	108.56	106.71
20	3	3014	CLA	CHD-C4C-NC	4.13	130.58	124.21
20	B	1741	CLA	C1B-C2B-C3B	-4.13	103.08	106.92
21	A	7037	LMU	C1B-O1B-C4'	-4.13	107.74	117.96
22	B	1776	BCR	C34-C9-C10	-4.13	117.14	122.92
20	A	1762	CLA	CHC-C1C-NC	4.13	130.47	124.20
20	J	1044	CLA	CAC-C3C-C4C	4.13	130.16	124.81
21	A	7036	LMU	O3B-C3B-C4B	-4.12	100.82	110.35
22	A	1807	BCR	C24-C23-C22	-4.12	120.00	126.23
20	4	4003	CLA	C3A-C4A-CHB	-4.12	118.86	123.91
20	B	1742	CLA	CMD-C2D-C3D	-4.12	118.13	127.61
20	3	1214	CLA	C3B-C2B-C1B	-4.12	102.76	106.29
20	4	1199	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
20	2	1214	CLA	C3B-C2B-C1B	-4.12	102.76	106.29
22	B	1778	BCR	C7-C8-C9	-4.12	120.01	126.23
21	A	7022	LMU	C6B-C5B-C4B	-4.12	103.36	113.00
20	A	1767	CLA	CAA-C2A-C3A	-4.12	101.51	112.78
20	2	1218	CLA	C6-C5-C3	-4.12	102.66	113.45
22	A	1807	BCR	C33-C5-C6	-4.11	119.91	124.53
22	B	1775	BCR	C7-C8-C9	-4.11	120.02	126.23
20	A	1784	CLA	C4D-C3D-CAD	4.11	112.94	108.10
22	A	1803	BCR	C38-C26-C25	-4.11	119.91	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	4003	CLA	C4C-CHD-C1D	-4.11	115.94	126.11
20	A	1778	CLA	CAA-C2A-C1A	4.11	121.24	112.14
20	B	1742	CLA	CHC-C1C-NC	4.11	130.44	124.20
20	4	1209	CLA	C4A-NA-C1A	4.11	108.55	106.71
21	A	7021	LMU	C1B-O5B-C5B	4.11	121.75	113.69
20	B	1786	CLA	CHD-C4C-C3C	-4.11	118.80	124.84
20	4	1198	CLA	C1-C2-C3	-4.11	118.94	126.04
20	A	1785	CLA	CHD-C4C-C3C	-4.11	118.81	124.84
20	B	1758	CLA	O2D-CGD-O1D	-4.11	115.81	123.84
20	L	1167	CLA	CHC-C1C-NC	4.10	130.43	124.20
20	2	1215	CLA	CMD-C2D-C3D	-4.10	118.18	127.61
22	A	1807	BCR	C7-C8-C9	-4.10	120.04	126.23
22	A	1804	BCR	C38-C26-C25	-4.10	119.92	124.53
20	4	1208	CLA	C2B-C1B-NB	4.10	113.70	110.11
20	A	1773	CLA	CMD-C2D-C3D	-4.10	118.19	127.61
20	1	1199	CLA	C4A-NA-C1A	4.10	108.55	106.71
20	K	1146	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
21	A	7027	LMU	C6B-C5B-C4B	4.10	122.60	113.00
20	2	1224	CLA	CHD-C4C-C3C	-4.09	118.82	124.84
21	A	7042	LMU	C1B-O1B-C4'	-4.09	107.83	117.96
20	3	1218	CLA	CHC-C1C-NC	4.09	130.41	124.20
20	A	1790	CLA	CHD-C4C-NC	4.09	130.65	124.20
21	A	7037	LMU	O1B-C1B-C2B	4.09	118.70	108.10
20	B	1761	CLA	O2A-C1-C2	4.09	119.39	108.64
20	A	1776	CLA	CHC-C1C-NC	4.09	130.41	124.20
22	B	1777	BCR	C24-C23-C22	-4.09	120.06	126.23
22	A	1806	BCR	C7-C8-C9	-4.09	120.06	126.23
20	B	1748	CLA	CMD-C2D-C1D	4.09	131.91	124.71
20	1	1197	CLA	CAA-C2A-C1A	-4.08	98.60	111.97
20	4	1204	CLA	CMD-C2D-C3D	-4.08	118.23	127.61
20	2	1223	CLA	CHD-C4C-NC	4.08	130.63	124.20
20	3	1216	CLA	C2A-C1A-CHA	-4.08	115.67	122.63
20	A	1778	CLA	CMD-C2D-C3D	-4.08	118.23	127.61
21	A	7047	LMU	O1B-C4'-C5'	4.08	120.62	109.45
22	A	1805	BCR	C33-C5-C6	-4.08	119.95	124.53
22	A	1806	BCR	C38-C26-C25	-4.08	119.95	124.53
20	B	1787	CLA	CMD-C2D-C3D	-4.08	118.23	127.61
20	L	1167	CLA	CHB-C4A-NA	4.08	130.15	124.51
22	A	1808	BCR	C24-C23-C22	-4.08	120.07	126.23
20	3	3007	CLA	CAC-C3C-C4C	4.08	130.10	124.81
20	4	1203	CLA	C3A-C4A-CHB	-4.08	118.92	123.91
20	2	1216	CLA	C4C-CHD-C1D	-4.08	116.03	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1808	BCR	C38-C26-C25	-4.08	119.95	124.53
20	F	1155	CLA	C4A-NA-C1A	4.07	108.54	106.71
21	A	7038	LMU	C1B-O5B-C5B	4.07	121.69	113.69
20	A	1764	CLA	CMD-C2D-C3D	-4.07	118.24	127.61
20	4	1209	CLA	C4D-C3D-CAD	4.07	112.90	108.10
20	2	1217	CLA	CHC-C1C-NC	4.07	130.38	124.20
22	A	1806	BCR	C33-C5-C6	-4.07	119.96	124.53
20	L	1505	CLA	CHC-C1C-NC	4.07	130.38	124.20
20	B	1747	CLA	CHD-C4C-NC	4.07	130.61	124.20
20	A	1777	CLA	CHD-C4C-C3C	-4.07	118.86	124.84
20	B	1786	CLA	CAC-C3C-C4C	4.06	130.08	124.81
20	4	1198	CLA	C11-C10-C8	-4.06	102.78	115.92
20	4	1197	CLA	CAA-C2A-C3A	-4.06	106.61	116.10
20	A	1801	CLA	O2D-CGD-O1D	-4.06	115.89	123.84
20	A	1772	CLA	CHD-C4C-C3C	-4.06	118.87	124.84
20	A	1780	CLA	CMD-C2D-C3D	-4.06	118.27	127.61
20	3	3002	CLA	C4A-NA-C1A	4.06	108.53	106.71
20	L	1167	CLA	CMD-C2D-C3D	-4.06	118.27	127.61
20	A	1800	CLA	CHD-C4C-NC	4.06	130.60	124.20
20	2	1224	CLA	CHD-C4C-NC	4.06	130.60	124.20
20	3	3014	CLA	CHC-C1C-NC	4.06	130.22	124.23
20	I	1033	CLA	CHC-C1C-NC	4.06	130.36	124.20
22	B	1774	BCR	C33-C5-C6	-4.06	119.97	124.53
20	A	1762	CLA	CHD-C4C-C3C	-4.06	118.88	124.84
20	B	1766	CLA	CHD-C4C-C3C	-4.06	118.88	124.84
20	A	1811	CLA	CED-O2D-CGD	4.06	125.11	115.94
20	4	1202	CLA	CHC-C1C-NC	4.05	130.21	124.23
24	B	1783	LMG	O7-C10-C11	4.05	120.23	111.50
20	2	1219	CLA	C2D-C3D-C4D	-4.05	102.79	107.28
20	4	1208	CLA	C3A-C4A-CHB	-4.05	118.95	123.91
20	K	3009	CLA	O2D-CGD-O1D	-4.05	115.92	123.84
20	A	1767	CLA	C11-C12-C13	-4.05	102.83	115.92
20	B	1787	CLA	CHD-C4C-C3C	-4.05	118.89	124.84
20	3	1212	CLA	CHC-C1C-NC	4.05	130.34	124.20
20	B	1772	CLA	CHD-C4C-C3C	-4.05	118.66	124.98
22	A	1804	BCR	C24-C23-C22	-4.05	120.12	126.23
20	3	3011	CLA	CHD-C4C-NC	4.04	130.57	124.20
20	A	1772	CLA	CHC-C1C-NC	4.04	130.34	124.20
20	3	1212	CLA	C1B-C2B-C3B	-4.04	103.16	106.92
22	B	1774	BCR	C24-C23-C22	-4.04	120.13	126.23
21	A	7032	LMU	C1'-C2'-C3'	-4.04	101.58	110.00
20	1	1200	CLA	CAA-C2A-C1A	4.04	125.22	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1744	CLA	O2D-CGD-CBD	4.04	118.45	111.27
20	4	1200	CLA	CHD-C4C-C3C	-4.04	118.90	124.84
20	2	1213	CLA	CHD-C4C-C3C	-4.04	118.90	124.84
20	A	1812	CLA	CHC-C1C-NC	4.04	130.33	124.20
20	A	1775	CLA	C1B-C2B-C3B	-4.04	103.17	106.92
20	A	1770	CLA	CHC-C1C-NC	4.04	130.33	124.20
20	J	1044	CLA	CHD-C4C-NC	4.04	130.56	124.20
21	A	7032	LMU	O2B-C2B-C3B	-4.03	101.02	110.35
20	J	1045	CLA	CMD-C2D-C3D	-4.03	118.34	127.61
20	3	3001	CLA	C2D-C3D-C4D	-4.03	102.81	107.28
20	B	1760	CLA	O2D-CGD-CBD	4.03	118.43	111.27
20	A	1790	CLA	C1-C2-C3	-4.03	120.23	126.75
20	1	1200	CLA	O2A-CGA-CBA	4.03	124.55	111.91
22	A	1804	BCR	C33-C5-C6	-4.03	120.00	124.53
22	B	1774	BCR	C38-C26-C25	-4.03	120.01	124.53
20	3	1215	CLA	CHA-C4D-ND	4.03	128.40	124.52
22	B	1778	BCR	C33-C5-C6	-4.03	120.01	124.53
20	B	1739	CLA	C1-C2-C3	-4.02	119.08	126.04
20	A	1788	CLA	CHC-C1C-NC	4.02	130.31	124.20
22	B	1780	BCR	C33-C5-C6	-4.02	120.01	124.53
20	A	1815	CLA	CHD-C4C-NC	4.02	130.54	124.20
20	1	1199	CLA	CHC-C1C-NC	4.02	130.17	124.23
21	A	7032	LMU	O1'-C1'-C2'	-4.02	102.03	108.30
22	B	1777	BCR	C33-C5-C6	-4.02	120.02	124.53
20	1	1187	CLA	CAA-C2A-C3A	-4.02	101.78	112.78
22	B	1778	BCR	C38-C26-C25	-4.02	120.02	124.53
20	L	1168	CLA	O1D-CGD-CBD	-4.02	116.27	124.48
22	B	1775	BCR	C33-C5-C6	-4.01	120.02	124.53
21	A	7026	LMU	O4'-C4B-C3B	4.01	119.62	110.35
21	A	7043	LMU	C6'-C5'-C4'	-4.01	101.66	113.33
20	A	1761	CLA	CHD-C4C-C3C	-4.01	118.95	124.84
20	B	1772	CLA	CMA-C3A-C2A	-4.01	106.75	116.10
20	A	1817	CLA	CED-O2D-CGD	4.01	125.00	115.94
20	B	1767	CLA	CHD-C4C-C3C	-4.00	118.95	124.84
21	A	7017	LMU	C1B-O5B-C5B	-4.00	105.83	113.69
20	4	1201	CLA	C3C-C4C-NC	-4.00	106.08	110.57
20	B	1741	CLA	CHC-C1C-NC	4.00	130.27	124.20
21	A	7022	LMU	O2'-C2'-C1'	-4.00	100.33	110.05
21	A	7040	LMU	O1B-C1B-C2B	4.00	118.46	108.10
20	A	1763	CLA	CHD-C4C-NC	4.00	130.50	124.20
20	K	1146	CLA	CHD-C4C-NC	4.00	130.50	124.20
20	A	1788	CLA	O2D-CGD-CBD	4.00	118.37	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	4003	CLA	CHC-C1C-NC	4.00	130.13	124.23
20	A	1768	CLA	CHC-C1C-NC	3.99	130.26	124.20
20	1	1199	CLA	C2A-C1A-CHA	-3.99	115.82	122.63
21	A	7023	LMU	C2'-C3'-C4'	3.99	118.80	109.68
22	A	1805	BCR	C38-C26-C25	-3.99	120.05	124.53
20	L	1505	CLA	C4A-NA-C1A	3.99	108.50	106.71
22	B	1777	BCR	C38-C26-C25	-3.99	120.05	124.53
20	B	1760	CLA	CMD-C2D-C1D	3.99	131.74	124.71
20	A	1769	CLA	CHD-C4C-C3C	-3.99	118.98	124.84
22	A	1807	BCR	C38-C26-C25	-3.99	120.05	124.53
20	A	1787	CLA	C4D-C3D-CAD	3.98	112.79	108.10
20	B	1761	CLA	C4D-C3D-CAD	3.98	112.79	108.10
20	1	1191	CLA	C1B-C2B-C3B	-3.98	103.22	106.92
20	A	1770	CLA	CHD-C4C-NC	3.98	130.48	124.20
20	2	1227	CLA	C4C-CHD-C1D	-3.98	116.27	126.11
21	A	7021	LMU	C6B-C5B-C4B	-3.98	103.68	113.00
21	4	1210	LMU	C1B-O5B-C5B	3.98	121.50	113.69
21	A	7032	LMU	C4B-C3B-C2B	-3.98	103.88	110.82
22	B	1781	BCR	C24-C25-C26	-3.97	111.83	121.46
20	3	1217	CLA	C3D-C4D-CHA	-3.97	116.61	124.98
20	B	1748	CLA	C1-C2-C3	-3.97	119.17	126.04
20	2	1222	CLA	CHC-C1C-NC	3.97	130.23	124.20
20	B	1764	CLA	O2D-CGD-CBD	3.97	118.32	111.27
21	A	7040	LMU	O2'-C2'-C3'	-3.97	101.18	110.35
20	1	1193	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
20	B	1751	CLA	O2D-CGD-CBD	3.97	118.31	111.27
20	A	1798	CLA	C4A-NA-C1A	3.96	108.49	106.71
20	B	1764	CLA	CMD-C2D-C3D	-3.96	118.51	127.61
20	B	1787	CLA	C4A-NA-C1A	3.96	108.48	106.71
20	2	1213	CLA	O2D-CGD-O1D	-3.96	116.10	123.84
20	4	1202	CLA	C2A-C1A-CHA	-3.96	115.89	122.63
22	A	1803	BCR	C33-C5-C6	-3.95	120.09	124.53
22	A	1808	BCR	C33-C5-C6	-3.95	120.09	124.53
20	B	1786	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
20	3	1216	CLA	C3B-C2B-C1B	-3.95	102.91	106.29
20	A	1799	CLA	CHD-C4C-NC	3.95	130.43	124.20
21	A	7025	LMU	C1B-O1B-C4'	-3.95	108.19	117.96
20	H	1079	CLA	CHD-C4C-C3C	-3.95	119.04	124.84
20	2	1217	CLA	CED-O2D-CGD	3.94	124.86	115.94
20	B	1786	CLA	CHC-C1C-NC	3.94	130.19	124.20
20	A	1776	CLA	CMD-C2D-C3D	-3.94	118.54	127.61
20	3	3007	CLA	C4A-NA-C1A	3.94	108.48	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1751	CLA	CMD-C2D-C3D	-3.94	118.55	127.61
20	4	1201	CLA	CGD-CBD-CAD	3.94	123.49	110.73
20	4	1205	CLA	CHD-C1D-ND	3.94	128.32	124.52
20	4	1208	CLA	CHD-C1D-ND	3.94	128.32	124.52
20	K	1146	CLA	O2A-CGA-CBA	3.93	124.26	111.91
22	I	1032	BCR	C30-C25-C24	3.93	126.90	115.78
20	4	1203	CLA	C3B-C2B-C1B	-3.93	102.92	106.29
20	1	1198	CLA	C1-C2-C3	-3.93	119.25	126.04
21	A	7028	LMU	O5'-C1'-C2'	-3.93	102.03	110.35
20	B	1757	CLA	CHD-C4C-C3C	-3.93	119.07	124.84
20	2	1215	CLA	CHC-C1C-NC	3.93	130.16	124.20
20	A	1773	CLA	CHC-C1C-NC	3.92	130.16	124.20
20	A	1762	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
20	1	1191	CLA	CMD-C2D-C3D	-3.92	118.59	127.61
20	3	3001	CLA	CHC-C1C-NC	3.92	130.02	124.23
20	B	1738	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
20	A	1765	CLA	O2A-CGA-CBA	3.92	124.20	111.91
20	1	1200	CLA	CMD-C2D-C1D	3.92	131.62	124.71
21	A	7038	LMU	O5B-C5B-C4B	3.92	116.81	109.69
21	A	7033	LMU	C3B-C4B-C5B	3.92	117.23	110.24
20	1	1198	CLA	CHC-C1C-NC	3.92	130.15	124.20
20	2	1213	CLA	C1-O2A-CGA	3.91	126.71	116.44
20	1	1188	CLA	CHD-C4C-C3C	-3.91	119.09	124.84
20	A	1764	CLA	C6-C5-C3	-3.91	103.20	113.45
20	4	1199	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
20	A	1789	CLA	CAC-C3C-C4C	3.91	129.88	124.81
20	B	1786	CLA	C5-C3-C2	-3.91	113.21	121.12
20	R	1055	CLA	C1-C2-C3	3.90	132.79	126.04
20	B	1754	CLA	CHD-C4C-NC	3.90	130.35	124.20
22	B	1775	BCR	C38-C26-C25	-3.90	120.15	124.53
20	A	1776	CLA	CHD-C4C-C3C	-3.90	119.11	124.84
20	A	1799	CLA	CHC-C1C-NC	3.90	130.12	124.20
20	A	1785	CLA	CHC-C1C-NC	3.90	130.12	124.20
21	A	7022	LMU	O2'-C2'-C3'	-3.89	101.35	110.35
20	4	4003	CLA	CHD-C4C-NC	3.89	130.21	124.21
20	3	3002	CLA	C3D-C4D-CHA	-3.89	116.79	124.98
20	R	1054	CLA	CHD-C4C-C3C	-3.89	119.12	124.84
21	A	7037	LMU	O5'-C1'-C2'	-3.89	102.12	110.35
21	R	1057	LMU	C1B-O1B-C4'	-3.89	108.35	117.96
20	A	1788	CLA	CHD-C4C-C3C	-3.89	119.13	124.84
20	A	1760	CLA	C4D-C3D-CAD	3.88	112.67	108.10
20	J	1044	CLA	CHC-C1C-NC	3.88	130.09	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	3015	CLA	C3B-C2B-C1B	-3.88	102.97	106.29
21	K	1086	LMU	O3'-C3'-C2'	-3.88	101.38	110.35
20	F	1155	CLA	CHD-C4C-C3C	-3.88	118.92	124.98
20	B	1762	CLA	CMD-C2D-C3D	-3.88	118.70	127.61
20	A	1780	CLA	CHD-C4C-NC	3.87	130.30	124.20
21	A	7036	LMU	C4B-C3B-C2B	-3.87	104.06	110.82
20	A	1779	CLA	CMD-C2D-C3D	-3.87	118.71	127.61
20	A	1771	CLA	O2D-CGD-CBD	3.87	118.14	111.27
20	B	1751	CLA	CHB-C4A-NA	3.87	129.86	124.51
21	A	7025	LMU	O3B-C3B-C4B	3.86	119.28	110.35
20	4	1198	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
22	B	1781	BCR	C31-C1-C6	3.86	116.56	110.30
20	B	1754	CLA	CAC-C3C-C4C	3.85	129.81	124.81
20	3	1212	CLA	CMD-C2D-C3D	-3.85	118.75	127.61
20	A	1773	CLA	O2A-CGA-CBA	3.85	123.99	111.91
20	1	1193	CLA	CHC-C1C-NC	3.85	130.04	124.20
21	A	7041	LMU	O6B-C6B-C5B	-3.85	98.10	111.29
20	4	1207	CLA	CHC-C1C-NC	3.84	130.04	124.20
20	A	1780	CLA	CHC-C1C-NC	3.84	130.03	124.20
20	3	1216	CLA	C4A-NA-C1A	3.84	108.43	106.71
20	B	1757	CLA	CHC-C1C-NC	3.84	130.03	124.20
20	4	4003	CLA	C3D-C4D-CHA	-3.84	116.90	124.98
20	A	1767	CLA	CMB-C2B-C1B	3.83	134.36	128.46
20	A	1770	CLA	CMD-C2D-C3D	-3.83	118.80	127.61
20	B	1753	CLA	C4D-C3D-CAD	3.83	112.61	108.10
20	K	1085	CLA	C1-C2-C3	-3.83	120.56	126.75
20	B	1763	CLA	CHC-C1C-NC	3.83	130.01	124.20
20	B	1759	CLA	O2D-CGD-O1D	-3.83	116.36	123.84
20	A	1766	CLA	C2A-C1A-CHA	-3.83	117.17	123.86
20	B	1753	CLA	O2D-CGD-CBD	3.82	118.06	111.27
20	B	1765	CLA	CHC-C1C-NC	3.82	130.00	124.20
20	4	1198	CLA	O2A-CGA-CBA	3.82	123.90	111.91
20	B	1758	CLA	CHB-C4A-NA	3.82	129.80	124.51
21	A	7026	LMU	O5B-C5B-C6B	3.82	115.94	106.44
20	2	1221	CLA	CHC-C1C-NC	3.82	129.87	124.23
20	4	1197	CLA	CHC-C1C-NC	3.82	130.00	124.20
20	2	1224	CLA	CHC-C1C-NC	3.82	129.99	124.20
20	A	1771	CLA	O2D-CGD-O1D	-3.82	116.38	123.84
20	B	1740	CLA	CHC-C1C-NC	3.82	129.99	124.20
20	B	1738	CLA	CMD-C2D-C3D	-3.82	118.83	127.61
20	2	1215	CLA	CHD-C4C-NC	3.81	130.21	124.20
20	2	1223	CLA	CGD-CBD-CAD	-3.81	98.39	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	1216	CLA	C4A-NA-C1A	3.81	108.42	106.71
20	A	1759	CLA	CHC-C1C-NC	3.81	129.98	124.20
20	H	1079	CLA	CHC-C1C-NC	3.81	129.98	124.20
20	A	1800	CLA	C6-C5-C3	-3.81	103.47	113.45
20	I	1033	CLA	C4-C3-C5	3.81	121.67	115.27
20	2	1227	CLA	CHD-C4C-NC	3.80	130.07	124.21
20	J	1044	CLA	CHD-C1D-ND	3.80	127.95	124.45
21	K	1086	LMU	O5B-C5B-C6B	3.80	115.88	106.44
20	A	1813	CLA	O2D-CGD-O1D	-3.80	116.42	123.84
20	R	1054	CLA	CHC-C1C-NC	3.80	129.96	124.20
20	A	1762	CLA	CMD-C2D-C3D	-3.80	118.88	127.61
20	2	1216	CLA	C3B-C2B-C1B	-3.80	103.04	106.29
20	A	1772	CLA	CMD-C2D-C3D	-3.80	118.88	127.61
20	F	1157	CLA	C4D-C3D-CAD	3.79	112.57	108.10
20	3	1214	CLA	C2A-C1A-CHA	-3.79	116.16	122.63
20	B	1758	CLA	CHC-C1C-NC	3.79	129.96	124.20
20	L	1167	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
20	B	1772	CLA	CBD-CHA-C1A	3.79	133.50	127.43
20	A	1788	CLA	CMD-C2D-C3D	-3.79	118.89	127.61
20	A	1813	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
20	1	1194	CLA	CHC-C1C-NC	3.79	129.82	124.23
20	2	1218	CLA	CHD-C4C-NC	3.79	130.17	124.20
20	1	1188	CLA	CHD-C4C-NC	3.79	130.17	124.20
20	L	1167	CLA	CGD-CBD-CAD	-3.79	98.47	110.73
20	B	1770	CLA	O2A-CGA-CBA	3.79	123.79	111.91
20	B	1758	CLA	O2A-CGA-CBA	3.78	123.78	111.91
20	A	1789	CLA	CHC-C1C-C2C	-3.78	116.26	126.72
22	B	1776	BCR	C35-C13-C14	-3.78	117.63	122.92
20	B	1746	CLA	O1D-CGD-CBD	-3.78	116.75	124.48
20	A	1787	CLA	CHD-C4C-C3C	-3.78	119.28	124.84
20	A	1787	CLA	CHC-C1C-NC	3.78	129.94	124.20
22	L	1169	BCR	C11-C10-C9	-3.78	121.92	127.31
20	4	1208	CLA	C3D-C4D-CHA	-3.78	117.03	124.98
22	B	1779	BCR	C27-C26-C25	-3.78	117.25	122.73
20	B	1745	CLA	O2D-CGD-CBD	3.78	117.98	111.27
20	H	1079	CLA	CMD-C2D-C3D	-3.78	118.93	127.61
20	B	1750	CLA	C4A-NA-C1A	3.77	108.40	106.71
23	B	1773	PQN	C2M-C2-C1	3.77	122.52	116.27
20	3	1215	CLA	C2A-C1A-CHA	-3.77	116.20	122.63
20	3	3011	CLA	CHB-C4A-NA	3.77	129.72	124.51
21	A	7036	LMU	C3'-C4'-C5'	-3.77	102.28	110.93
20	B	1787	CLA	C1-O2A-CGA	3.77	126.33	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1768	CLA	C4A-NA-C1A	3.77	108.40	106.71
20	B	1752	CLA	C4-C3-C5	3.76	121.60	115.27
20	4	1208	CLA	CHD-C4C-NC	3.76	130.01	124.21
20	B	1785	CLA	CAA-C2A-C3A	-3.76	102.48	112.78
20	A	1812	CLA	O2A-CGA-CBA	3.76	123.71	111.91
20	F	1157	CLA	O2D-CGD-CBD	3.76	117.95	111.27
20	J	1046	CLA	C4A-NA-C1A	3.76	108.40	106.71
20	B	1754	CLA	CGD-CBD-CAD	-3.76	98.56	110.73
20	B	1750	CLA	CHC-C1C-NC	3.76	129.90	124.20
20	4	1207	CLA	CHB-C4A-NA	3.76	129.71	124.51
20	B	1754	CLA	CAA-CBA-CGA	-3.76	102.28	113.25
20	1	1191	CLA	CBD-CHA-C1A	3.76	133.44	127.43
20	1	1195	CLA	CHC-C1C-NC	3.75	129.90	124.20
20	B	1760	CLA	CAC-C3C-C4C	3.75	129.68	124.81
20	A	1815	CLA	CMD-C2D-C3D	-3.75	118.98	127.61
20	B	1760	CLA	CHC-C1C-NC	3.75	129.89	124.20
22	B	1779	BCR	C40-C30-C25	-3.75	104.22	110.30
20	R	1055	CLA	CMA-C3A-C4A	3.74	121.84	111.77
20	B	1785	CLA	CMD-C2D-C1D	3.74	131.31	124.71
21	B	1782	LMU	O1'-C1'-C2'	3.74	114.14	108.30
21	A	7031	LMU	O1'-C1'-C2'	3.74	114.14	108.30
20	B	1747	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
20	A	1777	CLA	CHC-C1C-NC	3.74	129.87	124.20
20	J	1045	CLA	C4-C3-C5	3.73	121.55	115.27
20	A	1815	CLA	CMA-C3A-C2A	-3.73	98.77	113.83
20	B	1761	CLA	C1-C2-C3	-3.73	120.71	126.75
20	A	1798	CLA	CHC-C1C-NC	3.73	129.87	124.20
20	4	1208	CLA	C2A-C1A-CHA	-3.73	116.27	122.63
20	A	1766	CLA	CMB-C2B-C3B	3.73	131.66	124.68
20	A	1811	CLA	CMC-C2C-C1C	3.73	130.72	125.04
20	J	1046	CLA	C3D-C4D-CHA	-3.73	117.13	124.98
20	B	1746	CLA	CMD-C2D-C3D	-3.73	119.03	127.61
20	4	1200	CLA	CMD-C2D-C3D	-3.73	119.04	127.61
20	A	1780	CLA	CHD-C4C-C3C	-3.73	119.36	124.84
20	1	1188	CLA	CMB-C2B-C3B	3.72	131.64	124.68
20	J	1044	CLA	CHD-C4C-C3C	-3.72	119.37	124.84
20	4	1204	CLA	C4-C3-C5	3.72	121.53	115.27
20	A	1774	CLA	O2D-CGD-CBD	3.72	117.88	111.27
20	B	1740	CLA	O2A-CGA-O1A	-3.72	114.21	123.59
20	4	1197	CLA	CMB-C2B-C3B	3.72	131.97	124.69
20	B	1763	CLA	CMD-C2D-C3D	-3.72	119.07	127.61
20	B	1785	CLA	CBA-CAA-C2A	-3.72	102.90	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	1802	PQN	C2M-C2-C3	-3.71	118.34	124.40
20	B	1747	CLA	CMD-C2D-C3D	-3.71	119.08	127.61
20	I	1033	CLA	CHB-C4A-NA	3.71	129.64	124.51
20	A	1770	CLA	CHD-C4C-C3C	-3.71	119.39	124.84
20	A	1785	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
20	L	1166	CLA	CHC-C1C-NC	3.71	129.83	124.20
21	A	7021	LMU	O2B-C2B-C1B	3.71	119.05	110.05
20	4	4007	CLA	CMD-C2D-C3D	-3.70	119.09	127.61
20	4	1200	CLA	CHC-C1C-NC	3.70	129.82	124.20
20	A	1761	CLA	CMD-C2D-C3D	-3.70	119.10	127.61
20	B	1742	CLA	CHD-C4C-C3C	-3.70	119.40	124.84
20	2	1223	CLA	CHC-C1C-NC	3.70	129.81	124.20
20	4	1206	CLA	CHD-C4C-NC	3.70	129.91	124.21
20	1	1194	CLA	C2D-C3D-C4D	-3.70	103.18	107.28
22	B	1781	BCR	C19-C18-C17	3.70	124.61	118.94
21	A	7020	LMU	C1-O1'-C1'	-3.69	107.71	113.84
20	A	1771	CLA	CMD-C2D-C3D	-3.69	119.12	127.61
20	4	1206	CLA	CHC-C1C-NC	3.69	129.68	124.23
20	B	1751	CLA	CHC-C1C-NC	3.69	129.80	124.20
20	A	1789	CLA	CMA-C3A-C2A	-3.69	98.95	113.83
20	A	1801	CLA	CMD-C2D-C3D	-3.69	119.13	127.61
20	3	3011	CLA	CHC-C1C-NC	3.69	129.80	124.20
20	L	1167	CLA	CHD-C4C-C3C	-3.69	119.42	124.84
20	1	1195	CLA	C1B-C2B-C3B	-3.69	103.49	106.92
20	3	3007	CLA	CHD-C4C-NC	3.68	130.01	124.20
21	A	7022	LMU	O2B-C2B-C1B	3.68	119.00	110.05
21	K	1086	LMU	O2'-C2'-C1'	3.68	118.99	110.05
20	1	1201	CLA	C3D-C4D-ND	3.68	115.02	109.46
20	B	1740	CLA	CMB-C2B-C3B	3.68	131.57	124.68
21	A	1809	LMU	O5'-C5'-C4'	3.68	117.52	109.75
20	4	1203	CLA	C2D-C3D-C4D	-3.68	103.20	107.28
21	A	7033	LMU	C3'-C4'-C5'	-3.68	102.50	110.93
20	4	4003	CLA	C2D-C3D-C4D	-3.68	103.21	107.28
20	I	1033	CLA	CHD-C4C-NC	3.68	130.00	124.20
21	A	7033	LMU	O2B-C2B-C1B	-3.67	101.12	110.05
20	2	1214	CLA	C3D-C4D-CHA	-3.67	117.24	124.98
20	1	1197	CLA	C1-C2-C3	-3.67	119.69	126.04
20	1	1190	CLA	CED-O2D-CGD	3.67	124.25	115.94
20	A	1783	CLA	CHD-C4C-C3C	-3.67	119.45	124.84
21	A	7036	LMU	O5B-C5B-C6B	3.67	115.56	106.44
20	K	1146	CLA	C2D-C1D-ND	-3.67	107.40	110.10
21	A	7020	LMU	C3'-C4'-C5'	-3.67	102.52	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	1157	CLA	CMD-C2D-C1D	3.66	131.17	124.71
20	3	3011	CLA	CHD-C4C-C3C	-3.66	119.46	124.84
20	L	1166	CLA	CED-O2D-CGD	3.66	124.22	115.94
20	B	1748	CLA	C4A-NA-C1A	3.66	108.35	106.71
20	4	1204	CLA	C4-C3-C2	-3.66	114.29	123.68
20	B	1744	CLA	CHD-C4C-C3C	-3.66	119.46	124.84
20	1	1190	CLA	CHC-C1C-NC	3.65	129.75	124.20
20	B	1736	CLA	C4A-NA-C1A	3.65	108.35	106.71
20	A	1761	CLA	O2D-CGD-CBD	3.65	117.76	111.27
20	B	1762	CLA	C4-C3-C5	3.65	121.41	115.27
20	B	1744	CLA	CHC-C1C-NC	3.65	129.74	124.20
21	A	7024	LMU	C3B-C4B-C5B	-3.65	103.73	110.24
20	A	1772	CLA	C4-C3-C5	3.65	121.40	115.27
20	I	1031	CLA	CHC-C1C-NC	3.64	129.73	124.20
20	A	1790	CLA	CHC-C1C-NC	3.64	129.73	124.20
20	B	1740	CLA	CGD-CBD-CAD	3.64	122.52	110.73
21	A	7023	LMU	O2'-C2'-C3'	-3.64	101.94	110.35
20	3	3015	CLA	C3D-C4D-CHA	-3.64	117.32	124.98
20	2	1221	CLA	C2A-C1A-CHA	-3.64	116.43	122.63
20	B	1748	CLA	O2A-C1-C2	3.64	118.19	108.64
21	A	7033	LMU	O5'-C1'-C2'	3.64	118.05	110.35
20	B	1762	CLA	CHC-C1C-NC	3.64	129.72	124.20
20	1	1195	CLA	CAA-C2A-C3A	-3.64	107.61	116.10
20	4	1204	CLA	O2D-CGD-CBD	3.63	117.73	111.27
20	A	1785	CLA	C4-C3-C5	3.63	121.38	115.27
20	2	1218	CLA	CMD-C2D-C3D	-3.63	119.26	127.61
20	4	4003	CLA	C4A-NA-C1A	3.63	108.34	106.71
20	A	1775	CLA	CHC-C1C-NC	3.63	129.71	124.20
20	1	1188	CLA	O2A-CGA-CBA	3.63	123.29	111.91
20	A	1816	CLA	O2A-CGA-CBA	3.63	123.29	111.91
20	A	1768	CLA	CMD-C2D-C3D	-3.63	119.27	127.61
20	2	1223	CLA	CAA-C2A-C1A	3.63	123.86	111.97
20	4	1205	CLA	C3D-C4D-CHA	-3.62	117.35	124.98
21	A	7023	LMU	C3B-C4B-C5B	-3.62	103.78	110.24
21	A	7015	LMU	C1B-C2B-C3B	3.62	117.54	110.00
21	A	7032	LMU	O5B-C5B-C6B	3.62	115.43	106.44
22	B	1781	BCR	C38-C26-C25	-3.62	120.47	124.53
20	1	1187	CLA	C2D-C1D-ND	-3.61	107.44	110.10
20	4	1202	CLA	C2D-C3D-C4D	-3.61	103.28	107.28
21	A	7038	LMU	O5B-C5B-C6B	3.61	115.42	106.44
20	4	1199	CLA	CHC-C1C-C2C	-3.61	116.73	126.72
20	B	1739	CLA	CHD-C4C-NC	3.61	129.89	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	1216	CLA	C3D-C4D-ND	3.60	114.90	109.46
20	R	1055	CLA	CHC-C1C-NC	3.60	129.67	124.20
20	A	1765	CLA	C4A-NA-C1A	3.60	108.33	106.71
20	2	1215	CLA	CHD-C4C-C3C	-3.60	119.55	124.84
20	3	1217	CLA	C1D-ND-C4D	-3.60	103.78	106.33
20	B	1739	CLA	CHB-C4A-NA	3.60	129.49	124.51
20	A	1779	CLA	CHC-C1C-NC	3.60	129.66	124.20
20	A	1789	CLA	CHD-C4C-NC	3.60	129.87	124.20
20	1	1199	CLA	C2D-C3D-C4D	-3.59	103.30	107.28
21	A	7026	LMU	C1B-O5B-C5B	-3.59	106.64	113.69
20	3	1213	CLA	C2C-C1C-CHC	-3.59	117.07	125.67
20	R	1055	CLA	O2D-CGD-CBD	3.59	117.65	111.27
21	A	7038	LMU	C1'-O5'-C5'	3.59	120.73	113.69
20	G	1099	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
22	B	1779	BCR	C1-C6-C5	-3.59	117.56	122.61
20	1	1187	CLA	CHD-C4C-C3C	-3.59	119.57	124.84
20	B	1749	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
20	2	1217	CLA	C4-C3-C5	3.58	121.30	115.27
20	A	1817	CLA	CHC-C1C-C2C	-3.58	116.81	126.72
20	A	1787	CLA	CMD-C2D-C3D	-3.58	119.37	127.61
20	2	1217	CLA	CMD-C2D-C3D	-3.58	119.37	127.61
20	F	1157	CLA	C4-C3-C2	-3.58	114.50	123.68
20	2	1219	CLA	C3D-C4D-CHA	-3.58	117.45	124.98
20	A	1763	CLA	CHD-C4C-C3C	-3.58	119.58	124.84
20	B	1787	CLA	O2D-CGD-CBD	3.58	117.62	111.27
20	B	1771	CLA	CHD-C4C-NC	3.58	129.84	124.20
20	J	1046	CLA	C3B-C2B-C1B	-3.57	103.23	106.29
20	B	1754	CLA	CMD-C2D-C3D	-3.57	119.40	127.61
20	B	1738	CLA	O2A-CGA-CBA	3.57	123.11	111.91
20	1	1196	CLA	CHC-C1C-NC	3.57	129.62	124.20
23	A	1802	PQN	C21-C20-C18	-3.57	104.38	115.92
20	1	1192	CLA	CHC-C1C-NC	3.57	129.62	124.20
20	2	1218	CLA	CHC-C1C-C2C	-3.57	116.85	126.72
20	1	1187	CLA	CMC-C2C-C1C	3.57	130.47	125.04
20	1	1194	CLA	CHD-C1D-ND	3.57	127.96	124.52
21	A	7020	LMU	C1B-C2B-C3B	3.57	117.42	110.00
20	B	1739	CLA	O2A-CGA-CBA	3.57	123.10	111.91
22	B	1779	BCR	C28-C29-C30	-3.56	101.86	114.60
20	B	1743	CLA	CMD-C2D-C3D	-3.56	119.42	127.61
20	A	1771	CLA	CHD-C4C-C3C	-3.56	119.61	124.84
20	A	1765	CLA	C2D-C1D-ND	-3.56	107.48	110.10
20	A	1798	CLA	CMD-C2D-C3D	-3.56	119.43	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	1187	CLA	CBA-CAA-C2A	-3.56	103.36	113.86
20	3	3011	CLA	CMD-C2D-C3D	-3.56	119.43	127.61
20	F	1155	CLA	CHB-C4A-NA	3.56	129.43	124.51
20	A	1761	CLA	CHC-C1C-C2C	-3.55	116.89	126.72
22	B	1776	BCR	C38-C26-C27	3.55	120.44	113.62
20	2	1216	CLA	C3A-C4A-CHB	-3.55	119.56	123.91
20	A	1786	CLA	CMD-C2D-C3D	-3.55	119.44	127.61
21	A	7032	LMU	C1-O1'-C1'	-3.55	107.95	113.84
20	1	1198	CLA	CMD-C2D-C3D	-3.55	119.45	127.61
20	I	1031	CLA	C4A-NA-C1A	3.55	108.30	106.71
20	A	1784	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
20	3	1216	CLA	C3D-C4D-CHA	-3.55	117.51	124.98
20	A	1784	CLA	CHD-C4C-C3C	-3.55	119.63	124.84
20	B	1785	CLA	CHD-C4C-C3C	-3.54	119.63	124.84
20	B	1752	CLA	CED-O2D-CGD	3.54	123.95	115.94
20	1	1194	CLA	C3D-C4D-CHA	-3.54	117.52	124.98
20	2	1224	CLA	CMD-C2D-C3D	-3.54	119.47	127.61
20	A	1783	CLA	O2D-CGD-CBD	3.54	117.56	111.27
21	A	7022	LMU	C3B-C4B-C5B	-3.54	103.93	110.24
21	A	1810	LMU	O5B-C1B-C2B	3.54	117.84	110.35
20	2	1221	CLA	C2D-C3D-C4D	-3.54	103.36	107.28
20	A	1795	CLA	C4-C3-C5	3.54	120.03	115.98
20	A	1769	CLA	CMD-C2D-C3D	-3.54	119.48	127.61
20	4	1200	CLA	O2A-CGA-CBA	3.53	123.00	111.91
20	A	1812	CLA	O2D-CGD-CBD	3.53	117.55	111.27
21	A	7016	LMU	C1B-C2B-C3B	3.53	117.35	110.00
20	A	1769	CLA	CHB-C4A-NA	3.53	129.40	124.51
20	B	1765	CLA	CMD-C2D-C3D	-3.53	119.49	127.61
20	B	1738	CLA	CHC-C1C-C2C	-3.53	116.96	126.72
20	2	1221	CLA	C3D-C4D-CHA	-3.53	117.55	124.98
20	A	1762	CLA	CMB-C2B-C3B	3.53	131.28	124.68
20	B	1771	CLA	CHC-C1C-NC	3.52	129.55	124.20
20	1	1194	CLA	C2A-C1A-CHA	-3.52	116.63	122.63
20	A	1784	CLA	C1-O2A-CGA	3.52	125.68	116.44
20	2	1212	CLA	C4-C3-C5	3.52	120.00	115.98
20	A	1759	CLA	CMD-C2D-C3D	-3.52	119.53	127.61
20	2	1227	CLA	C3D-C4D-ND	3.52	114.77	109.46
20	1	1200	CLA	CHC-C1C-C2C	-3.52	117.00	126.72
20	A	1812	CLA	CHB-C4A-NA	3.51	129.37	124.51
21	A	7024	LMU	O1'-C1'-C2'	3.51	113.79	108.30
20	3	1218	CLA	C2A-C1A-CHA	-3.51	117.72	123.86
20	B	1760	CLA	CGD-CBD-CAD	3.51	122.10	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	1208	CLA	CHC-C1C-NC	3.51	129.41	124.23
20	A	1792	CLA	C4-C3-C5	3.50	119.99	115.98
20	A	1764	CLA	CHC-C1C-NC	3.50	129.51	124.20
20	B	1758	CLA	C16-C15-C13	-3.50	104.61	115.92
20	A	1759	CLA	C1-C2-C3	-3.50	121.09	126.75
20	J	1044	CLA	O2A-CGA-CBA	3.50	122.88	111.91
22	B	1779	BCR	C37-C22-C21	-3.50	118.03	122.92
20	3	1217	CLA	C3D-C4D-ND	3.50	114.74	109.46
20	A	1774	CLA	C1-C2-C3	-3.49	120.00	126.04
20	A	1801	CLA	C4-C3-C5	3.49	121.15	115.27
20	A	1767	CLA	CHC-C1C-C2C	-3.49	117.06	126.72
20	B	1754	CLA	C4A-NA-C1A	3.49	108.28	106.71
22	L	1170	BCR	C1-C6-C7	3.49	125.66	115.78
21	A	7028	LMU	C1B-O1B-C4'	-3.49	109.32	117.96
20	J	1045	CLA	CHB-C4A-NA	3.49	129.34	124.51
20	H	1079	CLA	CMB-C2B-C3B	3.49	131.21	124.68
20	A	1772	CLA	CAC-C3C-C4C	3.49	129.34	124.81
20	3	3015	CLA	C4A-NA-C1A	3.49	108.27	106.71
20	K	1146	CLA	CHB-C4A-NA	3.49	129.33	124.51
22	I	1032	BCR	C8-C7-C6	-3.49	117.41	127.20
20	1	1187	CLA	CHC-C1C-C2C	-3.49	117.08	126.72
21	A	7037	LMU	O5'-C5'-C6'	3.48	115.10	106.44
20	3	1217	CLA	C2C-C1C-CHC	-3.48	117.33	125.67
20	J	1045	CLA	C1-C2-C3	-3.48	120.02	126.04
20	A	1815	CLA	C1-O2A-CGA	3.48	125.58	116.44
20	3	3002	CLA	CHD-C1D-ND	3.48	127.88	124.52
20	A	1813	CLA	CHB-C4A-NA	3.48	129.32	124.51
20	B	1768	CLA	C4-C3-C5	3.48	121.12	115.27
20	A	1812	CLA	O2A-C1-C2	3.47	117.76	108.64
21	A	7017	LMU	C4B-C3B-C2B	3.47	116.88	110.82
20	K	1146	CLA	O2A-CGA-O1A	-3.47	114.85	123.59
20	3	3008	CLA	O2A-CGA-CBA	3.46	122.78	111.91
20	4	1202	CLA	C3D-C4D-CHA	-3.46	117.69	124.98
20	B	1763	CLA	CED-O2D-CGD	3.46	123.77	115.94
20	J	1044	CLA	CHB-C4A-NA	3.46	129.30	124.51
20	B	1739	CLA	CMD-C2D-C3D	-3.46	119.65	127.61
20	B	1769	CLA	CMD-C2D-C3D	-3.46	119.66	127.61
20	1	1199	CLA	C3D-C4D-CHA	-3.46	117.70	124.98
21	A	7020	LMU	C3B-C4B-C5B	-3.46	104.07	110.24
20	3	3008	CLA	C4A-NA-C1A	3.45	108.26	106.71
22	3	1220	BCR	C23-C24-C25	-3.45	117.51	127.20
22	L	1170	BCR	C7-C6-C5	-3.45	113.11	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1761	CLA	CHC-C1C-NC	3.45	129.43	124.20
20	B	1764	CLA	CED-O2D-CGD	3.45	123.73	115.94
20	B	1757	CLA	O2A-CGA-O1A	-3.44	114.90	123.59
20	4	1199	CLA	CHB-C4A-NA	3.44	129.28	124.51
21	A	7020	LMU	C1'-O5'-C5'	-3.44	106.93	113.69
20	4	1207	CLA	CHD-C4C-C3C	-3.44	119.60	124.98
20	4	1209	CLA	CHB-C4A-NA	3.44	129.27	124.51
20	A	1812	CLA	O1D-CGD-CBD	-3.44	117.44	124.48
20	1	1199	CLA	CHD-C1D-ND	3.44	127.84	124.52
20	1	1187	CLA	C4D-CHA-C1A	-3.44	117.06	121.25
20	A	1798	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
20	3	3001	CLA	C3D-C4D-CHA	-3.44	117.74	124.98
20	2	1223	CLA	CHB-C4A-NA	3.43	129.26	124.51
20	4	1202	CLA	CHD-C1D-ND	3.43	127.83	124.52
20	4	1198	CLA	C7-C6-C5	-3.43	104.04	113.36
20	1	1195	CLA	CBD-CHA-C1A	3.43	132.92	127.43
20	2	1213	CLA	O2A-CGA-CBA	3.43	122.66	111.91
20	B	1748	CLA	O2A-CGA-CBA	3.42	122.66	111.91
22	L	1169	BCR	C15-C16-C17	-3.42	116.46	123.47
20	1	1188	CLA	CHC-C1C-C2C	-3.42	117.27	126.72
20	A	1765	CLA	CAC-C3C-C2C	-3.42	121.68	127.53
20	A	1759	CLA	O1D-CGD-CBD	-3.42	117.49	124.48
20	A	1760	CLA	OBD-CAD-C3D	-3.41	120.30	128.52
20	L	1505	CLA	O2D-CGD-CBD	3.41	117.33	111.27
20	2	1222	CLA	CHD-C4C-NC	3.41	129.58	124.20
20	1	1201	CLA	C1D-ND-C4D	-3.41	103.91	106.33
20	4	1207	CLA	CAA-C2A-C3A	-3.41	108.14	116.10
20	R	1054	CLA	CED-O2D-CGD	3.41	123.65	115.94
20	R	1055	CLA	OBD-CAD-C3D	-3.41	120.32	128.52
20	4	1199	CLA	CAC-C3C-C2C	-3.41	121.70	127.53
20	A	1786	CLA	CHD-C4C-NC	3.41	129.57	124.20
20	A	1764	CLA	CHB-C4A-NA	3.41	129.22	124.51
20	3	1213	CLA	C3D-C4D-CHA	-3.40	117.81	124.98
20	B	1748	CLA	O2D-CGD-CBD	3.40	117.32	111.27
20	2	1219	CLA	C3C-C4C-CHD	-3.40	117.77	125.22
22	B	1781	BCR	C36-C18-C19	-3.40	112.72	118.08
20	B	1749	CLA	C1-C2-C3	-3.40	120.16	126.04
20	3	3011	CLA	CMB-C2B-C3B	3.40	131.04	124.68
20	2	1213	CLA	C4A-NA-C1A	3.40	108.23	106.71
20	2	1213	CLA	C4-C3-C2	-3.40	114.96	123.68
20	A	1788	CLA	O2A-CGA-CBA	3.40	122.58	111.91
20	A	1762	CLA	C1-C2-C3	-3.40	120.17	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1789	CLA	C2D-C1D-ND	-3.40	107.60	110.10
20	L	1505	CLA	CED-O2D-CGD	3.39	123.61	115.94
20	2	1213	CLA	C1D-ND-C4D	-3.39	103.92	106.33
20	A	1812	CLA	O2A-CGA-O1A	-3.39	115.03	123.59
20	J	1046	CLA	C2D-C3D-C4D	-3.39	103.53	107.28
21	A	7031	LMU	O1B-C1B-C2B	3.39	116.88	108.10
20	B	1745	CLA	CHC-C1C-NC	3.39	129.34	124.20
20	1	1191	CLA	CHC-C1C-NC	3.39	129.34	124.20
20	J	1044	CLA	C3A-C2A-C1A	3.38	106.41	101.34
20	1	1187	CLA	CHD-C1D-ND	3.38	127.56	124.45
20	A	1779	CLA	CHD-C4C-C3C	-3.38	119.87	124.84
21	A	7028	LMU	O5B-C5B-C4B	-3.38	103.55	109.69
20	1	1197	CLA	CMB-C2B-C1B	3.38	133.66	128.46
20	A	1790	CLA	CHD-C4C-C3C	-3.38	119.87	124.84
21	A	7020	LMU	O1'-C1'-C2'	3.38	113.58	108.30
20	B	1767	CLA	CHC-C1C-NC	3.38	129.33	124.20
20	3	3001	CLA	CHD-C1D-ND	3.38	127.78	124.52
20	A	1800	CLA	CAC-C3C-C4C	3.38	129.19	124.81
20	B	1767	CLA	C1-O2A-CGA	3.38	125.30	116.44
20	4	1209	CLA	CMD-C2D-C1D	3.37	130.66	124.71
22	I	1032	BCR	C19-C18-C17	3.37	124.12	118.94
21	A	7017	LMU	O5B-C5B-C6B	3.37	114.82	106.44
20	4	1201	CLA	C6-C5-C3	-3.37	109.10	114.62
20	B	1768	CLA	CHD-C4C-C3C	-3.37	119.89	124.84
20	A	1763	CLA	CHC-C1C-NC	3.37	129.32	124.20
20	4	4007	CLA	C1-C2-C3	-3.37	120.22	126.04
21	A	7020	LMU	C1B-O5B-C5B	3.37	120.30	113.69
20	B	1753	CLA	C3A-C2A-C1A	-3.37	96.30	101.34
20	B	1787	CLA	CMA-C3A-C4A	-3.37	102.73	111.77
20	A	1815	CLA	CHD-C4C-C3C	-3.36	119.90	124.84
20	3	1213	CLA	C2D-C3D-C4D	-3.36	103.56	107.28
20	A	1799	CLA	CAC-C3C-C4C	3.36	129.17	124.81
20	A	1780	CLA	O2A-CGA-CBA	3.36	122.45	111.91
22	A	1805	BCR	C38-C26-C27	3.36	120.07	113.62
20	A	1811	CLA	CMD-C2D-C3D	-3.36	119.89	127.61
20	G	1099	CLA	CMD-C2D-C3D	-3.36	119.89	127.61
20	3	3002	CLA	C3B-C2B-C1B	-3.36	103.41	106.29
22	A	1803	BCR	C38-C26-C27	3.36	120.07	113.62
20	B	1754	CLA	CHB-C4A-NA	3.36	129.16	124.51
22	A	1807	BCR	C33-C5-C4	3.35	120.06	113.62
20	4	1209	CLA	CHC-C1C-NC	3.35	129.29	124.20
22	B	1777	BCR	C38-C26-C27	3.35	120.05	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	1205	CLA	C4A-NA-C1A	3.35	108.21	106.71
20	K	3009	CLA	C4A-NA-C1A	3.35	108.21	106.71
22	B	1778	BCR	C38-C26-C27	3.35	120.05	113.62
22	B	1774	BCR	C38-C26-C27	3.35	120.05	113.62
21	K	1086	LMU	O1B-C4'-C5'	3.35	118.62	109.45
21	A	7031	LMU	O5'-C1'-O1'	3.35	117.90	109.97
22	A	1805	BCR	C33-C5-C4	3.35	120.05	113.62
20	3	1214	CLA	C2D-C3D-C4D	-3.35	103.57	107.28
21	R	1057	LMU	O5'-C1'-O1'	3.34	117.89	109.97
20	A	1767	CLA	CHD-C4C-C3C	-3.34	119.92	124.84
20	3	1213	CLA	C3B-C2B-C1B	-3.34	103.43	106.29
21	A	7013	LMU	O4'-C4B-C5B	3.34	117.59	109.30
22	B	1774	BCR	C33-C5-C4	3.34	120.03	113.62
22	A	1808	BCR	C38-C26-C27	3.34	120.03	113.62
22	B	1780	BCR	C38-C26-C27	3.34	120.03	113.62
20	4	4003	CLA	C3B-C2B-C1B	-3.34	103.43	106.29
22	A	1804	BCR	C38-C26-C27	3.34	120.03	113.62
22	B	1776	BCR	C23-C22-C21	3.34	124.06	118.94
20	3	1214	CLA	C3C-C4C-CHD	-3.33	117.92	125.22
20	4	1198	CLA	CMA-C3A-C4A	3.33	120.73	111.77
21	A	7037	LMU	C1'-C2'-C3'	3.33	116.94	110.00
20	A	1817	CLA	C3A-C2A-C1A	3.33	106.33	101.34
20	A	1766	CLA	CMA-C3A-C2A	-3.33	100.38	113.83
20	F	1157	CLA	CAA-C2A-C3A	-3.33	103.65	112.78
22	B	1777	BCR	C33-C5-C4	3.33	120.02	113.62
22	A	1806	BCR	C38-C26-C27	3.33	120.01	113.62
21	A	7016	LMU	C2'-C3'-C4'	3.33	117.28	109.68
20	B	1764	CLA	CHB-C4A-NA	3.33	129.11	124.51
21	A	7017	LMU	C1'-C2'-C3'	3.33	116.92	110.00
20	2	1221	CLA	CHD-C1D-ND	3.33	127.73	124.52
22	B	1775	BCR	C33-C5-C4	3.33	120.00	113.62
20	L	1168	CLA	C4D-CHA-C1A	3.32	125.29	121.25
21	K	1086	LMU	O2B-C2B-C1B	-3.32	101.98	110.05
22	A	1806	BCR	C33-C5-C4	3.32	120.00	113.62
22	3	1220	BCR	C15-C14-C13	-3.32	122.57	127.31
20	A	1778	CLA	CHD-C4C-C3C	-3.32	119.96	124.84
20	B	1760	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
20	B	1739	CLA	O2A-CGA-O1A	-3.32	115.22	123.59
22	A	1803	BCR	C33-C5-C4	3.32	119.99	113.62
21	A	7030	LMU	O5B-C5B-C6B	3.32	114.69	106.44
20	3	1218	CLA	CAC-C3C-C4C	-3.32	120.51	124.81
20	A	1767	CLA	CAA-C2A-C1A	-3.32	101.11	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	1217	CLA	O2D-CGD-CBD	3.32	117.16	111.27
20	B	1769	CLA	O1D-CGD-CBD	-3.32	117.70	124.48
20	A	1774	CLA	CMD-C2D-C3D	-3.31	119.99	127.61
20	3	1215	CLA	C3C-C4C-CHD	-3.31	117.97	125.22
22	B	1780	BCR	C33-C5-C4	3.31	119.98	113.62
20	B	1759	CLA	CMA-C3A-C2A	-3.31	100.47	113.83
20	B	1753	CLA	CMC-C2C-C1C	3.31	130.08	125.04
21	A	7032	LMU	C1'-O5'-C5'	-3.31	107.19	113.69
22	B	1781	BCR	C33-C5-C4	3.31	119.97	113.62
21	A	7024	LMU	C1'-C2'-C3'	3.31	116.88	110.00
21	A	7041	LMU	O5'-C1'-C2'	-3.31	103.35	110.35
20	A	1815	CLA	O2A-CGA-CBA	3.30	122.28	111.91
22	A	1804	BCR	C33-C5-C4	3.30	119.96	113.62
20	B	1760	CLA	C2D-C1D-ND	-3.30	107.67	110.10
20	B	1751	CLA	C4A-NA-C1A	3.30	108.19	106.71
21	A	7032	LMU	O1B-C1B-C2B	-3.30	99.54	108.10
20	4	1201	CLA	CED-O2D-CGD	3.30	123.40	115.94
22	L	1170	BCR	C29-C30-C25	3.30	115.56	110.48
22	B	1781	BCR	C27-C26-C25	-3.30	117.94	122.73
22	A	1807	BCR	C38-C26-C27	3.30	119.95	113.62
20	1	1192	CLA	O2A-CGA-CBA	3.30	122.26	111.91
22	A	1808	BCR	C33-C5-C4	3.30	119.95	113.62
22	B	1775	BCR	C38-C26-C27	3.30	119.95	113.62
20	3	1216	CLA	C2D-C3D-C4D	-3.29	103.63	107.28
21	A	1810	LMU	O1'-C1'-C2'	3.29	113.44	108.30
20	B	1751	CLA	O1D-CGD-CBD	-3.29	117.75	124.48
20	B	1747	CLA	CHD-C4C-C3C	-3.29	120.00	124.84
20	A	1783	CLA	CHC-C1C-NC	3.29	129.20	124.20
20	B	1770	CLA	CMB-C2B-C3B	3.29	130.84	124.68
20	F	1155	CLA	CAA-C2A-C1A	-3.29	103.68	111.81
22	3	1220	BCR	C38-C26-C27	3.29	119.94	113.62
21	A	7025	LMU	C1'-O5'-C5'	3.29	120.14	113.69
20	B	1786	CLA	CMD-C2D-C3D	-3.29	120.05	127.61
21	A	7026	LMU	O3'-C3'-C4'	3.29	118.65	109.94
20	4	1197	CLA	C2D-C1D-ND	-3.29	107.68	110.10
20	B	1766	CLA	CHC-C1C-NC	3.29	129.19	124.20
20	A	1786	CLA	O2A-CGA-CBA	3.29	122.22	111.91
20	B	1760	CLA	CED-O2D-CGD	3.28	123.36	115.94
20	B	1737	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
20	K	3009	CLA	CMD-C2D-C3D	-3.28	120.06	127.61
20	J	1045	CLA	CAA-CBA-CGA	-3.28	103.66	113.25
20	2	1216	CLA	C2C-C1C-CHC	-3.28	117.81	125.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	1198	CLA	O1D-CGD-CBD	-3.28	117.77	124.48
20	B	1737	CLA	CHD-C4C-C3C	-3.28	120.02	124.84
20	A	1816	CLA	C2A-C1A-CHA	-3.28	118.12	123.86
20	1	1191	CLA	C4A-NA-C1A	3.28	108.18	106.71
20	1	1195	CLA	C4A-NA-C1A	3.28	108.18	106.71
20	B	1768	CLA	C4A-NA-C1A	3.28	108.18	106.71
20	4	1204	CLA	C1D-ND-C4D	-3.28	104.01	106.33
20	A	1765	CLA	O2A-C1-C2	3.28	117.25	108.64
20	B	1785	CLA	CHB-C4A-NA	3.28	129.04	124.51
20	I	1033	CLA	CMD-C2D-C3D	-3.27	120.08	127.61
21	A	7036	LMU	O3'-C3'-C2'	3.27	117.92	110.35
20	I	1033	CLA	CED-O2D-CGD	3.27	123.34	115.94
20	B	1740	CLA	C4-C3-C5	3.27	120.77	115.27
20	A	1778	CLA	CHC-C1C-C2C	-3.27	117.67	126.72
20	B	1772	CLA	C1B-C2B-C3B	-3.27	103.88	106.92
22	B	1778	BCR	C33-C5-C4	3.27	119.90	113.62
20	4	1198	CLA	C16-C15-C13	-3.27	105.36	115.92
21	A	7022	LMU	O1B-C1B-O5B	-3.27	101.55	110.67
20	A	1773	CLA	CED-O2D-CGD	3.26	123.32	115.94
20	3	1215	CLA	C2D-C3D-C4D	-3.26	103.66	107.28
20	A	1817	CLA	CBA-CAA-C2A	3.26	123.50	113.86
21	A	7027	LMU	C2'-C3'-C4'	3.26	117.13	109.68
20	4	1198	CLA	CBC-CAC-C3C	-3.26	103.44	112.43
20	G	1099	CLA	CHC-C1C-NC	3.26	129.15	124.20
20	A	1787	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
21	A	7037	LMU	C6'-C5'-C4'	-3.26	103.84	113.33
20	I	1031	CLA	O2A-CGA-CBA	3.26	122.13	111.91
20	B	1786	CLA	C1-O2A-CGA	3.26	124.99	116.44
20	A	1800	CLA	CHC-C1C-NC	3.25	129.14	124.20
22	3	1220	BCR	C36-C18-C17	-3.25	118.37	122.92
20	A	1817	CLA	CHD-C4C-NC	3.25	129.32	124.20
21	A	7027	LMU	O1B-C1B-C2B	3.25	116.52	108.10
20	1	1188	CLA	C3A-C2A-C1A	3.25	106.20	101.34
20	J	1043	CLA	C1-C2-C3	-3.25	120.43	126.04
20	B	1764	CLA	CHC-C1C-NC	3.25	129.13	124.20
20	A	1762	CLA	C4A-NA-C1A	3.25	108.17	106.71
21	A	7039	LMU	O1B-C1B-O5B	3.24	119.74	110.67
20	J	1044	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
21	A	7016	LMU	O5'-C1'-O1'	-3.24	102.30	109.97
20	A	1811	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
21	A	7030	LMU	C1'-O5'-C5'	-3.24	107.33	113.69
20	A	1771	CLA	O2A-CGA-CBA	3.24	122.07	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1781	CLA	C1-C2-C3	-3.24	120.44	126.04
20	4	1198	CLA	CHC-C1C-C2C	-3.24	117.77	126.72
20	A	1763	CLA	CMD-C2D-C3D	-3.24	120.17	127.61
20	A	1765	CLA	C4-C3-C5	3.24	120.71	115.27
20	4	1208	CLA	C1C-NC-C4C	-3.23	105.25	106.71
20	A	1783	CLA	CHB-C4A-NA	3.23	128.98	124.51
22	B	1779	BCR	C38-C26-C27	3.23	119.83	113.62
20	A	1790	CLA	CHB-C4A-NA	3.23	128.98	124.51
21	A	7037	LMU	O1B-C1B-O5B	3.23	119.70	110.67
20	A	1798	CLA	C7-C6-C5	-3.23	104.58	113.36
20	A	1795	CLA	C1-C2-C3	-3.23	120.45	126.04
21	A	1809	LMU	C1B-O5B-C5B	3.23	120.03	113.69
20	B	1754	CLA	CHD-C4C-C3C	-3.23	120.09	124.84
20	B	1772	CLA	CHC-C1C-NC	3.23	129.10	124.20
22	B	1776	BCR	C16-C15-C14	-3.23	116.86	123.47
20	B	1765	CLA	O1D-CGD-CBD	-3.23	117.88	124.48
21	A	7021	LMU	O5B-C5B-C4B	3.23	115.56	109.69
21	A	7036	LMU	O5'-C1'-C2'	-3.23	103.52	110.35
20	B	1756	CLA	C1-C2-C3	-3.22	120.47	126.04
20	I	1033	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
21	A	7043	LMU	C1'-C2'-C3'	3.22	116.71	110.00
20	4	1208	CLA	C4A-NA-C1A	3.22	108.16	106.71
20	B	1745	CLA	O2A-CGA-CBA	3.22	122.02	111.91
20	B	1754	CLA	CHC-C1C-NC	3.22	129.09	124.20
20	A	1792	CLA	C1-C2-C3	-3.22	120.47	126.04
20	A	1785	CLA	CMD-C2D-C3D	-3.22	120.21	127.61
20	A	1811	CLA	CHB-C4A-NA	3.22	128.96	124.51
20	A	1797	CLA	C1-C2-C3	-3.22	120.48	126.04
20	A	1811	CLA	C4A-NA-C1A	3.22	108.15	106.71
20	A	1793	CLA	C1-C2-C3	-3.22	120.48	126.04
20	J	1044	CLA	CBC-CAC-C3C	-3.22	103.56	112.43
22	L	1170	BCR	C36-C18-C17	-3.22	118.42	122.92
20	2	1227	CLA	CHC-C1C-NC	3.22	128.98	124.23
20	3	3011	CLA	C1-C2-C3	-3.21	120.48	126.04
20	B	1736	CLA	CHB-C4A-NA	3.21	128.96	124.51
20	1	1192	CLA	CAC-C3C-C4C	3.21	128.98	124.81
22	L	1170	BCR	C24-C23-C22	-3.21	121.38	126.23
20	1	1199	CLA	C2A-C3A-C4A	-3.21	99.14	104.18
21	A	7026	LMU	C6B-C5B-C4B	3.21	120.52	113.00
20	4	4003	CLA	CHD-C1D-ND	3.21	127.61	124.52
20	G	1099	CLA	C4A-NA-C1A	3.21	108.15	106.71
20	B	1768	CLA	O2A-CGA-CBA	3.21	121.97	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1744	CLA	CHB-C4A-NA	3.21	128.95	124.51
20	A	1796	CLA	C1-C2-C3	-3.21	120.50	126.04
21	A	7028	LMU	O3'-C3'-C4'	-3.21	101.45	109.94
20	B	1763	CLA	O2A-CGA-CBA	3.21	121.97	111.91
20	B	1755	CLA	C1-C2-C3	-3.20	120.50	126.04
20	3	1213	CLA	C3B-C4B-NB	3.20	112.91	110.11
21	A	7030	LMU	O3'-C3'-C2'	-3.20	102.94	110.35
20	A	1786	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
20	B	1763	CLA	O2A-CGA-O1A	-3.20	115.51	123.59
20	A	1769	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
22	B	1779	BCR	C4-C5-C6	-3.20	118.08	122.73
20	3	1218	CLA	C4-C3-C5	3.20	120.65	115.27
20	4	1196	CLA	C1-C2-C3	-3.20	120.51	126.04
20	B	1769	CLA	CAA-C2A-C3A	-3.20	104.02	112.78
20	A	1817	CLA	CGD-CBD-CAD	3.19	121.08	110.73
20	B	1735	CLA	C1-C2-C3	-3.19	120.52	126.04
20	A	1779	CLA	CAC-C3C-C4C	3.19	128.95	124.81
20	R	1055	CLA	C4A-NA-C1A	3.19	108.14	106.71
21	A	7042	LMU	C1'-C2'-C3'	-3.19	103.35	110.00
20	B	1771	CLA	O2A-CGA-O1A	-3.19	115.54	123.59
20	L	1167	CLA	CMA-C3A-C4A	-3.19	103.20	111.77
20	L	1167	CLA	C4A-NA-C1A	3.19	108.14	106.71
20	A	1782	CLA	C1-C2-C3	-3.19	120.53	126.04
21	A	7019	LMU	O5B-C5B-C6B	3.19	114.36	106.44
20	K	1146	CLA	CHD-C4C-C3C	-3.19	120.15	124.84
20	A	1774	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
20	3	1219	CLA	C1-C2-C3	-3.19	120.53	126.04
20	A	1760	CLA	CMB-C2B-C3B	3.19	130.64	124.68
20	A	1776	CLA	CGD-CBD-CAD	3.18	121.05	110.73
20	B	1759	CLA	C2A-C1A-CHA	-3.18	118.30	123.86
20	A	1784	CLA	C4A-NA-C1A	3.18	108.14	106.71
20	A	1799	CLA	C2D-C1D-ND	-3.18	107.76	110.10
20	B	1741	CLA	CHD-C4C-C3C	-3.18	120.17	124.84
20	2	1214	CLA	C3C-C4C-CHD	-3.18	118.26	125.22
20	B	1738	CLA	CMA-C3A-C2A	-3.18	101.01	113.83
20	3	1213	CLA	CHB-C4A-NA	3.18	129.20	124.34
21	A	7013	LMU	O5B-C1B-C2B	-3.18	103.63	110.35
20	F	1157	CLA	CMA-C3A-C4A	3.17	120.30	111.77
20	R	1054	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
20	B	1785	CLA	CBC-CAC-C3C	-3.17	103.69	112.43
20	2	2010	CLA	C3C-C4C-CHD	-3.17	118.28	125.22
20	B	1737	CLA	CHC-C1C-C2C	-3.17	117.95	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	I	1031	CLA	CMD-C2D-C3D	-3.17	120.32	127.61
20	A	1784	CLA	O1D-CGD-CBD	-3.17	118.01	124.48
20	2	1218	CLA	C4A-NA-C1A	3.17	108.13	106.71
20	1	1189	CLA	CMC-C2C-C1C	3.17	129.86	125.04
20	A	1783	CLA	O2A-CGA-CBA	3.16	121.84	111.91
20	2	1216	CLA	C3C-C4C-CHD	-3.16	118.30	125.22
20	A	1813	CLA	CHC-C1C-NC	3.16	129.00	124.20
20	R	1054	CLA	C4-C3-C5	3.16	120.58	115.27
21	A	7024	LMU	O5'-C5'-C6'	3.16	114.28	106.44
20	A	1817	CLA	CAC-C3C-C2C	-3.16	122.13	127.53
20	2	2010	CLA	C3B-C2B-C1B	-3.16	103.59	106.29
20	4	1202	CLA	C2A-C3A-C4A	-3.15	99.23	104.18
20	3	3002	CLA	C3C-C4C-CHD	-3.15	118.31	125.22
21	A	7022	LMU	O5B-C1B-C2B	-3.15	103.68	110.35
20	A	1798	CLA	CED-O2D-CGD	3.15	123.06	115.94
20	4	1205	CLA	C2D-C3D-C4D	-3.15	103.79	107.28
21	A	7039	LMU	O3'-C3'-C4'	-3.15	101.61	109.94
23	A	1802	PQN	C2M-C2-C1	3.15	121.48	116.27
20	A	1780	CLA	O2A-CGA-O1A	-3.14	115.66	123.59
20	A	1783	CLA	C4A-NA-C1A	3.14	108.12	106.71
20	A	1788	CLA	C4A-NA-C1A	3.14	108.12	106.71
20	A	1801	CLA	O2A-CGA-CBA	3.14	121.77	111.91
20	B	1760	CLA	CMD-C2D-C3D	-3.14	120.39	127.61
22	B	1776	BCR	C15-C14-C13	-3.14	122.83	127.31
20	4	1208	CLA	C2D-C3D-C4D	-3.14	103.80	107.28
22	L	1169	BCR	C19-C18-C17	-3.14	114.13	118.94
22	I	1032	BCR	C32-C1-C6	-3.14	105.21	110.30
20	2	1212	CLA	C1-C2-C3	-3.13	120.62	126.04
20	A	1811	CLA	C6-C7-C8	-3.13	105.79	115.92
20	A	1774	CLA	C4-C3-C5	3.13	120.54	115.27
22	B	1779	BCR	C23-C22-C21	3.13	123.74	118.94
20	B	1741	CLA	C2D-C1D-ND	-3.13	107.80	110.10
20	A	1766	CLA	CHD-C4C-C3C	-3.13	120.25	124.84
20	F	1157	CLA	C2A-C1A-CHA	-3.12	118.40	123.86
20	1	1201	CLA	CHB-C4A-NA	3.12	129.12	124.34
20	F	1157	CLA	CBA-CAA-C2A	-3.12	104.65	113.86
20	3	1214	CLA	CHD-C1D-ND	3.12	127.53	124.52
21	A	7024	LMU	C4B-C3B-C2B	-3.12	105.38	110.82
20	B	1743	CLA	CMB-C2B-C3B	3.12	130.51	124.68
20	B	1763	CLA	C4A-NA-C1A	3.12	108.11	106.71
21	A	7028	LMU	O5'-C1'-O1'	-3.11	102.60	109.97
20	G	1099	CLA	C1D-ND-C4D	-3.11	104.12	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1742	CLA	C4-C3-C2	-3.11	115.69	123.68
20	A	1788	CLA	CMB-C2B-C3B	3.11	130.50	124.68
20	B	1763	CLA	CMB-C2B-C3B	3.11	130.50	124.68
21	A	7027	LMU	C1'-C2'-C3'	3.11	116.48	110.00
20	3	3007	CLA	CHD-C4C-C3C	-3.11	120.27	124.84
20	J	1044	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
20	4	1201	CLA	O2D-CGD-CBD	3.11	116.79	111.27
20	2	2010	CLA	C1C-NC-C4C	-3.11	105.31	106.71
20	3	3007	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
20	B	1754	CLA	O2A-CGA-CBA	3.11	121.65	111.91
20	1	1194	CLA	C3C-C4C-CHD	-3.10	118.42	125.22
20	B	1742	CLA	C5-C3-C2	3.10	127.40	121.12
20	4	1201	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
20	L	1167	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
22	B	1776	BCR	C33-C5-C6	-3.10	121.05	124.53
20	B	1772	CLA	CGD-CBD-CAD	-3.10	101.59	114.30
20	B	1745	CLA	CMB-C2B-C3B	3.10	130.48	124.68
20	2	1221	CLA	C4A-NA-C1A	3.10	108.10	106.71
20	B	1768	CLA	CHC-C1C-C2C	-3.10	118.16	126.72
21	A	7013	LMU	C3B-C4B-C5B	-3.09	104.72	110.24
20	1	1190	CLA	CGD-CBD-CAD	3.09	120.75	110.73
20	B	1752	CLA	C5-C3-C2	-3.09	114.86	121.12
20	A	1785	CLA	CAA-C2A-C1A	-3.09	101.84	111.97
20	2	1222	CLA	CHB-C4A-NA	3.09	128.79	124.51
20	4	1204	CLA	CHC-C1C-NC	3.09	128.89	124.20
20	A	1780	CLA	CMB-C2B-C3B	3.09	130.46	124.68
21	A	7030	LMU	O5'-C5'-C4'	-3.09	103.24	109.75
21	A	7028	LMU	O5B-C1B-C2B	-3.09	103.81	110.35
20	4	1205	CLA	C3C-C4C-CHD	-3.09	118.46	125.22
20	B	1741	CLA	CAA-C2A-C3A	-3.09	104.32	112.78
20	B	1741	CLA	CAC-C3C-C4C	3.09	128.82	124.81
20	A	1775	CLA	CBD-CHA-C1A	3.09	132.37	127.43
20	B	1762	CLA	C1-C2-C3	-3.08	120.71	126.04
21	A	7030	LMU	C1B-O5B-C5B	3.08	119.73	113.69
20	B	1771	CLA	CMD-C2D-C3D	-3.08	120.53	127.61
20	A	1762	CLA	C2A-C1A-CHA	-3.08	118.47	123.86
20	1	1194	CLA	C4A-NA-C1A	3.08	108.09	106.71
21	A	7020	LMU	O5B-C1B-C2B	3.08	116.86	110.35
22	L	1169	BCR	C15-C14-C13	3.08	131.70	127.31
20	2	1218	CLA	CGD-CBD-CAD	3.08	120.70	110.73
20	3	1218	CLA	O2A-CGA-CBA	3.07	121.56	111.91
21	A	7026	LMU	O1B-C1B-C2B	3.07	116.06	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	7026	LMU	O5'-C5'-C6'	3.07	114.08	106.44
21	A	7028	LMU	O5B-C5B-C6B	3.07	114.08	106.44
20	A	1815	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
20	1	1197	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
20	A	1767	CLA	CHB-C4A-NA	3.07	128.76	124.51
20	3	3015	CLA	C3C-C4C-CHD	-3.07	118.50	125.22
20	B	1787	CLA	O2A-CGA-CBA	3.07	121.54	111.91
20	3	3015	CLA	C2C-C1C-CHC	-3.07	118.33	125.67
21	A	7015	LMU	C4B-C3B-C2B	3.06	116.17	110.82
20	R	1054	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
20	3	1213	CLA	C3C-C4C-CHD	-3.06	118.51	125.22
21	A	7023	LMU	C6B-C5B-C4B	-3.06	105.83	113.00
20	A	1773	CLA	O1D-CGD-CBD	-3.06	118.22	124.48
20	1	1197	CLA	C1D-ND-C4D	-3.06	104.16	106.33
20	1	1195	CLA	C1D-ND-C4D	-3.06	104.16	106.33
20	B	1739	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
20	B	1757	CLA	CHB-C4A-NA	3.06	128.74	124.51
20	2	1224	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
20	B	1770	CLA	C4-C3-C5	3.05	120.41	115.27
20	A	1763	CLA	CAA-C2A-C1A	-3.05	101.96	111.97
20	3	3011	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
21	A	7021	LMU	C1'-O5'-C5'	-3.05	107.69	113.69
20	A	1764	CLA	C4A-NA-C1A	3.05	108.08	106.71
20	2	1224	CLA	O2A-CGA-CBA	3.05	121.48	111.91
20	1	1194	CLA	C2A-C3A-C4A	-3.05	99.39	104.18
20	4	1198	CLA	C3C-C4C-NC	-3.05	107.15	110.57
20	B	1753	CLA	C1D-ND-C4D	-3.05	104.17	106.33
20	B	1740	CLA	C4A-NA-C1A	3.05	108.08	106.71
20	A	1759	CLA	CMB-C2B-C3B	3.05	130.38	124.68
20	A	1789	CLA	O2A-CGA-O1A	-3.05	115.91	123.59
20	B	1768	CLA	CBC-CAC-C3C	-3.05	104.04	112.43
20	A	1775	CLA	C4A-NA-C1A	3.05	108.08	106.71
20	1	1200	CLA	C1D-ND-C4D	3.04	108.50	106.33
20	3	1215	CLA	CHD-C1D-ND	3.04	127.46	124.52
20	2	1221	CLA	C3C-C4C-CHD	-3.04	118.56	125.22
20	B	1785	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
21	A	7016	LMU	O3'-C3'-C4'	-3.04	101.89	109.94
20	B	1770	CLA	CAA-C2A-C3A	-3.04	104.45	112.78
20	4	1201	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
20	A	1780	CLA	CAC-C3C-C4C	3.03	128.75	124.81
20	2	1213	CLA	C4-C3-C5	3.03	120.37	115.27
20	1	1193	CLA	CMB-C2B-C3B	3.03	130.35	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	1166	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
20	B	1752	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
20	A	1783	CLA	CMA-C3A-C4A	-3.03	103.64	111.77
20	3	1217	CLA	C4C-CHD-C1D	-3.03	118.62	126.11
20	2	1219	CLA	C1D-ND-C4D	-3.03	104.19	106.33
20	A	1780	CLA	O2D-CGD-CBD	3.03	116.64	111.27
20	3	1212	CLA	C4A-NA-C1A	3.03	108.07	106.71
21	L	1171	LMU	O5'-C5'-C6'	3.02	113.95	106.44
20	B	1771	CLA	CAA-CBA-CGA	3.02	122.09	113.25
20	A	1784	CLA	CMA-C3A-C4A	-3.02	103.65	111.77
21	2	1225	LMU	O1B-C4'-C3'	3.02	115.32	107.28
21	A	7037	LMU	C3'-C4'-C5'	-3.02	104.00	110.93
20	A	1786	CLA	C2D-C1D-ND	-3.02	107.88	110.10
20	B	1745	CLA	C4-C3-C5	3.02	120.35	115.27
20	B	1759	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
21	A	1809	LMU	C2'-C3'-C4'	3.02	116.58	109.68
20	B	1744	CLA	C4A-NA-C1A	3.02	108.06	106.71
20	A	1813	CLA	C2A-C1A-CHA	-3.02	118.58	123.86
20	B	1746	CLA	C1D-ND-C4D	-3.02	104.19	106.33
20	3	1214	CLA	C2A-C3A-C4A	-3.02	99.45	104.18
20	4	1208	CLA	C3C-C4C-CHD	-3.01	118.62	125.22
20	R	1054	CLA	C1-O2A-CGA	3.01	124.35	116.44
20	2	1220	CLA	O2A-CGA-CBA	3.01	121.36	111.91
21	A	7030	LMU	C3'-C4'-C5'	-3.01	104.02	110.93
20	A	1777	CLA	C4-C3-C5	3.01	119.43	115.98
20	2	2010	CLA	C3D-C4D-CHA	-3.01	118.64	124.98
20	4	4007	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
20	A	1768	CLA	CHB-C4A-NA	3.01	128.67	124.51
20	A	1779	CLA	C4-C3-C5	3.00	120.32	115.27
20	B	1739	CLA	CAA-C2A-C3A	-3.00	104.55	112.78
20	3	3014	CLA	C3D-C4D-ND	3.00	113.99	109.46
20	A	1763	CLA	C2A-C1A-CHA	-3.00	118.61	123.86
20	B	1752	CLA	CHD-C4C-C3C	-3.00	120.43	124.84
20	L	1166	CLA	CMD-C2D-C3D	-3.00	120.72	127.61
20	A	1765	CLA	O2A-CGA-O1A	-2.99	116.03	123.59
20	B	1763	CLA	CAA-CBA-CGA	-2.99	104.50	113.25
20	A	1789	CLA	O2A-CGA-CBA	2.99	121.30	111.91
20	3	3001	CLA	CHB-C4A-NA	2.99	128.92	124.34
20	B	1748	CLA	CGD-CBD-CAD	-2.99	101.05	110.73
20	B	1747	CLA	CMB-C2B-C3B	2.99	130.27	124.68
20	1	1189	CLA	C4A-NA-C1A	2.99	108.05	106.71
21	A	7025	LMU	O1B-C1B-C2B	2.99	115.84	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	1208	CLA	C3B-C2B-C1B	-2.99	103.73	106.29
21	A	7037	LMU	O1B-C4'-C3'	2.98	115.22	107.28
21	A	7033	LMU	O1B-C1B-O5B	-2.98	102.34	110.67
20	A	1798	CLA	C1-O2A-CGA	2.98	124.27	116.44
21	K	1086	LMU	C1B-O5B-C5B	-2.98	107.83	113.69
20	A	1779	CLA	CHB-C4A-NA	2.98	128.64	124.51
20	4	1207	CLA	CMC-C2C-C1C	2.98	129.58	125.04
20	3	1214	CLA	C2C-C1C-CHC	-2.98	118.53	125.67
20	2	1223	CLA	O2A-CGA-CBA	2.98	121.25	111.91
20	A	1789	CLA	CAC-C3C-C2C	-2.98	122.44	127.53
20	A	1777	CLA	CHB-C4A-NA	2.98	128.63	124.51
20	1	1191	CLA	CHB-C4A-NA	2.97	128.62	124.51
20	3	1215	CLA	C2A-C3A-C4A	-2.97	99.52	104.18
20	K	3009	CLA	CHC-C1C-NC	2.97	128.71	124.20
21	A	7040	LMU	C1'-C2'-C3'	2.97	116.19	110.00
22	I	1032	BCR	C40-C30-C25	-2.97	105.48	110.30
20	1	1187	CLA	CMA-C3A-C4A	2.97	119.76	111.77
20	1	1198	CLA	C4A-NA-C1A	2.97	108.04	106.71
20	B	1749	CLA	CHC-C1C-NC	2.97	128.71	124.20
20	2	2010	CLA	CHD-C1D-ND	2.97	127.38	124.52
20	A	1779	CLA	C1-C2-C3	-2.97	120.91	126.04
20	2	1221	CLA	C2A-C3A-C4A	-2.97	99.52	104.18
20	2	2010	CLA	C4A-NA-C1A	2.96	108.04	106.71
20	3	1216	CLA	C2A-C3A-C4A	-2.96	99.53	104.18
20	4	1201	CLA	O1D-CGD-CBD	-2.96	118.42	124.48
20	B	1760	CLA	CHD-C4C-NC	2.96	128.87	124.20
20	4	4007	CLA	CHB-C4A-NA	2.96	128.61	124.51
20	J	1046	CLA	C3C-C4C-CHD	-2.96	118.74	125.22
20	B	1753	CLA	CBA-CAA-C2A	2.96	122.60	113.86
20	B	1787	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
20	B	1738	CLA	C16-C15-C13	-2.96	106.35	115.92
20	B	1754	CLA	OBD-CAD-C3D	-2.96	121.40	128.52
21	A	7024	LMU	C2'-C3'-C4'	2.96	116.44	109.68
20	3	1215	CLA	C2C-C1C-CHC	-2.96	118.58	125.67
20	A	1765	CLA	CHD-C4C-NC	2.96	128.87	124.20
20	1	1196	CLA	CBD-CHA-C1A	2.96	132.17	127.43
20	4	1200	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
20	J	1044	CLA	CMD-C2D-C3D	-2.96	120.81	127.61
21	A	7037	LMU	O3'-C3'-C4'	2.96	117.78	109.94
20	2	1219	CLA	C3B-C2B-C1B	-2.96	103.76	106.29
20	A	1780	CLA	CHB-C4A-NA	2.96	128.60	124.51
22	L	1170	BCR	C32-C1-C6	2.95	115.09	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1811	CLA	CMB-C2B-C3B	2.95	130.21	124.68
20	B	1770	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
21	A	7031	LMU	O1B-C4'-C3'	2.95	115.14	107.28
20	B	1767	CLA	CMC-C2C-C1C	2.95	129.54	125.04
20	2	1223	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
20	1	1187	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
20	3	1216	CLA	CHD-C1D-ND	2.95	127.37	124.52
20	3	3002	CLA	C2D-C3D-C4D	-2.95	104.01	107.28
22	B	1776	BCR	C36-C18-C19	2.95	122.72	118.08
21	A	7013	LMU	O1B-C4'-C3'	2.95	115.13	107.28
20	A	1776	CLA	C1-O2A-CGA	2.95	124.18	116.44
20	B	1745	CLA	CMD-C2D-C3D	-2.95	120.83	127.61
20	A	1777	CLA	O2A-CGA-CBA	2.95	121.16	111.91
20	A	1789	CLA	CED-O2D-CGD	2.95	122.60	115.94
20	A	1769	CLA	CAA-C2A-C1A	-2.95	102.32	111.97
20	A	1812	CLA	CMD-C2D-C3D	-2.94	120.84	127.61
20	B	1740	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
20	B	1742	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
20	J	1044	CLA	CMB-C2B-C3B	2.94	130.18	124.68
23	B	1773	PQN	C16-C15-C13	-2.94	105.74	113.45
20	A	1813	CLA	C4A-NA-C1A	2.94	108.03	106.71
20	A	1817	CLA	CAA-C2A-C1A	2.94	121.61	111.97
20	A	1799	CLA	O2D-CGD-CBD	2.94	116.49	111.27
20	J	1046	CLA	CHD-C1D-ND	2.94	127.35	124.52
20	B	1785	CLA	C7-C6-C5	-2.94	105.38	113.36
21	A	7037	LMU	O3B-C3B-C4B	-2.94	103.56	110.35
20	B	1758	CLA	C11-C12-C13	-2.94	106.42	115.92
20	1	1192	CLA	CMD-C2D-C3D	-2.94	120.86	127.61
20	B	1738	CLA	O2A-CGA-O1A	-2.94	116.18	123.59
20	B	1771	CLA	C4-C3-C5	2.94	120.21	115.27
20	B	1749	CLA	CMC-C2C-C1C	2.94	129.51	125.04
20	A	1774	CLA	O2A-CGA-CBA	2.94	121.12	111.91
20	K	3009	CLA	CAA-CBA-CGA	-2.94	104.68	113.25
20	1	1198	CLA	C6-C5-C3	-2.93	105.76	113.45
20	B	1771	CLA	CHC-C1C-C2C	-2.93	118.60	126.72
20	B	1741	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
20	1	1200	CLA	CAC-C3C-C4C	2.93	128.61	124.81
20	A	1764	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
20	A	1762	CLA	CHB-C4A-NA	2.93	128.56	124.51
20	B	1748	CLA	CHB-C4A-NA	2.93	128.56	124.51
21	A	7024	LMU	O5B-C5B-C6B	2.93	113.72	106.44
20	4	1207	CLA	CMD-C2D-C3D	-2.93	120.88	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	1057	LMU	C1B-C2B-C3B	2.93	116.09	110.00
20	1	1193	CLA	CAA-CBA-CGA	2.93	121.81	113.25
20	B	1747	CLA	C4A-NA-C1A	2.92	108.02	106.71
20	B	1758	CLA	CHD-C1D-ND	2.92	127.14	124.45
20	A	1784	CLA	CHB-C4A-NA	2.92	128.55	124.51
20	L	1505	CLA	O2A-CGA-CBA	2.92	121.07	111.91
20	B	1747	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
20	B	1770	CLA	C4A-NA-C1A	2.92	108.02	106.71
20	R	1054	CLA	C4A-NA-C1A	2.92	108.02	106.71
20	B	1745	CLA	C4-C3-C2	-2.92	116.19	123.68
20	B	1772	CLA	CMD-C2D-C3D	-2.92	120.90	127.61
20	2	1216	CLA	C3D-C2D-C1D	2.92	110.51	107.28
21	A	7030	LMU	O1B-C4'-C3'	2.92	115.05	107.28
21	L	1171	LMU	O5'-C5'-C4'	-2.92	103.60	109.75
21	A	1810	LMU	C2'-C3'-C4'	2.92	116.34	109.68
20	B	1763	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
21	A	1810	LMU	C1B-O5B-C5B	2.92	119.41	113.69
20	A	1776	CLA	C4-C3-C5	2.92	120.18	115.27
20	B	1761	CLA	C1D-ND-C4D	-2.92	104.26	106.33
21	A	7023	LMU	C1B-C2B-C3B	2.91	116.06	110.00
20	2	1220	CLA	O1D-CGD-CBD	-2.91	118.52	124.48
20	G	1099	CLA	CHB-C4A-NA	2.91	128.54	124.51
20	A	1786	CLA	CAC-C3C-C4C	2.91	128.59	124.81
20	A	1760	CLA	CBA-CAA-C2A	2.91	122.45	113.86
20	1	1193	CLA	C1D-ND-C4D	-2.91	104.27	106.33
20	B	1738	CLA	CAC-C3C-C4C	2.91	128.58	124.81
21	A	7043	LMU	O3B-C3B-C2B	2.91	117.07	110.35
20	3	3015	CLA	CHD-C1D-ND	2.90	127.32	124.52
20	2	1220	CLA	C1-C2-C3	-2.90	121.02	126.04
20	4	4007	CLA	CMB-C2B-C3B	2.90	130.11	124.68
20	A	1763	CLA	CMC-C2C-C1C	2.90	129.46	125.04
20	1	1197	CLA	O2A-C1-C2	2.90	116.27	108.64
20	B	1738	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
20	I	1031	CLA	O1D-CGD-CBD	-2.90	118.55	124.48
22	I	1032	BCR	C24-C25-C26	2.90	128.48	121.46
20	2	1215	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
20	I	1033	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
20	B	1750	CLA	C1D-ND-C4D	-2.90	104.28	106.33
22	B	1781	BCR	C15-C16-C17	2.89	129.40	123.47
20	B	1754	CLA	CHC-C1C-C2C	-2.89	118.71	126.72
20	4	1202	CLA	CHB-C4A-NA	2.89	128.77	124.34
21	A	7023	LMU	C1'-O5'-C5'	-2.89	108.01	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1762	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
20	3	3014	CLA	CHD-C1D-ND	2.89	127.31	124.52
21	A	7033	LMU	C6B-C5B-C4B	2.89	119.78	113.00
20	A	1776	CLA	CED-O2D-CGD	2.89	122.48	115.94
20	2	1214	CLA	CHD-C1D-ND	2.89	127.31	124.52
20	B	1758	CLA	CMA-C3A-C2A	-2.89	102.16	113.83
21	A	7035	LMU	O3'-C3'-C4'	2.89	117.60	109.94
21	4	1210	LMU	O1'-C1'-C2'	2.89	112.82	108.30
20	A	1771	CLA	CGD-CBD-CAD	2.89	120.09	110.73
20	A	1801	CLA	CHC-C1C-NC	2.89	128.59	124.20
20	K	3009	CLA	O2A-CGA-CBA	2.89	120.97	111.91
20	A	1788	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
20	B	1761	CLA	CHB-C4A-NA	2.89	128.50	124.51
20	4	1201	CLA	CMA-C3A-C2A	-2.89	102.19	113.83
20	B	1753	CLA	CMA-C3A-C4A	-2.88	104.02	111.77
21	A	7032	LMU	O1B-C4'-C3'	-2.88	99.62	107.28
20	A	1761	CLA	O2A-CGA-CBA	2.88	120.95	111.91
20	H	1079	CLA	CAC-C3C-C4C	2.88	128.54	124.81
20	3	1214	CLA	C3D-C4D-CHA	-2.88	118.92	124.98
20	3	3008	CLA	C2A-C1A-CHA	-2.88	118.83	123.86
20	B	1786	CLA	CAA-C2A-C1A	2.88	121.40	111.97
20	2	1223	CLA	C1-O2A-CGA	2.88	123.99	116.44
20	B	1754	CLA	CAC-C3C-C2C	-2.88	122.61	127.53
20	2	1219	CLA	C2C-C1C-CHC	-2.87	118.79	125.67
20	A	1779	CLA	CMC-C2C-C1C	2.87	129.42	125.04
20	B	1751	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
20	2	1222	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
20	B	1758	CLA	C1-C2-C3	-2.87	121.08	126.04
21	A	7025	LMU	C4B-C3B-C2B	-2.87	105.81	110.82
20	L	1166	CLA	O1D-CGD-CBD	-2.87	118.61	124.48
20	2	1221	CLA	C2B-C3B-C4B	2.87	108.74	106.29
21	A	7025	LMU	O3B-C3B-C2B	-2.87	103.72	110.35
21	A	7019	LMU	O5'-C5'-C4'	2.87	115.80	109.75
20	K	1146	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
20	B	1786	CLA	C6-C5-C3	2.87	120.97	113.45
20	4	1199	CLA	CHD-C4C-NC	2.86	128.72	124.20
22	3	1220	BCR	C24-C23-C22	-2.86	121.91	126.23
20	J	1046	CLA	C2C-C1C-CHC	-2.86	118.81	125.67
21	A	7028	LMU	O2'-C2'-C1'	-2.86	103.09	110.05
20	B	1742	CLA	CHB-C4A-NA	2.86	128.47	124.51
20	A	1766	CLA	O1D-CGD-CBD	-2.86	118.63	124.48
20	A	1764	CLA	C1-C2-C3	-2.86	121.10	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1810	LMU	O2B-C2B-C1B	-2.86	103.10	110.05
20	B	1752	CLA	CAC-C3C-C4C	2.86	128.52	124.81
20	B	1785	CLA	O2D-CGD-CBD	2.86	116.35	111.27
20	3	1215	CLA	C2B-C3B-C4B	2.86	108.73	106.29
20	L	1168	CLA	CHC-C1C-NC	2.86	128.54	124.20
21	A	7036	LMU	C1B-O5B-C5B	2.86	119.29	113.69
20	A	1801	CLA	C1D-ND-C4D	-2.85	104.31	106.33
20	A	1801	CLA	CMC-C2C-C1C	2.85	129.38	125.04
20	3	1218	CLA	CAC-C3C-C2C	2.85	132.41	127.53
20	4	4007	CLA	CAA-C2A-C1A	-2.85	102.63	111.97
21	A	7027	LMU	O5B-C5B-C4B	-2.85	104.51	109.69
21	A	7033	LMU	O5'-C5'-C4'	-2.85	103.74	109.75
20	3	3014	CLA	CHB-C4A-NA	2.85	128.71	124.34
20	A	1770	CLA	O1D-CGD-CBD	-2.85	118.65	124.48
20	A	1773	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
20	3	1218	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
20	1	1192	CLA	C4-C3-C5	2.85	120.06	115.27
20	B	1762	CLA	CHB-C4A-NA	2.85	128.45	124.51
20	A	1763	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
20	A	1811	CLA	C3B-C4B-NB	-2.85	105.53	109.21
21	A	7042	LMU	O2'-C2'-C1'	2.85	116.96	110.05
20	K	3009	CLA	C4-C3-C5	2.85	120.06	115.27
20	2	1220	CLA	C4A-NA-C1A	2.85	107.99	106.71
20	A	1772	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
20	1	1199	CLA	CHB-C4A-NA	2.85	128.70	124.34
20	A	1817	CLA	C1B-C2B-C3B	-2.84	104.27	106.92
20	B	1738	CLA	CHD-C4C-C3C	-2.84	120.66	124.84
20	A	1763	CLA	CAC-C3C-C4C	2.84	128.50	124.81
20	B	1749	CLA	C4A-NA-C1A	2.84	107.98	106.71
20	3	1216	CLA	C2C-C1C-CHC	-2.84	118.86	125.67
20	I	1033	CLA	CHD-C4C-C3C	-2.84	120.66	124.84
20	A	1801	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
20	A	1771	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
21	A	7019	LMU	C1'-C2'-C3'	2.84	115.91	110.00
20	A	1767	CLA	CAA-CBA-CGA	2.84	121.55	113.25
21	A	7022	LMU	O1B-C4'-C3'	2.84	114.83	107.28
20	B	1755	CLA	C4-C3-C5	2.84	120.05	115.27
20	1	1201	CLA	C2C-C1C-CHC	-2.84	118.87	125.67
21	A	7035	LMU	O5'-C1'-C2'	2.84	116.36	110.35
20	4	1207	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
20	A	1774	CLA	CMB-C2B-C3B	2.84	129.99	124.68
20	R	1054	CLA	C1D-ND-C4D	-2.84	104.32	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1800	CLA	CMD-C2D-C3D	-2.84	121.09	127.61
20	A	1800	CLA	C6-C7-C8	-2.84	106.75	115.92
20	B	1785	CLA	O2A-CGA-CBA	2.83	120.80	111.91
20	B	1770	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
22	B	1781	BCR	C32-C1-C31	-2.83	99.83	108.53
20	I	1033	CLA	O2A-CGA-CBA	2.83	120.80	111.91
20	A	1785	CLA	CED-O2D-CGD	2.83	122.34	115.94
20	3	1215	CLA	C3D-C4D-CHA	-2.83	119.02	124.98
20	J	1044	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
20	1	1200	CLA	CMB-C2B-C3B	2.83	129.97	124.68
20	J	1045	CLA	CED-O2D-CGD	2.83	122.34	115.94
20	J	1043	CLA	C4-C3-C5	2.83	120.03	115.27
20	B	1748	CLA	CAC-C3C-C4C	2.83	128.48	124.81
20	1	1200	CLA	C2D-C1D-ND	-2.83	108.02	110.10
20	4	1204	CLA	CED-O2D-CGD	2.83	122.34	115.94
20	H	1079	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
20	B	1761	CLA	CED-O2D-CGD	2.83	122.33	115.94
20	A	1782	CLA	C4-C3-C5	2.83	120.03	115.27
20	B	1735	CLA	C4-C3-C5	2.83	120.03	115.27
20	B	1744	CLA	CMC-C2C-C1C	2.83	129.34	125.04
20	A	1770	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
20	A	1764	CLA	CMB-C2B-C3B	2.83	129.97	124.68
20	1	1197	CLA	CMA-C3A-C4A	-2.83	104.18	111.77
20	3	1219	CLA	C4-C3-C5	2.83	120.02	115.27
21	A	1810	LMU	O3B-C3B-C2B	2.83	116.88	110.35
20	4	1209	CLA	CBA-CAA-C2A	-2.82	105.53	113.86
20	B	1756	CLA	C4-C3-C5	2.82	120.02	115.27
20	3	3011	CLA	CAC-C3C-C4C	2.82	128.47	124.81
20	2	1218	CLA	CHD-C4C-C3C	-2.82	120.69	124.84
20	H	1079	CLA	CMC-C2C-C1C	2.82	129.34	125.04
20	4	1196	CLA	C4-C3-C5	2.82	120.02	115.27
20	4	4003	CLA	C2C-C1C-CHC	-2.82	118.91	125.67
20	A	1781	CLA	C4-C3-C5	2.82	120.02	115.27
20	B	1753	CLA	C3D-C4D-ND	2.82	114.80	110.24
20	A	1793	CLA	C4-C3-C5	2.82	120.01	115.27
21	A	7038	LMU	O3B-C3B-C2B	2.82	116.87	110.35
20	A	1761	CLA	CED-O2D-CGD	2.82	122.31	115.94
21	A	7037	LMU	O5'-C5'-C4'	-2.82	103.81	109.75
20	3	1214	CLA	CHB-C4A-NA	2.82	128.65	124.34
20	1	1192	CLA	C1-C2-C3	-2.82	121.17	126.04
20	B	1738	CLA	C11-C12-C13	-2.82	106.81	115.92
21	A	7017	LMU	O5'-C5'-C6'	2.82	113.44	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	1214	CLA	C2C-C1C-CHC	-2.81	118.93	125.67
20	3	1215	CLA	CHB-C4A-NA	2.81	128.65	124.34
20	A	1773	CLA	C1-O2A-CGA	2.81	123.82	116.44
20	4	1203	CLA	C2C-C1C-CHC	-2.81	118.94	125.67
20	A	1796	CLA	C4-C3-C5	2.81	120.00	115.27
22	3	1220	BCR	C34-C9-C10	-2.81	118.99	122.92
20	B	1771	CLA	CHB-C4A-NA	2.81	128.40	124.51
20	A	1816	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
20	A	1790	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
20	B	1749	CLA	C4-C3-C5	2.81	119.99	115.27
20	4	1205	CLA	C2C-C1C-CHC	-2.81	118.95	125.67
20	1	1192	CLA	C1-O2A-CGA	2.81	123.81	116.44
21	B	1782	LMU	O5B-C5B-C4B	2.81	114.79	109.69
20	1	1188	CLA	CHB-C4A-NA	2.80	128.39	124.51
21	A	7026	LMU	C1B-O1B-C4'	-2.80	111.02	117.96
20	G	1099	CLA	CMB-C2B-C3B	2.80	129.92	124.68
20	3	1212	CLA	CBD-CHA-C1A	2.80	131.92	127.43
20	B	1746	CLA	CHB-C4A-NA	2.80	128.39	124.51
20	B	1742	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
20	A	1779	CLA	O2D-CGD-CBD	2.80	116.25	111.27
20	A	1776	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
22	L	1169	BCR	C33-C5-C4	2.80	118.99	113.62
21	A	7017	LMU	O5'-C1'-C2'	2.80	116.27	110.35
20	2	1227	CLA	C1D-ND-C4D	-2.80	104.35	106.33
20	3	3008	CLA	CAA-C2A-C3A	2.80	120.43	112.78
20	A	1790	CLA	C4A-NA-C1A	2.80	107.96	106.71
21	A	7027	LMU	C4B-C3B-C2B	-2.80	105.94	110.82
22	B	1779	BCR	C33-C5-C4	2.80	118.99	113.62
20	B	1749	CLA	CMD-C2D-C3D	-2.80	121.18	127.61
20	A	1799	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
20	A	1797	CLA	C4-C3-C5	2.79	119.97	115.27
20	B	1739	CLA	CMA-C3A-C4A	-2.79	104.26	111.77
20	A	1798	CLA	CHB-C4A-NA	2.79	128.38	124.51
20	3	3014	CLA	C2C-C1C-CHC	-2.79	118.98	125.67
20	F	1157	CLA	O2A-CGA-CBA	2.79	120.67	111.91
20	3	3008	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
20	2	1224	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
20	B	1748	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
20	B	1741	CLA	O2A-CGA-CBA	2.79	120.65	111.91
21	L	1171	LMU	O5B-C5B-C4B	2.79	114.75	109.69
20	2	1214	CLA	C3D-C4D-ND	2.79	113.67	109.46
20	B	1765	CLA	C4A-NA-C1A	2.78	107.96	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1779	BCR	C2-C3-C4	-2.78	105.15	111.38
20	B	1760	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
21	A	7017	LMU	C6'-C5'-C4'	-2.78	105.22	113.33
20	3	1216	CLA	C3C-C4C-CHD	-2.78	119.12	125.22
20	A	1784	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
20	1	1200	CLA	O1D-CGD-CBD	-2.78	118.79	124.48
20	2	1219	CLA	C3D-C4D-ND	2.78	113.66	109.46
20	A	1799	CLA	CHD-C4C-C3C	-2.78	120.75	124.84
21	A	1809	LMU	C3'-C4'-C5'	2.78	117.30	110.93
20	K	1146	CLA	C5-C3-C4	2.78	120.74	114.60
20	L	1167	CLA	CED-O2D-CGD	2.78	122.22	115.94
20	4	1203	CLA	CHB-C4A-NA	2.78	128.59	124.34
21	A	7034	LMU	C3B-C4B-C5B	2.78	115.19	110.24
20	B	1785	CLA	CMD-C2D-C3D	-2.77	121.23	127.61
20	B	1744	CLA	O1D-CGD-CBD	-2.77	118.81	124.48
20	B	1746	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
20	B	1738	CLA	CMB-C2B-C1B	2.77	132.72	128.46
20	R	1055	CLA	CGD-CBD-CAD	-2.77	101.76	110.73
20	1	1199	CLA	C2C-C1C-CHC	-2.77	119.04	125.67
20	2	2010	CLA	C2C-C1C-CHC	-2.77	119.04	125.67
20	1	1189	CLA	CHC-C1C-NC	2.77	128.41	124.20
20	3	3014	CLA	C2A-C3A-C4A	-2.77	99.83	104.18
20	2	1223	CLA	O1D-CGD-CBD	-2.77	118.82	124.48
20	A	1759	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
20	B	1757	CLA	CMB-C2B-C3B	2.77	129.86	124.68
20	2	1222	CLA	CHD-C4C-C3C	-2.77	120.77	124.84
20	4	1202	CLA	C2C-C1C-CHC	-2.77	119.05	125.67
20	G	1099	CLA	CED-O2D-CGD	2.76	122.19	115.94
20	R	1055	CLA	CMB-C2B-C1B	2.76	132.71	128.46
20	J	1045	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
21	R	1057	LMU	O2B-C2B-C1B	2.76	116.75	110.05
20	4	1206	CLA	C3D-C4D-ND	2.76	113.63	109.46
20	B	1759	CLA	O1D-CGD-CBD	-2.76	118.84	124.48
20	A	1761	CLA	CAC-C3C-C4C	2.76	128.39	124.81
20	A	1768	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
20	A	1771	CLA	C2D-C1D-ND	-2.76	108.07	110.10
20	3	1212	CLA	CMB-C2B-C3B	2.76	130.09	124.69
20	A	1788	CLA	CHB-C4A-NA	2.76	128.33	124.51
20	1	1190	CLA	C4D-C3D-CAD	2.76	111.34	108.10
21	A	7040	LMU	C4B-C3B-C2B	-2.76	106.01	110.82
20	G	1099	CLA	CAA-CBA-CGA	-2.76	105.20	113.25
20	3	3015	CLA	C2D-C3D-C4D	-2.76	104.23	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	1168	CLA	CAA-C2A-C1A	2.75	121.00	111.97
20	A	1779	CLA	CAA-C2A-C3A	-2.75	105.24	112.78
21	A	7013	LMU	O5'-C5'-C6'	2.75	113.28	106.44
20	A	1762	CLA	O2A-CGA-CBA	2.75	120.54	111.91
20	B	1749	CLA	CAA-C2A-C1A	2.75	120.99	111.97
20	B	1758	CLA	O1D-CGD-CBD	-2.75	118.86	124.48
20	3	3008	CLA	CED-O2D-CGD	2.75	122.15	115.94
20	B	1741	CLA	O2A-C1-C2	2.75	115.85	108.64
20	A	1783	CLA	C6-C7-C8	-2.75	107.04	115.92
20	R	1055	CLA	CHC-C1C-C2C	-2.75	119.13	126.72
20	A	1764	CLA	O2A-C1-C2	2.74	115.85	108.64
21	A	7043	LMU	O2B-C2B-C3B	-2.74	104.00	110.35
20	B	1758	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
21	A	7037	LMU	O6B-C6B-C5B	-2.74	101.89	111.29
20	1	1198	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
20	3	1213	CLA	C1C-NC-C4C	2.74	107.94	106.71
21	A	7016	LMU	O5B-C5B-C4B	-2.74	104.72	109.69
20	2	1219	CLA	CHD-C1D-ND	2.74	127.16	124.52
21	A	7043	LMU	O2'-C2'-C1'	-2.74	103.39	110.05
20	H	1079	CLA	O2A-CGA-CBA	2.74	120.50	111.91
20	B	1752	CLA	O2D-CGD-CBD	2.74	116.13	111.27
20	A	1771	CLA	CMB-C2B-C3B	2.74	129.80	124.68
20	B	1750	CLA	O2A-CGA-CBA	2.74	120.49	111.91
20	B	1785	CLA	C16-C17-C18	-2.74	103.09	115.98
20	B	1754	CLA	C1-O2A-CGA	2.74	123.62	116.44
21	A	7041	LMU	C1B-O5B-C5B	-2.73	108.32	113.69
20	B	1749	CLA	O1D-CGD-CBD	-2.73	118.89	124.48
20	1	1190	CLA	C4A-NA-C1A	2.73	107.94	106.71
21	A	7042	LMU	O6'-C6'-C5'	2.73	120.67	111.29
20	B	1762	CLA	CAA-CBA-CGA	-2.73	105.27	113.25
21	A	7013	LMU	O3'-C3'-C4'	-2.73	102.70	109.94
20	J	1044	CLA	C11-C12-C13	-2.73	107.09	115.92
20	B	1785	CLA	C1D-ND-C4D	-2.73	104.39	106.33
21	A	7043	LMU	O5'-C5'-C6'	2.73	113.23	106.44
20	B	1748	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
20	A	1799	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
22	B	1779	BCR	C34-C9-C10	-2.73	119.10	122.92
20	A	1767	CLA	O2D-CGD-CBD	2.73	116.11	111.27
20	A	1767	CLA	C3A-C2A-C1A	2.73	105.42	101.34
21	A	7023	LMU	C1-O1'-C1'	-2.72	109.32	113.84
21	A	7032	LMU	C1B-O1B-C4'	-2.72	111.22	117.96
20	1	1200	CLA	O2D-CGD-O1D	-2.72	118.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1799	CLA	CHB-C4A-NA	2.72	128.28	124.51
20	2	1217	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
21	A	7041	LMU	O2B-C2B-C1B	-2.72	103.43	110.05
20	A	1789	CLA	CHB-C4A-NA	2.72	128.28	124.51
20	A	1768	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
20	K	3009	CLA	C6-C7-C8	-2.72	107.12	115.92
20	1	1197	CLA	CHB-C4A-NA	2.72	128.28	124.51
21	B	1782	LMU	C3B-C4B-C5B	2.72	115.09	110.24
20	A	1771	CLA	C1-C2-C3	-2.72	122.35	126.75
20	A	1800	CLA	CMC-C2C-C1C	2.72	129.18	125.04
20	A	1813	CLA	O2A-C1-C2	2.72	115.78	108.64
20	A	1767	CLA	C2D-C1D-ND	-2.72	108.10	110.10
20	I	1031	CLA	CHB-C4A-NA	2.72	128.27	124.51
21	A	7023	LMU	O5B-C5B-C6B	2.72	113.19	106.44
20	3	3001	CLA	C3C-C4C-CHD	-2.72	119.27	125.22
21	A	7032	LMU	C3'-C4'-C5'	2.71	117.15	110.93
20	A	1815	CLA	C4A-NA-C1A	2.71	107.93	106.71
20	A	1817	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
20	A	1799	CLA	O1D-CGD-CBD	-2.71	118.94	124.48
20	1	1201	CLA	C3C-C4C-CHD	-2.71	119.28	125.22
20	1	1192	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
20	B	1772	CLA	CMC-C2C-C1C	2.71	129.16	125.04
20	A	1769	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
20	B	1786	CLA	CMC-C2C-C1C	2.70	129.16	125.04
20	A	1811	CLA	CHC-C1C-NC	2.70	128.30	124.20
20	2	1215	CLA	CHB-C4A-NA	2.70	128.25	124.51
20	B	1772	CLA	CHB-C4A-NA	2.70	128.25	124.51
20	3	3007	CLA	CAC-C3C-C2C	-2.70	122.91	127.53
20	J	1044	CLA	CAC-C3C-C2C	-2.70	122.91	127.53
20	B	1744	CLA	CED-O2D-CGD	2.70	122.04	115.94
20	R	1054	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
21	A	7028	LMU	C1B-C2B-C3B	-2.70	104.38	110.00
20	B	1744	CLA	CAC-C3C-C4C	2.70	128.31	124.81
20	B	1762	CLA	C1-O2A-CGA	2.70	123.52	116.44
20	A	1782	CLA	C4A-NA-C1A	2.70	107.92	106.71
21	A	7043	LMU	C1'-O5'-C5'	2.70	118.98	113.69
21	A	7043	LMU	C1B-O5B-C5B	2.70	118.98	113.69
22	I	1032	BCR	C23-C22-C21	2.69	123.08	118.94
21	A	7041	LMU	O2'-C2'-C1'	-2.69	103.50	110.05
20	1	1197	CLA	C2A-C3A-C4A	2.69	106.22	101.87
20	B	1742	CLA	CAC-C3C-C4C	2.69	128.30	124.81
21	A	7038	LMU	O3'-C3'-C2'	2.69	116.57	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	3001	CLA	C2C-C1C-CHC	-2.69	119.22	125.67
20	A	1811	CLA	O2A-CGA-CBA	2.69	120.36	111.91
20	L	1167	CLA	O2A-CGA-CBA	2.69	120.36	111.91
20	3	3011	CLA	C4-C3-C5	2.69	119.80	115.27
20	B	1761	CLA	O1D-CGD-CBD	-2.69	118.98	124.48
20	B	1736	CLA	C1D-ND-C4D	-2.69	104.42	106.33
21	A	7028	LMU	C3B-C4B-C5B	-2.69	105.44	110.24
20	1	1190	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
20	F	1155	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
20	B	1761	CLA	CMD-C2D-C3D	-2.69	121.43	127.61
20	4	1206	CLA	C3C-C4C-CHD	-2.69	119.33	125.22
20	L	1505	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
21	A	7042	LMU	C3B-C4B-C5B	-2.69	105.45	110.24
20	L	1168	CLA	CMD-C2D-C3D	-2.69	121.44	127.61
21	A	7033	LMU	C4B-C3B-C2B	2.68	115.51	110.82
20	B	1747	CLA	CED-O2D-CGD	2.68	122.01	115.94
20	A	1816	CLA	CMA-C3A-C4A	2.68	118.99	111.77
20	B	1740	CLA	C4D-CHA-C1A	2.68	124.52	121.25
20	B	1750	CLA	C1-O2A-CGA	2.68	123.48	116.44
20	A	1759	CLA	C5-C3-C4	2.68	120.53	114.60
21	K	1086	LMU	O3B-C3B-C2B	2.68	116.55	110.35
20	B	1743	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
20	A	1816	CLA	CMB-C2B-C3B	2.68	129.69	124.68
20	4	1201	CLA	C3D-C4D-ND	2.68	114.57	110.24
21	A	7033	LMU	O1'-C1'-C2'	2.68	112.49	108.30
21	A	7042	LMU	C1-O1'-C1'	-2.68	109.39	113.84
20	2	1227	CLA	CHB-C4A-NA	2.68	128.44	124.34
20	B	1743	CLA	C4A-NA-C1A	2.68	107.91	106.71
20	B	1737	CLA	O2A-CGA-CBA	2.68	120.32	111.91
20	3	1214	CLA	C2B-C3B-C4B	2.68	108.58	106.29
20	A	1813	CLA	CGD-CBD-CAD	2.68	119.41	110.73
20	J	1045	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
20	4	1209	CLA	C1D-ND-C4D	-2.68	104.43	106.33
20	3	1219	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
20	B	1763	CLA	C3A-C2A-C1A	2.67	105.34	101.34
21	L	1171	LMU	O3B-C3B-C2B	-2.67	104.17	110.35
20	1	1190	CLA	C2A-C1A-CHA	-2.67	119.18	123.86
20	1	1194	CLA	C2C-C1C-CHC	-2.67	119.27	125.67
20	1	1190	CLA	OBD-CAD-C3D	-2.67	122.09	128.52
20	L	1166	CLA	C1D-ND-C4D	-2.67	104.44	106.33
20	3	1218	CLA	CAA-C2A-C1A	-2.67	103.23	111.97
20	1	1189	CLA	CAC-C3C-C4C	2.67	128.27	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1750	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
20	A	1762	CLA	CAA-C2A-C1A	-2.67	103.23	111.97
20	1	1200	CLA	CHA-C1A-NA	-2.67	120.29	126.40
20	J	1044	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
20	B	1760	CLA	C1-C2-C3	-2.67	122.44	126.75
20	3	3008	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
20	A	1787	CLA	O2A-CGA-CBA	2.67	120.28	111.91
20	A	1768	CLA	O2A-CGA-CBA	2.67	120.28	111.91
22	B	1777	BCR	C3-C4-C5	-2.67	109.32	114.08
20	1	1197	CLA	C3A-C2A-C1A	-2.67	97.35	101.34
20	F	1156	CLA	CHC-C1C-C2C	-2.67	119.35	126.72
20	B	1747	CLA	O2A-CGA-CBA	2.67	120.27	111.91
20	1	1200	CLA	CHA-C4D-ND	2.66	138.07	132.50
20	4	1205	CLA	C2A-C3A-C4A	-2.66	100.00	104.18
20	B	1741	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
22	L	1169	BCR	C37-C22-C21	-2.66	119.19	122.92
20	4	1198	CLA	C1D-ND-C4D	-2.66	104.44	106.33
20	A	1759	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
20	B	1757	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
20	A	1798	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
20	1	1196	CLA	C4A-NA-C1A	2.66	107.90	106.71
21	A	7023	LMU	O1B-C1B-C2B	2.66	115.00	108.10
20	K	1085	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
20	4	1209	CLA	CHD-C1D-ND	2.66	126.90	124.45
20	A	1817	CLA	CMA-C3A-C4A	2.66	118.92	111.77
20	1	1189	CLA	O2A-CGA-CBA	2.66	120.26	111.91
20	B	1755	CLA	O2A-CGA-CBA	2.66	120.26	111.91
20	A	1775	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
20	J	1045	CLA	CGD-CBD-CAD	-2.66	102.12	110.73
20	4	1197	CLA	CHD-C1D-ND	2.66	126.90	124.45
20	I	1033	CLA	O1D-CGD-CBD	-2.66	119.05	124.48
20	3	3002	CLA	C2C-C1C-CHC	-2.66	119.31	125.67
20	B	1755	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
21	A	7033	LMU	O5'-C5'-C6'	2.66	113.04	106.44
20	B	1756	CLA	CHC-C1C-C2C	-2.66	119.38	126.72
20	B	1759	CLA	C7-C6-C5	-2.66	106.15	113.36
20	2	1213	CLA	CHC-C1C-C2C	-2.66	119.38	126.72
20	1	1196	CLA	C1B-C2B-C3B	-2.66	104.45	106.92
20	A	1782	CLA	CHC-C1C-C2C	-2.66	119.38	126.72
20	A	1800	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
20	A	1801	CLA	C4-C3-C2	-2.65	116.87	123.68
20	4	1197	CLA	CHB-C4A-NA	2.65	128.18	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1769	CLA	CAA-CBA-CGA	-2.65	105.50	113.25
21	A	7025	LMU	O5'-C5'-C4'	2.65	115.35	109.75
20	B	1737	CLA	CBC-CAC-C3C	-2.65	105.12	112.43
20	1	1192	CLA	C1D-ND-C4D	-2.65	104.45	106.33
20	2	1220	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
20	K	1085	CLA	O2A-CGA-CBA	2.65	120.22	111.91
20	A	1776	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
20	2	1218	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	B	1783	LMG	O8-C28-C29	2.65	120.22	111.91
20	3	3014	CLA	C2B-C3B-C4B	2.65	108.55	106.29
20	B	1761	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
20	4	1203	CLA	C3C-C4C-CHD	-2.65	119.42	125.22
20	A	1760	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
20	B	1745	CLA	CHB-C4A-NA	2.65	128.17	124.51
20	A	1793	CLA	C4A-NA-C1A	2.65	107.90	106.71
20	K	1085	CLA	C4A-NA-C1A	2.65	107.90	106.71
20	4	1209	CLA	CMB-C2B-C3B	2.65	129.63	124.68
20	A	1793	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
21	A	7033	LMU	O2'-C2'-C1'	2.65	116.47	110.05
20	4	1196	CLA	O2A-CGA-CBA	2.65	120.21	111.91
20	B	1735	CLA	CHC-C1C-C2C	-2.65	119.41	126.72
20	G	1099	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
20	A	1794	CLA	CHC-C1C-C2C	-2.64	119.41	126.72
20	A	1788	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
21	A	7026	LMU	O3'-C3'-C2'	2.64	116.46	110.35
20	B	1756	CLA	O2A-CGA-CBA	2.64	120.20	111.91
20	4	4007	CLA	C1D-ND-C4D	-2.64	104.46	106.33
22	L	1169	BCR	C8-C7-C6	-2.64	119.79	127.20
20	A	1784	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
20	2	1212	CLA	O2A-CGA-CBA	2.64	120.19	111.91
20	2	1213	CLA	CAC-C3C-C4C	2.64	128.23	124.81
21	A	7035	LMU	O5'-C5'-C4'	-2.64	104.19	109.75
20	K	1142	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
22	B	1774	BCR	C3-C4-C5	-2.64	109.37	114.08
21	A	7040	LMU	O2B-C2B-C1B	2.64	116.45	110.05
20	A	1791	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
20	I	1033	CLA	C4-C3-C2	-2.64	116.91	123.68
22	L	1170	BCR	C19-C18-C17	-2.64	114.89	118.94
20	A	1795	CLA	O2A-CGA-CBA	2.64	120.18	111.91
20	A	1792	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
20	A	1817	CLA	C2D-C1D-ND	-2.63	108.16	110.10
20	A	1769	CLA	C1D-ND-C4D	-2.63	104.46	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1794	CLA	O2A-CGA-CBA	2.63	120.17	111.91
20	B	1735	CLA	O2A-CGA-CBA	2.63	120.17	111.91
20	J	1043	CLA	O2A-CGA-CBA	2.63	120.17	111.91
20	A	1795	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
20	A	1797	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
20	A	1793	CLA	O2A-CGA-CBA	2.63	120.17	111.91
20	A	1761	CLA	C1-O2A-CGA	2.63	123.35	116.44
20	1	1192	CLA	C4A-NA-C1A	2.63	107.89	106.71
20	A	1781	CLA	C4A-NA-C1A	2.63	107.89	106.71
20	A	1792	CLA	O2A-CGA-CBA	2.63	120.17	111.91
20	3	3007	CLA	CHB-C4A-NA	2.63	128.15	124.51
21	A	7023	LMU	C4B-C3B-C2B	-2.63	106.23	110.82
20	A	1766	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
20	2	1212	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
20	4	1198	CLA	CHA-C1A-NA	-2.63	120.38	126.40
20	A	1797	CLA	O2A-CGA-CBA	2.63	120.16	111.91
22	3	1220	BCR	C37-C22-C21	-2.63	119.24	122.92
20	A	1796	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
20	A	1781	CLA	O2A-CGA-CBA	2.63	120.15	111.91
20	A	1781	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
21	A	7027	LMU	O3'-C3'-C4'	-2.63	102.98	109.94
20	A	1811	CLA	CMA-C3A-C2A	-2.63	103.23	113.83
20	4	1196	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
20	B	1766	CLA	O2A-C1-C2	2.63	115.54	108.64
21	A	7023	LMU	C8-C7-C6	-2.63	101.09	114.42
21	A	7041	LMU	C6'-C5'-C4'	-2.62	105.69	113.33
20	A	1816	CLA	CHC-C1C-NC	2.62	128.18	124.20
20	F	1155	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
20	A	1777	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
20	B	1752	CLA	C2D-C1D-ND	-2.62	108.17	110.10
20	A	1796	CLA	O2A-CGA-CBA	2.62	120.14	111.91
20	R	1055	CLA	CAA-CBA-CGA	2.62	120.91	113.25
21	A	7028	LMU	O4'-C4B-C5B	-2.62	102.79	109.30
20	3	1219	CLA	O2A-CGA-CBA	2.62	120.13	111.91
20	B	1785	CLA	CGD-CBD-CAD	2.62	119.22	110.73
22	B	1779	BCR	C12-C13-C14	2.62	122.96	118.94
21	A	7037	LMU	O2B-C2B-C3B	-2.62	104.30	110.35
20	B	1756	CLA	C4A-NA-C1A	2.62	107.88	106.71
20	2	1227	CLA	C2C-C1C-CHC	-2.61	119.41	125.67
22	B	1781	BCR	C8-C9-C10	2.61	122.95	118.94
20	2	1224	CLA	CMB-C2B-C3B	2.61	129.57	124.68
21	A	7026	LMU	C4B-C3B-C2B	-2.61	106.26	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	1207	CLA	CAC-C3C-C2C	-2.61	121.33	126.75
20	2	1218	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	B	1761	CLA	O2A-CGA-CBA	2.61	120.11	111.91
20	A	1783	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
22	B	1778	BCR	C28-C27-C26	-2.61	109.41	114.08
20	4	1196	CLA	C4A-NA-C1A	2.61	107.88	106.71
20	A	1815	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
20	2	2010	CLA	C2A-C3A-C4A	-2.61	100.08	104.18
20	A	1772	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
20	B	1744	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
20	4	4007	CLA	CED-O2D-CGD	2.61	121.84	115.94
20	A	1772	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	4	4014	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
20	A	1816	CLA	C4A-NA-C1A	-2.61	105.53	106.71
22	B	1779	BCR	C32-C1-C6	-2.61	106.07	110.30
20	K	3009	CLA	C1-O2A-CGA	2.61	123.28	116.44
22	B	1780	BCR	C23-C24-C25	-2.61	119.88	127.20
22	B	1778	BCR	C3-C4-C5	-2.61	109.42	114.08
20	A	1780	CLA	CHC-C1C-C2C	-2.61	119.52	126.72
20	A	1777	CLA	C4A-NA-C1A	2.60	107.88	106.71
20	B	1762	CLA	C4A-NA-C1A	2.60	107.88	106.71
20	4	4014	CLA	O2A-CGA-CBA	2.60	120.08	111.91
21	A	7017	LMU	O2B-C2B-C3B	2.60	116.37	110.35
20	B	1738	CLA	CBC-CAC-C3C	-2.60	105.25	112.43
20	A	1771	CLA	C1-O2A-CGA	2.60	123.27	116.44
20	B	1741	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
20	B	1754	CLA	CMC-C2C-C1C	2.60	129.00	125.04
22	B	1776	BCR	C39-C30-C25	-2.60	106.08	110.30
20	2	1224	CLA	CAC-C3C-C4C	2.60	128.18	124.81
20	4	1200	CLA	CED-O2D-CGD	2.60	121.81	115.94
21	A	7023	LMU	O5'-C5'-C6'	-2.60	99.98	106.44
20	A	1770	CLA	C1D-ND-C4D	-2.60	104.49	106.33
20	A	1769	CLA	C3D-C4D-ND	2.59	114.43	110.24
22	A	1803	BCR	C28-C27-C26	-2.59	109.44	114.08
20	B	1767	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
22	A	1806	BCR	C3-C4-C5	-2.59	109.45	114.08
20	J	1043	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
21	A	7039	LMU	O3B-C3B-C2B	-2.59	104.35	110.35
20	A	1782	CLA	O2A-CGA-CBA	2.59	120.04	111.91
20	A	1766	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
20	B	1740	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
20	A	1815	CLA	CGD-CBD-CAD	2.59	119.13	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1775	BCR	C23-C24-C25	-2.59	119.92	127.20
20	A	1765	CLA	C2C-C1C-NC	2.59	112.40	109.97
20	2	1224	CLA	O1D-CGD-CBD	-2.59	119.18	124.48
20	2	1224	CLA	C4-C3-C5	2.59	119.63	115.27
20	L	1505	CLA	CGD-CBD-CAD	-2.59	102.35	110.73
20	K	3009	CLA	CMC-C2C-C1C	2.59	128.98	125.04
20	A	1776	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
20	4	1202	CLA	C3C-C4C-CHD	-2.59	119.55	125.22
22	B	1774	BCR	C28-C27-C26	-2.59	109.46	114.08
20	A	1774	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
20	2	1213	CLA	CHB-C4A-NA	2.59	128.09	124.51
20	K	1142	CLA	C4A-NA-C1A	2.59	107.87	106.71
20	A	1817	CLA	CHB-C4A-NA	2.59	128.09	124.51
21	A	7032	LMU	O6'-C6'-C5'	-2.58	102.42	111.29
20	A	1791	CLA	C4A-NA-C1A	2.58	107.87	106.71
22	A	1808	BCR	C28-C27-C26	-2.58	109.47	114.08
21	A	7022	LMU	O4'-C4B-C5B	2.58	115.71	109.30
20	J	1045	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
20	B	1740	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	B	1774	BCR	C8-C7-C6	-2.58	119.95	127.20
20	3	1218	CLA	CMD-C2D-C3D	-2.58	121.68	127.61
22	A	1805	BCR	C23-C24-C25	-2.58	119.96	127.20
21	A	7043	LMU	C3'-C4'-C5'	-2.58	105.02	110.93
20	A	1773	CLA	O2A-C1-C2	2.58	115.41	108.64
20	B	1745	CLA	CED-O2D-CGD	2.58	121.76	115.94
22	A	1805	BCR	C8-C7-C6	-2.58	119.97	127.20
20	1	1199	CLA	C3C-C4C-CHD	-2.58	119.58	125.22
20	3	3014	CLA	C3D-C2D-C1D	2.57	110.13	107.28
20	3	1217	CLA	CHB-C4A-NA	2.57	128.28	124.34
20	J	1044	CLA	CED-O2D-CGD	2.57	121.76	115.94
22	B	1780	BCR	C8-C7-C6	-2.57	119.98	127.20
22	A	1804	BCR	C3-C4-C5	-2.57	109.48	114.08
22	B	1775	BCR	C28-C27-C26	-2.57	109.48	114.08
20	A	1761	CLA	C6-C7-C8	-2.57	107.61	115.92
20	I	1033	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
20	4	1199	CLA	C1-O2A-CGA	2.57	123.19	116.44
20	1	1201	CLA	C2A-C3A-C4A	-2.57	100.15	104.18
20	A	1770	CLA	CED-O2D-CGD	2.57	121.75	115.94
20	3	3002	CLA	CHB-C4A-NA	2.57	128.27	124.34
22	B	1775	BCR	C3-C4-C5	-2.57	109.49	114.08
21	A	7035	LMU	C2'-C3'-C4'	-2.57	103.82	109.68
20	B	1743	CLA	CBA-CAA-C2A	-2.57	106.28	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1804	BCR	C8-C7-C6	-2.57	119.99	127.20
20	L	1167	CLA	CAC-C3C-C4C	2.57	128.14	124.81
20	B	1735	CLA	C4A-NA-C1A	2.57	107.86	106.71
22	A	1803	BCR	C23-C24-C25	-2.57	120.00	127.20
22	A	1806	BCR	C23-C24-C25	-2.57	120.00	127.20
22	B	1780	BCR	C3-C4-C5	-2.56	109.50	114.08
21	A	7021	LMU	O1B-C1B-C2B	2.56	114.74	108.10
20	2	1227	CLA	C3D-C2D-C1D	2.56	110.12	107.28
22	B	1777	BCR	C23-C24-C25	-2.56	120.00	127.20
22	B	1779	BCR	C7-C8-C9	2.56	130.11	126.23
20	2	1212	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
20	2	1221	CLA	C2C-C1C-CHC	-2.56	119.54	125.67
22	B	1778	BCR	C23-C24-C25	-2.56	120.01	127.20
21	R	1057	LMU	O5B-C5B-C6B	2.56	112.80	106.44
22	A	1808	BCR	C8-C7-C6	-2.56	120.01	127.20
20	4	1197	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
21	A	7028	LMU	O5'-C5'-C6'	-2.56	100.07	106.44
21	A	7034	LMU	O2B-C2B-C3B	-2.56	104.43	110.35
22	B	1777	BCR	C8-C7-C6	-2.56	120.02	127.20
22	A	1803	BCR	C8-C7-C6	-2.56	120.02	127.20
20	B	1756	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
20	2	1223	CLA	CHD-C1D-ND	2.56	126.80	124.45
22	A	1807	BCR	C23-C24-C25	-2.56	120.02	127.20
20	2	1215	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
20	H	1079	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
20	1	1189	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	2	1213	CLA	C3D-C4D-ND	2.56	114.37	110.24
22	A	1806	BCR	C8-C7-C6	-2.56	120.03	127.20
21	A	7038	LMU	C4B-C3B-C2B	-2.56	106.36	110.82
21	A	7027	LMU	C3'-C4'-C5'	2.56	116.78	110.93
20	A	1778	CLA	CAA-C2A-C3A	2.55	120.64	114.26
20	B	1771	CLA	CMA-C3A-C2A	-2.55	103.53	113.83
22	B	1779	BCR	C39-C30-C25	2.55	114.44	110.30
20	A	1785	CLA	C1-C2-C3	-2.55	121.63	126.04
20	4	1201	CLA	C2C-C1C-NC	-2.55	107.58	109.97
20	1	1193	CLA	O2A-CGA-CBA	2.55	119.92	111.91
20	B	1738	CLA	C3C-C4C-NC	-2.55	107.71	110.57
20	B	1743	CLA	C11-C10-C8	-2.55	107.67	115.92
20	A	1792	CLA	C4A-NA-C1A	2.55	107.85	106.71
20	1	1187	CLA	CMA-C3A-C2A	2.55	124.12	113.83
20	G	1099	CLA	C1-C2-C3	-2.55	121.63	126.04
22	A	1807	BCR	C3-C4-C5	-2.55	109.52	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1807	BCR	C28-C27-C26	-2.55	109.52	114.08
22	B	1777	BCR	C28-C27-C26	-2.55	109.52	114.08
20	4	1201	CLA	CMA-C3A-C4A	-2.55	104.92	111.77
20	B	1757	CLA	O2A-C1-C2	2.55	115.34	108.64
20	1	1198	CLA	C6-C7-C8	-2.55	107.68	115.92
20	2	1219	CLA	CHB-C4A-NA	2.55	128.24	124.34
20	A	1780	CLA	C4A-NA-C1A	2.55	107.85	106.71
20	A	1796	CLA	C4A-NA-C1A	2.55	107.85	106.71
21	1	1202	LMU	C1B-O1B-C4'	-2.55	111.66	117.96
20	A	1782	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
20	A	1783	CLA	C11-C10-C8	-2.55	107.68	115.92
20	A	1773	CLA	CHB-C4A-NA	2.55	128.03	124.51
20	3	3001	CLA	C3D-C2D-C1D	2.55	110.10	107.28
22	A	1807	BCR	C8-C7-C6	-2.55	120.05	127.20
20	L	1168	CLA	C1-C2-C3	-2.55	122.63	126.75
20	2	1216	CLA	C1D-ND-C4D	-2.55	104.53	106.33
20	B	1770	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
21	A	7030	LMU	O5B-C5B-C4B	-2.54	105.08	109.69
20	4	1201	CLA	C1D-ND-C4D	-2.54	104.53	106.33
20	A	1791	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
22	L	1169	BCR	C30-C25-C24	2.54	122.97	115.78
22	A	1808	BCR	C23-C24-C25	-2.54	120.07	127.20
20	1	1194	CLA	C1C-NC-C4C	-2.54	105.56	106.71
21	A	7035	LMU	O5'-C5'-C6'	2.54	112.75	106.44
20	A	1763	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
20	A	1799	CLA	C5-C3-C4	2.54	120.21	114.60
20	J	1043	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
20	1	1194	CLA	C2B-C3B-C4B	2.54	108.46	106.29
22	A	1805	BCR	C3-C4-C5	-2.54	109.54	114.08
20	A	1793	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
20	A	1784	CLA	CGD-CBD-CAD	2.54	118.95	110.73
20	B	1771	CLA	CMB-C2B-C1B	2.54	132.37	128.46
20	2	1222	CLA	C5-C3-C4	2.54	120.21	114.60
20	I	1031	CLA	CHC-C1C-C2C	-2.54	119.70	126.72
21	A	7027	LMU	O5'-C5'-C6'	2.54	112.74	106.44
21	2	7006	LMU	C1B-O1B-C4'	-2.54	111.69	117.96
20	R	1055	CLA	CED-O2D-CGD	2.54	121.67	115.94
20	A	1787	CLA	O2A-CGA-O1A	-2.53	117.19	123.59
20	A	1780	CLA	C4-C3-C2	-2.53	117.18	123.68
20	A	1785	CLA	CHC-C1C-C2C	-2.53	119.71	126.72
20	B	1787	CLA	C1-C2-C3	-2.53	121.66	126.04
22	A	1806	BCR	C28-C27-C26	-2.53	109.55	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1778	BCR	C8-C7-C6	-2.53	120.09	127.20
20	B	1785	CLA	C11-C10-C8	-2.53	107.73	115.92
20	A	1770	CLA	CMB-C2B-C1B	2.53	132.35	128.46
20	K	3009	CLA	C4-C3-C2	-2.53	117.19	123.68
20	B	1770	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	1	1188	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
20	A	1812	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
20	A	1796	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
20	A	1775	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	F	1156	CLA	C2A-C1A-CHA	-2.53	119.44	123.85
20	K	1085	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
20	3	1219	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
22	B	1775	BCR	C8-C7-C6	-2.53	120.11	127.20
22	B	1779	BCR	C24-C25-C26	2.53	127.58	121.46
20	K	1142	CLA	C2A-C1A-CHA	-2.52	119.44	123.86
21	A	7009	LMU	C1B-O1B-C4'	-2.52	111.72	117.96
22	B	1774	BCR	C23-C24-C25	-2.52	120.11	127.20
20	B	1755	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
20	F	1155	CLA	CBD-CHA-C1A	2.52	131.47	127.43
22	A	1804	BCR	C28-C27-C26	-2.52	109.57	114.08
20	4	1205	CLA	CHB-C4A-NA	2.52	128.20	124.34
20	B	1745	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	A	1805	BCR	C28-C27-C26	-2.52	109.58	114.08
20	B	1757	CLA	C2D-C1D-ND	-2.52	108.25	110.10
20	3	1212	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
20	A	1759	CLA	O2A-CGA-CBA	2.52	119.82	111.91
20	B	1769	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
20	A	1797	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
20	3	1212	CLA	CHB-C4A-NA	2.52	128.00	124.51
20	B	1739	CLA	O2A-C1-C2	2.52	115.26	108.64
20	B	1743	CLA	C16-C15-C13	-2.52	107.78	115.92
22	A	1803	BCR	C3-C4-C5	-2.52	109.58	114.08
20	A	1781	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
20	B	1746	CLA	CAC-C3C-C4C	2.52	128.08	124.81
20	A	1795	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
21	K	1086	LMU	O2'-C2'-C3'	-2.52	104.53	110.35
20	B	1760	CLA	CHD-C4C-C3C	-2.52	121.14	124.84
20	4	1199	CLA	C4-C3-C5	2.52	119.50	115.27
20	B	1735	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
22	A	1804	BCR	C23-C24-C25	-2.52	120.14	127.20
22	B	1780	BCR	C28-C27-C26	-2.52	109.59	114.08
20	B	1762	CLA	C3A-C2A-C1A	2.51	105.11	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1778	CLA	CHB-C4A-NA	2.51	127.99	124.51
20	B	1785	CLA	CMB-C2B-C3B	2.51	129.38	124.68
22	B	1781	BCR	C40-C30-C25	2.51	114.38	110.30
20	F	1156	CLA	C4A-NA-C1A	2.51	107.84	106.71
20	4	1199	CLA	O2A-CGA-CBA	2.51	119.80	111.91
21	A	7015	LMU	O5B-C5B-C4B	-2.51	105.13	109.69
20	3	3001	CLA	C2A-C3A-C4A	-2.51	100.24	104.18
20	B	1766	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
20	B	1765	CLA	C1D-ND-C4D	-2.51	104.55	106.33
20	B	1744	CLA	O2A-CGA-CBA	2.51	119.79	111.91
20	4	1204	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
20	B	1737	CLA	C6-C7-C8	-2.51	107.81	115.92
20	H	1079	CLA	C1-C2-C3	2.51	130.38	126.04
20	A	1772	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
20	A	1794	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
20	A	1797	CLA	C4A-NA-C1A	2.51	107.83	106.71
21	A	7010	LMU	C1B-O1B-C4'	-2.51	111.75	117.96
20	B	1751	CLA	CMB-C2B-C3B	2.51	129.37	124.68
20	A	1787	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
20	A	1792	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
20	A	1773	CLA	C1D-ND-C4D	-2.51	104.55	106.33
20	K	3009	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	L	1171	LMU	O3'-C3'-C4'	-2.50	103.31	109.94
20	A	1760	CLA	C1D-ND-C4D	-2.50	104.56	106.33
20	A	1772	CLA	CAC-C3C-C2C	-2.50	123.25	127.53
20	R	1054	CLA	C4-C3-C2	-2.50	117.25	123.68
20	A	1800	CLA	CMB-C2B-C1B	2.50	132.31	128.46
20	A	1811	CLA	O2A-C1-C2	2.50	115.21	108.64
20	A	1790	CLA	O2A-CGA-CBA	2.50	119.76	111.91
20	B	1737	CLA	C1-C2-C3	2.50	130.37	126.04
20	A	1789	CLA	C2C-C1C-NC	2.50	112.32	109.97
20	4	1206	CLA	C3D-C2D-C1D	2.50	110.05	107.28
20	A	1766	CLA	C2D-C1D-ND	-2.50	108.26	110.10
20	B	1764	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
20	4	1204	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
20	B	1754	CLA	CHD-C1D-ND	2.50	126.75	124.45
20	B	1750	CLA	C3D-C4D-ND	2.50	114.28	110.24
20	1	1192	CLA	CMB-C2B-C3B	2.50	129.35	124.68
21	A	7038	LMU	O1B-C1B-C2B	2.50	114.57	108.10
21	A	7039	LMU	C1'-O5'-C5'	2.50	118.59	113.69
20	3	3007	CLA	CED-O2D-CGD	2.50	121.58	115.94
20	4	1201	CLA	CHB-C4A-NA	2.50	127.96	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1764	CLA	O2A-CGA-CBA	2.50	122.05	114.03
22	A	1808	BCR	C3-C4-C5	-2.49	109.62	114.08
22	B	1781	BCR	C34-C9-C8	-2.49	114.15	118.08
21	1	7004	LMU	C1B-O1B-C4'	-2.49	111.79	117.96
20	4	4014	CLA	C4A-NA-C1A	2.49	107.83	106.71
22	L	1170	BCR	C11-C10-C9	2.49	130.87	127.31
20	B	1785	CLA	C12-C11-C10	-2.49	101.78	113.24
20	A	1812	CLA	CMB-C2B-C3B	2.49	129.34	124.68
20	B	1785	CLA	CAC-C3C-C4C	2.49	128.04	124.81
20	B	1739	CLA	CAC-C3C-C4C	2.49	128.04	124.81
20	2	1213	CLA	CAA-C2A-C1A	-2.49	103.81	111.97
20	3	3007	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
20	B	1765	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
20	A	1788	CLA	C4-C3-C5	2.49	119.46	115.27
20	4	1200	CLA	CAC-C3C-C4C	2.49	128.04	124.81
20	A	1766	CLA	C3D-C4D-ND	2.49	114.26	110.24
20	K	1085	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	R	1056	LMU	C1B-O1B-C4'	-2.49	111.81	117.96
20	A	1785	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
20	K	1146	CLA	C4D-CHA-C1A	-2.48	118.22	121.25
22	B	1781	BCR	C20-C19-C18	2.48	133.40	126.42
20	B	1736	CLA	CMB-C2B-C3B	2.48	129.33	124.68
20	1	1197	CLA	C3D-C2D-C1D	-2.48	102.44	105.83
21	L	1171	LMU	C1B-O1B-C4'	-2.48	111.82	117.96
20	B	1761	CLA	CMC-C2C-C1C	2.48	128.82	125.04
20	4	1197	CLA	C4A-NA-C1A	2.48	107.82	106.71
20	J	1043	CLA	C4A-NA-C1A	2.48	107.82	106.71
20	4	4014	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
20	B	1763	CLA	C1D-ND-C4D	-2.48	104.57	106.33
22	B	1776	BCR	C32-C1-C6	2.48	114.32	110.30
22	3	1220	BCR	C8-C7-C6	-2.48	120.25	127.20
20	A	1764	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
20	4	1196	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
20	K	1142	CLA	CHB-C4A-NA	2.47	127.93	124.51
20	3	3015	CLA	CHB-C4A-NA	2.47	128.13	124.34
20	3	3014	CLA	C3C-C4C-CHD	-2.47	119.80	125.22
22	L	1170	BCR	C23-C22-C21	2.47	122.74	118.94
21	A	7030	LMU	O3'-C3'-C4'	-2.47	103.39	109.94
20	B	1748	CLA	CMD-C2D-C3D	-2.47	121.93	127.61
21	A	7042	LMU	O5B-C5B-C6B	2.47	112.57	106.44
20	4	1201	CLA	C3B-C4B-NB	2.47	112.40	109.21
21	A	7043	LMU	O1B-C1B-C2B	2.47	114.49	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	1195	CLA	CMB-C2B-C1B	2.47	132.25	128.46
21	3	7005	LMU	C1B-O1B-C4'	-2.47	111.86	117.96
20	B	1755	CLA	C4A-NA-C1A	2.46	107.81	106.71
20	A	1760	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
20	2	1227	CLA	C3C-C4C-CHD	-2.46	119.83	125.22
24	B	1783	LMG	C8-O7-C10	-2.46	111.73	117.79
20	A	1816	CLA	CHD-C1D-ND	2.46	126.72	124.45
20	B	1751	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
20	1	1195	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
20	L	1168	CLA	O2A-CGA-CBA	2.46	119.63	111.91
20	B	1757	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
20	B	1737	CLA	C4-C3-C5	2.46	119.41	115.27
20	A	1771	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
20	A	1811	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
20	A	1815	CLA	CMA-C3A-C4A	-2.46	105.16	111.77
20	B	1772	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
20	A	1796	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	A	1763	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
20	A	1794	CLA	C4A-NA-C1A	2.46	107.81	106.71
20	1	1193	CLA	CHC-C1C-C2C	-2.46	119.93	126.72
20	A	1782	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	A	1793	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	B	1763	CLA	CAA-C2A-C1A	-2.45	103.93	111.97
22	B	1779	BCR	C35-C13-C12	2.45	121.94	118.08
20	G	1099	CLA	O2A-CGA-CBA	2.45	119.61	111.91
21	A	7028	LMU	O4'-C4B-C3B	2.45	116.02	110.35
20	B	1750	CLA	CMA-C3A-C2A	-2.45	103.93	113.83
20	B	1757	CLA	CAA-C2A-C1A	-2.45	103.94	111.97
20	A	1813	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
20	2	1223	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
20	A	1783	CLA	C4-C3-C2	-2.45	117.39	123.68
20	A	1795	CLA	C4A-NA-C1A	2.45	107.81	106.71
20	B	1737	CLA	CAA-C2A-C1A	-2.45	103.95	111.97
20	A	1815	CLA	C3B-C4B-NB	2.45	112.38	109.21
21	4	1210	LMU	C4B-C3B-C2B	-2.45	106.55	110.82
20	J	1044	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
21	A	7031	LMU	C1-O1'-C1'	2.45	117.90	113.84
20	B	1766	CLA	O2A-CGA-CBA	2.45	119.58	111.91
20	A	1770	CLA	C3D-C4D-ND	2.45	114.19	110.24
20	A	1769	CLA	CMB-C2B-C3B	2.45	129.25	124.68
20	B	1735	CLA	CHB-C4A-NA	2.44	127.89	124.51
20	4	4003	CLA	C3C-C4C-CHD	-2.44	119.87	125.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1766	CLA	CED-O2D-CGD	2.44	121.47	115.94
20	1	1198	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
20	B	1753	CLA	C7-C6-C5	-2.44	106.72	113.36
20	A	1801	CLA	CMA-C3A-C4A	2.44	118.34	111.77
20	A	1781	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	A	7035	LMU	O1B-C4'-C5'	2.44	116.14	109.45
20	3	3007	CLA	C3D-C4D-ND	2.44	114.19	110.24
20	A	1761	CLA	C4-C3-C5	2.44	119.38	115.27
20	A	1772	CLA	CBC-CAC-C3C	-2.44	105.70	112.43
20	1	1200	CLA	CED-O2D-CGD	2.44	121.45	115.94
21	A	7043	LMU	O4'-C4B-C5B	2.44	115.35	109.30
20	B	1736	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
20	A	1816	CLA	CMC-C2C-C1C	-2.44	121.33	125.04
20	A	1772	CLA	CMB-C2B-C3B	2.44	129.24	124.68
20	A	1776	CLA	CMB-C2B-C3B	2.44	129.24	124.68
21	2	7003	LMU	C1B-O1B-C4'	-2.44	111.94	117.96
20	2	1220	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	4	1196	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	B	1739	CLA	CHD-C4C-C3C	-2.43	121.26	124.84
20	3	1219	CLA	CHB-C4A-NA	2.43	127.88	124.51
20	3	3011	CLA	C4A-NA-C1A	2.43	107.80	106.71
20	A	1779	CLA	CAC-C3C-C2C	-2.43	123.37	127.53
20	2	1220	CLA	CHC-C1C-C2C	-2.43	119.99	126.72
20	J	1043	CLA	CHB-C4A-NA	2.43	127.88	124.51
20	1	1197	CLA	C6-C5-C3	-2.43	101.72	113.58
20	L	1168	CLA	CAA-CBA-CGA	-2.43	106.15	113.25
20	B	1753	CLA	O2A-C1-C2	2.43	115.02	108.64
20	A	1776	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
20	A	1761	CLA	O1A-CGA-CBA	-2.43	114.25	123.73
20	L	1167	CLA	CMB-C2B-C3B	2.43	129.22	124.68
20	G	1099	CLA	C3D-C4D-ND	2.43	114.16	110.24
20	A	1776	CLA	CHB-C4A-NA	2.43	127.87	124.51
20	A	1795	CLA	CHB-C4A-NA	2.43	127.87	124.51
20	2	1214	CLA	CHB-C4A-NA	2.43	128.05	124.34
20	R	1055	CLA	C4-C3-C2	-2.43	117.46	123.68
20	F	1157	CLA	C2C-C1C-NC	2.43	112.24	109.97
20	1	1198	CLA	C11-C12-C13	-2.43	108.08	115.92
22	L	1169	BCR	C28-C27-C26	-2.42	109.75	114.08
20	4	4014	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
20	A	1792	CLA	CHB-C4A-NA	2.42	127.86	124.51
20	2	1218	CLA	C1-O2A-CGA	2.42	122.80	116.44
20	A	1774	CLA	CED-O2D-CGD	2.42	121.42	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	1200	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
20	A	1789	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
20	2	1215	CLA	CED-O2D-CGD	2.42	121.41	115.94
20	A	1764	CLA	CAA-CBA-CGA	2.42	120.33	113.25
20	L	1505	CLA	C1-O2A-CGA	2.42	122.79	116.44
20	L	1505	CLA	CAC-C3C-C4C	2.42	127.95	124.81
21	R	1057	LMU	C1'-O5'-C5'	-2.42	108.94	113.69
20	B	1762	CLA	CHC-C1C-C2C	-2.42	120.03	126.72
20	B	1767	CLA	O2A-CGA-CBA	2.42	119.50	111.91
20	3	1219	CLA	C4A-NA-C1A	2.42	107.79	106.71
20	A	1774	CLA	CAA-CBA-CGA	-2.42	106.19	113.25
21	A	7022	LMU	O5'-C5'-C4'	2.42	114.85	109.75
20	A	1800	CLA	C1D-ND-C4D	-2.42	104.62	106.33
20	B	1762	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
22	3	1220	BCR	C35-C13-C12	2.42	121.89	118.08
20	B	1756	CLA	CHB-C4A-NA	2.42	127.85	124.51
20	A	1763	CLA	C3D-C4D-ND	2.42	114.15	110.24
20	A	1812	CLA	CED-O2D-CGD	2.42	121.40	115.94
22	B	1781	BCR	C16-C15-C14	-2.42	118.52	123.47
20	3	3011	CLA	CHC-C1C-C2C	-2.42	120.04	126.72
20	A	1784	CLA	O2A-CGA-CBA	2.42	119.49	111.91
20	A	1782	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
20	K	1085	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
20	A	1786	CLA	CHB-C4A-NA	2.41	127.85	124.51
20	B	1758	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
20	A	1783	CLA	CMB-C2B-C3B	2.41	129.19	124.68
21	A	7041	LMU	O1'-C1-C2	-2.41	101.11	109.56
20	2	1214	CLA	C1D-ND-C4D	-2.41	104.62	106.33
20	A	1797	CLA	CHB-C4A-NA	2.41	127.85	124.51
20	B	1769	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
20	A	1780	CLA	C14-C13-C12	2.41	120.02	111.29
20	F	1156	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	1	1201	CLA	CHD-C1D-ND	2.41	126.84	124.52
20	K	1142	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
20	2	1215	CLA	C4A-NA-C1A	2.41	107.79	106.71
20	A	1783	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
20	A	1791	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	K	1085	CLA	C5-C3-C4	2.41	119.92	114.60
20	J	1043	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
20	B	1743	CLA	C4-C3-C5	2.41	119.32	115.27
20	B	1760	CLA	CHB-C4A-NA	2.41	127.84	124.51
21	A	7023	LMU	O4'-C4B-C5B	-2.40	103.33	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1793	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
20	A	1813	CLA	O2A-CGA-CBA	2.40	119.45	111.91
20	A	1773	CLA	C3D-C4D-ND	2.40	114.12	110.24
20	H	1079	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	A	1792	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
21	A	7021	LMU	C3B-C4B-C5B	-2.40	105.96	110.24
20	1	1191	CLA	CMA-C3A-C2A	-2.40	110.50	116.10
20	A	1798	CLA	C1-C2-C3	-2.40	121.90	126.04
22	L	1170	BCR	C2-C1-C6	2.40	114.17	110.48
20	A	1795	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
20	A	1794	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
20	B	1746	CLA	CED-O2D-CGD	2.39	121.35	115.94
20	4	1202	CLA	C2B-C3B-C4B	2.39	108.34	106.29
20	B	1761	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
21	A	7016	LMU	C4B-C3B-C2B	2.39	115.00	110.82
20	4	1206	CLA	C2B-C3B-C4B	2.39	108.33	106.29
20	4	1204	CLA	C3D-C4D-ND	2.39	114.11	110.24
20	B	1739	CLA	C11-C12-C13	-2.39	108.19	115.92
20	B	1745	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
20	A	1797	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
20	A	1764	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
20	A	1796	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
20	B	1759	CLA	CMB-C2B-C1B	2.39	132.13	128.46
21	A	7022	LMU	O5B-C5B-C4B	2.39	114.03	109.69
21	A	7015	LMU	C6B-C5B-C4B	2.39	118.59	113.00
20	F	1156	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
20	4	4014	CLA	CHB-C4A-NA	2.38	127.81	124.51
20	2	1224	CLA	CED-O2D-CGD	2.38	121.33	115.94
20	2	1222	CLA	CAC-C3C-C2C	-2.38	123.45	127.53
20	1	1199	CLA	C3D-C4D-ND	2.38	113.06	109.46
20	A	1791	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
20	B	1749	CLA	O2A-CGA-CBA	2.38	119.38	111.91
20	4	1204	CLA	O2A-CGA-CBA	2.38	119.38	111.91
20	B	1735	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
20	B	1736	CLA	C3D-C4D-ND	2.38	114.09	110.24
20	L	1166	CLA	C1-O2A-CGA	2.38	122.69	116.44
20	2	1212	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
20	4	1200	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
20	3	3008	CLA	CHB-C4A-NA	2.38	127.80	124.51
21	A	7039	LMU	O5'-C1'-C2'	-2.38	105.31	110.35
20	2	1212	CLA	C4A-NA-C1A	2.38	107.78	106.71
20	2	1213	CLA	C3A-C2A-C1A	2.38	104.90	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1786	CLA	CAC-C3C-C2C	-2.37	123.47	127.53
20	B	1740	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
20	B	1743	CLA	O2A-CGA-CBA	2.37	119.36	111.91
21	A	7027	LMU	C1'-O5'-C5'	2.37	118.34	113.69
20	K	1146	CLA	CED-O2D-CGD	2.37	121.30	115.94
20	B	1740	CLA	O2D-CGD-CBD	2.37	115.48	111.27
20	B	1754	CLA	C2C-C1C-NC	2.37	112.19	109.97
21	A	7022	LMU	C1B-O1B-C4'	2.37	123.83	117.96
20	A	1794	CLA	CHB-C4A-NA	2.37	127.79	124.51
20	A	1774	CLA	C1-O2A-CGA	2.37	122.66	116.44
20	L	1166	CLA	CMB-C2B-C3B	2.37	129.11	124.68
20	3	1219	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
20	B	1755	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	B	1776	BCR	C1-C6-C7	2.37	122.47	115.78
20	4	1196	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
20	B	1787	CLA	C6-C7-C8	-2.37	108.27	115.92
20	B	1764	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
20	2	1216	CLA	CHB-C4A-NA	2.36	127.96	124.34
20	2	1212	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	4	1206	CLA	CHB-C4A-NA	2.36	127.96	124.34
20	B	1771	CLA	CAC-C3C-C4C	2.36	127.88	124.81
20	B	1740	CLA	O2A-CGA-CBA	2.36	119.32	111.91
21	B	1782	LMU	O1B-C4'-C3'	2.36	113.56	107.28
20	A	1761	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	4	1199	CLA	C4D-CHA-C1A	-2.36	118.38	121.25
20	B	1787	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
21	A	7034	LMU	C1B-C2B-C3B	2.36	114.91	110.00
20	4	1202	CLA	C3D-C4D-ND	2.36	113.02	109.46
20	4	1198	CLA	C1C-C2C-C3C	2.36	109.43	106.96
22	3	1220	BCR	C28-C27-C26	-2.36	109.87	114.08
20	A	1788	CLA	C2D-C1D-ND	-2.36	108.37	110.10
21	A	7022	LMU	C1'-C2'-C3'	2.36	114.90	110.00
20	A	1801	CLA	CED-O2D-CGD	2.36	121.27	115.94
20	A	1788	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
20	4	1208	CLA	C2C-C1C-CHC	-2.35	120.03	125.67
20	B	1749	CLA	CHC-C1C-C2C	-2.35	120.21	126.72
20	2	1220	CLA	C3D-C4D-ND	2.35	114.04	110.24
20	A	1781	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
20	B	1787	CLA	CED-O2D-CGD	2.35	121.26	115.94
20	B	1737	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
20	A	1767	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
20	B	1770	CLA	C1-C2-C3	-2.35	121.98	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1787	CLA	C4A-NA-C1A	2.35	107.76	106.71
20	A	1769	CLA	CAC-C3C-C4C	2.35	127.86	124.81
20	B	1756	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
20	B	1749	CLA	CMB-C2B-C3B	2.35	129.07	124.68
20	1	1187	CLA	CHA-C4D-ND	2.35	137.41	132.50
20	1	1192	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
21	A	7021	LMU	C1-O1'-C1'	-2.35	109.95	113.84
21	A	7023	LMU	O1'-C1'-C2'	2.34	111.96	108.30
22	3	1220	BCR	C33-C5-C4	2.34	118.12	113.62
20	1	1192	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
20	4	1198	CLA	CAC-C3C-C4C	2.34	127.85	124.81
20	A	1760	CLA	O2D-CGD-CBD	2.34	115.43	111.27
20	1	1195	CLA	C3D-C4D-ND	2.34	114.02	110.24
21	A	7028	LMU	O3'-C3'-C2'	2.34	115.76	110.35
20	A	1784	CLA	C4-C3-C5	2.34	119.21	115.27
20	A	1772	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	A	7013	LMU	O1B-C4'-C5'	2.34	115.86	109.45
20	A	1773	CLA	C4A-NA-C1A	2.34	107.76	106.71
22	A	1803	BCR	C11-C12-C13	-2.34	119.85	126.42
20	A	1766	CLA	CED-O2D-CGD	2.34	121.22	115.94
20	J	1044	CLA	C2A-C3A-C4A	-2.34	98.10	101.87
20	B	1766	CLA	C1D-ND-C4D	-2.34	104.68	106.33
20	B	1737	CLA	C3C-C4C-NC	-2.33	107.95	110.57
21	A	7017	LMU	O5'-C5'-C4'	2.33	114.67	109.75
20	1	1200	CLA	C4D-CHA-C1A	2.33	124.09	121.25
21	A	7025	LMU	O4'-C4B-C3B	2.33	115.74	110.35
22	B	1776	BCR	C35-C13-C12	2.33	121.75	118.08
20	B	1758	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
20	2	1221	CLA	C3A-C4A-NA	2.33	114.81	109.92
20	B	1761	CLA	CHC-C1C-C2C	-2.33	120.27	126.72
20	3	3001	CLA	C3D-C4D-ND	2.33	112.98	109.46
20	L	1166	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
20	B	1762	CLA	C9-C8-C10	2.33	119.73	111.29
20	B	1767	CLA	CAC-C3C-C4C	2.33	127.83	124.81
20	I	1031	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
20	B	1744	CLA	O2A-C1-C2	2.33	114.75	108.64
20	B	1762	CLA	CAA-C2A-C1A	-2.33	104.35	111.97
22	B	1780	BCR	C11-C12-C13	-2.33	119.88	126.42
20	B	1752	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
20	1	1187	CLA	CAA-C2A-C1A	2.33	119.60	111.97
20	1	1196	CLA	C3D-C4D-ND	2.33	114.00	110.24
20	2	1218	CLA	C11-C10-C8	-2.32	108.41	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	1146	CLA	CHA-C4D-ND	2.32	137.36	132.50
20	R	1054	CLA	C3D-C4D-ND	2.32	113.99	110.24
20	4	1201	CLA	C4C-C3C-C2C	2.32	110.28	106.90
20	A	1786	CLA	CHD-C4C-C3C	-2.32	121.43	124.84
20	B	1743	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
20	L	1168	CLA	CMC-C2C-C1C	2.32	128.57	125.04
20	J	1045	CLA	O2A-CGA-CBA	2.32	119.19	111.91
20	A	1811	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
22	A	1804	BCR	C11-C12-C13	-2.32	119.90	126.42
20	1	1199	CLA	C3A-C4A-NA	2.32	114.78	109.92
20	B	1750	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
20	A	1763	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
20	A	1779	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
20	A	1764	CLA	C1D-ND-C4D	-2.32	104.69	106.33
20	2	1224	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
20	B	1741	CLA	C1-O2A-CGA	2.32	122.52	116.44
20	2	1217	CLA	C1-C2-C3	-2.32	122.04	126.04
22	L	1170	BCR	C32-C1-C31	-2.32	101.42	108.53
20	B	1748	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
21	A	1809	LMU	O6'-C6'-C5'	-2.31	103.35	111.29
21	A	7024	LMU	C1B-O5B-C5B	2.31	118.23	113.69
20	A	1785	CLA	CMC-C2C-C1C	2.31	128.56	125.04
20	B	1750	CLA	CMC-C2C-C1C	2.31	128.56	125.04
22	B	1777	BCR	C11-C12-C13	-2.31	119.92	126.42
22	A	1807	BCR	C20-C19-C18	-2.31	119.92	126.42
20	4	1198	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
20	2	1215	CLA	CMB-C2B-C3B	2.31	129.00	124.68
20	B	1738	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
20	A	1787	CLA	CBA-CAA-C2A	2.31	120.68	113.86
20	1	1194	CLA	C3A-C4A-NA	2.31	114.77	109.92
20	F	1155	CLA	CGD-CBD-CAD	-2.31	104.83	114.30
20	B	1737	CLA	C11-C12-C13	-2.31	108.46	115.92
20	A	1772	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
20	A	1786	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
21	A	7019	LMU	C3'-C4'-C5'	2.31	116.22	110.93
20	I	1033	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
21	2	1225	LMU	O5'-C5'-C6'	2.31	112.17	106.44
20	3	1216	CLA	C3A-C4A-NA	2.31	114.76	109.92
20	2	1218	CLA	CAA-CBA-CGA	-2.31	106.52	113.25
20	2	1216	CLA	CHD-C1D-ND	2.31	126.74	124.52
21	A	1809	LMU	C3B-C4B-C5B	2.30	114.35	110.24
20	2	1220	CLA	CED-O2D-CGD	2.30	121.15	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1782	LMU	C2'-C3'-C4'	2.30	114.94	109.68
20	K	3009	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
21	A	7042	LMU	O4'-C4B-C5B	2.30	115.02	109.30
20	1	1197	CLA	CMB-C2B-C3B	-2.30	120.37	124.68
20	A	1765	CLA	C5-C3-C2	-2.30	116.46	121.12
20	A	1790	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
20	4	1209	CLA	C3A-C2A-C1A	2.30	104.79	101.34
22	A	1805	BCR	C20-C19-C18	-2.30	119.95	126.42
21	A	7026	LMU	O5'-C5'-C4'	2.30	114.60	109.75
20	A	1763	CLA	CGD-CBD-CAD	-2.30	103.28	110.73
20	A	1785	CLA	CAA-CBA-CGA	2.30	119.97	113.25
20	B	1750	CLA	CMB-C2B-C3B	2.30	128.98	124.68
20	B	1765	CLA	O2A-CGA-CBA	2.30	121.41	114.03
20	A	1816	CLA	CHB-C4A-NA	2.30	127.69	124.51
20	I	1031	CLA	C1-O2A-CGA	2.30	122.47	116.44
21	B	1782	LMU	O5'-C5'-C4'	2.30	114.59	109.75
20	A	1769	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
22	A	1808	BCR	C20-C19-C18	-2.29	119.97	126.42
22	B	1774	BCR	C11-C12-C13	-2.29	119.97	126.42
20	F	1155	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
21	A	1810	LMU	C1B-C2B-C3B	2.29	114.77	110.00
22	B	1778	BCR	C11-C12-C13	-2.29	119.97	126.42
20	B	1755	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
20	I	1033	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
20	B	1766	CLA	CHB-C4A-NA	2.29	127.68	124.51
20	B	1754	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	A	1807	BCR	C11-C12-C13	-2.29	119.98	126.42
20	2	1218	CLA	C6-C7-C8	-2.29	108.52	115.92
20	4	1202	CLA	C3A-C4A-NA	2.29	114.72	109.92
20	A	1759	CLA	C4A-NA-C1A	2.29	107.73	106.71
21	A	7041	LMU	O5'-C5'-C4'	2.29	114.58	109.75
20	A	1800	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
20	B	1764	CLA	CHD-C1D-ND	2.29	126.56	124.45
20	B	1787	CLA	CMA-C3A-C2A	-2.29	104.60	113.83
21	A	7031	LMU	O5'-C5'-C6'	2.29	112.12	106.44
22	B	1774	BCR	C20-C19-C18	-2.29	120.00	126.42
20	B	1765	CLA	O2A-CGA-O1A	-2.28	117.61	123.30
20	A	1785	CLA	C2A-C1A-CHA	-2.28	119.86	123.86
20	B	1749	CLA	C4-C3-C2	-2.28	117.82	123.68
20	B	1745	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
20	2	1220	CLA	C4-C3-C5	2.28	119.11	115.27
20	A	1772	CLA	C4A-NA-C1A	2.28	107.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	1199	CLA	C2B-C3B-C4B	2.28	108.24	106.29
20	J	1044	CLA	CMA-C3A-C4A	-2.28	105.65	111.77
20	3	3007	CLA	C1D-ND-C4D	-2.28	104.72	106.33
20	A	1765	CLA	C1-C2-C3	2.28	129.98	126.04
21	A	7026	LMU	O5B-C1B-C2B	2.28	115.17	110.35
22	A	1808	BCR	C11-C12-C13	-2.28	120.02	126.42
20	2	1218	CLA	CMB-C2B-C3B	2.28	128.94	124.68
20	A	1786	CLA	C1-O2A-CGA	2.28	122.42	116.44
20	B	1772	CLA	CAC-C3C-C4C	2.28	128.50	125.04
22	A	1806	BCR	C11-C12-C13	-2.27	120.03	126.42
20	4	1206	CLA	C2C-C1C-CHC	-2.27	120.22	125.67
20	A	1762	CLA	CED-O2D-CGD	2.27	121.08	115.94
20	4	1205	CLA	C2B-C3B-C4B	2.27	108.23	106.29
22	B	1780	BCR	C20-C19-C18	-2.27	120.03	126.42
20	B	1759	CLA	CHB-C4A-NA	2.27	127.65	124.51
20	B	1745	CLA	C3D-C4D-ND	2.27	113.91	110.24
20	B	1785	CLA	C3D-C4D-ND	2.27	113.91	110.24
21	A	7036	LMU	C6'-C5'-C4'	-2.27	106.72	113.33
20	B	1737	CLA	C2D-C1D-ND	-2.27	108.43	110.10
20	B	1741	CLA	CAC-C3C-C2C	-2.27	123.65	127.53
20	B	1787	CLA	C3D-C4D-ND	2.27	113.91	110.24
21	A	7036	LMU	O5'-C5'-C4'	-2.27	104.97	109.75
21	A	7030	LMU	O2'-C2'-C1'	-2.27	104.54	110.05
20	L	1166	CLA	C3D-C4D-ND	2.27	113.90	110.24
22	A	1806	BCR	C20-C19-C18	-2.27	120.05	126.42
20	B	1760	CLA	C3D-C4D-ND	2.27	113.90	110.24
20	3	3008	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
20	3	3011	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
20	B	1744	CLA	CAC-C3C-C2C	-2.26	123.66	127.53
20	4	1209	CLA	CMA-C3A-C4A	-2.26	105.69	111.77
20	A	1764	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
20	A	1787	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	A	1804	BCR	C20-C19-C18	-2.26	120.06	126.42
21	A	7036	LMU	O3'-C3'-C4'	-2.26	103.95	109.94
20	1	1189	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
22	A	1803	BCR	C20-C19-C18	-2.26	120.06	126.42
20	3	3008	CLA	C3D-C4D-ND	2.26	113.89	110.24
20	B	1760	CLA	CMB-C2B-C3B	2.26	128.91	124.68
22	B	1775	BCR	C11-C12-C13	-2.26	120.06	126.42
20	B	1770	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
20	3	3008	CLA	CMB-C2B-C3B	2.26	128.91	124.68
20	B	1758	CLA	C12-C11-C10	-2.26	102.85	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1777	BCR	C20-C19-C18	-2.26	120.07	126.42
22	B	1778	BCR	C20-C19-C18	-2.26	120.07	126.42
20	A	1813	CLA	C3D-C4D-ND	2.26	113.89	110.24
20	B	1787	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	A	7021	LMU	O1'-C1'-C2'	2.26	111.83	108.30
23	A	1802	PQN	O1-C1-C2	2.26	123.19	120.25
20	B	1751	CLA	O2A-CGA-CBA	2.26	121.15	112.23
21	A	1810	LMU	C4B-C3B-C2B	-2.26	106.88	110.82
22	B	1779	BCR	C8-C9-C10	-2.26	115.48	118.94
22	B	1776	BCR	C33-C5-C4	2.26	117.95	113.62
20	F	1155	CLA	C3D-C4D-ND	2.26	113.89	110.24
22	B	1775	BCR	C20-C19-C18	-2.26	120.08	126.42
20	B	1742	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
20	4	4003	CLA	C2A-C3A-C4A	-2.26	100.64	104.18
20	B	1771	CLA	CED-O2D-CGD	2.26	121.04	115.94
20	A	1761	CLA	C1D-ND-C4D	-2.26	104.73	106.33
20	R	1055	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
22	B	1779	BCR	C15-C16-C17	-2.25	118.86	123.47
20	A	1777	CLA	CHC-C1C-C2C	-2.25	120.49	126.72
20	I	1033	CLA	C2D-C1D-ND	-2.25	108.44	110.10
20	B	1765	CLA	CED-O2D-CGD	2.25	121.03	115.94
20	2	1213	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
20	A	1813	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
20	B	1766	CLA	C1-C2-C3	-2.25	122.15	126.04
20	B	1765	CLA	CMB-C2B-C3B	2.25	128.89	124.68
20	A	1786	CLA	CGD-CBD-CAD	2.25	118.02	110.73
20	A	1777	CLA	CED-O2D-CGD	2.25	121.02	115.94
21	A	7019	LMU	O2'-C2'-C3'	-2.25	105.15	110.35
20	A	1785	CLA	C5-C3-C2	-2.25	116.57	121.12
20	1	1189	CLA	C2D-C1D-ND	-2.25	108.45	110.10
20	B	1785	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
20	A	1813	CLA	C16-C15-C13	-2.25	108.66	115.92
20	4	1196	CLA	C3D-C4D-ND	2.24	113.87	110.24
21	A	7027	LMU	O5'-C1'-C2'	2.24	115.10	110.35
20	1	1196	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
20	B	1738	CLA	C1-C2-C3	-2.24	122.17	126.04
21	A	7016	LMU	C4-C3-C2	-2.24	103.05	114.42
20	R	1055	CLA	C1D-ND-C4D	-2.24	104.74	106.33
20	B	1741	CLA	CHB-C4A-NA	2.24	127.61	124.51
20	A	1815	CLA	C1-C2-C3	2.24	129.91	126.04
20	B	1755	CLA	C3D-C4D-ND	2.24	113.86	110.24
20	B	1786	CLA	CBA-CAA-C2A	-2.24	107.26	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1810	LMU	C1'-C2'-C3'	2.24	114.66	110.00
20	4	1203	CLA	C3D-C2D-C1D	2.24	109.76	107.28
22	B	1776	BCR	C2-C1-C6	2.24	113.92	110.48
20	A	1783	CLA	C1-O2A-CGA	2.24	122.31	116.44
21	A	7042	LMU	C5-C4-C3	-2.24	103.08	114.42
20	1	1198	CLA	O2A-CGA-CBA	2.24	118.92	111.91
20	A	1764	CLA	C1-O2A-CGA	2.23	122.31	116.44
22	A	1805	BCR	C11-C12-C13	-2.23	120.14	126.42
20	B	1769	CLA	CED-O2D-CGD	2.23	120.99	115.94
20	A	1787	CLA	C4-C3-C2	-2.23	117.95	123.68
20	A	1778	CLA	CED-O2D-CGD	2.23	120.98	115.94
20	B	1753	CLA	CHC-C1C-NC	2.23	127.59	124.20
20	3	1217	CLA	C3D-C2D-C1D	2.23	109.75	107.28
20	3	3014	CLA	C3A-C4A-NA	2.23	114.60	109.92
20	B	1754	CLA	CAA-C2A-C1A	2.23	119.28	111.97
20	A	1760	CLA	C3B-C4B-NB	-2.23	106.33	109.21
21	R	1057	LMU	O5B-C5B-C4B	2.23	113.74	109.69
20	R	1054	CLA	CGD-CBD-CAD	-2.23	103.52	110.73
20	B	1763	CLA	CAC-C3C-C4C	2.23	127.70	124.81
20	4	1201	CLA	C4-C3-C2	-2.22	117.97	123.68
20	H	1079	CLA	C1-O2A-CGA	2.22	122.28	116.44
20	J	1046	CLA	CHB-C4A-NA	2.22	127.74	124.34
20	B	1748	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
20	A	1772	CLA	O2A-CGA-CBA	2.22	118.88	111.91
20	A	1759	CLA	CHB-C4A-NA	2.22	127.58	124.51
20	A	1773	CLA	C4-C3-C5	2.22	119.01	115.27
21	A	7013	LMU	O5'-C1'-C2'	-2.22	105.65	110.35
20	A	1800	CLA	CHB-C4A-NA	2.22	127.58	124.51
20	B	1786	CLA	O2A-CGA-CBA	2.22	118.87	111.91
20	B	1758	CLA	O2A-C1-C2	2.22	114.46	108.64
20	2	1215	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
20	B	1738	CLA	C2D-C1D-ND	-2.22	108.47	110.10
21	A	7016	LMU	C6B-C5B-C4B	-2.22	107.81	113.00
20	3	3008	CLA	C1D-ND-C4D	-2.22	104.76	106.33
21	A	7042	LMU	C6B-C5B-C4B	-2.22	107.81	113.00
20	1	1191	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
21	A	7023	LMU	C1'-C2'-C3'	2.21	114.61	110.00
20	3	1214	CLA	C3A-C4A-NA	2.21	114.57	109.92
20	A	1781	CLA	C3D-C4D-ND	2.21	113.82	110.24
20	A	1788	CLA	C3D-C4D-ND	2.21	113.82	110.24
20	2	1227	CLA	CHD-C1D-ND	2.21	126.65	124.52
20	B	1743	CLA	C3D-C4D-ND	2.21	113.82	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1779	BCR	C20-C19-C18	-2.21	120.20	126.42
21	A	7020	LMU	C8-C7-C6	-2.21	103.20	114.42
20	4	1204	CLA	CHB-C4A-NA	2.21	127.57	124.51
20	4	1208	CLA	C2A-C3A-C4A	-2.21	100.72	104.18
21	A	7021	LMU	O5'-C5'-C6'	-2.21	100.94	106.44
20	2	1217	CLA	CHB-C4A-NA	2.21	127.56	124.51
20	B	1766	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
20	A	1767	CLA	CAC-C3C-C4C	2.21	127.67	124.81
20	F	1157	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
20	L	1168	CLA	CMA-C3A-C4A	2.21	117.70	111.77
20	4	4003	CLA	C3D-C4D-ND	2.21	112.79	109.46
20	4	1198	CLA	C3D-C4D-ND	2.21	113.81	110.24
20	A	1764	CLA	O2A-CGA-CBA	2.20	118.83	111.91
20	2	1214	CLA	C2A-C3A-C4A	-2.20	100.72	104.18
20	4	4007	CLA	CAA-CBA-CGA	-2.20	106.81	113.25
20	B	1742	CLA	C1D-ND-C4D	-2.20	104.77	106.33
20	3	1215	CLA	C3A-C4A-NA	2.20	114.54	109.92
20	F	1157	CLA	CMC-C2C-C1C	2.20	128.39	125.04
20	4	1197	CLA	CAC-C3C-C4C	2.20	128.39	125.04
20	4	1197	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
20	A	1790	CLA	C1-O2A-CGA	2.20	122.22	116.44
20	H	1079	CLA	C4-C3-C5	2.20	118.97	115.27
20	2	1220	CLA	C1D-ND-C4D	-2.20	104.77	106.33
20	B	1770	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
20	B	1747	CLA	C1-O2A-CGA	2.20	122.21	116.44
20	A	1785	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
20	B	1757	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
20	3	1218	CLA	C1-O2A-CGA	2.20	122.21	116.44
20	A	1760	CLA	CHB-C4A-NA	2.20	127.55	124.51
20	J	1044	CLA	C6-C5-C3	-2.20	107.70	113.45
22	I	1032	BCR	C3-C2-C1	-2.20	106.75	114.60
20	B	1765	CLA	CHB-C4A-NA	2.19	127.55	124.51
22	L	1169	BCR	C23-C24-C25	-2.19	121.04	127.20
20	1	1188	CLA	C1-O2A-CGA	2.19	123.10	116.73
20	2	1220	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
20	A	1765	CLA	C3D-C4D-ND	2.19	113.78	110.24
20	B	1760	CLA	CAA-CBA-CGA	-2.19	106.85	113.25
20	B	1742	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
21	A	7041	LMU	O4'-C4B-C3B	2.19	115.41	110.35
20	B	1768	CLA	C3D-C4D-ND	2.19	113.78	110.24
21	A	7028	LMU	O2B-C2B-C1B	-2.19	104.73	110.05
22	B	1776	BCR	C8-C7-C6	-2.19	121.06	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	1200	CLA	CMA-C3A-C2A	-2.18	105.02	113.83
20	1	1188	CLA	O2D-CGD-CBD	2.18	115.15	111.27
20	1	1193	CLA	C4D-CHA-C1A	-2.18	118.59	121.25
20	B	1748	CLA	CED-O2D-CGD	2.18	120.87	115.94
20	B	1752	CLA	CHB-C4A-NA	2.18	127.53	124.51
21	A	7017	LMU	O1B-C1B-C2B	2.18	113.75	108.10
20	A	1786	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
20	K	1085	CLA	C3D-C4D-ND	2.18	113.77	110.24
20	B	1737	CLA	C3D-C4D-ND	2.18	113.76	110.24
20	B	1744	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
20	3	3011	CLA	CED-O2D-CGD	2.18	120.87	115.94
20	A	1783	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
21	A	7041	LMU	C1'-O5'-C5'	2.18	117.96	113.69
21	L	1171	LMU	C1'-C2'-C3'	-2.18	105.46	110.00
20	A	1777	CLA	CMB-C2B-C3B	2.18	128.75	124.68
20	A	1788	CLA	C1-O2A-CGA	2.18	122.15	116.44
20	3	3011	CLA	C5-C3-C2	-2.18	116.71	121.12
20	4	4003	CLA	C1C-NC-C4C	-2.18	105.73	106.71
20	4	1199	CLA	O1D-CGD-CBD	-2.17	120.03	124.48
20	A	1765	CLA	C3B-C4B-NB	2.17	112.02	109.21
20	A	1799	CLA	O2A-CGA-CBA	2.17	118.73	111.91
21	A	7028	LMU	C1-O1'-C1'	-2.17	110.23	113.84
20	2	1224	CLA	C4A-NA-C1A	2.17	107.68	106.71
21	A	7037	LMU	C6-C5-C4	-2.17	103.39	114.42
20	3	1213	CLA	C3D-C4D-ND	2.17	112.74	109.46
20	H	1079	CLA	C2D-C1D-ND	-2.17	108.50	110.10
20	A	1800	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
21	A	7015	LMU	O4'-C4B-C5B	2.17	114.69	109.30
20	A	1783	CLA	C4-C3-C5	2.17	118.92	115.27
21	A	7028	LMU	O1B-C4'-C5'	2.17	115.39	109.45
20	2	1212	CLA	C3D-C4D-ND	2.17	113.75	110.24
20	A	1760	CLA	C1-C2-C3	2.17	129.79	126.04
20	4	1200	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
20	2	1221	CLA	C3D-C4D-ND	2.17	112.73	109.46
20	1	1192	CLA	CBC-CAC-C3C	2.17	118.40	112.43
20	B	1768	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
21	A	7041	LMU	O5B-C1B-C2B	-2.17	105.77	110.35
20	A	1771	CLA	CED-O2D-CGD	2.16	120.83	115.94
22	I	1032	BCR	C4-C5-C6	-2.16	119.59	122.73
20	B	1769	CLA	O2A-CGA-CBA	2.16	118.69	111.91
21	A	7027	LMU	C3B-C4B-C5B	2.16	114.10	110.24
21	A	7040	LMU	O4'-C4B-C3B	2.16	115.35	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	7023	LMU	O5B-C5B-C4B	-2.16	105.77	109.69
20	L	1166	CLA	C4A-NA-C1A	2.16	107.68	106.71
20	1	1189	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
20	4	1203	CLA	C3D-C4D-ND	2.16	112.72	109.46
20	2	1215	CLA	C4D-CHA-C1A	-2.16	118.62	121.25
20	F	1157	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
20	A	1761	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
20	B	1739	CLA	C3A-C2A-C1A	2.16	104.57	101.34
20	2	1224	CLA	C4-C3-C2	-2.16	118.14	123.68
20	A	1789	CLA	C4A-NA-C1A	2.16	107.68	106.71
21	A	7022	LMU	C6'-C5'-C4'	-2.16	107.05	113.33
20	3	1219	CLA	C3D-C4D-ND	2.16	113.72	110.24
20	B	1736	CLA	C3A-C2A-C1A	2.16	104.57	101.34
20	J	1045	CLA	CAA-C2A-C1A	-2.15	104.91	111.97
20	F	1157	CLA	CHC-C1C-C2C	-2.15	120.76	126.72
20	1	1196	CLA	C1D-ND-C4D	-2.15	104.81	106.33
20	B	1743	CLA	C1D-ND-C4D	-2.15	104.81	106.33
21	A	7040	LMU	O5'-C5'-C4'	-2.15	105.21	109.75
20	B	1757	CLA	C1-C2-C3	-2.15	122.32	126.04
20	A	1812	CLA	CMA-C3A-C4A	-2.15	105.99	111.77
20	1	1193	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
20	A	1816	CLA	C4C-C3C-C2C	-2.15	103.76	106.90
21	A	7017	LMU	C3B-C4B-C5B	2.15	114.08	110.24
20	1	1198	CLA	CBA-CAA-C2A	-2.15	107.51	113.86
22	B	1777	BCR	C34-C9-C10	-2.15	119.91	122.92
20	A	1786	CLA	CBA-CAA-C2A	2.15	120.21	113.86
20	A	1793	CLA	C3D-C4D-ND	2.15	113.72	110.24
23	B	1773	PQN	C14-C13-C12	-2.15	118.16	123.68
20	B	1764	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
20	3	3002	CLA	C3D-C4D-ND	2.15	112.71	109.46
21	A	7020	LMU	O2B-C2B-C3B	-2.15	105.38	110.35
22	B	1777	BCR	C37-C22-C21	-2.15	119.91	122.92
20	2	1222	CLA	C2D-C1D-ND	-2.15	108.52	110.10
20	A	1796	CLA	C3D-C4D-ND	2.15	113.71	110.24
20	4	1201	CLA	C5-C3-C2	2.15	125.46	121.12
22	B	1774	BCR	C34-C9-C10	-2.15	119.92	122.92
20	B	1735	CLA	C3D-C4D-ND	2.15	113.71	110.24
20	L	1167	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
20	A	1791	CLA	C3D-C4D-ND	2.15	113.71	110.24
20	A	1775	CLA	C2A-C1A-CHA	-2.15	120.11	123.85
20	A	1816	CLA	CAC-C3C-C2C	2.15	131.20	127.53
20	1	1198	CLA	CHB-C4A-NA	2.15	127.48	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1781	BCR	C10-C11-C12	-2.15	116.52	123.22
22	B	1776	BCR	C36-C18-C17	-2.15	119.92	122.92
22	B	1781	BCR	C15-C14-C13	2.14	130.37	127.31
20	F	1156	CLA	C3D-C4D-ND	2.14	113.71	110.24
20	B	1757	CLA	C7-C6-C5	-2.14	107.54	113.36
21	A	7021	LMU	O5B-C5B-C6B	2.14	111.77	106.44
20	A	1759	CLA	O2A-C1-C2	2.14	114.27	108.64
21	A	7038	LMU	O5'-C1'-C2'	2.14	114.89	110.35
20	4	1204	CLA	CBC-CAC-C3C	-2.14	106.52	112.43
20	4	1198	CLA	C2C-C1C-NC	-2.14	107.97	109.97
20	A	1772	CLA	C6-C7-C8	-2.14	109.00	115.92
20	B	1747	CLA	C1-C2-C3	-2.14	122.34	126.04
21	A	7030	LMU	O2B-C2B-C3B	-2.14	105.40	110.35
20	3	3008	CLA	C2D-C1D-ND	-2.14	108.53	110.10
20	A	1783	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
20	A	1792	CLA	C3D-C4D-ND	2.14	113.69	110.24
22	L	1169	BCR	C24-C23-C22	-2.14	123.01	126.23
22	B	1781	BCR	C29-C30-C25	-2.14	107.19	110.48
20	A	1817	CLA	CHD-C4C-C3C	-2.14	121.70	124.84
20	A	1795	CLA	C3D-C4D-ND	2.14	113.69	110.24
20	H	1079	CLA	O2A-C1-C2	2.14	114.25	108.64
20	B	1737	CLA	CMB-C2B-C1B	2.14	131.75	128.46
21	A	7015	LMU	O1B-C1B-C2B	2.13	113.63	108.10
21	A	7043	LMU	O3'-C3'-C2'	2.13	115.28	110.35
21	A	7025	LMU	O2B-C2B-C1B	2.13	115.23	110.05
20	A	1800	CLA	O2A-CGA-CBA	2.13	118.60	111.91
20	A	1786	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
20	B	1746	CLA	C3D-C4D-ND	2.13	113.69	110.24
20	I	1031	CLA	C4-C3-C5	2.13	118.86	115.27
21	A	7030	LMU	O1'-C1'-C2'	2.13	111.63	108.30
20	4	4007	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
20	J	1046	CLA	C3D-C4D-ND	2.13	112.68	109.46
20	A	1785	CLA	CHB-C4A-NA	2.13	127.46	124.51
20	K	1146	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
22	B	1777	BCR	C36-C18-C17	-2.13	119.94	122.92
20	B	1786	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
20	A	1797	CLA	C3D-C4D-ND	2.13	113.68	110.24
20	G	1099	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
21	A	7042	LMU	O1B-C1B-C2B	-2.13	102.58	108.10
21	A	1809	LMU	C1-O1'-C1'	-2.13	110.31	113.84
20	B	1771	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
20	H	1079	CLA	CAC-C3C-C2C	-2.13	123.89	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1786	CLA	C1D-ND-C4D	-2.13	104.82	106.33
20	A	1759	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
20	B	1750	CLA	CHB-C4A-NA	2.13	127.45	124.51
20	I	1031	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
20	3	1217	CLA	C2B-C3B-C4B	2.12	108.11	106.29
21	A	7032	LMU	O3'-C3'-C4'	-2.12	104.31	109.94
20	L	1167	CLA	CMC-C2C-C1C	2.12	128.27	125.04
20	1	1200	CLA	CHD-C1D-ND	2.12	126.41	124.45
20	A	1770	CLA	CHB-C4A-NA	2.12	127.45	124.51
22	A	1807	BCR	C35-C13-C14	-2.12	119.95	122.92
20	A	1815	CLA	C2D-C1D-ND	-2.12	108.54	110.10
22	A	1807	BCR	C37-C22-C21	-2.12	119.95	122.92
20	F	1155	CLA	CAA-C2A-C3A	-2.12	111.15	116.10
22	B	1777	BCR	C35-C13-C14	-2.12	119.95	122.92
20	1	1195	CLA	CHB-C4A-NA	2.12	127.44	124.51
20	A	1768	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
20	A	1794	CLA	C3D-C4D-ND	2.12	113.67	110.24
20	2	1217	CLA	CMB-C2B-C3B	2.12	128.64	124.68
20	A	1798	CLA	C4-C3-C2	-2.12	118.25	123.68
20	1	1194	CLA	C3D-C4D-ND	2.12	112.66	109.46
20	4	4014	CLA	C3D-C4D-ND	2.12	113.66	110.24
20	2	1213	CLA	CED-O2D-CGD	2.12	120.72	115.94
20	B	1754	CLA	C2D-C1D-ND	-2.12	108.55	110.10
20	3	1218	CLA	C3A-C2A-C1A	-2.11	98.17	101.34
20	A	1774	CLA	C4-C3-C2	-2.11	118.25	123.68
20	2	1221	CLA	CHB-C4A-NA	2.11	127.58	124.34
20	A	1789	CLA	C3C-C4C-NC	-2.11	108.20	110.57
20	A	1762	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
20	3	3008	CLA	C5-C3-C4	2.11	119.27	114.60
22	A	1808	BCR	C36-C18-C17	-2.11	119.96	122.92
20	A	1760	CLA	C3D-C4D-ND	2.11	113.65	110.24
22	A	1803	BCR	C35-C13-C14	-2.11	119.97	122.92
20	1	1190	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
20	J	1043	CLA	C3D-C4D-ND	2.11	113.65	110.24
22	A	1804	BCR	C35-C13-C14	-2.11	119.97	122.92
20	A	1783	CLA	C3A-C2A-C1A	2.11	104.50	101.34
20	A	1777	CLA	C1-C2-C3	-2.11	122.40	126.04
20	L	1168	CLA	CHB-C4A-NA	2.11	127.43	124.51
20	3	3011	CLA	O2A-C1-C2	2.11	114.17	108.64
20	1	1198	CLA	CED-O2D-CGD	2.11	120.70	115.94
20	A	1779	CLA	CGD-CBD-CAD	2.11	117.56	110.73
20	1	1198	CLA	CGD-CBD-CAD	-2.11	103.91	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1775	BCR	C37-C22-C21	-2.11	119.97	122.92
22	A	1803	BCR	C34-C9-C10	-2.11	119.97	122.92
20	B	1749	CLA	O2A-C1-C2	2.10	114.17	108.64
22	B	1774	BCR	C36-C18-C17	-2.10	119.97	122.92
20	1	1193	CLA	CAC-C3C-C4C	2.10	127.54	124.81
22	A	1804	BCR	C37-C22-C21	-2.10	119.98	122.92
20	2	1227	CLA	C1C-NC-C4C	-2.10	105.76	106.71
20	1	1200	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
20	K	3009	CLA	C1D-ND-C4D	-2.10	104.84	106.33
20	1	1197	CLA	C3B-C4B-NB	2.10	111.92	109.21
22	A	1804	BCR	C34-C9-C10	-2.10	119.98	122.92
20	3	1216	CLA	CHB-C4A-NA	2.10	127.55	124.34
20	4	1209	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
20	B	1737	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
20	A	1774	CLA	CAA-C2A-C1A	-2.10	105.10	111.97
20	A	1785	CLA	C3A-C2A-C1A	2.10	104.48	101.34
20	A	1767	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
20	B	1747	CLA	CHB-C4A-NA	2.10	127.41	124.51
20	1	1187	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
20	4	1197	CLA	CAA-C2A-C1A	-2.10	106.63	111.81
20	4	1205	CLA	C3A-C4A-NA	2.10	114.32	109.92
20	1	1190	CLA	CHB-C4A-NA	2.09	127.41	124.51
20	A	1789	CLA	C5-C3-C2	-2.09	116.88	121.12
20	B	1743	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
21	A	7024	LMU	C1'-O5'-C5'	-2.09	109.58	113.69
22	B	1775	BCR	C34-C9-C10	-2.09	119.99	122.92
22	A	1806	BCR	C37-C22-C21	-2.09	119.99	122.92
22	A	1805	BCR	C36-C18-C17	-2.09	120.00	122.92
20	A	1782	CLA	C3D-C4D-ND	2.09	113.62	110.24
20	A	1766	CLA	C3B-C4B-NB	-2.09	106.51	109.21
20	2	1219	CLA	C3B-C4B-NB	2.09	111.94	110.11
20	2	1220	CLA	CGD-CBD-CAD	-2.09	103.97	110.73
20	B	1738	CLA	C3D-C4D-ND	2.09	113.61	110.24
20	A	1801	CLA	CHB-C4A-NA	2.09	127.40	124.51
20	A	1786	CLA	CAC-C3C-C2C	-2.09	123.96	127.53
20	3	3007	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
22	A	1808	BCR	C34-C9-C10	-2.09	120.00	122.92
20	B	1756	CLA	C3D-C4D-ND	2.08	113.61	110.24
20	3	1218	CLA	C4-C3-C2	-2.08	118.33	123.68
20	2	1224	CLA	C2D-C1D-ND	-2.08	108.57	110.10
20	A	1787	CLA	CMB-C2B-C1B	-2.08	125.26	128.46
20	B	1757	CLA	C4-C3-C5	2.08	118.78	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	1190	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
20	B	1747	CLA	CMB-C2B-C1B	-2.08	125.26	128.46
20	3	3015	CLA	C3D-C4D-ND	2.08	112.60	109.46
22	B	1780	BCR	C35-C13-C14	-2.08	120.01	122.92
20	R	1055	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
22	B	1780	BCR	C37-C22-C21	-2.08	120.01	122.92
20	R	1055	CLA	CAA-C2A-C1A	2.08	118.79	111.97
20	B	1737	CLA	C4D-CHA-C1A	-2.08	118.72	121.25
20	B	1740	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
20	G	1099	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
20	A	1769	CLA	C4-C3-C5	2.08	118.77	115.27
22	B	1775	BCR	C35-C13-C14	-2.08	120.01	122.92
20	L	1167	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
20	2	1222	CLA	O2A-CGA-CBA	2.08	118.42	111.91
21	A	7020	LMU	O6B-C6B-C5B	-2.07	104.17	111.29
20	A	1768	CLA	C3D-C4D-ND	2.07	113.59	110.24
20	A	1785	CLA	C6-C7-C8	-2.07	109.22	115.92
22	A	1806	BCR	C36-C18-C17	-2.07	120.02	122.92
20	2	1220	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
20	1	1191	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
20	R	1054	CLA	CAC-C3C-C4C	2.07	127.50	124.81
20	B	1747	CLA	C4-C3-C5	2.07	118.75	115.27
22	A	1803	BCR	C37-C22-C21	-2.07	120.02	122.92
22	3	1220	BCR	C39-C30-C25	-2.07	106.94	110.30
20	A	1776	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
22	B	1778	BCR	C34-C9-C10	-2.07	120.02	122.92
20	B	1749	CLA	C11-C10-C8	-2.07	109.23	115.92
20	B	1755	CLA	C1D-ND-C4D	-2.07	104.86	106.33
20	2	1217	CLA	CHD-C1D-ND	2.07	126.36	124.45
22	B	1774	BCR	C35-C13-C14	-2.07	120.03	122.92
20	2	1222	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
20	2	1215	CLA	O2A-CGA-CBA	2.07	118.40	111.91
22	A	1808	BCR	C35-C13-C14	-2.07	120.03	122.92
20	L	1168	CLA	CMB-C2B-C3B	2.07	128.55	124.68
20	B	1738	CLA	CAC-C3C-C2C	-2.07	123.99	127.53
21	A	7019	LMU	O5B-C5B-C4B	-2.07	105.94	109.69
20	3	3015	CLA	C1D-ND-C4D	-2.07	104.87	106.33
20	B	1747	CLA	CAC-C3C-C4C	2.07	127.49	124.81
20	4	1209	CLA	C1-O2A-CGA	2.07	122.92	116.11
21	A	7019	LMU	C4B-C3B-C2B	2.07	114.43	110.82
21	A	7036	LMU	O5'-C1'-O1'	-2.07	105.08	109.97
20	B	1743	CLA	C5-C3-C2	-2.07	116.94	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1738	CLA	C1B-CHB-C4A	-2.07	126.03	130.12
20	1	1191	CLA	C1D-ND-C4D	-2.07	104.87	106.33
20	B	1751	CLA	CGD-CBD-CAD	2.06	117.42	110.73
22	B	1775	BCR	C36-C18-C17	-2.06	120.03	122.92
20	B	1772	CLA	C1D-ND-C4D	-2.06	104.87	106.33
21	A	7020	LMU	O5B-C5B-C4B	2.06	113.44	109.69
20	3	1215	CLA	C3D-C4D-ND	2.06	112.58	109.46
22	A	1808	BCR	C37-C22-C21	-2.06	120.03	122.92
20	A	1779	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
20	4	1207	CLA	CHD-C1D-ND	2.06	126.35	124.45
20	B	1759	CLA	O2A-CGA-CBA	2.06	118.38	111.91
20	A	1777	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
21	A	7042	LMU	O3'-C3'-C2'	-2.06	105.58	110.35
20	4	1199	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
22	A	1805	BCR	C35-C13-C14	-2.06	120.04	122.92
20	4	1198	CLA	C9-C8-C10	-2.06	103.83	111.29
20	A	1799	CLA	CMB-C2B-C3B	2.06	128.53	124.68
20	A	1789	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
22	B	1774	BCR	C37-C22-C21	-2.06	120.04	122.92
22	A	1805	BCR	C37-C22-C21	-2.06	120.04	122.92
22	A	1806	BCR	C35-C13-C14	-2.05	120.05	122.92
20	A	1779	CLA	CMB-C2B-C3B	2.05	128.52	124.68
20	B	1741	CLA	C5-C3-C2	-2.05	116.96	121.12
22	A	1807	BCR	C36-C18-C17	-2.05	120.05	122.92
20	2	1217	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
20	A	1817	CLA	CMA-C3A-C2A	2.05	122.10	113.83
22	B	1781	BCR	C2-C1-C6	-2.05	107.32	110.48
20	4	1205	CLA	C3D-C4D-ND	2.05	112.56	109.46
20	A	1760	CLA	O2A-C1-C2	2.05	114.02	108.64
20	2	1217	CLA	O2A-CGA-CBA	2.05	118.34	111.91
20	2	1223	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
21	A	7032	LMU	O1'-C1-C2	2.05	116.74	109.56
20	B	1769	CLA	C4A-NA-C1A	2.05	107.63	106.71
20	B	1737	CLA	O2A-C1-C2	-2.05	103.26	108.64
20	A	1787	CLA	C1-O2A-CGA	2.05	121.81	116.44
22	3	1220	BCR	C20-C19-C18	-2.05	120.67	126.42
20	A	1767	CLA	O2A-CGA-CBA	2.04	118.33	111.91
20	B	1766	CLA	C4A-NA-C1A	2.04	107.62	106.71
20	A	1771	CLA	CHB-C4A-NA	2.04	127.34	124.51
20	A	1759	CLA	CGD-CBD-CAD	2.04	117.35	110.73
20	F	1157	CLA	CGD-CBD-CAD	-2.04	104.12	110.73
20	B	1749	CLA	CAA-C2A-C3A	-2.04	107.18	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	1212	CLA	CAA-C2A-C3A	-2.04	111.33	116.10
20	2	1217	CLA	CAC-C3C-C4C	2.04	127.46	124.81
20	B	1771	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
20	A	1790	CLA	C2D-C1D-ND	-2.04	108.60	110.10
20	2	2010	CLA	C1D-ND-C4D	-2.04	104.89	106.33
20	A	1774	CLA	C3D-C4D-ND	2.04	113.54	110.24
22	B	1778	BCR	C37-C22-C21	-2.04	120.06	122.92
20	A	1790	CLA	CED-O2D-CGD	2.04	120.55	115.94
20	B	1752	CLA	CAC-C3C-C2C	-2.04	124.04	127.53
20	1	1193	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
20	2	1215	CLA	CGD-CBD-CAD	-2.04	104.13	110.73
22	A	1807	BCR	C34-C9-C10	-2.04	120.07	122.92
22	B	1778	BCR	C35-C13-C14	-2.04	120.07	122.92
22	B	1778	BCR	C36-C18-C17	-2.04	120.07	122.92
20	B	1752	CLA	C3D-C4D-ND	2.04	113.53	110.24
20	1	1192	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
20	F	1155	CLA	C3C-C4C-NC	-2.04	108.35	110.57
20	B	1770	CLA	CBA-CAA-C2A	2.04	119.87	113.86
22	A	1804	BCR	C36-C18-C17	-2.03	120.08	122.92
22	B	1780	BCR	C36-C18-C17	-2.03	120.08	122.92
20	K	1142	CLA	C3D-C4D-ND	2.03	113.53	110.24
20	4	1201	CLA	C2D-C1D-ND	-2.03	108.61	110.10
21	A	7025	LMU	C3'-C4'-C5'	2.03	115.59	110.93
20	A	1771	CLA	C3D-C4D-ND	2.03	113.53	110.24
20	B	1764	CLA	CMB-C2B-C3B	2.03	128.48	124.68
20	1	1193	CLA	CMC-C2C-C1C	2.03	128.13	125.04
22	A	1806	BCR	C34-C9-C10	-2.03	120.08	122.92
20	B	1762	CLA	C1D-ND-C4D	-2.03	104.89	106.33
20	B	1759	CLA	C3D-C4D-ND	2.03	113.52	110.24
20	F	1157	CLA	CHD-C1D-ND	2.03	126.32	124.45
20	A	1771	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
20	3	1218	CLA	C11-C12-C13	-2.03	109.37	115.92
20	L	1167	CLA	CAC-C3C-C2C	-2.03	124.06	127.53
20	A	1780	CLA	C2D-C1D-ND	-2.03	108.61	110.10
20	3	1214	CLA	C3D-C4D-ND	2.03	112.52	109.46
22	B	1780	BCR	C34-C9-C10	-2.03	120.09	122.92
20	B	1785	CLA	CMA-C3A-C2A	-2.03	105.66	113.83
20	K	3009	CLA	C3D-C4D-ND	2.02	113.51	110.24
20	1	1200	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
20	B	1748	CLA	CMB-C2B-C3B	2.02	128.46	124.68
20	2	1213	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
20	4	1196	CLA	C1D-ND-C4D	-2.02	104.90	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1790	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
20	1	1196	CLA	C2A-C1A-CHA	-2.02	120.32	123.85
20	1	1198	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
21	R	1057	LMU	O1B-C4'-C3'	2.02	112.65	107.28
23	A	1802	PQN	C17-C16-C15	-2.02	107.88	113.36
21	A	7043	LMU	O3B-C3B-C4B	-2.02	105.68	110.35
22	L	1170	BCR	C23-C24-C25	-2.02	121.53	127.20
20	A	1765	CLA	C3C-C4C-NC	-2.02	108.31	110.57
20	1	1198	CLA	C11-C10-C8	-2.02	109.40	115.92
22	I	1032	BCR	C36-C18-C19	-2.02	114.90	118.08
21	A	7036	LMU	O1B-C4'-C3'	-2.02	101.92	107.28
20	4	4007	CLA	C3D-C4D-ND	2.02	113.50	110.24
21	A	7026	LMU	O1B-C1B-O5B	2.02	116.31	110.67
20	1	1194	CLA	CHB-C4A-NA	2.02	127.43	124.34
20	3	1217	CLA	C3C-C4C-CHD	-2.02	120.81	125.22
20	4	1198	CLA	C9-C8-C7	2.02	118.59	111.29
20	A	1774	CLA	CHB-C4A-NA	2.01	127.30	124.51
20	B	1769	CLA	CHB-C4A-NA	2.01	127.30	124.51
21	R	1057	LMU	O5'-C1'-C2'	-2.01	106.09	110.35
20	B	1785	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
20	1	1192	CLA	C3D-C4D-ND	2.01	113.49	110.24
20	1	1193	CLA	C3D-C4D-ND	2.01	113.49	110.24
20	B	1744	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
23	B	1773	PQN	C11-C3-C4	2.01	120.65	118.50
20	A	1776	CLA	C3A-C2A-C1A	2.01	104.35	101.34
22	L	1170	BCR	C27-C26-C25	-2.01	119.81	122.73
20	A	1780	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
20	I	1033	CLA	CHD-C1D-ND	2.01	126.30	124.45
20	B	1763	CLA	C1-O2A-CGA	2.01	121.71	116.44
22	A	1805	BCR	C34-C9-C10	-2.01	120.11	122.92
20	3	3015	CLA	C2B-C3B-C4B	2.01	108.00	106.29
20	2	2010	CLA	CHB-C4A-NA	2.01	127.41	124.34
20	A	1799	CLA	CAC-C3C-C2C	-2.00	124.10	127.53
20	A	1784	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
20	A	1815	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
20	A	1800	CLA	CED-O2D-CGD	2.00	120.47	115.94
20	B	1740	CLA	C1-C2-C3	-2.00	122.58	126.04
20	B	1738	CLA	CBA-CAA-C2A	-2.00	107.95	113.86
21	A	7047	LMU	O5B-C5B-C6B	2.00	111.42	106.44
20	B	1770	CLA	CMA-C3A-C2A	-2.00	105.75	113.83
20	A	1789	CLA	CGD-CBD-CAD	-2.00	104.25	110.73
20	A	1786	CLA	C4A-NA-C1A	2.00	107.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	1189	CLA	C1D-ND-C4D	-2.00	104.91	106.33
20	R	1054	CLA	CMB-C2B-C3B	2.00	128.42	124.68
20	2	1224	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
20	B	1771	CLA	C2C-C1C-NC	2.00	111.85	109.97
20	2	1218	CLA	C2C-C1C-NC	2.00	111.85	109.97

All (271) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	1187	CLA	ND
20	1	1188	CLA	ND
20	1	1189	CLA	ND
20	1	1190	CLA	ND
20	1	1191	CLA	ND
20	1	1192	CLA	C8
20	1	1192	CLA	ND
20	1	1193	CLA	C2A
20	1	1193	CLA	ND
20	1	1194	CLA	ND
20	1	1195	CLA	ND
20	1	1196	CLA	ND
20	1	1197	CLA	ND
20	1	1197	CLA	CBD
20	1	1198	CLA	C8
20	1	1198	CLA	ND
20	1	1199	CLA	ND
20	1	1200	CLA	C3A
20	1	1200	CLA	C2A
20	1	1200	CLA	ND
20	1	1201	CLA	ND
20	2	1212	CLA	ND
20	2	1213	CLA	C8
20	2	1213	CLA	ND
20	2	1214	CLA	ND
20	2	1215	CLA	ND
20	2	1216	CLA	ND
20	2	1217	CLA	C8
20	2	1217	CLA	ND
20	2	1218	CLA	C8
20	2	1218	CLA	ND
20	2	1219	CLA	ND
20	2	1220	CLA	C8

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Mol	Chain	Res	Type	Atom
20	2	1220	CLA	ND
20	2	1221	CLA	ND
20	2	1222	CLA	ND
20	2	1223	CLA	ND
20	2	1224	CLA	C8
20	2	1224	CLA	ND
20	2	1227	CLA	ND
20	2	2010	CLA	ND
20	3	1212	CLA	ND
20	3	1213	CLA	ND
20	3	1214	CLA	ND
20	3	1215	CLA	ND
20	3	1216	CLA	ND
20	3	1217	CLA	ND
20	3	1218	CLA	C8
20	3	1218	CLA	ND
20	3	1219	CLA	C8
20	3	1219	CLA	ND
20	3	3001	CLA	ND
20	3	3002	CLA	ND
20	3	3007	CLA	ND
20	3	3008	CLA	ND
20	3	3011	CLA	C8
20	3	3011	CLA	ND
20	3	3014	CLA	ND
20	3	3015	CLA	ND
20	4	1196	CLA	C8
20	4	1196	CLA	ND
20	4	1197	CLA	ND
20	4	1198	CLA	C8
20	4	1198	CLA	ND
20	4	1198	CLA	CBD
20	4	1199	CLA	C8
20	4	1199	CLA	ND
20	4	1200	CLA	ND
20	4	1201	CLA	C2A
20	4	1201	CLA	ND
20	4	1202	CLA	ND
20	4	1203	CLA	ND
20	4	1204	CLA	C8
20	4	1204	CLA	ND
20	4	1205	CLA	ND

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Mol	Chain	Res	Type	Atom
20	4	1206	CLA	ND
20	4	1207	CLA	ND
20	4	1208	CLA	ND
20	4	1209	CLA	ND
20	4	4003	CLA	ND
20	4	4007	CLA	ND
20	4	4014	CLA	ND
20	A	1759	CLA	ND
20	A	1760	CLA	C8
20	A	1760	CLA	ND
20	A	1761	CLA	C8
20	A	1761	CLA	ND
20	A	1762	CLA	C8
20	A	1762	CLA	ND
20	A	1763	CLA	ND
20	A	1764	CLA	C8
20	A	1764	CLA	ND
20	A	1765	CLA	C8
20	A	1765	CLA	ND
20	A	1766	CLA	ND
20	A	1767	CLA	C8
20	A	1767	CLA	ND
20	A	1768	CLA	ND
20	A	1769	CLA	ND
20	A	1770	CLA	ND
20	A	1771	CLA	ND
20	A	1772	CLA	C8
20	A	1772	CLA	ND
20	A	1773	CLA	ND
20	A	1774	CLA	C8
20	A	1774	CLA	ND
20	A	1775	CLA	ND
20	A	1776	CLA	C8
20	A	1776	CLA	ND
20	A	1777	CLA	ND
20	A	1778	CLA	ND
20	A	1779	CLA	C8
20	A	1779	CLA	ND
20	A	1780	CLA	C8
20	A	1780	CLA	ND
20	A	1781	CLA	C8
20	A	1781	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	1782	CLA	C8
20	A	1782	CLA	ND
20	A	1783	CLA	C8
20	A	1783	CLA	ND
20	A	1784	CLA	C8
20	A	1784	CLA	ND
20	A	1785	CLA	C8
20	A	1785	CLA	ND
20	A	1786	CLA	ND
20	A	1787	CLA	C8
20	A	1787	CLA	ND
20	A	1788	CLA	C8
20	A	1788	CLA	ND
20	A	1789	CLA	C8
20	A	1789	CLA	ND
20	A	1790	CLA	ND
20	A	1791	CLA	ND
20	A	1792	CLA	ND
20	A	1793	CLA	C8
20	A	1793	CLA	ND
20	A	1794	CLA	ND
20	A	1795	CLA	ND
20	A	1796	CLA	C8
20	A	1796	CLA	ND
20	A	1797	CLA	C8
20	A	1797	CLA	ND
20	A	1798	CLA	C8
20	A	1798	CLA	ND
20	A	1799	CLA	ND
20	A	1800	CLA	C8
20	A	1800	CLA	ND
20	A	1801	CLA	C8
20	A	1801	CLA	ND
20	A	1811	CLA	C8
20	A	1811	CLA	ND
20	A	1812	CLA	C8
20	A	1812	CLA	ND
20	A	1813	CLA	C8
20	A	1813	CLA	ND
20	A	1815	CLA	C8
20	A	1815	CLA	ND
20	A	1815	CLA	CBD

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Mol	Chain	Res	Type	Atom
20	A	1816	CLA	C3A
20	A	1816	CLA	C2A
20	A	1816	CLA	ND
20	A	1817	CLA	C2A
20	A	1817	CLA	ND
20	A	1817	CLA	CBD
20	B	1735	CLA	C8
20	B	1735	CLA	ND
20	B	1736	CLA	ND
20	B	1737	CLA	C8
20	B	1737	CLA	ND
20	B	1738	CLA	C8
20	B	1738	CLA	ND
20	B	1739	CLA	C8
20	B	1739	CLA	ND
20	B	1740	CLA	C8
20	B	1740	CLA	ND
20	B	1741	CLA	C8
20	B	1741	CLA	ND
20	B	1742	CLA	C8
20	B	1742	CLA	ND
20	B	1743	CLA	C8
20	B	1743	CLA	ND
20	B	1744	CLA	C8
20	B	1744	CLA	ND
20	B	1745	CLA	C8
20	B	1745	CLA	ND
20	B	1746	CLA	ND
20	B	1747	CLA	C8
20	B	1747	CLA	ND
20	B	1748	CLA	C8
20	B	1748	CLA	ND
20	B	1749	CLA	C8
20	B	1749	CLA	ND
20	B	1750	CLA	ND
20	B	1751	CLA	ND
20	B	1752	CLA	C8
20	B	1752	CLA	ND
20	B	1753	CLA	ND
20	B	1754	CLA	ND
20	B	1755	CLA	C8
20	B	1755	CLA	ND

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Mol	Chain	Res	Type	Atom
20	B	1756	CLA	C8
20	B	1756	CLA	ND
20	B	1757	CLA	C8
20	B	1757	CLA	ND
20	B	1758	CLA	C8
20	B	1758	CLA	ND
20	B	1759	CLA	C8
20	B	1759	CLA	ND
20	B	1760	CLA	ND
20	B	1761	CLA	ND
20	B	1762	CLA	C8
20	B	1762	CLA	ND
20	B	1763	CLA	ND
20	B	1764	CLA	ND
20	B	1765	CLA	ND
20	B	1766	CLA	ND
20	B	1767	CLA	C8
20	B	1767	CLA	ND
20	B	1768	CLA	C8
20	B	1768	CLA	ND
20	B	1769	CLA	ND
20	B	1770	CLA	C8
20	B	1770	CLA	ND
20	B	1771	CLA	C8
20	B	1771	CLA	ND
20	B	1772	CLA	ND
20	B	1785	CLA	C8
20	B	1785	CLA	ND
20	B	1786	CLA	C8
20	B	1786	CLA	ND
20	B	1787	CLA	C8
20	B	1787	CLA	ND
20	F	1155	CLA	ND
20	F	1156	CLA	ND
20	F	1157	CLA	C3A
20	F	1157	CLA	C2A
20	F	1157	CLA	CBD
20	F	1157	CLA	ND
20	G	1099	CLA	ND
20	H	1079	CLA	C8
20	H	1079	CLA	ND
20	I	1031	CLA	C8

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Mol	Chain	Res	Type	Atom
20	I	1031	CLA	ND
20	I	1033	CLA	C8
20	I	1033	CLA	ND
20	J	1043	CLA	C8
20	J	1043	CLA	ND
20	J	1044	CLA	C8
20	J	1044	CLA	ND
20	J	1045	CLA	C8
20	J	1045	CLA	ND
20	J	1046	CLA	ND
20	K	1085	CLA	ND
20	K	1142	CLA	ND
20	K	1146	CLA	ND
20	K	3009	CLA	C8
20	K	3009	CLA	ND
20	L	1166	CLA	ND
20	L	1167	CLA	ND
20	L	1168	CLA	ND
20	L	1168	CLA	CBD
20	L	1505	CLA	C8
20	L	1505	CLA	ND
20	R	1054	CLA	C8
20	R	1054	CLA	ND
20	R	1055	CLA	C8
20	R	1055	CLA	ND
21	R	1057	LMU	C2B
23	A	1802	PQN	C23
23	B	1773	PQN	C23

All (2727) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	1187	CLA	C1A-C2A-CAA-CBA
20	1	1187	CLA	C3A-C2A-CAA-CBA
20	1	1187	CLA	CBA-CGA-O2A-C1
20	1	1187	CLA	CHA-CBD-CGD-O1D
20	1	1187	CLA	CHA-CBD-CGD-O2D
20	1	1188	CLA	C3A-C2A-CAA-CBA
20	1	1188	CLA	CBD-CGD-O2D-CED
20	1	1190	CLA	C1A-C2A-CAA-CBA
20	1	1190	CLA	CBD-CGD-O2D-CED
20	1	1190	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	1	1192	CLA	C1A-C2A-CAA-CBA
20	1	1192	CLA	C2C-C3C-CAC-CBC
20	1	1192	CLA	C4C-C3C-CAC-CBC
20	1	1192	CLA	CHA-CBD-CGD-O1D
20	1	1192	CLA	CHA-CBD-CGD-O2D
20	1	1193	CLA	C2-C3-C5-C6
20	1	1193	CLA	C4-C3-C5-C6
20	1	1197	CLA	CBD-CGD-O2D-CED
20	1	1197	CLA	C2-C3-C5-C6
20	1	1197	CLA	C4-C3-C5-C6
20	1	1198	CLA	C2-C3-C5-C6
20	1	1198	CLA	C4-C3-C5-C6
20	1	1200	CLA	C3A-C2A-CAA-CBA
20	1	1200	CLA	CBD-CGD-O2D-CED
20	1	1200	CLA	C2-C3-C5-C6
20	2	1212	CLA	C1A-C2A-CAA-CBA
20	2	1212	CLA	C3A-C2A-CAA-CBA
20	2	1212	CLA	O2A-C1-C2-C3
20	2	1213	CLA	C1A-C2A-CAA-CBA
20	2	1213	CLA	C3A-C2A-CAA-CBA
20	2	1213	CLA	CAD-CBD-CGD-O1D
20	2	1213	CLA	CAD-CBD-CGD-O2D
20	2	1213	CLA	C4-C3-C5-C6
20	2	1215	CLA	C2-C1-O2A-CGA
20	2	1217	CLA	C1A-C2A-CAA-CBA
20	2	1217	CLA	CBD-CGD-O2D-CED
20	2	1218	CLA	CBA-CGA-O2A-C1
20	2	1218	CLA	O1A-CGA-O2A-C1
20	2	1220	CLA	C1A-C2A-CAA-CBA
20	2	1220	CLA	C2-C3-C5-C6
20	2	1220	CLA	C4-C3-C5-C6
20	2	1222	CLA	CHA-CBD-CGD-O1D
20	2	1222	CLA	CHA-CBD-CGD-O2D
20	2	1223	CLA	CBA-CGA-O2A-C1
20	2	1223	CLA	O1A-CGA-O2A-C1
20	2	1224	CLA	C2-C1-O2A-CGA
20	2	1224	CLA	CBD-CGD-O2D-CED
20	2	1224	CLA	C14-C13-C15-C16
20	3	1218	CLA	C1A-C2A-CAA-CBA
20	3	1218	CLA	C3A-C2A-CAA-CBA
20	3	1218	CLA	CAD-CBD-CGD-O1D
20	3	1218	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	3	3007	CLA	C1A-C2A-CAA-CBA
20	3	3008	CLA	C1A-C2A-CAA-CBA
20	3	3011	CLA	C2-C3-C5-C6
20	3	3011	CLA	C4-C3-C5-C6
20	4	1196	CLA	C2C-C3C-CAC-CBC
20	4	1196	CLA	C4C-C3C-CAC-CBC
20	4	1196	CLA	C2-C3-C5-C6
20	4	1196	CLA	C4-C3-C5-C6
20	4	1198	CLA	C1A-C2A-CAA-CBA
20	4	1198	CLA	C3A-C2A-CAA-CBA
20	4	1198	CLA	CHA-CBD-CGD-O1D
20	4	1198	CLA	CHA-CBD-CGD-O2D
20	4	1204	CLA	CBD-CGD-O2D-CED
20	4	1209	CLA	C1A-C2A-CAA-CBA
20	4	4014	CLA	CHA-CBD-CGD-O1D
20	4	4014	CLA	CHA-CBD-CGD-O2D
20	4	4014	CLA	CBD-CGD-O2D-CED
20	A	1760	CLA	C3A-C2A-CAA-CBA
20	A	1760	CLA	CBA-CGA-O2A-C1
20	A	1760	CLA	O1A-CGA-O2A-C1
20	A	1761	CLA	C1A-C2A-CAA-CBA
20	A	1761	CLA	C3A-C2A-CAA-CBA
20	A	1761	CLA	C2-C3-C5-C6
20	A	1761	CLA	C4-C3-C5-C6
20	A	1762	CLA	CBA-CGA-O2A-C1
20	A	1762	CLA	O1A-CGA-O2A-C1
20	A	1762	CLA	CBD-CGD-O2D-CED
20	A	1763	CLA	C1A-C2A-CAA-CBA
20	A	1763	CLA	C3A-C2A-CAA-CBA
20	A	1763	CLA	CBA-CGA-O2A-C1
20	A	1764	CLA	C1A-C2A-CAA-CBA
20	A	1764	CLA	C3A-C2A-CAA-CBA
20	A	1765	CLA	C1A-C2A-CAA-CBA
20	A	1765	CLA	O2A-C1-C2-C3
20	A	1766	CLA	CBD-CGD-O2D-CED
20	A	1767	CLA	CBD-CGD-O2D-CED
20	A	1769	CLA	C1A-C2A-CAA-CBA
20	A	1769	CLA	C3A-C2A-CAA-CBA
20	A	1769	CLA	CBD-CGD-O2D-CED
20	A	1770	CLA	C1A-C2A-CAA-CBA
20	A	1771	CLA	C1A-C2A-CAA-CBA
20	A	1771	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	1771	CLA	O1A-CGA-O2A-C1
20	A	1771	CLA	CHA-CBD-CGD-O1D
20	A	1771	CLA	CHA-CBD-CGD-O2D
20	A	1771	CLA	CBD-CGD-O2D-CED
20	A	1772	CLA	CBA-CGA-O2A-C1
20	A	1772	CLA	O1A-CGA-O2A-C1
20	A	1772	CLA	C2-C3-C5-C6
20	A	1772	CLA	C4-C3-C5-C6
20	A	1773	CLA	C1A-C2A-CAA-CBA
20	A	1773	CLA	C3A-C2A-CAA-CBA
20	A	1773	CLA	O1A-CGA-O2A-C1
20	A	1773	CLA	CHA-CBD-CGD-O1D
20	A	1773	CLA	CHA-CBD-CGD-O2D
20	A	1773	CLA	CBD-CGD-O2D-CED
20	A	1774	CLA	C1A-C2A-CAA-CBA
20	A	1774	CLA	C3A-C2A-CAA-CBA
20	A	1774	CLA	CBA-CGA-O2A-C1
20	A	1774	CLA	O1A-CGA-O2A-C1
20	A	1774	CLA	CAD-CBD-CGD-O1D
20	A	1774	CLA	CAD-CBD-CGD-O2D
20	A	1774	CLA	CBD-CGD-O2D-CED
20	A	1777	CLA	C1A-C2A-CAA-CBA
20	A	1777	CLA	CAD-CBD-CGD-O1D
20	A	1777	CLA	CAD-CBD-CGD-O2D
20	A	1778	CLA	C1A-C2A-CAA-CBA
20	A	1778	CLA	C3A-C2A-CAA-CBA
20	A	1779	CLA	C1A-C2A-CAA-CBA
20	A	1781	CLA	C2-C1-O2A-CGA
20	A	1781	CLA	C2C-C3C-CAC-CBC
20	A	1781	CLA	C4C-C3C-CAC-CBC
20	A	1781	CLA	CBD-CGD-O2D-CED
20	A	1782	CLA	C1A-C2A-CAA-CBA
20	A	1782	CLA	O2A-C1-C2-C3
20	A	1785	CLA	C1A-C2A-CAA-CBA
20	A	1785	CLA	C3A-C2A-CAA-CBA
20	A	1785	CLA	CHA-CBD-CGD-O1D
20	A	1785	CLA	CHA-CBD-CGD-O2D
20	A	1785	CLA	CBD-CGD-O2D-CED
20	A	1787	CLA	C1A-C2A-CAA-CBA
20	A	1787	CLA	CHA-CBD-CGD-O1D
20	A	1787	CLA	CHA-CBD-CGD-O2D
20	A	1787	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1787	CLA	C4-C3-C5-C6
20	A	1788	CLA	CBD-CGD-O2D-CED
20	A	1789	CLA	C14-C13-C15-C16
20	A	1790	CLA	C1A-C2A-CAA-CBA
20	A	1790	CLA	C3A-C2A-CAA-CBA
20	A	1790	CLA	CAD-CBD-CGD-O1D
20	A	1791	CLA	C1A-C2A-CAA-CBA
20	A	1792	CLA	C1A-C2A-CAA-CBA
20	A	1793	CLA	CAD-CBD-CGD-O1D
20	A	1793	CLA	CAD-CBD-CGD-O2D
20	A	1794	CLA	C1A-C2A-CAA-CBA
20	A	1795	CLA	C1A-C2A-CAA-CBA
20	A	1795	CLA	CBD-CGD-O2D-CED
20	A	1795	CLA	O2A-C1-C2-C3
20	A	1796	CLA	C1A-C2A-CAA-CBA
20	A	1796	CLA	C3A-C2A-CAA-CBA
20	A	1797	CLA	C4-C3-C5-C6
20	A	1798	CLA	C3A-C2A-CAA-CBA
20	A	1798	CLA	CBD-CGD-O2D-CED
20	A	1798	CLA	O1D-CGD-O2D-CED
20	A	1799	CLA	C3A-C2A-CAA-CBA
20	A	1799	CLA	CHA-CBD-CGD-O1D
20	A	1799	CLA	CHA-CBD-CGD-O2D
20	A	1799	CLA	CBD-CGD-O2D-CED
20	A	1799	CLA	O1D-CGD-O2D-CED
20	A	1801	CLA	CBD-CGD-O2D-CED
20	A	1801	CLA	C2-C3-C5-C6
20	A	1801	CLA	C4-C3-C5-C6
20	A	1811	CLA	C3A-C2A-CAA-CBA
20	A	1811	CLA	CBA-CGA-O2A-C1
20	A	1812	CLA	CBD-CGD-O2D-CED
20	A	1812	CLA	O1D-CGD-O2D-CED
20	A	1812	CLA	C6-C7-C8-C9
20	A	1813	CLA	CHA-CBD-CGD-O1D
20	A	1813	CLA	CHA-CBD-CGD-O2D
20	A	1813	CLA	O2A-C1-C2-C3
20	A	1815	CLA	C1A-C2A-CAA-CBA
20	A	1815	CLA	C3A-C2A-CAA-CBA
20	A	1815	CLA	CAD-CBD-CGD-O1D
20	A	1815	CLA	CBD-CGD-O2D-CED
20	A	1816	CLA	C1A-C2A-CAA-CBA
20	A	1816	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	1816	CLA	C2-C1-O2A-CGA
20	A	1816	CLA	C2C-C3C-CAC-CBC
20	A	1816	CLA	C4C-C3C-CAC-CBC
20	A	1817	CLA	CAD-CBD-CGD-O1D
20	A	1817	CLA	CAD-CBD-CGD-O2D
20	A	1817	CLA	CBD-CGD-O2D-CED
20	B	1735	CLA	C14-C13-C15-C16
20	B	1736	CLA	C1A-C2A-CAA-CBA
20	B	1736	CLA	C3A-C2A-CAA-CBA
20	B	1737	CLA	C1A-C2A-CAA-CBA
20	B	1737	CLA	C2-C1-O2A-CGA
20	B	1737	CLA	CAD-CBD-CGD-O1D
20	B	1737	CLA	CAD-CBD-CGD-O2D
20	B	1738	CLA	CBD-CGD-O2D-CED
20	B	1739	CLA	C11-C10-C8-C9
20	B	1739	CLA	C12-C13-C15-C16
20	B	1740	CLA	C1A-C2A-CAA-CBA
20	B	1740	CLA	O2A-C1-C2-C3
20	B	1741	CLA	C1A-C2A-CAA-CBA
20	B	1741	CLA	C3A-C2A-CAA-CBA
20	B	1741	CLA	CBA-CGA-O2A-C1
20	B	1741	CLA	O1A-CGA-O2A-C1
20	B	1743	CLA	C1A-C2A-CAA-CBA
20	B	1743	CLA	CHA-CBD-CGD-O1D
20	B	1743	CLA	CHA-CBD-CGD-O2D
20	B	1743	CLA	CAD-CBD-CGD-O1D
20	B	1743	CLA	CAD-CBD-CGD-O2D
20	B	1744	CLA	C1A-C2A-CAA-CBA
20	B	1744	CLA	C3A-C2A-CAA-CBA
20	B	1745	CLA	C1A-C2A-CAA-CBA
20	B	1745	CLA	CHA-CBD-CGD-O1D
20	B	1745	CLA	CHA-CBD-CGD-O2D
20	B	1745	CLA	CAD-CBD-CGD-O1D
20	B	1745	CLA	CAD-CBD-CGD-O2D
20	B	1746	CLA	C3A-C2A-CAA-CBA
20	B	1746	CLA	C2C-C3C-CAC-CBC
20	B	1746	CLA	C4C-C3C-CAC-CBC
20	B	1746	CLA	CBD-CGD-O2D-CED
20	B	1747	CLA	C1A-C2A-CAA-CBA
20	B	1747	CLA	C3A-C2A-CAA-CBA
20	B	1747	CLA	C2A-CAA-CBA-CGA
20	B	1747	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	1748	CLA	C1A-C2A-CAA-CBA
20	B	1748	CLA	C3A-C2A-CAA-CBA
20	B	1749	CLA	C1A-C2A-CAA-CBA
20	B	1749	CLA	C3A-C2A-CAA-CBA
20	B	1749	CLA	CBD-CGD-O2D-CED
20	B	1749	CLA	C4-C3-C5-C6
20	B	1750	CLA	CBD-CGD-O2D-CED
20	B	1750	CLA	O1D-CGD-O2D-CED
20	B	1751	CLA	CBA-CGA-O2A-C1
20	B	1751	CLA	CBD-CGD-O2D-CED
20	B	1752	CLA	C1A-C2A-CAA-CBA
20	B	1752	CLA	C3A-C2A-CAA-CBA
20	B	1753	CLA	CBA-CGA-O2A-C1
20	B	1753	CLA	O1A-CGA-O2A-C1
20	B	1753	CLA	CBD-CGD-O2D-CED
20	B	1753	CLA	C6-C7-C8-C9
20	B	1755	CLA	C1A-C2A-CAA-CBA
20	B	1755	CLA	C3A-C2A-CAA-CBA
20	B	1755	CLA	C2C-C3C-CAC-CBC
20	B	1755	CLA	C4C-C3C-CAC-CBC
20	B	1755	CLA	CBD-CGD-O2D-CED
20	B	1755	CLA	C2-C3-C5-C6
20	B	1755	CLA	C4-C3-C5-C6
20	B	1755	CLA	C11-C10-C8-C9
20	B	1756	CLA	C1A-C2A-CAA-CBA
20	B	1756	CLA	C3A-C2A-CAA-CBA
20	B	1757	CLA	C3A-C2A-CAA-CBA
20	B	1757	CLA	CBD-CGD-O2D-CED
20	B	1758	CLA	C3A-C2A-CAA-CBA
20	B	1759	CLA	CHA-CBD-CGD-O1D
20	B	1759	CLA	CHA-CBD-CGD-O2D
20	B	1759	CLA	CAD-CBD-CGD-O1D
20	B	1760	CLA	C1A-C2A-CAA-CBA
20	B	1760	CLA	C3A-C2A-CAA-CBA
20	B	1760	CLA	CHA-CBD-CGD-O1D
20	B	1760	CLA	CHA-CBD-CGD-O2D
20	B	1760	CLA	CBD-CGD-O2D-CED
20	B	1760	CLA	O1D-CGD-O2D-CED
20	B	1761	CLA	C1A-C2A-CAA-CBA
20	B	1761	CLA	C2C-C3C-CAC-CBC
20	B	1761	CLA	C4C-C3C-CAC-CBC
20	B	1761	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	B	1761	CLA	CHA-CBD-CGD-O2D
20	B	1762	CLA	C1A-C2A-CAA-CBA
20	B	1763	CLA	C1A-C2A-CAA-CBA
20	B	1763	CLA	C3A-C2A-CAA-CBA
20	B	1763	CLA	CBD-CGD-O2D-CED
20	B	1763	CLA	O2A-C1-C2-C3
20	B	1764	CLA	C1A-C2A-CAA-CBA
20	B	1764	CLA	C3A-C2A-CAA-CBA
20	B	1764	CLA	CHA-CBD-CGD-O1D
20	B	1764	CLA	CHA-CBD-CGD-O2D
20	B	1764	CLA	CAD-CBD-CGD-O1D
20	B	1764	CLA	CAD-CBD-CGD-O2D
20	B	1764	CLA	CBD-CGD-O2D-CED
20	B	1765	CLA	CBD-CGD-O2D-CED
20	B	1766	CLA	C3A-C2A-CAA-CBA
20	B	1766	CLA	C2-C3-C5-C6
20	B	1766	CLA	C4-C3-C5-C6
20	B	1770	CLA	C2A-CAA-CBA-CGA
20	B	1771	CLA	C3A-C2A-CAA-CBA
20	B	1786	CLA	C2-C3-C5-C6
20	B	1786	CLA	C4-C3-C5-C6
20	F	1156	CLA	CBD-CGD-O2D-CED
20	F	1157	CLA	C1A-C2A-CAA-CBA
20	F	1157	CLA	C3A-C2A-CAA-CBA
20	F	1157	CLA	CBD-CGD-O2D-CED
20	F	1157	CLA	O1D-CGD-O2D-CED
20	G	1099	CLA	CAD-CBD-CGD-O1D
20	G	1099	CLA	CAD-CBD-CGD-O2D
20	G	1099	CLA	CBD-CGD-O2D-CED
20	G	1099	CLA	C2-C3-C5-C6
20	G	1099	CLA	C4-C3-C5-C6
20	H	1079	CLA	O2A-C1-C2-C3
20	I	1031	CLA	CHA-CBD-CGD-O1D
20	I	1031	CLA	CHA-CBD-CGD-O2D
20	I	1033	CLA	CAD-CBD-CGD-O1D
20	I	1033	CLA	CAD-CBD-CGD-O2D
20	I	1033	CLA	CBD-CGD-O2D-CED
20	J	1043	CLA	C3A-C2A-CAA-CBA
20	J	1043	CLA	C2A-CAA-CBA-CGA
20	J	1043	CLA	CHA-CBD-CGD-O1D
20	J	1043	CLA	CHA-CBD-CGD-O2D
20	J	1043	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	J	1044	CLA	C1A-C2A-CAA-CBA
20	J	1044	CLA	C3A-C2A-CAA-CBA
20	J	1044	CLA	CHA-CBD-CGD-O1D
20	J	1044	CLA	CHA-CBD-CGD-O2D
20	J	1044	CLA	CAD-CBD-CGD-O1D
20	J	1044	CLA	CBD-CGD-O2D-CED
20	J	1045	CLA	C2C-C3C-CAC-CBC
20	J	1045	CLA	C4C-C3C-CAC-CBC
20	J	1045	CLA	CAD-CBD-CGD-O1D
20	J	1045	CLA	CAD-CBD-CGD-O2D
20	J	1045	CLA	CBD-CGD-O2D-CED
20	K	1085	CLA	O2A-C1-C2-C3
20	K	3009	CLA	C1A-C2A-CAA-CBA
20	K	3009	CLA	C3A-C2A-CAA-CBA
20	K	3009	CLA	C2-C1-O2A-CGA
20	K	3009	CLA	CHA-CBD-CGD-O1D
20	K	3009	CLA	CHA-CBD-CGD-O2D
20	L	1166	CLA	C1A-C2A-CAA-CBA
20	L	1166	CLA	C3A-C2A-CAA-CBA
20	L	1166	CLA	CBD-CGD-O2D-CED
20	L	1167	CLA	CBD-CGD-O2D-CED
20	L	1168	CLA	C1A-C2A-CAA-CBA
20	L	1168	CLA	C3A-C2A-CAA-CBA
20	L	1168	CLA	C2C-C3C-CAC-CBC
20	L	1168	CLA	C4C-C3C-CAC-CBC
20	L	1505	CLA	C2A-CAA-CBA-CGA
20	L	1505	CLA	C2-C3-C5-C6
20	L	1505	CLA	C4-C3-C5-C6
20	R	1054	CLA	C1A-C2A-CAA-CBA
20	R	1054	CLA	CHA-CBD-CGD-O1D
20	R	1054	CLA	CHA-CBD-CGD-O2D
20	R	1054	CLA	CBD-CGD-O2D-CED
20	R	1054	CLA	C2-C3-C5-C6
20	R	1054	CLA	C4-C3-C5-C6
20	R	1055	CLA	C1A-C2A-CAA-CBA
20	R	1055	CLA	CAD-CBD-CGD-O1D
20	R	1055	CLA	O2A-C1-C2-C3
21	1	1202	LMU	O5'-C1'-O1'-C1
21	1	7004	LMU	C2'-C1'-O1'-C1
21	1	7004	LMU	O5'-C1'-O1'-C1
21	2	1225	LMU	C2-C1-O1'-C1'
21	2	7003	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
21	2	7003	LMU	O5'-C1'-O1'-C1
21	2	7006	LMU	O5'-C1'-O1'-C1
21	3	7005	LMU	O5'-C1'-O1'-C1
21	4	1210	LMU	C2'-C1'-O1'-C1
21	4	1210	LMU	O5'-C1'-O1'-C1
21	A	1809	LMU	C2-C1-O1'-C1'
21	A	1810	LMU	C2-C1-O1'-C1'
21	A	7009	LMU	O5'-C1'-O1'-C1
21	A	7010	LMU	C2'-C1'-O1'-C1
21	A	7010	LMU	O5'-C1'-O1'-C1
21	A	7010	LMU	C2-C1-O1'-C1'
21	A	7013	LMU	C2-C1-O1'-C1'
21	A	7015	LMU	C2'-C1'-O1'-C1
21	A	7015	LMU	O5'-C1'-O1'-C1
21	A	7017	LMU	C2-C1-O1'-C1'
21	A	7019	LMU	C2'-C1'-O1'-C1
21	A	7019	LMU	O5'-C1'-O1'-C1
21	A	7020	LMU	C2-C1-O1'-C1'
21	A	7022	LMU	O5'-C1'-O1'-C1
21	A	7022	LMU	C2-C1-O1'-C1'
21	A	7023	LMU	C2'-C1'-O1'-C1
21	A	7023	LMU	O5'-C1'-O1'-C1
21	A	7024	LMU	C2'-C1'-O1'-C1
21	A	7024	LMU	O5'-C1'-O1'-C1
21	A	7025	LMU	C2'-C1'-O1'-C1
21	A	7025	LMU	O5'-C1'-O1'-C1
21	A	7025	LMU	C2-C1-O1'-C1'
21	A	7026	LMU	C2'-C1'-O1'-C1
21	A	7026	LMU	O5'-C1'-O1'-C1
21	A	7026	LMU	C2-C1-O1'-C1'
21	A	7027	LMU	C2'-C1'-O1'-C1
21	A	7027	LMU	O5'-C1'-O1'-C1
21	A	7028	LMU	C2-C1-O1'-C1'
21	A	7030	LMU	O5'-C1'-O1'-C1
21	A	7030	LMU	C2-C1-O1'-C1'
21	A	7031	LMU	C2B-C1B-O1B-C4'
21	A	7032	LMU	O5'-C1'-O1'-C1
21	A	7034	LMU	C2'-C1'-O1'-C1
21	A	7034	LMU	O5'-C1'-O1'-C1
21	A	7036	LMU	C2'-C1'-O1'-C1
21	A	7036	LMU	O5'-C1'-O1'-C1
21	A	7037	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
21	A	7037	LMU	O5'-C1'-O1'-C1
21	A	7040	LMU	O5'-C1'-O1'-C1
21	A	7041	LMU	C2B-C1B-O1B-C4'
21	A	7041	LMU	C2'-C1'-O1'-C1
21	A	7041	LMU	O5'-C1'-O1'-C1
21	A	7042	LMU	C2'-C1'-O1'-C1
21	A	7042	LMU	O5'-C1'-O1'-C1
21	A	7043	LMU	O5'-C1'-O1'-C1
21	A	7047	LMU	O5'-C1'-O1'-C1
21	A	7047	LMU	C2-C1-O1'-C1'
21	L	1171	LMU	C2'-C1'-O1'-C1
21	L	1171	LMU	O5'-C1'-O1'-C1
21	L	1171	LMU	C2-C1-O1'-C1'
21	R	1056	LMU	O5B-C1B-O1B-C4'
21	R	1056	LMU	O5'-C1'-O1'-C1
21	R	1056	LMU	C2-C1-O1'-C1'
21	R	1057	LMU	C2'-C1'-O1'-C1
21	R	1057	LMU	O5'-C1'-O1'-C1
22	3	1220	BCR	C18-C19-C20-C21
22	3	1220	BCR	C20-C21-C22-C23
22	3	1220	BCR	C20-C21-C22-C37
22	3	1220	BCR	C21-C22-C23-C24
22	3	1220	BCR	C37-C22-C23-C24
22	A	1803	BCR	C18-C19-C20-C21
22	A	1803	BCR	C20-C21-C22-C23
22	A	1803	BCR	C20-C21-C22-C37
22	A	1803	BCR	C21-C22-C23-C24
22	A	1803	BCR	C37-C22-C23-C24
22	A	1804	BCR	C1-C6-C7-C8
22	A	1804	BCR	C5-C6-C7-C8
22	A	1804	BCR	C7-C8-C9-C10
22	A	1804	BCR	C7-C8-C9-C34
22	A	1804	BCR	C11-C12-C13-C14
22	A	1804	BCR	C11-C12-C13-C35
22	A	1804	BCR	C20-C21-C22-C23
22	A	1804	BCR	C20-C21-C22-C37
22	A	1804	BCR	C21-C22-C23-C24
22	A	1804	BCR	C37-C22-C23-C24
22	A	1805	BCR	C5-C6-C7-C8
22	A	1805	BCR	C7-C8-C9-C10
22	A	1805	BCR	C11-C12-C13-C14
22	A	1805	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
22	A	1805	BCR	C36-C18-C19-C20
22	A	1805	BCR	C20-C21-C22-C23
22	A	1805	BCR	C20-C21-C22-C37
22	A	1805	BCR	C21-C22-C23-C24
22	A	1805	BCR	C37-C22-C23-C24
22	A	1806	BCR	C1-C6-C7-C8
22	A	1806	BCR	C5-C6-C7-C8
22	A	1806	BCR	C7-C8-C9-C10
22	A	1806	BCR	C7-C8-C9-C34
22	A	1806	BCR	C11-C12-C13-C35
22	A	1806	BCR	C18-C19-C20-C21
22	A	1806	BCR	C37-C22-C23-C24
22	A	1806	BCR	C23-C24-C25-C30
22	A	1807	BCR	C17-C18-C19-C20
22	A	1807	BCR	C36-C18-C19-C20
22	A	1807	BCR	C18-C19-C20-C21
22	A	1807	BCR	C19-C20-C21-C22
22	A	1807	BCR	C20-C21-C22-C23
22	A	1807	BCR	C20-C21-C22-C37
22	A	1807	BCR	C23-C24-C25-C26
22	A	1807	BCR	C23-C24-C25-C30
22	A	1808	BCR	C5-C6-C7-C8
22	A	1808	BCR	C7-C8-C9-C10
22	A	1808	BCR	C7-C8-C9-C34
22	A	1808	BCR	C18-C19-C20-C21
22	A	1808	BCR	C20-C21-C22-C23
22	A	1808	BCR	C20-C21-C22-C37
22	B	1774	BCR	C7-C8-C9-C10
22	B	1774	BCR	C7-C8-C9-C34
22	B	1774	BCR	C17-C18-C19-C20
22	B	1774	BCR	C36-C18-C19-C20
22	B	1774	BCR	C18-C19-C20-C21
22	B	1775	BCR	C1-C6-C7-C8
22	B	1775	BCR	C5-C6-C7-C8
22	B	1775	BCR	C18-C19-C20-C21
22	B	1775	BCR	C20-C21-C22-C23
22	B	1775	BCR	C20-C21-C22-C37
22	B	1775	BCR	C23-C24-C25-C30
22	B	1776	BCR	C20-C21-C22-C23
22	B	1776	BCR	C20-C21-C22-C37
22	B	1776	BCR	C37-C22-C23-C24
22	B	1776	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	B	1776	BCR	C23-C24-C25-C30
22	B	1777	BCR	C9-C10-C11-C12
22	B	1777	BCR	C17-C18-C19-C20
22	B	1777	BCR	C36-C18-C19-C20
22	B	1777	BCR	C21-C22-C23-C24
22	B	1777	BCR	C37-C22-C23-C24
22	B	1778	BCR	C5-C6-C7-C8
22	B	1778	BCR	C18-C19-C20-C21
22	B	1779	BCR	C7-C8-C9-C10
22	B	1779	BCR	C7-C8-C9-C34
22	B	1779	BCR	C15-C16-C17-C18
22	B	1779	BCR	C18-C19-C20-C21
22	B	1779	BCR	C20-C21-C22-C23
22	B	1779	BCR	C20-C21-C22-C37
22	B	1780	BCR	C1-C6-C7-C8
22	B	1780	BCR	C5-C6-C7-C8
22	B	1780	BCR	C7-C8-C9-C34
22	B	1780	BCR	C18-C19-C20-C21
22	B	1780	BCR	C19-C20-C21-C22
22	B	1780	BCR	C20-C21-C22-C23
22	B	1780	BCR	C20-C21-C22-C37
22	B	1780	BCR	C21-C22-C23-C24
22	B	1780	BCR	C37-C22-C23-C24
22	B	1781	BCR	C1-C6-C7-C8
22	B	1781	BCR	C5-C6-C7-C8
22	B	1781	BCR	C17-C18-C19-C20
22	B	1781	BCR	C19-C20-C21-C22
22	I	1032	BCR	C11-C12-C13-C14
22	I	1032	BCR	C11-C12-C13-C35
22	I	1032	BCR	C17-C18-C19-C20
22	I	1032	BCR	C36-C18-C19-C20
22	I	1032	BCR	C18-C19-C20-C21
22	I	1032	BCR	C19-C20-C21-C22
22	I	1032	BCR	C20-C21-C22-C23
22	I	1032	BCR	C20-C21-C22-C37
22	L	1169	BCR	C1-C6-C7-C8
22	L	1169	BCR	C7-C8-C9-C10
22	L	1169	BCR	C7-C8-C9-C34
22	L	1169	BCR	C20-C21-C22-C23
22	L	1169	BCR	C20-C21-C22-C37
22	L	1169	BCR	C21-C22-C23-C24
22	L	1169	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	L	1170	BCR	C11-C12-C13-C14
22	L	1170	BCR	C11-C12-C13-C35
22	L	1170	BCR	C20-C21-C22-C23
22	L	1170	BCR	C20-C21-C22-C37
22	L	1170	BCR	C21-C22-C23-C24
22	L	1170	BCR	C37-C22-C23-C24
23	A	1802	PQN	C12-C13-C15-C16
23	A	1802	PQN	C14-C13-C15-C16
23	B	1773	PQN	C12-C13-C15-C16
23	B	1773	PQN	C14-C13-C15-C16
24	B	1783	LMG	O6-C1-O1-C7
24	B	1783	LMG	C11-C10-O7-C8
20	1	1188	CLA	C4C-C3C-CAC-CBC
20	1	1198	CLA	C2C-C3C-CAC-CBC
21	1	1202	LMU	C5'-C4'-O1B-C1B
21	A	7042	LMU	C3'-C4'-O1B-C1B
21	A	7043	LMU	C3'-C4'-O1B-C1B
20	1	1188	CLA	O1D-CGD-O2D-CED
20	1	1200	CLA	O1D-CGD-O2D-CED
20	2	1217	CLA	O1D-CGD-O2D-CED
20	3	3007	CLA	O1D-CGD-O2D-CED
20	4	4007	CLA	O1D-CGD-O2D-CED
20	4	4014	CLA	O1D-CGD-O2D-CED
20	A	1762	CLA	O1D-CGD-O2D-CED
20	A	1772	CLA	O1D-CGD-O2D-CED
20	A	1780	CLA	O1D-CGD-O2D-CED
20	A	1787	CLA	O1D-CGD-O2D-CED
20	A	1815	CLA	O1D-CGD-O2D-CED
20	A	1817	CLA	O1D-CGD-O2D-CED
20	B	1741	CLA	O1D-CGD-O2D-CED
20	B	1746	CLA	O1D-CGD-O2D-CED
20	B	1747	CLA	O1D-CGD-O2D-CED
20	F	1156	CLA	O1D-CGD-O2D-CED
20	G	1099	CLA	O1D-CGD-O2D-CED
20	L	1166	CLA	O1D-CGD-O2D-CED
20	L	1505	CLA	O1D-CGD-O2D-CED
21	A	7037	LMU	O5B-C1B-O1B-C4'
21	A	7038	LMU	O5B-C1B-O1B-C4'
21	A	7042	LMU	O5B-C1B-O1B-C4'
20	1	1187	CLA	C2C-C3C-CAC-CBC
20	1	1188	CLA	C2C-C3C-CAC-CBC
20	2	1213	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	4	1199	CLA	C2C-C3C-CAC-CBC
20	4	4014	CLA	C2C-C3C-CAC-CBC
20	A	1771	CLA	C2C-C3C-CAC-CBC
20	A	1817	CLA	C2C-C3C-CAC-CBC
20	B	1751	CLA	C2C-C3C-CAC-CBC
20	B	1757	CLA	C2C-C3C-CAC-CBC
20	B	1757	CLA	C4C-C3C-CAC-CBC
20	B	1771	CLA	C2C-C3C-CAC-CBC
20	B	1771	CLA	C4C-C3C-CAC-CBC
20	K	1146	CLA	C2C-C3C-CAC-CBC
20	K	1146	CLA	C4C-C3C-CAC-CBC
21	2	7006	LMU	C5'-C4'-O1B-C1B
21	A	7021	LMU	C3'-C4'-O1B-C1B
21	R	1057	LMU	C3'-C4'-O1B-C1B
20	1	1189	CLA	O1D-CGD-O2D-CED
20	1	1192	CLA	O1D-CGD-O2D-CED
20	4	1209	CLA	O1D-CGD-O2D-CED
20	A	1763	CLA	O1D-CGD-O2D-CED
20	A	1767	CLA	O1D-CGD-O2D-CED
20	A	1771	CLA	O1D-CGD-O2D-CED
20	A	1773	CLA	O1D-CGD-O2D-CED
20	A	1774	CLA	O1D-CGD-O2D-CED
20	A	1788	CLA	O1D-CGD-O2D-CED
20	A	1795	CLA	O1D-CGD-O2D-CED
20	A	1801	CLA	O1D-CGD-O2D-CED
20	B	1751	CLA	O1D-CGD-O2D-CED
20	B	1755	CLA	O1D-CGD-O2D-CED
20	B	1763	CLA	O1D-CGD-O2D-CED
20	J	1044	CLA	O1D-CGD-O2D-CED
20	L	1167	CLA	O1D-CGD-O2D-CED
20	R	1054	CLA	O1D-CGD-O2D-CED
20	1	1187	CLA	CBD-CGD-O2D-CED
20	1	1189	CLA	CBD-CGD-O2D-CED
20	1	1192	CLA	CBD-CGD-O2D-CED
20	1	1193	CLA	CBD-CGD-O2D-CED
20	1	1198	CLA	CBD-CGD-O2D-CED
20	2	1223	CLA	CBD-CGD-O2D-CED
20	3	3007	CLA	CBD-CGD-O2D-CED
20	4	1200	CLA	CBD-CGD-O2D-CED
20	4	1209	CLA	CBD-CGD-O2D-CED
20	4	4007	CLA	CBD-CGD-O2D-CED
20	A	1760	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	1763	CLA	CBD-CGD-O2D-CED
20	A	1765	CLA	CBD-CGD-O2D-CED
20	A	1770	CLA	CBD-CGD-O2D-CED
20	A	1772	CLA	CBD-CGD-O2D-CED
20	A	1779	CLA	CBD-CGD-O2D-CED
20	A	1780	CLA	CBD-CGD-O2D-CED
20	A	1782	CLA	CBD-CGD-O2D-CED
20	A	1783	CLA	CBD-CGD-O2D-CED
20	A	1792	CLA	CBD-CGD-O2D-CED
20	A	1796	CLA	CBD-CGD-O2D-CED
20	B	1735	CLA	CBD-CGD-O2D-CED
20	B	1737	CLA	CBD-CGD-O2D-CED
20	B	1741	CLA	CBD-CGD-O2D-CED
20	B	1745	CLA	CBD-CGD-O2D-CED
20	B	1759	CLA	CBD-CGD-O2D-CED
20	B	1762	CLA	CBD-CGD-O2D-CED
20	B	1767	CLA	CBD-CGD-O2D-CED
20	B	1785	CLA	CBD-CGD-O2D-CED
20	B	1786	CLA	CBD-CGD-O2D-CED
20	B	1787	CLA	CBD-CGD-O2D-CED
20	H	1079	CLA	CBD-CGD-O2D-CED
20	I	1031	CLA	CBD-CGD-O2D-CED
20	K	3009	CLA	CBD-CGD-O2D-CED
20	L	1168	CLA	CBD-CGD-O2D-CED
20	L	1505	CLA	CBD-CGD-O2D-CED
20	3	1219	CLA	O1A-CGA-O2A-C1
20	3	3011	CLA	O1A-CGA-O2A-C1
20	A	1790	CLA	O1A-CGA-O2A-C1
20	A	1811	CLA	O1A-CGA-O2A-C1
20	B	1740	CLA	O1A-CGA-O2A-C1
20	B	1747	CLA	O1A-CGA-O2A-C1
20	B	1769	CLA	O1A-CGA-O2A-C1
20	L	1505	CLA	O1A-CGA-O2A-C1
20	R	1054	CLA	O1A-CGA-O2A-C1
20	4	1209	CLA	O1A-CGA-O2A-C1
20	A	1763	CLA	O1A-CGA-O2A-C1
21	A	7037	LMU	C2B-C1B-O1B-C4'
21	A	7038	LMU	C2B-C1B-O1B-C4'
21	A	7042	LMU	C2B-C1B-O1B-C4'
20	1	1187	CLA	C4C-C3C-CAC-CBC
20	1	1190	CLA	C2C-C3C-CAC-CBC
20	1	1198	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	1	1200	CLA	C2C-C3C-CAC-CBC
20	1	1200	CLA	C4C-C3C-CAC-CBC
20	3	1219	CLA	C2C-C3C-CAC-CBC
20	3	1219	CLA	C4C-C3C-CAC-CBC
20	3	3008	CLA	C2C-C3C-CAC-CBC
20	3	3008	CLA	C4C-C3C-CAC-CBC
20	4	1199	CLA	C4C-C3C-CAC-CBC
20	4	4014	CLA	C4C-C3C-CAC-CBC
20	A	1771	CLA	C4C-C3C-CAC-CBC
20	A	1772	CLA	C2C-C3C-CAC-CBC
20	A	1772	CLA	C4C-C3C-CAC-CBC
20	A	1815	CLA	C2C-C3C-CAC-CBC
20	A	1815	CLA	C4C-C3C-CAC-CBC
20	A	1817	CLA	C4C-C3C-CAC-CBC
20	B	1753	CLA	C2C-C3C-CAC-CBC
20	B	1753	CLA	C4C-C3C-CAC-CBC
21	A	7013	LMU	C3'-C4'-O1B-C1B
21	A	7034	LMU	C5'-C4'-O1B-C1B
21	A	7047	LMU	C5'-C4'-O1B-C1B
21	B	1782	LMU	C3'-C4'-O1B-C1B
21	A	1809	LMU	C4B-C5B-C6B-O6B
20	1	1193	CLA	O1D-CGD-O2D-CED
20	1	1197	CLA	O1D-CGD-O2D-CED
20	4	1200	CLA	O1D-CGD-O2D-CED
20	A	1765	CLA	O1D-CGD-O2D-CED
20	A	1783	CLA	O1D-CGD-O2D-CED
20	B	1735	CLA	O1D-CGD-O2D-CED
20	B	1737	CLA	O1D-CGD-O2D-CED
20	B	1738	CLA	O1D-CGD-O2D-CED
20	B	1745	CLA	O1D-CGD-O2D-CED
20	B	1757	CLA	O1D-CGD-O2D-CED
20	J	1043	CLA	O1D-CGD-O2D-CED
20	J	1045	CLA	O1D-CGD-O2D-CED
20	K	3009	CLA	O1D-CGD-O2D-CED
20	4	1209	CLA	CBA-CGA-O2A-C1
20	1	1189	CLA	C2-C1-O2A-CGA
20	1	1190	CLA	C4C-C3C-CAC-CBC
20	2	1213	CLA	C4C-C3C-CAC-CBC
20	A	1767	CLA	C4C-C3C-CAC-CBC
20	A	1776	CLA	C4C-C3C-CAC-CBC
20	A	1794	CLA	C4C-C3C-CAC-CBC
21	A	1810	LMU	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
21	K	1086	LMU	C5'-C4'-O1B-C1B
24	B	1783	LMG	C8-C9-O8-C28
21	1	7004	LMU	O5B-C1B-O1B-C4'
21	2	1225	LMU	O5B-C1B-O1B-C4'
21	A	1810	LMU	O5B-C1B-O1B-C4'
21	A	7020	LMU	O5B-C1B-O1B-C4'
21	A	7024	LMU	O5B-C1B-O1B-C4'
21	A	7039	LMU	O5B-C1B-O1B-C4'
21	L	1171	LMU	O5B-C1B-O1B-C4'
20	4	1204	CLA	O1D-CGD-O2D-CED
20	A	1770	CLA	O1D-CGD-O2D-CED
20	A	1781	CLA	O1D-CGD-O2D-CED
20	A	1792	CLA	O1D-CGD-O2D-CED
20	B	1764	CLA	O1D-CGD-O2D-CED
20	B	1765	CLA	O1D-CGD-O2D-CED
20	I	1033	CLA	O1D-CGD-O2D-CED
20	3	1219	CLA	CBA-CGA-O2A-C1
20	3	3011	CLA	CBA-CGA-O2A-C1
20	A	1790	CLA	CBA-CGA-O2A-C1
20	B	1754	CLA	CBA-CGA-O2A-C1
20	B	1766	CLA	CBA-CGA-O2A-C1
20	B	1769	CLA	CBA-CGA-O2A-C1
20	L	1505	CLA	CBA-CGA-O2A-C1
20	R	1054	CLA	CBA-CGA-O2A-C1
20	2	1220	CLA	CBD-CGD-O2D-CED
20	3	1219	CLA	CBD-CGD-O2D-CED
20	3	3011	CLA	CBD-CGD-O2D-CED
20	4	1199	CLA	CBD-CGD-O2D-CED
20	A	1768	CLA	CBD-CGD-O2D-CED
20	A	1789	CLA	CBD-CGD-O2D-CED
20	A	1791	CLA	CBD-CGD-O2D-CED
20	A	1793	CLA	CBD-CGD-O2D-CED
20	B	1748	CLA	CBD-CGD-O2D-CED
20	2	1212	CLA	C2C-C3C-CAC-CBC
20	2	1212	CLA	C4C-C3C-CAC-CBC
20	2	1223	CLA	C2C-C3C-CAC-CBC
20	A	1776	CLA	C2C-C3C-CAC-CBC
20	A	1790	CLA	C2C-C3C-CAC-CBC
20	A	1790	CLA	C4C-C3C-CAC-CBC
20	B	1751	CLA	C4C-C3C-CAC-CBC
20	B	1767	CLA	C4C-C3C-CAC-CBC
20	B	1787	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	B	1787	CLA	C4C-C3C-CAC-CBC
20	1	1192	CLA	O1A-CGA-O2A-C1
20	1	1193	CLA	O1A-CGA-O2A-C1
20	2	1224	CLA	O1A-CGA-O2A-C1
20	A	1783	CLA	O1A-CGA-O2A-C1
20	A	1799	CLA	O1A-CGA-O2A-C1
20	A	1800	CLA	O1A-CGA-O2A-C1
20	A	1813	CLA	O1A-CGA-O2A-C1
20	B	1750	CLA	O1A-CGA-O2A-C1
20	B	1754	CLA	O1A-CGA-O2A-C1
20	B	1761	CLA	O1A-CGA-O2A-C1
20	B	1766	CLA	O1A-CGA-O2A-C1
20	B	1785	CLA	O1A-CGA-O2A-C1
20	J	1043	CLA	O1A-CGA-O2A-C1
20	K	1085	CLA	O1A-CGA-O2A-C1
20	R	1055	CLA	O1A-CGA-O2A-C1
20	1	1187	CLA	O1A-CGA-O2A-C1
20	A	1766	CLA	O1D-CGD-O2D-CED
20	A	1769	CLA	O1D-CGD-O2D-CED
20	A	1785	CLA	O1D-CGD-O2D-CED
20	B	1753	CLA	O1D-CGD-O2D-CED
20	2	1217	CLA	C15-C16-C17-C18
20	2	1223	CLA	C4C-C3C-CAC-CBC
20	A	1767	CLA	C2C-C3C-CAC-CBC
20	A	1773	CLA	C4C-C3C-CAC-CBC
20	A	1794	CLA	C2C-C3C-CAC-CBC
21	4	1210	LMU	O5'-C5'-C6'-O6'
20	2	1224	CLA	O1D-CGD-O2D-CED
20	A	1782	CLA	C2C-C3C-CAC-CBC
20	A	1782	CLA	C4C-C3C-CAC-CBC
20	B	1759	CLA	C2C-C3C-CAC-CBC
20	B	1759	CLA	C4C-C3C-CAC-CBC
21	A	7040	LMU	C3'-C4'-O1B-C1B
20	4	1201	CLA	CBD-CGD-O2D-CED
20	A	1790	CLA	CBD-CGD-O2D-CED
20	B	1749	CLA	O1D-CGD-O2D-CED
24	B	1783	LMG	O9-C10-O7-C8
20	B	1746	CLA	CBA-CGA-O2A-C1
20	B	1767	CLA	C2C-C3C-CAC-CBC
21	A	7033	LMU	C3'-C4'-O1B-C1B
20	B	1746	CLA	O1A-CGA-O2A-C1
20	4	1196	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	4	1199	CLA	C3-C5-C6-C7
20	A	1761	CLA	C3-C5-C6-C7
20	A	1776	CLA	C3-C5-C6-C7
20	A	1783	CLA	C3-C5-C6-C7
20	A	1785	CLA	C3-C5-C6-C7
20	A	1788	CLA	C3-C5-C6-C7
20	B	1737	CLA	C3-C5-C6-C7
20	B	1741	CLA	C3-C5-C6-C7
20	B	1767	CLA	C3-C5-C6-C7
20	B	1770	CLA	C3-C5-C6-C7
20	B	1771	CLA	C3-C5-C6-C7
20	1	1192	CLA	CBA-CGA-O2A-C1
20	A	1773	CLA	CBA-CGA-O2A-C1
20	A	1800	CLA	CBA-CGA-O2A-C1
20	A	1813	CLA	CBA-CGA-O2A-C1
20	A	1817	CLA	CBA-CGA-O2A-C1
20	B	1740	CLA	CBA-CGA-O2A-C1
20	B	1747	CLA	CBA-CGA-O2A-C1
20	B	1761	CLA	CBA-CGA-O2A-C1
20	B	1785	CLA	CBA-CGA-O2A-C1
20	F	1157	CLA	CBA-CGA-O2A-C1
20	K	1085	CLA	CBA-CGA-O2A-C1
20	R	1055	CLA	CBA-CGA-O2A-C1
20	A	1773	CLA	C2C-C3C-CAC-CBC
20	A	1797	CLA	C2C-C3C-CAC-CBC
21	A	7010	LMU	C3'-C4'-O1B-C1B
21	A	7035	LMU	C3'-C4'-O1B-C1B
21	A	7022	LMU	O5B-C5B-C6B-O6B
20	2	1220	CLA	C5-C6-C7-C8
20	2	1223	CLA	O1D-CGD-O2D-CED
20	B	1761	CLA	CBD-CGD-O2D-CED
20	1	1193	CLA	C2C-C3C-CAC-CBC
20	4	4007	CLA	O1A-CGA-O2A-C1
21	R	1057	LMU	C4'-C5'-C6'-O6'
21	B	1782	LMU	O5'-C5'-C6'-O6'
20	1	1192	CLA	C4-C3-C5-C6
21	A	7042	LMU	C4B-C5B-C6B-O6B
20	A	1787	CLA	C2-C3-C5-C6
20	A	1797	CLA	C2-C3-C5-C6
20	A	1777	CLA	CBD-CGD-O2D-CED
20	A	1794	CLA	CBD-CGD-O2D-CED
20	B	1744	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	1769	CLA	CBD-CGD-O2D-CED
20	2	1217	CLA	C2A-CAA-CBA-CGA
20	2	1220	CLA	C2A-CAA-CBA-CGA
20	A	1761	CLA	C2A-CAA-CBA-CGA
20	A	1763	CLA	C2A-CAA-CBA-CGA
20	A	1770	CLA	C2A-CAA-CBA-CGA
20	A	1773	CLA	C2A-CAA-CBA-CGA
20	A	1787	CLA	C2A-CAA-CBA-CGA
20	A	1790	CLA	C2A-CAA-CBA-CGA
20	A	1795	CLA	C2A-CAA-CBA-CGA
20	A	1797	CLA	C2A-CAA-CBA-CGA
20	A	1811	CLA	C2A-CAA-CBA-CGA
20	B	1735	CLA	C2A-CAA-CBA-CGA
20	B	1743	CLA	C2A-CAA-CBA-CGA
20	B	1752	CLA	C2A-CAA-CBA-CGA
20	B	1760	CLA	C2A-CAA-CBA-CGA
20	H	1079	CLA	C2A-CAA-CBA-CGA
20	K	1146	CLA	C2A-CAA-CBA-CGA
20	R	1054	CLA	C2A-CAA-CBA-CGA
20	2	1220	CLA	O1A-CGA-O2A-C1
20	A	1765	CLA	O1A-CGA-O2A-C1
20	B	1759	CLA	O1D-CGD-O2D-CED
20	B	1762	CLA	O1D-CGD-O2D-CED
20	2	1224	CLA	C3-C5-C6-C7
20	A	1784	CLA	C3-C5-C6-C7
20	A	1796	CLA	C3-C5-C6-C7
20	B	1752	CLA	C3-C5-C6-C7
20	B	1786	CLA	C3-C5-C6-C7
20	J	1045	CLA	C3-C5-C6-C7
20	1	1193	CLA	CBA-CGA-O2A-C1
20	2	1224	CLA	CBA-CGA-O2A-C1
20	A	1783	CLA	CBA-CGA-O2A-C1
20	A	1799	CLA	CBA-CGA-O2A-C1
20	B	1742	CLA	CBA-CGA-O2A-C1
20	B	1749	CLA	CBA-CGA-O2A-C1
20	B	1750	CLA	CBA-CGA-O2A-C1
20	I	1033	CLA	CBA-CGA-O2A-C1
20	J	1043	CLA	CBA-CGA-O2A-C1
20	L	1168	CLA	CBA-CGA-O2A-C1
21	2	1225	LMU	O5'-C5'-C6'-O6'
21	3	7005	LMU	O5'-C5'-C6'-O6'
21	A	7025	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	A	7009	LMU	C4'-C5'-C6'-O6'
21	A	7021	LMU	C4B-C5B-C6B-O6B
21	A	7026	LMU	C2B-C1B-O1B-C4'
21	A	7030	LMU	C3-C4-C5-C6
20	A	1760	CLA	O1D-CGD-O2D-CED
20	A	1797	CLA	C4C-C3C-CAC-CBC
20	J	1043	CLA	C2C-C3C-CAC-CBC
21	A	7016	LMU	C2-C3-C4-C5
21	A	7039	LMU	C11-C10-C9-C8
21	A	7019	LMU	O5B-C1B-O1B-C4'
20	A	1779	CLA	O1D-CGD-O2D-CED
20	A	1782	CLA	O1D-CGD-O2D-CED
21	A	7039	LMU	O5'-C5'-C6'-O6'
21	A	7038	LMU	C4B-C5B-C6B-O6B
21	A	7041	LMU	C4'-C5'-C6'-O6'
20	4	4014	CLA	O1A-CGA-O2A-C1
20	A	1817	CLA	O1A-CGA-O2A-C1
20	B	1749	CLA	O1A-CGA-O2A-C1
20	F	1157	CLA	O1A-CGA-O2A-C1
20	I	1033	CLA	O1A-CGA-O2A-C1
21	A	7037	LMU	C1-C2-C3-C4
20	B	1751	CLA	O1A-CGA-O2A-C1
22	3	1220	BCR	C19-C20-C21-C22
22	A	1803	BCR	C9-C10-C11-C12
22	A	1805	BCR	C19-C20-C21-C22
22	B	1776	BCR	C19-C20-C21-C22
22	B	1779	BCR	C13-C14-C15-C16
22	B	1779	BCR	C19-C20-C21-C22
22	L	1170	BCR	C19-C20-C21-C22
21	A	7019	LMU	C2B-C1B-O1B-C4'
21	A	7019	LMU	O5B-C5B-C6B-O6B
21	A	7022	LMU	O5'-C5'-C6'-O6'
21	A	7024	LMU	O5B-C5B-C6B-O6B
21	A	7036	LMU	O5B-C5B-C6B-O6B
20	A	1784	CLA	CBD-CGD-O2D-CED
20	3	1219	CLA	C3-C5-C6-C7
20	A	1779	CLA	C3-C5-C6-C7
20	L	1505	CLA	C3-C5-C6-C7
20	2	1215	CLA	CBA-CGA-O2A-C1
20	4	1204	CLA	CBA-CGA-O2A-C1
20	4	4007	CLA	CBA-CGA-O2A-C1
20	A	1765	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	1785	CLA	CBA-CGA-O2A-C1
20	B	1735	CLA	CBA-CGA-O2A-C1
20	H	1079	CLA	CBA-CGA-O2A-C1
21	A	7022	LMU	C3'-C4'-O1B-C1B
20	L	1168	CLA	O1A-CGA-O2A-C1
21	A	7021	LMU	O5'-C5'-C6'-O6'
21	A	7024	LMU	O5'-C5'-C6'-O6'
21	A	7033	LMU	O5'-C5'-C6'-O6'
21	1	7004	LMU	C4'-C5'-C6'-O6'
21	4	1210	LMU	C4'-C5'-C6'-O6'
20	B	1767	CLA	O1D-CGD-O2D-CED
20	B	1786	CLA	O1D-CGD-O2D-CED
20	I	1031	CLA	O1D-CGD-O2D-CED
20	B	1741	CLA	C5-C6-C7-C8
20	K	1085	CLA	C2C-C3C-CAC-CBC
21	A	7010	LMU	O5B-C1B-O1B-C4'
20	2	1222	CLA	CBD-CGD-O2D-CED
20	A	1813	CLA	CBD-CGD-O2D-CED
21	A	7017	LMU	O5'-C5'-C6'-O6'
21	A	7027	LMU	O5B-C5B-C6B-O6B
21	A	7036	LMU	O5'-C5'-C6'-O6'
20	1	1193	CLA	C4C-C3C-CAC-CBC
20	4	4014	CLA	C2-C1-O2A-CGA
21	A	1809	LMU	C2-C3-C4-C5
21	A	7020	LMU	C6-C7-C8-C9
21	A	7020	LMU	C11-C10-C9-C8
21	A	7022	LMU	C11-C10-C9-C8
21	A	7032	LMU	C5-C6-C7-C8
21	A	7033	LMU	C7-C8-C9-C10
21	A	7036	LMU	C7-C8-C9-C10
20	B	1735	CLA	O1A-CGA-O2A-C1
21	A	7010	LMU	C2-C3-C4-C5
21	A	7016	LMU	C4-C5-C6-C7
21	A	7019	LMU	C7-C8-C9-C10
21	A	7025	LMU	C2-C3-C4-C5
21	A	7030	LMU	C6-C7-C8-C9
21	A	7043	LMU	C7-C8-C9-C10
21	K	1086	LMU	C5-C6-C7-C8
21	A	7019	LMU	O5'-C5'-C6'-O6'
21	A	7035	LMU	O5'-C5'-C6'-O6'
21	A	7021	LMU	C4'-C5'-C6'-O6'
21	A	7022	LMU	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	A	7025	LMU	C4B-C5B-C6B-O6B
21	A	7033	LMU	C4'-C5'-C6'-O6'
21	A	7034	LMU	C4B-C5B-C6B-O6B
21	A	7039	LMU	C4'-C5'-C6'-O6'
20	A	1796	CLA	O1D-CGD-O2D-CED
21	A	1809	LMU	C3'-C4'-O1B-C1B
21	A	7013	LMU	C1-C2-C3-C4
20	A	1801	CLA	C3-C5-C6-C7
20	K	3009	CLA	C3-C5-C6-C7
23	A	1802	PQN	C13-C15-C16-C17
20	2	1220	CLA	CBA-CGA-O2A-C1
20	4	4014	CLA	CBA-CGA-O2A-C1
21	1	7004	LMU	O5'-C5'-C6'-O6'
21	A	7009	LMU	O5'-C5'-C6'-O6'
21	A	7010	LMU	O5'-C5'-C6'-O6'
21	R	1057	LMU	O5'-C5'-C6'-O6'
21	2	7006	LMU	C4'-C5'-C6'-O6'
21	3	7005	LMU	C4'-C5'-C6'-O6'
21	A	7024	LMU	C4B-C5B-C6B-O6B
21	L	1171	LMU	C5-C6-C7-C8
20	2	1215	CLA	O1A-CGA-O2A-C1
20	A	1785	CLA	O1A-CGA-O2A-C1
20	B	1742	CLA	O1A-CGA-O2A-C1
20	4	4007	CLA	C3-C5-C6-C7
20	A	1813	CLA	C2C-C3C-CAC-CBC
21	A	7032	LMU	O1'-C1-C2-C3
21	A	7037	LMU	C3-C4-C5-C6
21	2	7003	LMU	O5'-C5'-C6'-O6'
21	A	1809	LMU	O5B-C5B-C6B-O6B
21	A	7023	LMU	O5B-C5B-C6B-O6B
21	A	7028	LMU	O5B-C5B-C6B-O6B
21	A	7030	LMU	O5'-C5'-C6'-O6'
21	A	7038	LMU	O5B-C5B-C6B-O6B
20	3	1219	CLA	C4-C3-C5-C6
20	A	1789	CLA	C4-C3-C5-C6
20	A	1812	CLA	C4-C3-C5-C6
20	B	1756	CLA	C4-C3-C5-C6
21	A	7028	LMU	C4B-C5B-C6B-O6B
20	2	1213	CLA	C2-C3-C5-C6
20	3	1219	CLA	C2-C3-C5-C6
20	A	1789	CLA	C2-C3-C5-C6
20	A	1812	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	B	1749	CLA	C2-C3-C5-C6
20	B	1756	CLA	C2-C3-C5-C6
21	A	7041	LMU	O5B-C1B-O1B-C4'
20	A	1791	CLA	C2A-CAA-CBA-CGA
20	B	1744	CLA	C2A-CAA-CBA-CGA
20	B	1751	CLA	C2A-CAA-CBA-CGA
20	H	1079	CLA	O1D-CGD-O2D-CED
21	3	7005	LMU	O5B-C5B-C6B-O6B
21	A	7017	LMU	O5B-C5B-C6B-O6B
21	A	7021	LMU	O5B-C5B-C6B-O6B
21	A	7041	LMU	O5'-C5'-C6'-O6'
21	A	7042	LMU	O5B-C5B-C6B-O6B
20	4	1204	CLA	O1A-CGA-O2A-C1
21	A	7036	LMU	C4B-C5B-C6B-O6B
21	A	7036	LMU	C4'-C5'-C6'-O6'
21	A	7016	LMU	O5'-C1'-O1'-C1
21	A	7028	LMU	O5'-C1'-O1'-C1
21	A	7025	LMU	C6-C7-C8-C9
20	A	1795	CLA	CBA-CGA-O2A-C1
20	2	1215	CLA	C2C-C3C-CAC-CBC
21	A	7042	LMU	C3-C4-C5-C6
21	R	1056	LMU	C7-C8-C9-C10
21	K	1086	LMU	O5'-C5'-C6'-O6'
21	A	7017	LMU	C4'-C5'-C6'-O6'
20	L	1167	CLA	C2C-C3C-CAC-CBC
20	4	1201	CLA	O1D-CGD-O2D-CED
20	B	1748	CLA	O1D-CGD-O2D-CED
20	B	1785	CLA	O1D-CGD-O2D-CED
20	H	1079	CLA	O1A-CGA-O2A-C1
21	2	7006	LMU	O5B-C1B-O1B-C4'
21	A	1809	LMU	C4'-C5'-C6'-O6'
21	A	7023	LMU	C4B-C5B-C6B-O6B
21	A	7043	LMU	C4B-C5B-C6B-O6B
20	B	1770	CLA	C2C-C3C-CAC-CBC
21	A	7027	LMU	C3-C4-C5-C6
20	1	1187	CLA	O1D-CGD-O2D-CED
20	1	1198	CLA	O1D-CGD-O2D-CED
20	A	1789	CLA	O1D-CGD-O2D-CED
20	L	1168	CLA	O1D-CGD-O2D-CED
20	2	1212	CLA	CBD-CGD-O2D-CED
20	B	1770	CLA	CBD-CGD-O2D-CED
20	B	1787	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	R	1057	LMU	C4B-C5B-C6B-O6B
21	2	1225	LMU	C5'-C4'-O1B-C1B
20	A	1768	CLA	C3-C5-C6-C7
20	1	1197	CLA	CBA-CGA-O2A-C1
20	2	1212	CLA	CBA-CGA-O2A-C1
20	2	1222	CLA	CBA-CGA-O2A-C1
20	4	1199	CLA	CBA-CGA-O2A-C1
20	A	1768	CLA	CBA-CGA-O2A-C1
20	A	1794	CLA	CBA-CGA-O2A-C1
20	A	1796	CLA	CBA-CGA-O2A-C1
20	K	1146	CLA	CBA-CGA-O2A-C1
20	L	1166	CLA	CBA-CGA-O2A-C1
24	B	1783	LMG	C29-C28-O8-C9
21	A	7026	LMU	C1-C2-C3-C4
20	4	1196	CLA	CBD-CGD-O2D-CED
20	A	1776	CLA	CBD-CGD-O2D-CED
20	B	1742	CLA	CBD-CGD-O2D-CED
21	A	7031	LMU	C2-C3-C4-C5
21	A	7041	LMU	C11-C10-C9-C8
22	A	1803	BCR	C19-C20-C21-C22
22	A	1804	BCR	C19-C20-C21-C22
20	B	1735	CLA	C13-C15-C16-C17
20	B	1762	CLA	C13-C15-C16-C17
21	A	7022	LMU	C4'-C5'-C6'-O6'
21	A	7024	LMU	C4'-C5'-C6'-O6'
21	A	7030	LMU	C4'-C5'-C6'-O6'
21	A	7035	LMU	C4'-C5'-C6'-O6'
21	A	7023	LMU	C5-C6-C7-C8
21	A	7038	LMU	C6-C7-C8-C9
20	3	1219	CLA	O1D-CGD-O2D-CED
20	A	1789	CLA	C2C-C3C-CAC-CBC
21	A	1809	LMU	C5'-C4'-O1B-C1B
21	A	7009	LMU	C7-C8-C9-C10
21	A	7033	LMU	C3-C4-C5-C6
21	2	1225	LMU	C4'-C5'-C6'-O6'
21	2	7003	LMU	C4'-C5'-C6'-O6'
21	A	7017	LMU	C4B-C5B-C6B-O6B
21	A	7030	LMU	C4B-C5B-C6B-O6B
21	B	1782	LMU	C4'-C5'-C6'-O6'
20	A	1764	CLA	C5-C6-C7-C8
20	A	1776	CLA	C10-C11-C12-C13
20	A	1783	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	A	1797	CLA	C5-C6-C7-C8
20	A	1800	CLA	C15-C16-C17-C18
20	B	1757	CLA	C8-C10-C11-C12
20	A	1773	CLA	C3-C5-C6-C7
21	2	7006	LMU	C2'-C1'-O1'-C1
21	A	7009	LMU	C2'-C1'-O1'-C1
21	A	7031	LMU	C2'-C1'-O1'-C1
21	A	7040	LMU	C2'-C1'-O1'-C1
21	A	7043	LMU	C2'-C1'-O1'-C1
21	R	1056	LMU	C2'-C1'-O1'-C1
21	A	7021	LMU	C7-C8-C9-C10
24	B	1783	LMG	O10-C28-O8-C9
21	2	7006	LMU	O5'-C5'-C6'-O6'
21	A	7034	LMU	O5B-C5B-C6B-O6B
21	A	7040	LMU	O5B-C5B-C6B-O6B
20	1	1198	CLA	C11-C12-C13-C14
20	2	1220	CLA	C6-C7-C8-C9
20	4	1198	CLA	C6-C7-C8-C9
20	A	1772	CLA	C14-C13-C15-C16
20	A	1774	CLA	C6-C7-C8-C9
20	A	1780	CLA	C11-C10-C8-C9
20	A	1780	CLA	C14-C13-C15-C16
20	A	1782	CLA	C11-C10-C8-C9
20	A	1782	CLA	C14-C13-C15-C16
20	A	1813	CLA	C11-C10-C8-C9
20	B	1735	CLA	C11-C10-C8-C9
20	B	1740	CLA	C11-C10-C8-C9
20	B	1744	CLA	C14-C13-C15-C16
20	B	1753	CLA	C14-C13-C15-C16
20	B	1756	CLA	C11-C12-C13-C14
20	B	1757	CLA	C6-C7-C8-C9
20	B	1759	CLA	C11-C10-C8-C9
20	B	1762	CLA	C11-C10-C8-C9
20	B	1768	CLA	C11-C12-C13-C14
20	B	1785	CLA	C11-C12-C13-C14
20	B	1787	CLA	C14-C13-C15-C16
20	J	1043	CLA	C11-C12-C13-C14
20	R	1055	CLA	C11-C10-C8-C9
20	R	1055	CLA	C11-C12-C13-C14
23	A	1802	PQN	C21-C22-C23-C24
20	1	1198	CLA	C10-C11-C12-C13
20	A	1800	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	4	1196	CLA	C2A-CAA-CBA-CGA
20	A	1772	CLA	C2A-CAA-CBA-CGA
22	3	1220	BCR	C36-C18-C19-C20
22	A	1803	BCR	C7-C8-C9-C34
22	A	1805	BCR	C7-C8-C9-C34
22	A	1806	BCR	C36-C18-C19-C20
22	A	1808	BCR	C36-C18-C19-C20
22	B	1776	BCR	C11-C12-C13-C35
22	B	1778	BCR	C37-C22-C23-C24
22	B	1781	BCR	C36-C18-C19-C20
22	I	1032	BCR	C37-C22-C23-C24
21	A	7010	LMU	C2B-C1B-O1B-C4'
22	3	1220	BCR	C17-C18-C19-C20
22	A	1805	BCR	C17-C18-C19-C20
22	A	1806	BCR	C21-C22-C23-C24
22	B	1776	BCR	C21-C22-C23-C24
22	B	1778	BCR	C21-C22-C23-C24
22	B	1780	BCR	C7-C8-C9-C10
22	I	1032	BCR	C21-C22-C23-C24
21	L	1171	LMU	O5B-C5B-C6B-O6B
20	4	1209	CLA	C2C-C3C-CAC-CBC
21	3	7005	LMU	C4B-C5B-C6B-O6B
21	A	7010	LMU	C4B-C5B-C6B-O6B
20	2	1222	CLA	O1A-CGA-O2A-C1
20	A	1796	CLA	O1A-CGA-O2A-C1
20	A	1789	CLA	C5-C6-C7-C8
20	A	1811	CLA	C10-C11-C12-C13
20	R	1055	CLA	CBD-CGD-O2D-CED
21	A	7013	LMU	O5'-C5'-C6'-O6'
21	A	7010	LMU	C4'-C5'-C6'-O6'
21	K	1086	LMU	C4'-C5'-C6'-O6'
20	J	1043	CLA	C4C-C3C-CAC-CBC
21	A	7038	LMU	C7-C8-C9-C10
21	R	1056	LMU	C5'-C4'-O1B-C1B
20	3	3011	CLA	O1D-CGD-O2D-CED
20	A	1767	CLA	C3-C5-C6-C7
20	A	1774	CLA	C3-C5-C6-C7
20	A	1797	CLA	C3-C5-C6-C7
20	2	1217	CLA	CBA-CGA-O2A-C1
20	A	1765	CLA	C5-C6-C7-C8
20	A	1774	CLA	C10-C11-C12-C13
20	A	1787	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	B	1759	CLA	C15-C16-C17-C18
20	B	1762	CLA	C10-C11-C12-C13
20	B	1771	CLA	C15-C16-C17-C18
20	B	1787	CLA	C10-C11-C12-C13
20	B	1787	CLA	C13-C15-C16-C17
20	R	1055	CLA	C8-C10-C11-C12
23	B	1773	PQN	C15-C16-C17-C18
21	A	7026	LMU	C4-C5-C6-C7
21	A	7015	LMU	O5'-C5'-C6'-O6'
21	R	1057	LMU	C1-C2-C3-C4
20	1	1192	CLA	C8-C10-C11-C12
20	4	1204	CLA	C5-C6-C7-C8
20	A	1767	CLA	C5-C6-C7-C8
20	A	1784	CLA	C5-C6-C7-C8
20	A	1787	CLA	C5-C6-C7-C8
20	A	1796	CLA	C5-C6-C7-C8
20	A	1796	CLA	C10-C11-C12-C13
20	A	1796	CLA	C13-C15-C16-C17
20	A	1813	CLA	C8-C10-C11-C12
20	B	1735	CLA	C15-C16-C17-C18
20	B	1737	CLA	C15-C16-C17-C18
20	B	1739	CLA	C8-C10-C11-C12
20	B	1739	CLA	C15-C16-C17-C18
20	B	1740	CLA	C10-C11-C12-C13
20	B	1749	CLA	C10-C11-C12-C13
21	R	1056	LMU	C3'-C4'-O1B-C1B
20	A	1768	CLA	O1D-CGD-O2D-CED
20	A	1791	CLA	O1D-CGD-O2D-CED
21	A	7010	LMU	O1'-C1-C2-C3
20	A	1811	CLA	C5-C6-C7-C8
20	B	1740	CLA	C5-C6-C7-C8
20	B	1742	CLA	C5-C6-C7-C8
20	B	1744	CLA	C13-C15-C16-C17
20	B	1752	CLA	C5-C6-C7-C8
20	B	1770	CLA	C10-C11-C12-C13
20	J	1045	CLA	C5-C6-C7-C8
20	L	1505	CLA	C5-C6-C7-C8
21	A	7028	LMU	O1'-C1-C2-C3
20	A	1793	CLA	O1D-CGD-O2D-CED
20	B	1769	CLA	O1D-CGD-O2D-CED
21	4	1210	LMU	O5B-C5B-C6B-O6B
21	R	1057	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
20	1	1192	CLA	C2-C1-O2A-CGA
20	4	1201	CLA	C2-C1-O2A-CGA
20	A	1761	CLA	C2-C1-O2A-CGA
20	A	1780	CLA	C2-C1-O2A-CGA
20	A	1795	CLA	C2-C1-O2A-CGA
21	A	7028	LMU	C4'-C5'-C6'-O6'
21	A	7036	LMU	O1'-C1-C2-C3
20	A	1767	CLA	C10-C11-C12-C13
20	B	1748	CLA	C10-C11-C12-C13
20	B	1756	CLA	C15-C16-C17-C18
20	B	1768	CLA	C8-C10-C11-C12
23	A	1802	PQN	C25-C26-C27-C28
20	R	1054	CLA	C8-C10-C11-C12
20	A	1765	CLA	C2C-C3C-CAC-CBC
20	I	1031	CLA	C5-C6-C7-C8
20	J	1043	CLA	C8-C10-C11-C12
20	A	1790	CLA	O1D-CGD-O2D-CED
20	1	1198	CLA	C6-C7-C8-C10
20	2	1217	CLA	C11-C10-C8-C7
20	2	1218	CLA	C12-C13-C15-C16
20	3	3011	CLA	C11-C10-C8-C7
20	4	1198	CLA	C12-C13-C15-C16
20	A	1764	CLA	C12-C13-C15-C16
20	A	1787	CLA	C12-C13-C15-C16
20	A	1800	CLA	C11-C10-C8-C7
20	A	1811	CLA	C12-C13-C15-C16
20	B	1738	CLA	C11-C10-C8-C7
20	B	1753	CLA	C11-C12-C13-C15
20	B	1757	CLA	C6-C7-C8-C10
20	B	1759	CLA	C11-C10-C8-C7
20	J	1043	CLA	C6-C7-C8-C10
20	J	1044	CLA	C11-C12-C13-C15
20	B	1753	CLA	C3-C5-C6-C7
20	A	1794	CLA	O1A-CGA-O2A-C1
20	L	1166	CLA	O1A-CGA-O2A-C1
22	A	1806	BCR	C19-C20-C21-C22
22	B	1779	BCR	C9-C10-C11-C12
22	I	1032	BCR	C9-C10-C11-C12
22	L	1169	BCR	C19-C20-C21-C22
20	A	1764	CLA	C2A-CAA-CBA-CGA
20	A	1768	CLA	C2A-CAA-CBA-CGA
20	A	1780	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	A	1781	CLA	C2A-CAA-CBA-CGA
20	A	1792	CLA	C2A-CAA-CBA-CGA
20	B	1759	CLA	C2A-CAA-CBA-CGA
20	2	1220	CLA	O1D-CGD-O2D-CED
20	4	1199	CLA	O1D-CGD-O2D-CED
20	B	1761	CLA	O1D-CGD-O2D-CED
20	3	1218	CLA	C5-C6-C7-C8
20	3	1219	CLA	C13-C15-C16-C17
20	A	1793	CLA	C5-C6-C7-C8
20	B	1738	CLA	C13-C15-C16-C17
23	A	1802	PQN	C20-C21-C22-C23
23	B	1773	PQN	C18-C20-C21-C22
20	A	1813	CLA	C4C-C3C-CAC-CBC
21	A	7027	LMU	C1-C2-C3-C4
21	2	1225	LMU	O1'-C1-C2-C3
21	A	7023	LMU	O1'-C1-C2-C3
21	A	7038	LMU	O1'-C1-C2-C3
20	2	1212	CLA	O1A-CGA-O2A-C1
20	A	1768	CLA	O1A-CGA-O2A-C1
20	K	1146	CLA	O1A-CGA-O2A-C1
21	1	1202	LMU	C4'-C5'-C6'-O6'
21	2	1225	LMU	O5'-C1'-O1'-C1
20	A	1776	CLA	C5-C6-C7-C8
20	B	1744	CLA	C5-C6-C7-C8
20	B	1744	CLA	C10-C11-C12-C13
20	H	1079	CLA	C8-C10-C11-C12
21	3	7005	LMU	O1'-C1-C2-C3
21	A	7032	LMU	C3'-C4'-O1B-C1B
22	A	1804	BCR	C18-C19-C20-C21
22	A	1805	BCR	C18-C19-C20-C21
22	L	1169	BCR	C18-C19-C20-C21
21	A	7023	LMU	O5'-C5'-C6'-O6'
21	A	7028	LMU	O5'-C5'-C6'-O6'
21	R	1056	LMU	O5B-C5B-C6B-O6B
21	A	7019	LMU	C4B-C5B-C6B-O6B
20	A	1769	CLA	C3-C5-C6-C7
20	B	1759	CLA	C3-C5-C6-C7
20	2	1224	CLA	C8-C10-C11-C12
20	A	1789	CLA	C8-C10-C11-C12
20	A	1815	CLA	C5-C6-C7-C8
20	B	1747	CLA	C8-C10-C11-C12
20	B	1759	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	B	1785	CLA	C10-C11-C12-C13
20	1	1189	CLA	CBA-CGA-O2A-C1
20	4	1199	CLA	O1A-CGA-O2A-C1
20	A	1795	CLA	O1A-CGA-O2A-C1
21	A	7027	LMU	C4B-C5B-C6B-O6B
21	2	7006	LMU	O1'-C1-C2-C3
21	A	7013	LMU	O1'-C1-C2-C3
21	A	7026	LMU	C2-C3-C4-C5
20	4	1198	CLA	C8-C10-C11-C12
20	A	1762	CLA	C5-C6-C7-C8
20	A	1811	CLA	C8-C10-C11-C12
20	A	1813	CLA	C15-C16-C17-C18
20	B	1768	CLA	C13-C15-C16-C17
20	B	1786	CLA	C13-C15-C16-C17
21	A	7030	LMU	O5B-C5B-C6B-O6B
20	B	1744	CLA	O1D-CGD-O2D-CED
21	A	7033	LMU	C1-C2-C3-C4
20	2	1217	CLA	O1A-CGA-O2A-C1
20	B	1748	CLA	O1A-CGA-O2A-C1
20	B	1747	CLA	C10-C11-C12-C13
20	B	1770	CLA	C4C-C3C-CAC-CBC
20	3	1218	CLA	C10-C11-C12-C13
20	3	1219	CLA	C5-C6-C7-C8
20	A	1761	CLA	C13-C15-C16-C17
20	A	1774	CLA	C5-C6-C7-C8
20	A	1774	CLA	C15-C16-C17-C18
20	A	1780	CLA	C15-C16-C17-C18
20	A	1782	CLA	C8-C10-C11-C12
20	B	1753	CLA	C13-C15-C16-C17
20	B	1756	CLA	C8-C10-C11-C12
20	B	1767	CLA	C5-C6-C7-C8
20	K	3009	CLA	C13-C15-C16-C17
23	B	1773	PQN	C20-C21-C22-C23
20	A	1772	CLA	C3-C5-C6-C7
20	B	1744	CLA	C3-C5-C6-C7
20	B	1748	CLA	C3-C5-C6-C7
20	B	1770	CLA	CBA-CGA-O2A-C1
20	3	3011	CLA	C8-C10-C11-C12
20	B	1743	CLA	C15-C16-C17-C18
20	B	1736	CLA	C2C-C3C-CAC-CBC
20	K	1085	CLA	C4C-C3C-CAC-CBC
21	A	7042	LMU	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	R	1056	LMU	C4B-C5B-C6B-O6B
21	A	7025	LMU	O1'-C1-C2-C3
20	B	1740	CLA	C15-C16-C17-C18
20	B	1758	CLA	C10-C11-C12-C13
20	A	1788	CLA	C2A-CAA-CBA-CGA
20	B	1756	CLA	C2A-CAA-CBA-CGA
20	B	1764	CLA	C2A-CAA-CBA-CGA
20	G	1099	CLA	C2A-CAA-CBA-CGA
20	K	1142	CLA	C2A-CAA-CBA-CGA
20	A	1767	CLA	C16-C17-C18-C19
20	A	1793	CLA	C16-C17-C18-C19
20	B	1770	CLA	C16-C17-C18-C19
21	A	7037	LMU	O5'-C5'-C6'-O6'
20	A	1794	CLA	O1D-CGD-O2D-CED
20	A	1816	CLA	CBA-CGA-O2A-C1
20	B	1748	CLA	CBA-CGA-O2A-C1
20	B	1756	CLA	CBA-CGA-O2A-C1
20	G	1099	CLA	CBA-CGA-O2A-C1
20	B	1787	CLA	C15-C16-C17-C18
21	2	7003	LMU	O1'-C1-C2-C3
21	R	1056	LMU	C9-C10-C11-C12
20	R	1055	CLA	C10-C11-C12-C13
22	B	1775	BCR	C19-C20-C21-C22
22	B	1781	BCR	C9-C10-C11-C12
24	B	1783	LMG	C33-C34-C35-C36
20	B	1771	CLA	CBD-CGD-O2D-CED
22	B	1778	BCR	C20-C21-C22-C37
20	A	1789	CLA	C3-C5-C6-C7
20	F	1156	CLA	C2C-C3C-CAC-CBC
21	2	7003	LMU	C4-C5-C6-C7
21	4	1210	LMU	C2-C3-C4-C5
21	A	7010	LMU	C7-C8-C9-C10
21	A	7015	LMU	C11-C10-C9-C8
21	A	7016	LMU	C11-C10-C9-C8
21	A	7025	LMU	C3-C4-C5-C6
21	A	7035	LMU	C6-C7-C8-C9
21	A	7040	LMU	C4-C5-C6-C7
21	R	1056	LMU	C11-C10-C9-C8
21	A	7031	LMU	C4B-C5B-C6B-O6B
20	3	3011	CLA	C16-C17-C18-C19
20	A	1785	CLA	C16-C17-C18-C19
20	A	1800	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	1	1202	LMU	C3-C4-C5-C6
21	2	1225	LMU	C6-C7-C8-C9
21	A	1810	LMU	C5-C6-C7-C8
21	A	7026	LMU	C3-C4-C5-C6
21	A	7028	LMU	C6-C7-C8-C9
21	A	7031	LMU	C3-C4-C5-C6
21	A	7034	LMU	C4-C5-C6-C7
21	A	7038	LMU	C11-C10-C9-C8
21	L	1171	LMU	C6-C7-C8-C9
21	L	1171	LMU	C11-C10-C9-C8
21	A	7009	LMU	C3'-C4'-O1B-C1B
24	B	1783	LMG	C32-C33-C34-C35
20	A	1777	CLA	O1D-CGD-O2D-CED
21	A	1809	LMU	C11-C10-C9-C8
21	A	7013	LMU	C5-C6-C7-C8
21	A	7015	LMU	C7-C8-C9-C10
21	A	7023	LMU	C3-C4-C5-C6
21	A	7024	LMU	C2-C3-C4-C5
21	A	7042	LMU	C11-C10-C9-C8
21	L	1171	LMU	C4B-C5B-C6B-O6B
20	A	1769	CLA	C5-C6-C7-C8
20	B	1754	CLA	C5-C6-C7-C8
21	A	7024	LMU	O1'-C1-C2-C3
21	A	7039	LMU	C2-C3-C4-C5
21	1	1202	LMU	C2'-C1'-O1'-C1
21	3	7005	LMU	C2'-C1'-O1'-C1
21	A	7028	LMU	C2'-C1'-O1'-C1
21	A	7030	LMU	C2'-C1'-O1'-C1
21	A	7035	LMU	C2'-C1'-O1'-C1
22	B	1778	BCR	C20-C21-C22-C23
24	B	1783	LMG	C2-C1-O1-C7
21	A	1810	LMU	C6-C7-C8-C9
21	A	7015	LMU	C6-C7-C8-C9
21	A	7017	LMU	C6-C7-C8-C9
21	A	7022	LMU	O1'-C1-C2-C3
21	A	7035	LMU	C7-C8-C9-C10
20	A	1788	CLA	C15-C16-C17-C18
20	B	1743	CLA	C5-C6-C7-C8
20	1	1197	CLA	O1A-CGA-O2A-C1
20	B	1770	CLA	O1A-CGA-O2A-C1
20	4	1204	CLA	C6-C7-C8-C9
20	A	1784	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	1767	CLA	C11-C12-C13-C14
20	B	1768	CLA	C16-C17-C18-C19
21	A	7010	LMU	O5B-C5B-C6B-O6B
21	A	7016	LMU	O5'-C5'-C6'-O6'
20	B	1740	CLA	C4-C3-C5-C6
21	A	7009	LMU	C5'-C4'-O1B-C1B
21	A	7009	LMU	C4-C5-C6-C7
21	A	7037	LMU	C11-C10-C9-C8
21	A	7042	LMU	C6-C7-C8-C9
20	F	1157	CLA	C2-C3-C5-C6
20	A	1781	CLA	C11-C12-C13-C14
20	A	1787	CLA	C11-C10-C8-C9
20	A	1812	CLA	C11-C12-C13-C14
20	B	1738	CLA	C11-C10-C8-C9
20	B	1738	CLA	C11-C12-C13-C14
20	B	1785	CLA	C11-C10-C8-C9
20	J	1043	CLA	C11-C10-C8-C9
21	2	7006	LMU	C7-C8-C9-C10
21	4	1210	LMU	C7-C8-C9-C10
21	A	7013	LMU	C3-C4-C5-C6
21	A	7022	LMU	C5-C6-C7-C8
20	B	1740	CLA	C8-C10-C11-C12
20	A	1779	CLA	C2A-CAA-CBA-CGA
20	A	1786	CLA	C2A-CAA-CBA-CGA
20	A	1798	CLA	C2A-CAA-CBA-CGA
20	A	1815	CLA	C2A-CAA-CBA-CGA
20	B	1758	CLA	C2A-CAA-CBA-CGA
22	A	1808	BCR	C37-C22-C23-C24
22	B	1774	BCR	C37-C22-C23-C24
20	2	1215	CLA	C4C-C3C-CAC-CBC
21	3	7005	LMU	C5-C6-C7-C8
21	A	7041	LMU	C4-C5-C6-C7
21	A	7042	LMU	C4-C5-C6-C7
22	A	1803	BCR	C7-C8-C9-C10
22	A	1806	BCR	C11-C12-C13-C14
22	A	1808	BCR	C21-C22-C23-C24
22	B	1774	BCR	C21-C22-C23-C24
20	2	1218	CLA	C3-C5-C6-C7
20	A	1811	CLA	C3-C5-C6-C7
21	2	7003	LMU	C11-C10-C9-C8
21	A	7028	LMU	C2-C3-C4-C5
24	B	1783	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
20	A	1768	CLA	C5-C6-C7-C8
21	1	1202	LMU	C4-C5-C6-C7
21	4	1210	LMU	C11-C10-C9-C8
21	A	7010	LMU	C5-C6-C7-C8
21	A	7019	LMU	C6-C7-C8-C9
21	R	1057	LMU	C11-C10-C9-C8
24	B	1783	LMG	C37-C38-C39-C40
20	2	1218	CLA	C16-C17-C18-C20
20	3	1219	CLA	C16-C17-C18-C19
20	3	1219	CLA	C16-C17-C18-C20
20	A	1785	CLA	C16-C17-C18-C20
20	A	1812	CLA	C16-C17-C18-C20
20	B	1744	CLA	C16-C17-C18-C19
20	H	1079	CLA	C16-C17-C18-C19
20	H	1079	CLA	C16-C17-C18-C20
23	A	1802	PQN	C26-C27-C28-C30
20	2	1224	CLA	C10-C11-C12-C13
20	4	1198	CLA	C5-C6-C7-C8
20	B	1771	CLA	C10-C11-C12-C13
21	2	7003	LMU	C2-C3-C4-C5
21	A	7019	LMU	C3-C4-C5-C6
21	A	7024	LMU	C7-C8-C9-C10
21	A	7028	LMU	C5-C6-C7-C8
21	A	7032	LMU	C7-C8-C9-C10
21	A	7034	LMU	C2-C3-C4-C5
21	A	7035	LMU	C4-C5-C6-C7
21	A	7047	LMU	C7-C8-C9-C10
24	B	1783	LMG	C15-C16-C17-C18
21	3	7005	LMU	C1-C2-C3-C4
21	2	1225	LMU	C11-C10-C9-C8
21	A	7017	LMU	C4-C5-C6-C7
21	A	7027	LMU	C2-C3-C4-C5
21	A	7030	LMU	C4-C5-C6-C7
21	A	7033	LMU	C6-C7-C8-C9
21	A	7034	LMU	C3-C4-C5-C6
21	A	7047	LMU	C2-C3-C4-C5
20	A	1812	CLA	C13-C15-C16-C17
20	1	1189	CLA	O1A-CGA-O2A-C1
21	3	7005	LMU	C3-C4-C5-C6
21	A	7027	LMU	C4-C5-C6-C7
21	A	7040	LMU	C5-C6-C7-C8
21	A	7042	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
20	A	1780	CLA	CBA-CGA-O2A-C1
20	1	1189	CLA	C3A-C2A-CAA-CBA
20	1	1192	CLA	C3A-C2A-CAA-CBA
20	2	1217	CLA	C3A-C2A-CAA-CBA
20	2	1220	CLA	C3A-C2A-CAA-CBA
20	2	1224	CLA	C3A-C2A-CAA-CBA
20	4	1204	CLA	C3A-C2A-CAA-CBA
20	A	1759	CLA	C3A-C2A-CAA-CBA
20	A	1762	CLA	C3A-C2A-CAA-CBA
20	A	1765	CLA	C3A-C2A-CAA-CBA
20	A	1770	CLA	C3A-C2A-CAA-CBA
20	A	1782	CLA	C3A-C2A-CAA-CBA
20	A	1787	CLA	C3A-C2A-CAA-CBA
20	A	1795	CLA	C3A-C2A-CAA-CBA
20	B	1740	CLA	C3A-C2A-CAA-CBA
20	B	1743	CLA	C3A-C2A-CAA-CBA
20	B	1745	CLA	C3A-C2A-CAA-CBA
20	B	1761	CLA	C3A-C2A-CAA-CBA
20	L	1167	CLA	C3A-C2A-CAA-CBA
20	R	1054	CLA	C3A-C2A-CAA-CBA
20	A	1787	CLA	C10-C11-C12-C13
21	A	7021	LMU	C1-C2-C3-C4
21	A	7030	LMU	C1-C2-C3-C4
21	R	1056	LMU	C1-C2-C3-C4
21	A	7030	LMU	C2B-C1B-O1B-C4'
21	A	7016	LMU	C2-C1-O1'-C1'
21	A	7037	LMU	C2-C1-O1'-C1'
21	2	7006	LMU	C4-C5-C6-C7
21	A	1809	LMU	C5-C6-C7-C8
21	A	7010	LMU	C11-C10-C9-C8
21	A	7031	LMU	C5-C6-C7-C8
24	B	1783	LMG	C13-C14-C15-C16
24	B	1783	LMG	C35-C36-C37-C38
20	A	1764	CLA	C16-C17-C18-C19
20	A	1781	CLA	C16-C17-C18-C19
20	A	1800	CLA	C16-C17-C18-C19
20	A	1812	CLA	C16-C17-C18-C19
21	A	7017	LMU	C7-C8-C9-C10
21	A	7032	LMU	C4-C5-C6-C7
21	A	7016	LMU	C1-C2-C3-C4
21	A	1809	LMU	C3-C4-C5-C6
20	4	1200	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
20	A	1800	CLA	O2A-C1-C2-C3
20	4	1204	CLA	C3-C5-C6-C7
20	A	1782	CLA	C4-C3-C5-C6
20	B	1739	CLA	C4-C3-C5-C6
20	B	1744	CLA	C4-C3-C5-C6
20	F	1157	CLA	C4-C3-C5-C6
20	1	1192	CLA	C2-C3-C5-C6
20	A	1782	CLA	C2-C3-C5-C6
20	B	1739	CLA	C2-C3-C5-C6
20	B	1744	CLA	C2-C3-C5-C6
21	4	1210	LMU	C4-C5-C6-C7
21	A	7021	LMU	O1'-C1-C2-C3
21	A	7041	LMU	C6-C7-C8-C9
21	A	7039	LMU	O1'-C1-C2-C3
21	K	1086	LMU	C7-C8-C9-C10
21	L	1171	LMU	C3-C4-C5-C6
21	A	7032	LMU	O5'-C5'-C6'-O6'
20	4	1199	CLA	C6-C7-C8-C10
20	4	1204	CLA	C6-C7-C8-C10
20	B	1762	CLA	C16-C17-C18-C20
20	B	1770	CLA	C16-C17-C18-C20
21	A	7016	LMU	O1'-C1-C2-C3
20	A	1784	CLA	O1D-CGD-O2D-CED
20	A	1781	CLA	C10-C11-C12-C13
20	B	1749	CLA	C5-C6-C7-C8
21	1	1202	LMU	C1-C2-C3-C4
21	A	1810	LMU	C2-C3-C4-C5
20	B	1756	CLA	O1A-CGA-O2A-C1
20	B	1768	CLA	C15-C16-C17-C18
21	1	1202	LMU	C2-C3-C4-C5
21	A	1810	LMU	C11-C10-C9-C8
21	A	7010	LMU	C1-C2-C3-C4
20	3	1218	CLA	C2-C1-O2A-CGA
20	A	1792	CLA	C2-C1-O2A-CGA
20	B	1762	CLA	C2-C1-O2A-CGA
20	L	1167	CLA	C4C-C3C-CAC-CBC
21	2	1225	LMU	C4-C5-C6-C7
21	A	7015	LMU	C5-C6-C7-C8
20	3	1218	CLA	C13-C15-C16-C17
20	4	1199	CLA	C5-C6-C7-C8
20	A	1785	CLA	C8-C10-C11-C12
20	A	1811	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	B	1743	CLA	C10-C11-C12-C13
20	G	1099	CLA	O1A-CGA-O2A-C1
21	A	7025	LMU	C9-C10-C11-C12
20	A	1767	CLA	C16-C17-C18-C20
20	B	1786	CLA	C16-C17-C18-C19
20	1	1192	CLA	C3-C5-C6-C7
20	B	1754	CLA	C3-C5-C6-C7
22	A	1805	BCR	C1-C6-C7-C8
22	A	1805	BCR	C23-C24-C25-C26
22	A	1805	BCR	C23-C24-C25-C30
22	A	1806	BCR	C23-C24-C25-C26
22	A	1808	BCR	C1-C6-C7-C8
22	B	1774	BCR	C23-C24-C25-C26
22	B	1774	BCR	C23-C24-C25-C30
22	B	1775	BCR	C23-C24-C25-C26
22	B	1778	BCR	C1-C6-C7-C8
22	B	1778	BCR	C23-C24-C25-C26
22	B	1778	BCR	C23-C24-C25-C30
22	B	1780	BCR	C23-C24-C25-C26
21	A	7040	LMU	O5'-C5'-C6'-O6'
21	A	7042	LMU	O5'-C5'-C6'-O6'
21	A	7013	LMU	C6-C7-C8-C9
21	A	7021	LMU	C4-C5-C6-C7
21	A	7037	LMU	C4-C5-C6-C7
20	B	1759	CLA	CBA-CGA-O2A-C1
20	A	1812	CLA	C15-C16-C17-C18
20	B	1737	CLA	C10-C11-C12-C13
20	I	1031	CLA	C8-C10-C11-C12
21	A	7024	LMU	C1-C2-C3-C4
21	A	7025	LMU	C1-C2-C3-C4
21	L	1171	LMU	C1-C2-C3-C4
21	2	1225	LMU	C2-C3-C4-C5
21	A	7033	LMU	C5'-C4'-O1B-C1B
21	K	1086	LMU	C9-C10-C11-C12
21	R	1057	LMU	C2-C3-C4-C5
21	A	7020	LMU	O5'-C5'-C6'-O6'
21	A	7027	LMU	C7-C8-C9-C10
20	A	1780	CLA	C10-C11-C12-C13
20	A	1789	CLA	C13-C15-C16-C17
21	A	7032	LMU	C5'-C4'-O1B-C1B
21	A	7032	LMU	C9-C10-C11-C12
21	K	1086	LMU	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
20	A	1788	CLA	C4-C3-C5-C6
20	2	1220	CLA	C6-C7-C8-C10
20	A	1764	CLA	C6-C7-C8-C10
20	A	1764	CLA	C11-C12-C13-C15
20	A	1767	CLA	C6-C7-C8-C10
20	A	1767	CLA	C12-C13-C15-C16
20	A	1780	CLA	C11-C10-C8-C7
20	A	1780	CLA	C12-C13-C15-C16
20	A	1781	CLA	C11-C12-C13-C15
20	A	1782	CLA	C6-C7-C8-C10
20	A	1783	CLA	C11-C12-C13-C15
20	A	1788	CLA	C2-C3-C5-C6
20	A	1812	CLA	C11-C12-C13-C15
20	A	1813	CLA	C6-C7-C8-C10
20	A	1816	CLA	C2-C3-C5-C6
20	B	1738	CLA	C11-C12-C13-C15
20	B	1742	CLA	C2-C3-C5-C6
20	B	1743	CLA	C12-C13-C15-C16
20	B	1744	CLA	C11-C10-C8-C7
20	B	1744	CLA	C12-C13-C15-C16
20	B	1759	CLA	C6-C7-C8-C10
20	B	1762	CLA	C11-C12-C13-C15
20	B	1785	CLA	C6-C7-C8-C10
20	B	1785	CLA	C11-C10-C8-C7
20	B	1787	CLA	C6-C7-C8-C10
20	J	1043	CLA	C11-C10-C8-C7
20	R	1055	CLA	C6-C7-C8-C10
20	R	1055	CLA	C11-C12-C13-C15
23	B	1773	PQN	C21-C22-C23-C25
20	A	1780	CLA	O1A-CGA-O2A-C1
21	A	7033	LMU	C11-C10-C9-C8
20	B	1738	CLA	C10-C11-C12-C13
20	A	1784	CLA	C6-C7-C8-C10
20	I	1031	CLA	C11-C12-C13-C14
20	B	1743	CLA	CBA-CGA-O2A-C1
21	A	7021	LMU	C9-C10-C11-C12
21	A	7038	LMU	C5-C6-C7-C8
21	A	7017	LMU	C1-C2-C3-C4
20	A	1796	CLA	C2A-CAA-CBA-CGA
20	A	1799	CLA	C2A-CAA-CBA-CGA
20	B	1736	CLA	C2A-CAA-CBA-CGA
20	B	1761	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	2	1225	LMU	C7-C8-C9-C10
21	R	1056	LMU	C5-C6-C7-C8
20	A	1813	CLA	O1D-CGD-O2D-CED
21	A	7036	LMU	C5-C6-C7-C8
21	R	1056	LMU	C2-C3-C4-C5
20	J	1043	CLA	C12-C13-C15-C16
20	B	1749	CLA	C8-C10-C11-C12
21	A	1809	LMU	C6-C7-C8-C9
21	A	7025	LMU	C4-C5-C6-C7
21	A	7023	LMU	C4'-C5'-C6'-O6'
20	B	1740	CLA	C3-C5-C6-C7
20	2	1222	CLA	O1D-CGD-O2D-CED
20	A	1780	CLA	C2C-C3C-CAC-CBC
20	A	1816	CLA	O1A-CGA-O2A-C1
20	2	1224	CLA	C5-C6-C7-C8
21	K	1086	LMU	C1-C2-C3-C4
20	A	1789	CLA	C4C-C3C-CAC-CBC
21	A	1810	LMU	O1'-C1-C2-C3
21	A	7020	LMU	C2-C3-C4-C5
21	1	1202	LMU	O5'-C5'-C6'-O6'
22	B	1777	BCR	C18-C19-C20-C21
21	1	1202	LMU	C5-C6-C7-C8
20	A	1780	CLA	C5-C6-C7-C8
20	A	1813	CLA	C13-C15-C16-C17
20	B	1758	CLA	C5-C6-C7-C8
20	K	1142	CLA	CBD-CGD-O2D-CED
21	A	7032	LMU	C2'-C1'-O1'-C1
21	A	7035	LMU	C5-C6-C7-C8
20	B	1768	CLA	C16-C17-C18-C20
20	I	1031	CLA	C11-C12-C13-C15
20	A	1761	CLA	C15-C16-C17-C18
20	B	1770	CLA	C8-C10-C11-C12
20	B	1785	CLA	C5-C6-C7-C8
20	J	1044	CLA	C8-C10-C11-C12
20	A	1816	CLA	C4-C3-C5-C6
20	A	1768	CLA	C2-C3-C5-C6
20	B	1740	CLA	C2-C3-C5-C6
20	4	1209	CLA	C4C-C3C-CAC-CBC
21	A	7027	LMU	C5-C6-C7-C8
21	A	7043	LMU	C11-C10-C9-C8
20	2	1218	CLA	C14-C13-C15-C16
20	3	3011	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	1761	CLA	C11-C10-C8-C9
20	A	1767	CLA	C11-C12-C13-C14
20	A	1782	CLA	C6-C7-C8-C9
20	A	1783	CLA	C11-C12-C13-C14
20	A	1787	CLA	C14-C13-C15-C16
20	A	1800	CLA	C11-C12-C13-C14
20	B	1740	CLA	C14-C13-C15-C16
20	B	1743	CLA	C14-C13-C15-C16
20	B	1753	CLA	C11-C12-C13-C14
20	B	1759	CLA	C6-C7-C8-C9
20	B	1762	CLA	C11-C12-C13-C14
20	B	1787	CLA	C6-C7-C8-C9
20	J	1043	CLA	C6-C7-C8-C9
23	B	1773	PQN	C21-C22-C23-C24
21	A	7041	LMU	O1'-C1-C2-C3
20	2	1217	CLA	C3-C5-C6-C7
20	B	1762	CLA	C3-C5-C6-C7
21	2	1225	LMU	C1-C2-C3-C4
21	K	1086	LMU	C2-C3-C4-C5
20	B	1787	CLA	CBA-CGA-O2A-C1
20	B	1757	CLA	C5-C6-C7-C8
20	B	1759	CLA	C10-C11-C12-C13
21	L	1171	LMU	C2-C3-C4-C5
24	B	1783	LMG	C11-C12-C13-C14
22	3	1220	BCR	C11-C12-C13-C14
21	A	7020	LMU	C1-C2-C3-C4
20	B	1759	CLA	O1A-CGA-O2A-C1
20	R	1055	CLA	O1D-CGD-O2D-CED
20	1	1189	CLA	C1A-C2A-CAA-CBA
20	1	1200	CLA	C1A-C2A-CAA-CBA
20	4	1204	CLA	C1A-C2A-CAA-CBA
20	A	1759	CLA	C1A-C2A-CAA-CBA
20	A	1760	CLA	C1A-C2A-CAA-CBA
20	A	1798	CLA	C1A-C2A-CAA-CBA
20	A	1799	CLA	C1A-C2A-CAA-CBA
20	A	1811	CLA	C1A-C2A-CAA-CBA
20	A	1817	CLA	C1A-C2A-CAA-CBA
20	B	1746	CLA	C1A-C2A-CAA-CBA
20	B	1757	CLA	C1A-C2A-CAA-CBA
20	B	1758	CLA	C1A-C2A-CAA-CBA
20	B	1766	CLA	C1A-C2A-CAA-CBA
20	B	1769	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	B	1771	CLA	C1A-C2A-CAA-CBA
20	J	1043	CLA	C1A-C2A-CAA-CBA
20	J	1045	CLA	C1A-C2A-CAA-CBA
20	L	1167	CLA	C1A-C2A-CAA-CBA
20	3	3011	CLA	C16-C17-C18-C20
20	A	1774	CLA	C16-C17-C18-C20
20	B	1744	CLA	C16-C17-C18-C20
20	B	1758	CLA	C16-C17-C18-C20
22	B	1781	BCR	C15-C16-C17-C18
20	A	1761	CLA	C5-C6-C7-C8
20	2	1212	CLA	O1D-CGD-O2D-CED
21	A	7040	LMU	C11-C10-C9-C8
21	A	7039	LMU	C1-C2-C3-C4
20	A	1781	CLA	C5-C6-C7-C8
20	A	1785	CLA	C13-C15-C16-C17
20	A	1788	CLA	C13-C15-C16-C17
20	A	1813	CLA	C10-C11-C12-C13
20	R	1055	CLA	C5-C6-C7-C8
20	A	1788	CLA	CBA-CGA-O2A-C1
21	A	7035	LMU	C11-C10-C9-C8
21	1	7004	LMU	C5'-C4'-O1B-C1B
21	A	7028	LMU	C1-C2-C3-C4
20	A	1774	CLA	C16-C17-C18-C19
20	A	1781	CLA	C16-C17-C18-C20
20	B	1767	CLA	C11-C12-C13-C15
20	B	1771	CLA	O1D-CGD-O2D-CED
21	2	7006	LMU	C5-C6-C7-C8
21	A	7041	LMU	C3-C4-C5-C6
20	A	1782	CLA	CBA-CGA-O2A-C1
20	A	1789	CLA	CBA-CGA-O2A-C1
20	B	1743	CLA	O1A-CGA-O2A-C1
20	B	1742	CLA	C4-C3-C5-C6
21	A	7032	LMU	C4'-C5'-C6'-O6'
21	A	7042	LMU	C4'-C5'-C6'-O6'
21	B	1782	LMU	C4B-C5B-C6B-O6B
20	3	3007	CLA	C3A-C2A-CAA-CBA
20	B	1736	CLA	C4C-C3C-CAC-CBC
21	A	7017	LMU	C11-C10-C9-C8
20	B	1738	CLA	C15-C16-C17-C18
20	B	1786	CLA	C15-C16-C17-C18
21	A	7028	LMU	C11-C10-C9-C8
21	A	7033	LMU	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	A	1767	CLA	C8-C10-C11-C12
20	1	1197	CLA	C2A-CAA-CBA-CGA
20	L	1168	CLA	C2A-CAA-CBA-CGA
20	2	1218	CLA	C16-C17-C18-C19
20	3	1218	CLA	C16-C17-C18-C20
20	A	1793	CLA	C16-C17-C18-C20
20	A	1816	CLA	C6-C7-C8-C10
21	A	7047	LMU	O5B-C5B-C6B-O6B
20	R	1055	CLA	C3-C5-C6-C7
21	1	7004	LMU	C3'-C4'-O1B-C1B
21	1	7004	LMU	C2-C3-C4-C5
21	A	7039	LMU	C4-C5-C6-C7
21	A	7043	LMU	C9-C10-C11-C12
21	K	1086	LMU	O5B-C5B-C6B-O6B
21	A	7039	LMU	C5-C6-C7-C8
21	A	7043	LMU	C6-C7-C8-C9
21	A	7047	LMU	C9-C10-C11-C12
24	B	1783	LMG	C17-C18-C19-C20
20	4	1196	CLA	O1D-CGD-O2D-CED
20	B	1742	CLA	O1D-CGD-O2D-CED
21	3	7005	LMU	C7-C8-C9-C10
21	A	7031	LMU	C9-C10-C11-C12
21	A	7032	LMU	C2-C3-C4-C5
21	R	1057	LMU	C9-C10-C11-C12
20	J	1044	CLA	C14-C13-C15-C16
21	A	7016	LMU	C4'-C5'-C6'-O6'
21	2	7006	LMU	C9-C10-C11-C12
21	A	7036	LMU	C11-C10-C9-C8
20	A	1769	CLA	C6-C7-C8-C9
21	A	1810	LMU	C3-C4-C5-C6
20	A	1792	CLA	CBA-CGA-O2A-C1
21	A	7038	LMU	O5'-C5'-C6'-O6'
21	A	1809	LMU	C9-C10-C11-C12
20	B	1787	CLA	O1A-CGA-O2A-C1
21	A	7026	LMU	C6-C7-C8-C9
21	A	7026	LMU	C9-C10-C11-C12
21	A	1810	LMU	C9-C10-C11-C12
21	A	7025	LMU	O5'-C5'-C6'-O6'
21	A	7026	LMU	O5'-C5'-C6'-O6'
21	A	7031	LMU	O5'-C5'-C6'-O6'
21	A	7037	LMU	O5B-C5B-C6B-O6B
20	A	1768	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	B	1748	CLA	C4-C3-C5-C6
20	B	1785	CLA	C4-C3-C5-C6
21	A	7040	LMU	C3-C4-C5-C6
20	B	1748	CLA	C2-C3-C5-C6
24	B	1783	LMG	C10-C11-C12-C13
20	J	1044	CLA	CBA-CGA-O2A-C1
20	2	1218	CLA	C2C-C3C-CAC-CBC
20	B	1770	CLA	C5-C6-C7-C8
21	A	7010	LMU	C4-C5-C6-C7
24	B	1783	LMG	C9-C8-O7-C10
21	A	7022	LMU	O5B-C1B-O1B-C4'
21	A	7009	LMU	O5B-C5B-C6B-O6B
20	A	1784	CLA	C2A-CAA-CBA-CGA
20	A	1776	CLA	C8-C10-C11-C12
20	A	1797	CLA	C15-C16-C17-C18
20	A	1815	CLA	C2-C1-O2A-CGA
21	A	7022	LMU	C9-C10-C11-C12
21	A	7034	LMU	C5-C6-C7-C8
21	A	7024	LMU	C5'-C4'-O1B-C1B
20	B	1752	CLA	CBA-CGA-O2A-C1
20	3	1218	CLA	C16-C17-C18-C19
21	L	1171	LMU	C7-C8-C9-C10
20	A	1789	CLA	C10-C11-C12-C13
21	A	7022	LMU	C2'-C1'-O1'-C1
21	A	7039	LMU	C6-C7-C8-C9
20	A	1760	CLA	C2C-C3C-CAC-CBC
21	A	7027	LMU	O5B-C1B-O1B-C4'
20	A	1764	CLA	C15-C16-C17-C18
20	A	1797	CLA	C13-C15-C16-C17
20	A	1782	CLA	O1A-CGA-O2A-C1
20	J	1044	CLA	O1A-CGA-O2A-C1
21	A	7024	LMU	C5-C6-C7-C8
21	2	7006	LMU	O5B-C5B-C6B-O6B
20	B	1759	CLA	C4-C3-C5-C6
20	2	1218	CLA	C11-C10-C8-C7
20	3	1219	CLA	C11-C10-C8-C7
20	A	1761	CLA	C11-C10-C8-C7
20	A	1772	CLA	C12-C13-C15-C16
20	A	1780	CLA	C11-C12-C13-C15
20	A	1789	CLA	C11-C12-C13-C15
20	A	1797	CLA	C11-C10-C8-C7
20	A	1811	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	A	1812	CLA	C6-C7-C8-C10
20	A	1813	CLA	C11-C10-C8-C7
20	A	1813	CLA	C12-C13-C15-C16
20	B	1737	CLA	C6-C7-C8-C10
20	B	1738	CLA	C12-C13-C15-C16
20	B	1740	CLA	C11-C10-C8-C7
20	B	1740	CLA	C12-C13-C15-C16
20	B	1744	CLA	C6-C7-C8-C10
20	B	1749	CLA	C11-C12-C13-C15
20	B	1755	CLA	C6-C7-C8-C10
20	B	1757	CLA	C11-C10-C8-C7
20	B	1758	CLA	C11-C12-C13-C15
20	B	1762	CLA	C12-C13-C15-C16
20	B	1767	CLA	C6-C7-C8-C10
20	B	1768	CLA	C11-C10-C8-C7
20	B	1770	CLA	C11-C10-C8-C7
20	B	1787	CLA	C12-C13-C15-C16
20	H	1079	CLA	C12-C13-C15-C16
20	J	1043	CLA	C11-C12-C13-C15
20	J	1044	CLA	C11-C10-C8-C7
20	K	3009	CLA	C11-C10-C8-C7
20	K	3009	CLA	C12-C13-C15-C16
20	A	1759	CLA	CAA-CBA-CGA-O2A
20	A	1789	CLA	O1A-CGA-O2A-C1
20	A	1792	CLA	O1A-CGA-O2A-C1
21	A	7017	LMU	C5-C6-C7-C8
20	2	1217	CLA	C11-C12-C13-C14
20	3	1219	CLA	C11-C10-C8-C9
20	4	1198	CLA	C11-C12-C13-C14
20	4	1198	CLA	C14-C13-C15-C16
20	A	1767	CLA	C6-C7-C8-C9
20	A	1780	CLA	C11-C12-C13-C14
20	A	1783	CLA	C6-C7-C8-C9
20	A	1785	CLA	C11-C10-C8-C9
20	A	1800	CLA	C11-C10-C8-C9
20	A	1813	CLA	C6-C7-C8-C9
20	A	1813	CLA	C14-C13-C15-C16
20	B	1737	CLA	C6-C7-C8-C9
20	B	1738	CLA	C6-C7-C8-C9
20	B	1738	CLA	C14-C13-C15-C16
20	B	1743	CLA	C6-C7-C8-C9
20	B	1747	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	1757	CLA	C11-C10-C8-C9
20	B	1758	CLA	C11-C12-C13-C14
20	B	1767	CLA	C6-C7-C8-C9
20	B	1770	CLA	C11-C10-C8-C9
20	H	1079	CLA	C14-C13-C15-C16
20	J	1044	CLA	C11-C10-C8-C9
20	J	1044	CLA	C11-C12-C13-C14
20	K	3009	CLA	C11-C10-C8-C9
20	K	3009	CLA	C11-C12-C13-C14
20	K	3009	CLA	C14-C13-C15-C16
24	B	1783	LMG	C39-C40-C41-C42
21	A	7026	LMU	O5B-C1B-O1B-C4'
20	B	1786	CLA	C2A-CAA-CBA-CGA
21	A	7026	LMU	C5'-C4'-O1B-C1B
21	4	1210	LMU	C1-C2-C3-C4
22	B	1780	BCR	C36-C18-C19-C20
22	I	1032	BCR	C7-C8-C9-C34
20	B	1742	CLA	C6-C7-C8-C9
21	A	7016	LMU	C5-C6-C7-C8
22	A	1806	BCR	C17-C18-C19-C20
22	I	1032	BCR	C7-C8-C9-C10
20	B	1767	CLA	C10-C11-C12-C13
20	B	1754	CLA	C6-C7-C8-C9
21	A	7033	LMU	C5-C6-C7-C8
20	A	1788	CLA	O1A-CGA-O2A-C1
20	A	1779	CLA	CBA-CGA-O2A-C1
20	A	1786	CLA	CBA-CGA-O2A-C1
20	B	1737	CLA	CBA-CGA-O2A-C1
21	A	7035	LMU	C1-C2-C3-C4
21	A	7009	LMU	C5-C6-C7-C8
20	A	1765	CLA	C4C-C3C-CAC-CBC
21	A	7036	LMU	C3'-C4'-O1B-C1B
21	1	1202	LMU	O1'-C1-C2-C3
21	A	7017	LMU	C2-C3-C4-C5
20	B	1785	CLA	CAA-CBA-CGA-O2A
20	2	1215	CLA	O1D-CGD-O2D-CED
20	J	1043	CLA	C4-C3-C5-C6
20	B	1759	CLA	C2-C3-C5-C6
20	B	1785	CLA	C2-C3-C5-C6
21	A	7024	LMU	C3'-C4'-O1B-C1B
20	B	1755	CLA	C5-C6-C7-C8
20	B	1742	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	3	7005	LMU	C6-C7-C8-C9
21	A	7020	LMU	C3-C4-C5-C6
20	B	1735	CLA	C5-C6-C7-C8
20	A	1767	CLA	CBA-CGA-O2A-C1
20	A	1801	CLA	CBA-CGA-O2A-C1
20	B	1771	CLA	CBA-CGA-O2A-C1
21	2	1225	LMU	C3'-C4'-O1B-C1B
21	2	7003	LMU	C5-C6-C7-C8
21	A	7028	LMU	C7-C8-C9-C10
20	A	1777	CLA	C3A-C2A-CAA-CBA
20	A	1789	CLA	C3A-C2A-CAA-CBA
20	A	1791	CLA	C3A-C2A-CAA-CBA
20	A	1792	CLA	C3A-C2A-CAA-CBA
20	B	1737	CLA	C3A-C2A-CAA-CBA
21	A	7035	LMU	C2-C3-C4-C5
21	A	7013	LMU	C4'-C5'-C6'-O6'
21	2	7003	LMU	C2-C1-O1'-C1'
21	2	7006	LMU	C2-C1-O1'-C1'
21	A	7019	LMU	C2-C1-O1'-C1'
21	A	7021	LMU	C2-C1-O1'-C1'
21	A	7039	LMU	C2-C1-O1'-C1'
21	A	7042	LMU	C2-C1-O1'-C1'
20	B	1785	CLA	C8-C10-C11-C12
21	1	7004	LMU	C11-C10-C9-C8
20	B	1741	CLA	C6-C7-C8-C10
20	A	1777	CLA	CBA-CGA-O2A-C1
20	K	3009	CLA	CBA-CGA-O2A-C1
21	A	7038	LMU	C9-C10-C11-C12
20	A	1776	CLA	O1D-CGD-O2D-CED
20	B	1757	CLA	C10-C11-C12-C13
21	A	7017	LMU	C9-C10-C11-C12
21	A	7033	LMU	O1'-C1-C2-C3
20	B	1770	CLA	O1D-CGD-O2D-CED
20	B	1752	CLA	O1A-CGA-O2A-C1
20	B	1786	CLA	C16-C17-C18-C20
20	J	1043	CLA	C2-C3-C5-C6
21	K	1086	LMU	O1'-C1-C2-C3
21	2	7003	LMU	C7-C8-C9-C10
20	A	1776	CLA	C13-C15-C16-C17
21	A	7020	LMU	C5-C6-C7-C8
21	A	7042	LMU	C9-C10-C11-C12
21	A	7009	LMU	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
20	1	1198	CLA	C2A-CAA-CBA-CGA
21	A	7010	LMU	C5'-C4'-O1B-C1B
21	A	7016	LMU	C6-C7-C8-C9
21	A	7036	LMU	C2-C3-C4-C5
20	1	1200	CLA	CBA-CGA-O2A-C1
20	A	1769	CLA	CBA-CGA-O2A-C1
20	F	1156	CLA	C4C-C3C-CAC-CBC
21	A	7047	LMU	C6-C7-C8-C9
20	4	1198	CLA	C16-C17-C18-C20
20	4	1199	CLA	C6-C7-C8-C9
20	A	1761	CLA	C16-C17-C18-C20
20	A	1764	CLA	C16-C17-C18-C20
20	B	1753	CLA	C16-C17-C18-C20
20	J	1045	CLA	C6-C7-C8-C9
20	A	1793	CLA	C2C-C3C-CAC-CBC
20	A	1782	CLA	C5-C6-C7-C8
20	A	1786	CLA	O1A-CGA-O2A-C1
20	K	3009	CLA	O1A-CGA-O2A-C1
21	A	7041	LMU	C9-C10-C11-C12
21	A	7023	LMU	O5B-C1B-O1B-C4'
21	A	7030	LMU	O5B-C1B-O1B-C4'
20	B	1786	CLA	C5-C6-C7-C8
20	4	1198	CLA	C2C-C3C-CAC-CBC
22	A	1808	BCR	C19-C20-C21-C22
20	4	1196	CLA	C6-C7-C8-C10
20	A	1772	CLA	C16-C17-C18-C19
20	A	1788	CLA	C16-C17-C18-C19
20	B	1735	CLA	C16-C17-C18-C19
23	A	1802	PQN	C26-C27-C28-C29
21	A	7020	LMU	C3'-C4'-O1B-C1B
20	2	1224	CLA	C13-C15-C16-C17
20	3	3011	CLA	C5-C6-C7-C8
20	B	1738	CLA	C8-C10-C11-C12
20	B	1756	CLA	CBD-CGD-O2D-CED
20	A	1760	CLA	C2-C1-O2A-CGA
20	A	1790	CLA	C2-C1-O2A-CGA
20	B	1735	CLA	C2-C1-O2A-CGA
20	H	1079	CLA	C2-C1-O2A-CGA
24	B	1783	LMG	C41-C42-C43-C44
20	B	1759	CLA	C13-C15-C16-C17
21	A	1809	LMU	O5'-C5'-C6'-O6'
20	2	1217	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	3	1218	CLA	C11-C12-C13-C14
20	A	1764	CLA	C11-C10-C8-C9
20	A	1764	CLA	C11-C12-C13-C14
20	A	1767	CLA	C14-C13-C15-C16
20	A	1788	CLA	C6-C7-C8-C9
20	A	1793	CLA	C14-C13-C15-C16
20	A	1797	CLA	C14-C13-C15-C16
20	B	1737	CLA	C11-C10-C8-C9
20	B	1744	CLA	C6-C7-C8-C9
20	B	1749	CLA	C11-C10-C8-C9
20	B	1758	CLA	C6-C7-C8-C9
20	B	1762	CLA	C14-C13-C15-C16
20	B	1785	CLA	C6-C7-C8-C9
21	3	7005	LMU	C3'-C4'-O1B-C1B
21	A	1809	LMU	O1'-C1-C2-C3
21	A	7013	LMU	C7-C8-C9-C10
21	A	7034	LMU	C1-C2-C3-C4
20	2	1218	CLA	C13-C15-C16-C17
23	B	1773	PQN	C23-C25-C26-C27
20	1	1200	CLA	C4-C3-C5-C6
20	2	1212	CLA	C4-C3-C5-C6
20	A	1779	CLA	O1A-CGA-O2A-C1
21	A	7038	LMU	C3-C4-C5-C6
20	L	1167	CLA	C2A-CAA-CBA-CGA
20	A	1816	CLA	C6-C7-C8-C9
20	B	1758	CLA	C16-C17-C18-C19
23	B	1773	PQN	C26-C27-C28-C30
21	A	7043	LMU	O5B-C5B-C6B-O6B
22	A	1803	BCR	C23-C24-C25-C26
22	B	1777	BCR	C23-C24-C25-C26
22	B	1780	BCR	C23-C24-C25-C30
22	L	1169	BCR	C5-C6-C7-C8
22	3	1220	BCR	C11-C12-C13-C35
22	A	1808	BCR	C17-C18-C19-C20
22	B	1776	BCR	C11-C12-C13-C14
21	3	7005	LMU	C5'-C4'-O1B-C1B
20	1	1192	CLA	C14-C13-C15-C16
20	J	1043	CLA	C14-C13-C15-C16
21	A	7015	LMU	C3'-C4'-O1B-C1B
20	B	1786	CLA	C10-C11-C12-C13
20	A	1780	CLA	C4C-C3C-CAC-CBC
21	A	7031	LMU	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
20	B	1756	CLA	C5-C6-C7-C8
20	H	1079	CLA	C4-C3-C5-C6
20	1	1198	CLA	C11-C12-C13-C15
20	2	1217	CLA	C11-C12-C13-C15
20	3	1218	CLA	C11-C12-C13-C15
20	3	3011	CLA	C11-C12-C13-C15
20	4	1198	CLA	C11-C12-C13-C15
20	A	1764	CLA	C11-C10-C8-C7
20	A	1774	CLA	C12-C13-C15-C16
20	A	1783	CLA	C6-C7-C8-C10
20	A	1789	CLA	C12-C13-C15-C16
20	A	1793	CLA	C12-C13-C15-C16
20	A	1800	CLA	C11-C12-C13-C15
20	A	1813	CLA	C11-C12-C13-C15
20	B	1735	CLA	C11-C10-C8-C7
20	B	1735	CLA	C12-C13-C15-C16
20	B	1738	CLA	C6-C7-C8-C10
20	B	1739	CLA	C11-C10-C8-C7
20	B	1749	CLA	C11-C10-C8-C7
20	B	1753	CLA	C6-C7-C8-C10
20	B	1755	CLA	C11-C10-C8-C7
20	B	1758	CLA	C6-C7-C8-C10
20	B	1759	CLA	C11-C12-C13-C15
20	B	1771	CLA	C11-C12-C13-C15
20	B	1771	CLA	C12-C13-C15-C16
20	K	3009	CLA	C11-C12-C13-C15
20	R	1055	CLA	C11-C10-C8-C7
21	2	1225	LMU	C5-C6-C7-C8
22	B	1777	BCR	C19-C20-C21-C22
22	L	1170	BCR	C13-C14-C15-C16
22	L	1170	BCR	C15-C16-C17-C18
20	A	1796	CLA	C16-C17-C18-C20
20	1	1188	CLA	CBA-CGA-O2A-C1
20	1	1198	CLA	CBA-CGA-O2A-C1
20	A	1812	CLA	C2A-CAA-CBA-CGA
21	A	7040	LMU	C5'-C4'-O1B-C1B
21	A	7026	LMU	C4B-C5B-C6B-O6B
20	B	1757	CLA	C3-C5-C6-C7
20	4	1198	CLA	CBA-CGA-O2A-C1
20	1	1192	CLA	C12-C13-C15-C16
21	A	7038	LMU	C4-C5-C6-C7
20	A	1767	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	1	1189	CLA	CAD-CBD-CGD-O2D
20	1	1198	CLA	CAD-CBD-CGD-O2D
20	3	3007	CLA	CAD-CBD-CGD-O2D
20	4	1201	CLA	CAD-CBD-CGD-O2D
20	A	1760	CLA	CAD-CBD-CGD-O2D
20	A	1768	CLA	CAD-CBD-CGD-O2D
20	A	1792	CLA	CAD-CBD-CGD-O2D
20	B	1742	CLA	CAD-CBD-CGD-O2D
20	B	1766	CLA	CAD-CBD-CGD-O2D
20	B	1770	CLA	CAD-CBD-CGD-O2D
20	J	1044	CLA	CAD-CBD-CGD-O2D
20	K	1146	CLA	CAD-CBD-CGD-O2D
20	L	1168	CLA	CAD-CBD-CGD-O2D
24	B	1783	LMG	C38-C39-C40-C41
20	A	1797	CLA	CBA-CGA-O2A-C1
20	3	1218	CLA	C15-C16-C17-C18
20	A	1764	CLA	C13-C15-C16-C17
20	H	1079	CLA	C2-C3-C5-C6
20	1	1198	CLA	O1A-CGA-O2A-C1
20	A	1817	CLA	CAA-CBA-CGA-O2A
21	A	7019	LMU	C2-C3-C4-C5
20	A	1760	CLA	C6-C7-C8-C10
20	B	1741	CLA	C6-C7-C8-C9
20	B	1762	CLA	C16-C17-C18-C19
20	K	1142	CLA	O1D-CGD-O2D-CED
20	4	1199	CLA	CHA-CBD-CGD-O1D
20	4	1199	CLA	CHA-CBD-CGD-O2D
20	A	1764	CLA	CHA-CBD-CGD-O1D
20	A	1764	CLA	CHA-CBD-CGD-O2D
20	A	1772	CLA	CHA-CBD-CGD-O1D
20	A	1789	CLA	CHA-CBD-CGD-O1D
20	A	1789	CLA	CHA-CBD-CGD-O2D
20	A	1800	CLA	CHA-CBD-CGD-O1D
20	A	1800	CLA	CHA-CBD-CGD-O2D
20	A	1811	CLA	CHA-CBD-CGD-O1D
20	A	1811	CLA	CHA-CBD-CGD-O2D
20	A	1812	CLA	CHA-CBD-CGD-O1D
20	B	1751	CLA	CHA-CBD-CGD-O1D
20	B	1751	CLA	CHA-CBD-CGD-O2D
20	B	1753	CLA	CHA-CBD-CGD-O1D
20	B	1753	CLA	CHA-CBD-CGD-O2D
20	B	1765	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	B	1765	CLA	CHA-CBD-CGD-O2D
20	B	1768	CLA	CHA-CBD-CGD-O1D
20	B	1785	CLA	CHA-CBD-CGD-O1D
20	B	1785	CLA	CHA-CBD-CGD-O2D
22	3	1220	BCR	C15-C16-C17-C18
22	A	1806	BCR	C13-C14-C15-C16
20	3	1219	CLA	C10-C11-C12-C13
20	G	1099	CLA	C2C-C3C-CAC-CBC
20	A	1781	CLA	C3-C5-C6-C7
20	B	1758	CLA	C3-C5-C6-C7
20	1	1188	CLA	O1A-CGA-O2A-C1
20	A	1777	CLA	O1A-CGA-O2A-C1
20	B	1737	CLA	O1A-CGA-O2A-C1
21	1	7004	LMU	C4-C5-C6-C7
20	A	1801	CLA	O1A-CGA-O2A-C1
20	J	1045	CLA	CAA-CBA-CGA-O2A
20	A	1761	CLA	C16-C17-C18-C19
20	A	1764	CLA	C3-C5-C6-C7
21	A	7015	LMU	C5'-C4'-O1B-C1B
20	A	1764	CLA	C6-C7-C8-C9
20	A	1789	CLA	C11-C12-C13-C14
20	A	1796	CLA	C6-C7-C8-C9
20	A	1811	CLA	C14-C13-C15-C16
20	B	1739	CLA	C14-C13-C15-C16
20	B	1749	CLA	C11-C12-C13-C14
21	A	7009	LMU	C2-C3-C4-C5
20	A	1769	CLA	O1A-CGA-O2A-C1
20	B	1755	CLA	C2A-CAA-CBA-CGA
21	A	7009	LMU	C11-C10-C9-C8
20	2	1224	CLA	C1A-C2A-CAA-CBA
20	A	1789	CLA	C1A-C2A-CAA-CBA
20	B	1767	CLA	C1A-C2A-CAA-CBA
20	B	1786	CLA	C1A-C2A-CAA-CBA
20	B	1745	CLA	C11-C12-C13-C14
20	B	1752	CLA	C6-C7-C8-C9
20	B	1787	CLA	C16-C17-C18-C20
20	A	1764	CLA	C2-C1-O2A-CGA
20	J	1043	CLA	C2-C1-O2A-CGA
22	B	1778	BCR	C9-C10-C11-C12
22	L	1170	BCR	C9-C10-C11-C12
20	A	1770	CLA	C2C-C3C-CAC-CBC
21	A	7031	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	A	7030	LMU	C7-C8-C9-C10
20	B	1742	CLA	C3-C5-C6-C7
21	K	1086	LMU	C3'-C4'-O1B-C1B
20	A	1767	CLA	O1A-CGA-O2A-C1
20	3	3008	CLA	CAA-CBA-CGA-O2A
20	B	1745	CLA	C10-C11-C12-C13
20	A	1815	CLA	C3-C5-C6-C7
20	J	1045	CLA	C6-C7-C8-C10
20	2	1212	CLA	C2-C3-C5-C6
20	2	1218	CLA	CAD-CBD-CGD-O1D
20	4	1196	CLA	CAD-CBD-CGD-O1D
20	A	1783	CLA	CAD-CBD-CGD-O1D
20	A	1792	CLA	C2-C3-C5-C6
20	B	1738	CLA	CAD-CBD-CGD-O1D
20	B	1765	CLA	CAD-CBD-CGD-O1D
20	B	1767	CLA	CAD-CBD-CGD-O1D
20	B	1786	CLA	CAD-CBD-CGD-O1D
21	4	1210	LMU	C3-C4-C5-C6
20	B	1771	CLA	O1A-CGA-O2A-C1
20	A	1797	CLA	O1A-CGA-O2A-C1
21	A	7039	LMU	C9-C10-C11-C12
20	4	1196	CLA	C6-C7-C8-C9
20	4	1198	CLA	C16-C17-C18-C19
20	B	1748	CLA	C11-C12-C13-C15
20	2	1217	CLA	C6-C7-C8-C10
20	2	1224	CLA	C12-C13-C15-C16
20	3	1218	CLA	C11-C10-C8-C7
20	4	1201	CLA	C3A-C2A-CAA-CBA
20	A	1761	CLA	C11-C12-C13-C15
20	A	1782	CLA	C11-C10-C8-C7
20	A	1785	CLA	C6-C7-C8-C10
20	A	1788	CLA	C11-C10-C8-C7
20	A	1811	CLA	C6-C7-C8-C10
20	B	1737	CLA	C11-C12-C13-C15
20	B	1743	CLA	C11-C10-C8-C7
20	B	1744	CLA	C11-C12-C13-C15
20	B	1747	CLA	C11-C10-C8-C7
20	B	1756	CLA	C11-C12-C13-C15
20	B	1759	CLA	C12-C13-C15-C16
20	B	1762	CLA	C11-C10-C8-C7
20	B	1767	CLA	C3A-C2A-CAA-CBA
20	B	1785	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
20	I	1031	CLA	C11-C10-C8-C7
20	K	3009	CLA	C6-C7-C8-C10
23	A	1802	PQN	C22-C23-C25-C26
21	A	7022	LMU	C5'-C4'-O1B-C1B
21	A	7015	LMU	C2-C1-O1'-C1'
21	A	7023	LMU	C2-C3-C4-C5
20	B	1735	CLA	C16-C17-C18-C20
21	A	7038	LMU	C3'-C4'-O1B-C1B
20	B	1739	CLA	C3-C5-C6-C7
21	A	7017	LMU	C3'-C4'-O1B-C1B
20	B	1756	CLA	O1D-CGD-O2D-CED
20	1	1200	CLA	O1A-CGA-O2A-C1
20	A	1788	CLA	C16-C17-C18-C20
20	2	1218	CLA	C4C-C3C-CAC-CBC
20	3	1218	CLA	C2C-C3C-CAC-CBC
21	A	7015	LMU	O1'-C1-C2-C3
21	A	7043	LMU	C5-C6-C7-C8
21	4	1210	LMU	O1'-C1-C2-C3
21	A	1810	LMU	C7-C8-C9-C10
20	2	1217	CLA	C11-C10-C8-C9
20	A	1761	CLA	C11-C12-C13-C14
20	A	1764	CLA	C14-C13-C15-C16
20	A	1774	CLA	C14-C13-C15-C16
20	A	1813	CLA	C11-C12-C13-C14
20	B	1768	CLA	C11-C10-C8-C9
20	4	1198	CLA	O1A-CGA-O2A-C1
20	B	1755	CLA	C3-C5-C6-C7
21	3	7005	LMU	C9-C10-C11-C12
21	A	7038	LMU	C2-C3-C4-C5
20	3	3011	CLA	C10-C11-C12-C13
20	A	1796	CLA	C15-C16-C17-C18
20	L	1505	CLA	C6-C7-C8-C9
22	B	1780	BCR	C17-C18-C19-C20
20	A	1781	CLA	C13-C15-C16-C17
21	A	7034	LMU	C11-C10-C9-C8
20	2	1217	CLA	C10-C11-C12-C13
20	A	1783	CLA	C13-C15-C16-C17
20	A	1793	CLA	C13-C15-C16-C17
20	B	1738	CLA	C5-C6-C7-C8
21	1	1202	LMU	C6-C7-C8-C9
21	A	7036	LMU	C6-C7-C8-C9
21	A	7034	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	A	7037	LMU	C9-C10-C11-C12
21	R	1056	LMU	C3-C4-C5-C6
20	B	1769	CLA	C2A-CAA-CBA-CGA
20	L	1166	CLA	C2A-CAA-CBA-CGA
21	A	7033	LMU	C4-C5-C6-C7
20	4	1200	CLA	C2-C1-O2A-CGA
20	A	1765	CLA	C2-C1-O2A-CGA
20	A	1799	CLA	C2-C1-O2A-CGA
20	A	1800	CLA	C2-C1-O2A-CGA
20	B	1756	CLA	C2-C1-O2A-CGA
20	B	1761	CLA	C2-C1-O2A-CGA
20	B	1768	CLA	C2-C1-O2A-CGA
20	J	1044	CLA	C2-C1-O2A-CGA
20	B	1743	CLA	CAA-CBA-CGA-O2A
21	A	1810	LMU	C1-C2-C3-C4
21	A	7019	LMU	C4-C5-C6-C7
21	A	7038	LMU	C1-C2-C3-C4
21	A	7035	LMU	C5'-C4'-O1B-C1B
20	A	1796	CLA	C16-C17-C18-C19
20	3	3011	CLA	C13-C15-C16-C17
20	A	1800	CLA	C4-C3-C5-C6
21	A	7034	LMU	O1'-C1-C2-C3
20	B	1740	CLA	O1D-CGD-O2D-CED
20	A	1768	CLA	C6-C7-C8-C9
20	B	1746	CLA	CAA-CBA-CGA-O2A
21	A	7023	LMU	C2B-C1B-O1B-C4'
21	1	7004	LMU	C5-C6-C7-C8
20	B	1753	CLA	C16-C17-C18-C19
20	B	1763	CLA	C2A-CAA-CBA-CGA
20	3	1218	CLA	C8-C10-C11-C12
21	A	7024	LMU	C9-C10-C11-C12
20	A	1793	CLA	C4C-C3C-CAC-CBC
21	1	7004	LMU	C7-C8-C9-C10
21	A	7009	LMU	C6-C7-C8-C9
20	A	1767	CLA	C11-C12-C13-C15
20	A	1774	CLA	C6-C7-C8-C10
20	A	1785	CLA	C11-C10-C8-C7
20	A	1797	CLA	C12-C13-C15-C16
20	B	1743	CLA	C6-C7-C8-C10
20	B	1753	CLA	C12-C13-C15-C16
21	A	1809	LMU	C4-C5-C6-C7
21	A	7027	LMU	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
20	2	1218	CLA	C11-C10-C8-C9
20	A	1788	CLA	C11-C10-C8-C9
20	A	1811	CLA	C6-C7-C8-C9
20	B	1743	CLA	C11-C10-C8-C9
20	B	1744	CLA	C11-C10-C8-C9
20	B	1755	CLA	C6-C7-C8-C9
20	B	1759	CLA	C11-C12-C13-C14
20	B	1771	CLA	C11-C12-C13-C14
20	B	1785	CLA	C14-C13-C15-C16
20	K	3009	CLA	C6-C7-C8-C9
20	B	1756	CLA	C13-C15-C16-C17
22	L	1169	BCR	C15-C16-C17-C18
20	L	1505	CLA	C6-C7-C8-C10
23	B	1773	PQN	C26-C27-C28-C29
20	2	1220	CLA	C2C-C3C-CAC-CBC
21	A	1810	LMU	C4-C5-C6-C7
20	A	1816	CLA	C5-C6-C7-C8
20	I	1033	CLA	C5-C6-C7-C8
21	A	7022	LMU	C3-C4-C5-C6
21	A	7015	LMU	C9-C10-C11-C12
20	A	1770	CLA	C4C-C3C-CAC-CBC
20	J	1044	CLA	C12-C13-C15-C16
20	A	1776	CLA	CBA-CGA-O2A-C1
21	A	7020	LMU	C5'-C4'-O1B-C1B
20	A	1776	CLA	O1A-CGA-O2A-C1
21	A	7019	LMU	C1-C2-C3-C4
20	B	1757	CLA	CAA-CBA-CGA-O2A
20	B	1762	CLA	CBA-CGA-O2A-C1
20	1	1192	CLA	C2A-CAA-CBA-CGA
20	A	1791	CLA	CAA-CBA-CGA-O1A
21	A	7035	LMU	O5'-C1'-O1'-C1
22	A	1805	BCR	C13-C14-C15-C16
20	A	1784	CLA	O1A-CGA-O2A-C1
21	2	1225	LMU	C9-C10-C11-C12
20	B	1744	CLA	C8-C10-C11-C12
20	B	1762	CLA	O1A-CGA-O2A-C1
21	A	7036	LMU	C4-C5-C6-C7
20	A	1789	CLA	C16-C17-C18-C19
20	R	1055	CLA	CAA-CBA-CGA-O2A
20	A	1811	CLA	C4-C3-C5-C6
20	J	1044	CLA	C4-C3-C5-C6
21	A	7031	LMU	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
20	B	1747	CLA	C11-C12-C13-C14
20	B	1786	CLA	C2-C1-O2A-CGA
20	F	1157	CLA	C2-C1-O2A-CGA
20	B	1756	CLA	C16-C17-C18-C20
20	3	1218	CLA	C2A-CAA-CBA-CGA
20	B	1757	CLA	C2A-CAA-CBA-CGA
20	A	1784	CLA	CBA-CGA-O2A-C1
20	3	1219	CLA	C3A-C2A-CAA-CBA
20	3	3008	CLA	C3A-C2A-CAA-CBA
20	4	1196	CLA	C3A-C2A-CAA-CBA
20	4	1209	CLA	C3A-C2A-CAA-CBA
20	A	1768	CLA	C3A-C2A-CAA-CBA
20	A	1771	CLA	C3A-C2A-CAA-CBA
20	B	1735	CLA	C3A-C2A-CAA-CBA
22	B	1777	BCR	C13-C14-C15-C16
21	3	7005	LMU	C4-C5-C6-C7
21	A	7022	LMU	C2-C3-C4-C5
20	B	1743	CLA	C13-C15-C16-C17
20	A	1761	CLA	C14-C13-C15-C16
20	A	1779	CLA	C6-C7-C8-C10
20	K	1142	CLA	C2C-C3C-CAC-CBC
22	A	1807	BCR	C35-C13-C14-C15
22	B	1776	BCR	C11-C10-C9-C34
22	B	1777	BCR	C20-C21-C22-C37
22	B	1779	BCR	C16-C17-C18-C36
22	L	1170	BCR	C11-C10-C9-C34
20	A	1770	CLA	CAA-CBA-CGA-O1A
21	A	1809	LMU	C1-C2-C3-C4
20	A	1791	CLA	CAA-CBA-CGA-O2A
22	B	1779	BCR	C11-C12-C13-C35
21	A	7010	LMU	C6-C7-C8-C9
20	A	1767	CLA	C4-C3-C5-C6
20	A	1793	CLA	C4-C3-C5-C6
20	3	1219	CLA	C1A-C2A-CAA-CBA
20	4	1201	CLA	C1A-C2A-CAA-CBA
20	B	1765	CLA	C1A-C2A-CAA-CBA
21	A	7043	LMU	C2-C3-C4-C5
20	4	1198	CLA	C6-C7-C8-C10
20	A	1793	CLA	C2-C3-C5-C6
20	A	1796	CLA	C6-C7-C8-C10
20	A	1811	CLA	C11-C12-C13-C15
20	B	1767	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	A	1803	BCR	C13-C14-C15-C16
20	J	1045	CLA	C2A-CAA-CBA-CGA
20	B	1759	CLA	C8-C10-C11-C12
21	A	7042	LMU	O1'-C1-C2-C3
24	B	1783	LMG	C31-C32-C33-C34
20	A	1772	CLA	C16-C17-C18-C20
20	A	1813	CLA	C16-C17-C18-C20
20	B	1744	CLA	C15-C16-C17-C18
20	A	1770	CLA	CAA-CBA-CGA-O2A
21	A	7031	LMU	C1-C2-C3-C4
20	B	1743	CLA	C4-C3-C5-C6
20	A	1811	CLA	C2-C3-C5-C6
20	H	1079	CLA	C13-C15-C16-C17
21	A	7009	LMU	C2B-C1B-O1B-C4'
22	A	1807	BCR	C12-C13-C14-C15
22	B	1776	BCR	C11-C10-C9-C8
22	B	1777	BCR	C20-C21-C22-C23
22	B	1779	BCR	C16-C17-C18-C19
22	L	1170	BCR	C11-C10-C9-C8
21	2	7006	LMU	C3-C4-C5-C6
21	A	7040	LMU	C1-C2-C3-C4
20	3	1218	CLA	CAA-CBA-CGA-O2A
22	B	1778	BCR	C13-C14-C15-C16
20	B	1740	CLA	C13-C15-C16-C17
20	B	1735	CLA	C2C-C3C-CAC-CBC
21	A	7015	LMU	C4'-C5'-C6'-O6'
20	A	1788	CLA	C8-C10-C11-C12
20	A	1780	CLA	C3-C5-C6-C7
20	J	1044	CLA	C3-C5-C6-C7
20	4	4007	CLA	C4-C3-C5-C6
20	4	1196	CLA	C2-C1-O2A-CGA
20	4	1204	CLA	C2-C1-O2A-CGA
20	A	1812	CLA	C2-C1-O2A-CGA
20	B	1759	CLA	C2-C1-O2A-CGA
20	K	1146	CLA	C2-C1-O2A-CGA
20	R	1054	CLA	C2-C1-O2A-CGA
20	A	1800	CLA	C2-C3-C5-C6
20	A	1788	CLA	C10-C11-C12-C13
20	A	1812	CLA	C8-C10-C11-C12
20	B	1771	CLA	CAA-CBA-CGA-O2A
20	1	1198	CLA	C6-C7-C8-C9
20	A	1772	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	1788	CLA	C11-C12-C13-C14
20	B	1745	CLA	C6-C7-C8-C9
20	B	1748	CLA	C6-C7-C8-C9
20	B	1768	CLA	C14-C13-C15-C16
20	L	1167	CLA	C2-C1-O2A-CGA
20	H	1079	CLA	C3-C5-C6-C7
20	A	1792	CLA	C4-C3-C5-C6
20	4	1201	CLA	C2A-CAA-CBA-CGA
22	3	1220	BCR	C1-C6-C7-C8
22	A	1803	BCR	C23-C24-C25-C30
22	B	1777	BCR	C23-C24-C25-C30
20	B	1737	CLA	CAA-CBA-CGA-O2A
20	A	1781	CLA	C8-C10-C11-C12
22	A	1804	BCR	C13-C14-C15-C16
20	A	1783	CLA	C4-C3-C5-C6
20	B	1762	CLA	C4-C3-C5-C6
20	3	1219	CLA	C8-C10-C11-C12
20	B	1760	CLA	CAA-CBA-CGA-O2A
20	A	1783	CLA	C16-C17-C18-C19
21	A	7031	LMU	C7-C8-C9-C10
20	B	1785	CLA	CAA-CBA-CGA-O1A
20	A	1766	CLA	CAA-CBA-CGA-O2A
20	B	1740	CLA	C2A-CAA-CBA-CGA
21	A	7015	LMU	C3-C4-C5-C6
20	A	1766	CLA	CAA-CBA-CGA-O1A
20	B	1764	CLA	CAA-CBA-CGA-O1A
20	B	1748	CLA	C5-C6-C7-C8
20	A	1759	CLA	CAA-CBA-CGA-O1A
20	2	1224	CLA	C11-C10-C8-C7
20	4	4007	CLA	C2-C3-C5-C6
20	B	1785	CLA	C12-C13-C15-C16
22	B	1778	BCR	C15-C16-C17-C18
20	B	1735	CLA	CAA-CBA-CGA-O2A
20	B	1750	CLA	CAA-CBA-CGA-O2A
20	B	1765	CLA	CAA-CBA-CGA-O2A
20	B	1751	CLA	CAA-CBA-CGA-O2A
21	A	7022	LMU	C2B-C1B-O1B-C4'
20	A	1760	CLA	C4-C3-C5-C6
20	A	1781	CLA	C4-C3-C5-C6
20	B	1758	CLA	C4-C3-C5-C6
20	1	1198	CLA	C8-C10-C11-C12
20	B	1770	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	B	1737	CLA	C2-C3-C5-C6
20	A	1813	CLA	C16-C17-C18-C19
20	A	1811	CLA	CAA-CBA-CGA-O2A
20	3	1218	CLA	C11-C10-C8-C9
20	B	1737	CLA	C14-C13-C15-C16
20	B	1771	CLA	C14-C13-C15-C16
20	I	1031	CLA	C11-C10-C8-C9
20	R	1055	CLA	C14-C13-C15-C16
23	A	1802	PQN	C24-C23-C25-C26
20	2	1215	CLA	C3A-C2A-CAA-CBA
20	A	1767	CLA	C3A-C2A-CAA-CBA
20	A	1794	CLA	C3A-C2A-CAA-CBA
20	B	1751	CLA	C3A-C2A-CAA-CBA
20	K	1146	CLA	C3A-C2A-CAA-CBA
21	A	7032	LMU	C2B-C1B-O1B-C4'
20	2	1217	CLA	CAA-CBA-CGA-O2A
20	2	1223	CLA	CAA-CBA-CGA-O2A
20	A	1761	CLA	CAA-CBA-CGA-O2A
20	L	1505	CLA	CAA-CBA-CGA-O2A
20	2	1220	CLA	CAD-CBD-CGD-O2D
20	2	1223	CLA	CAD-CBD-CGD-O2D
20	3	3008	CLA	CAD-CBD-CGD-O2D
20	4	1204	CLA	CAD-CBD-CGD-O2D
20	A	1759	CLA	CAD-CBD-CGD-O2D
20	A	1769	CLA	CAD-CBD-CGD-O2D
20	A	1776	CLA	CAD-CBD-CGD-O2D
20	A	1780	CLA	CAD-CBD-CGD-O2D
20	A	1784	CLA	CAD-CBD-CGD-O2D
20	A	1790	CLA	CAD-CBD-CGD-O2D
20	A	1815	CLA	CAD-CBD-CGD-O2D
20	B	1754	CLA	CAD-CBD-CGD-O2D
20	B	1755	CLA	CAD-CBD-CGD-O2D
20	B	1759	CLA	CAD-CBD-CGD-O2D
20	H	1079	CLA	CAD-CBD-CGD-O2D
20	R	1055	CLA	CAD-CBD-CGD-O2D
20	I	1031	CLA	C2A-CAA-CBA-CGA
20	2	1213	CLA	C2-C1-O2A-CGA
20	B	1760	CLA	C2-C1-O2A-CGA
20	A	1795	CLA	CAA-CBA-CGA-O2A
20	B	1756	CLA	CAA-CBA-CGA-O2A
20	A	1783	CLA	C10-C11-C12-C13
20	J	1043	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	A	7039	LMU	C5'-C4'-O1B-C1B
20	B	1762	CLA	C5-C6-C7-C8
20	A	1767	CLA	C2-C3-C5-C6
20	A	1781	CLA	C2-C3-C5-C6
20	A	1783	CLA	C2-C3-C5-C6
20	B	1743	CLA	C2-C3-C5-C6
20	B	1762	CLA	C2-C3-C5-C6
20	I	1031	CLA	CAA-CBA-CGA-O2A
21	R	1056	LMU	O1'-C1-C2-C3
21	A	7027	LMU	C2B-C1B-O1B-C4'
21	4	1210	LMU	C4B-C5B-C6B-O6B
21	A	7035	LMU	C9-C10-C11-C12
20	4	1198	CLA	CAA-CBA-CGA-O2A
20	B	1766	CLA	CAA-CBA-CGA-O2A
20	B	1765	CLA	CAA-CBA-CGA-O1A
20	2	1215	CLA	CBD-CGD-O2D-CED
20	A	1782	CLA	C10-C11-C12-C13
20	1	1193	CLA	O2A-C1-C2-C3
20	A	1773	CLA	O2A-C1-C2-C3
20	B	1755	CLA	O2A-C1-C2-C3
20	B	1787	CLA	O2A-C1-C2-C3
20	A	1776	CLA	C2A-CAA-CBA-CGA
21	A	7034	LMU	C4'-C5'-C6'-O6'
20	2	1223	CLA	CHA-CBD-CGD-O1D
20	2	1223	CLA	CHA-CBD-CGD-O2D
20	2	1224	CLA	CHA-CBD-CGD-O1D
20	2	1224	CLA	CHA-CBD-CGD-O2D
20	3	1219	CLA	CHA-CBD-CGD-O1D
20	3	1219	CLA	CHA-CBD-CGD-O2D
20	3	3011	CLA	CHA-CBD-CGD-O1D
20	3	3011	CLA	CHA-CBD-CGD-O2D
20	4	1204	CLA	CHA-CBD-CGD-O2D
20	A	1761	CLA	CHA-CBD-CGD-O1D
20	A	1772	CLA	CHA-CBD-CGD-O2D
20	A	1782	CLA	CHA-CBD-CGD-O1D
20	A	1793	CLA	CHA-CBD-CGD-O1D
20	A	1793	CLA	CHA-CBD-CGD-O2D
20	A	1812	CLA	CHA-CBD-CGD-O2D
20	B	1735	CLA	CHA-CBD-CGD-O1D
20	B	1735	CLA	CHA-CBD-CGD-O2D
20	B	1737	CLA	CHA-CBD-CGD-O1D
20	B	1737	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	1749	CLA	CHA-CBD-CGD-O1D
20	B	1749	CLA	CHA-CBD-CGD-O2D
20	B	1758	CLA	CHA-CBD-CGD-O1D
20	B	1758	CLA	CHA-CBD-CGD-O2D
20	B	1768	CLA	CHA-CBD-CGD-O2D
20	B	1771	CLA	CHA-CBD-CGD-O1D
20	B	1771	CLA	CHA-CBD-CGD-O2D
20	J	1045	CLA	CHA-CBD-CGD-O1D
20	J	1045	CLA	CHA-CBD-CGD-O2D
20	L	1167	CLA	CHA-CBD-CGD-O1D
20	A	1798	CLA	C3-C5-C6-C7
20	A	1761	CLA	C2C-C3C-CAC-CBC
21	A	7019	LMU	C9-C10-C11-C12
20	1	1192	CLA	CAA-CBA-CGA-O2A
20	1	1197	CLA	CAA-CBA-CGA-O2A
20	1	1200	CLA	CAA-CBA-CGA-O2A
20	A	1782	CLA	CAA-CBA-CGA-O2A
20	A	1796	CLA	CAA-CBA-CGA-O2A
20	B	1742	CLA	C2A-CAA-CBA-CGA
20	A	1788	CLA	C5-C6-C7-C8
20	4	1198	CLA	C4C-C3C-CAC-CBC
20	A	1767	CLA	CAA-CBA-CGA-O2A
20	B	1758	CLA	C2-C3-C5-C6
20	H	1079	CLA	C11-C10-C8-C7
23	A	1802	PQN	C21-C22-C23-C25
20	A	1811	CLA	C16-C17-C18-C19
20	A	1780	CLA	C8-C10-C11-C12
20	R	1055	CLA	C13-C15-C16-C17
20	B	1764	CLA	CAA-CBA-CGA-O2A
20	B	1738	CLA	C2C-C3C-CAC-CBC
21	A	7037	LMU	O1'-C1-C2-C3
20	3	3011	CLA	C11-C12-C13-C14
20	A	1785	CLA	C6-C7-C8-C9
20	A	1811	CLA	C11-C12-C13-C14
20	B	1744	CLA	C11-C12-C13-C14
20	B	1735	CLA	C10-C11-C12-C13
20	B	1741	CLA	C2C-C3C-CAC-CBC
20	A	1776	CLA	C16-C17-C18-C20
20	A	1766	CLA	C2A-CAA-CBA-CGA
20	A	1813	CLA	C2A-CAA-CBA-CGA
20	I	1031	CLA	CAA-CBA-CGA-O1A
21	A	7039	LMU	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
20	K	3009	CLA	CAA-CBA-CGA-O2A
20	L	1166	CLA	C2C-C3C-CAC-CBC
20	B	1751	CLA	CAA-CBA-CGA-O1A
20	B	1756	CLA	CAA-CBA-CGA-O1A
20	B	1766	CLA	CAA-CBA-CGA-O1A
20	B	1754	CLA	C4-C3-C5-C6
21	1	7004	LMU	C9-C10-C11-C12
21	3	7005	LMU	C11-C10-C9-C8
20	2	1215	CLA	C1A-C2A-CAA-CBA
20	4	1196	CLA	C1A-C2A-CAA-CBA
20	A	1762	CLA	C1A-C2A-CAA-CBA
20	A	1768	CLA	C1A-C2A-CAA-CBA
20	A	1797	CLA	C1A-C2A-CAA-CBA
20	B	1735	CLA	C1A-C2A-CAA-CBA
20	B	1751	CLA	C1A-C2A-CAA-CBA
20	K	1146	CLA	C1A-C2A-CAA-CBA
20	A	1797	CLA	C2-C1-O2A-CGA
20	B	1753	CLA	C2-C1-O2A-CGA
20	4	1198	CLA	CAA-CBA-CGA-O1A
20	A	1795	CLA	CAA-CBA-CGA-O1A
20	B	1735	CLA	CAA-CBA-CGA-O1A
20	B	1750	CLA	CAA-CBA-CGA-O1A
20	4	1200	CLA	C2A-CAA-CBA-CGA
20	A	1797	CLA	C16-C17-C18-C20
24	B	1783	LMG	C28-C29-C30-C31
20	L	1505	CLA	CAA-CBA-CGA-O1A
20	2	1213	CLA	CBA-CGA-O2A-C1
20	I	1033	CLA	CAA-CBA-CGA-O2A
20	A	1811	CLA	C2C-C3C-CAC-CBC
20	1	1200	CLA	CAA-CBA-CGA-O1A
20	A	1761	CLA	CAA-CBA-CGA-O1A
20	A	1811	CLA	CAA-CBA-CGA-O1A
20	A	1767	CLA	CAA-CBA-CGA-O1A
20	K	3009	CLA	CAA-CBA-CGA-O1A
20	A	1797	CLA	CAA-CBA-CGA-O2A
21	A	7039	LMU	O5'-C1'-O1'-C1
21	A	7030	LMU	O1'-C1-C2-C3
22	3	1220	BCR	C5-C6-C7-C8
22	B	1777	BCR	C1-C6-C7-C8
22	B	1777	BCR	C5-C6-C7-C8
21	A	7023	LMU	C9-C10-C11-C12
20	A	1817	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	1	1202	LMU	C7-C8-C9-C10
20	1	1197	CLA	CAD-CBD-CGD-O1D
20	4	1200	CLA	CAD-CBD-CGD-O1D
20	A	1760	CLA	CAD-CBD-CGD-O1D
20	A	1761	CLA	CAD-CBD-CGD-O1D
20	A	1777	CLA	C2-C3-C5-C6
20	A	1782	CLA	CAD-CBD-CGD-O1D
20	A	1812	CLA	CAD-CBD-CGD-O1D
20	B	1736	CLA	CAD-CBD-CGD-O1D
20	B	1756	CLA	CAD-CBD-CGD-O1D
20	B	1768	CLA	CAD-CBD-CGD-O1D
20	F	1156	CLA	CAD-CBD-CGD-O1D
20	K	1142	CLA	CAD-CBD-CGD-O1D
20	L	1505	CLA	CAD-CBD-CGD-O1D
20	2	1223	CLA	CAA-CBA-CGA-O1A
20	A	1782	CLA	CAA-CBA-CGA-O1A
20	I	1033	CLA	CAA-CBA-CGA-O1A
20	2	1222	CLA	CAA-CBA-CGA-O2A
20	B	1787	CLA	CAA-CBA-CGA-O2A
20	2	1218	CLA	C11-C12-C13-C14
20	A	1776	CLA	C14-C13-C15-C16
20	B	1745	CLA	C11-C10-C8-C9
20	B	1770	CLA	C6-C7-C8-C9
20	B	1770	CLA	C14-C13-C15-C16
20	H	1079	CLA	C11-C10-C8-C9
20	A	1773	CLA	CAA-CBA-CGA-O2A
20	A	1788	CLA	CAA-CBA-CGA-O2A
20	B	1768	CLA	CAA-CBA-CGA-O2A
21	A	7037	LMU	C6-C7-C8-C9
20	2	1213	CLA	O1A-CGA-O2A-C1
20	3	3011	CLA	CAA-CBA-CGA-O2A
20	B	1787	CLA	C4-C3-C5-C6
22	L	1169	BCR	C36-C18-C19-C20
21	L	1171	LMU	C4'-C5'-C6'-O6'
20	1	1190	CLA	C3A-C2A-CAA-CBA
20	A	1767	CLA	C11-C10-C8-C7
20	A	1776	CLA	C12-C13-C15-C16
20	A	1779	CLA	C3A-C2A-CAA-CBA
20	B	1745	CLA	C6-C7-C8-C10
20	B	1745	CLA	C11-C10-C8-C7
20	B	1768	CLA	C6-C7-C8-C10
20	B	1768	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
20	B	1770	CLA	C6-C7-C8-C10
20	J	1044	CLA	C2-C3-C5-C6
20	1	1192	CLA	CAA-CBA-CGA-O1A
21	A	7023	LMU	C1-C2-C3-C4
20	A	1764	CLA	C2C-C3C-CAC-CBC
21	A	7021	LMU	C2-C3-C4-C5
20	2	1218	CLA	CAA-CBA-CGA-O2A
20	4	1209	CLA	CAA-CBA-CGA-O2A
20	A	1771	CLA	CAA-CBA-CGA-O2A
22	B	1777	BCR	C7-C8-C9-C10
20	A	1788	CLA	CAA-CBA-CGA-O1A
20	A	1797	CLA	CAA-CBA-CGA-O1A
22	B	1774	BCR	C15-C16-C17-C18
21	3	7005	LMU	C2-C1-O1'-C1'
20	4	4007	CLA	CAA-CBA-CGA-O2A
20	B	1744	CLA	CAA-CBA-CGA-O2A
21	A	7021	LMU	C5-C6-C7-C8
20	4	1209	CLA	CAA-CBA-CGA-O1A
20	A	1796	CLA	CAA-CBA-CGA-O1A
20	A	1817	CLA	CAA-CBA-CGA-O1A
20	A	1785	CLA	C10-C11-C12-C13
20	B	1756	CLA	C10-C11-C12-C13
21	A	7030	LMU	C3'-C4'-O1B-C1B
20	1	1188	CLA	CAA-CBA-CGA-O2A
20	B	1787	CLA	CAA-CBA-CGA-O1A
20	B	1754	CLA	CBD-CGD-O2D-CED
20	3	3011	CLA	C15-C16-C17-C18
20	A	1774	CLA	C8-C10-C11-C12
20	B	1737	CLA	C4-C3-C5-C6

There are no ring outliers.

222 monomers are involved in 3478 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	3007	CLA	2	0
20	3	3011	CLA	17	0
21	A	7010	LMU	8	0
21	L	1171	LMU	3	0
20	A	1766	CLA	5	0
20	I	1031	CLA	11	0
20	1	1192	CLA	9	0
20	2	1224	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	1213	CLA	1	0
20	A	1800	CLA	31	0
21	3	7005	LMU	3	0
25	C	1083	SF4	4	0
20	B	1748	CLA	14	0
20	2	1214	CLA	7	0
20	A	1787	CLA	26	0
20	B	1764	CLA	21	0
22	L	1169	BCR	48	0
20	1	1187	CLA	11	0
20	A	1790	CLA	16	0
20	I	1033	CLA	15	0
20	4	4014	CLA	11	0
22	B	1776	BCR	20	0
20	B	1745	CLA	12	0
21	A	7009	LMU	9	0
20	B	1735	CLA	33	0
20	B	1786	CLA	43	0
20	3	1212	CLA	9	0
20	B	1737	CLA	24	0
20	2	1212	CLA	18	0
21	2	7006	LMU	11	0
20	B	1736	CLA	9	0
20	3	1219	CLA	18	0
22	B	1779	BCR	46	0
20	1	1191	CLA	10	0
20	A	1799	CLA	7	0
20	B	1750	CLA	9	0
20	B	1769	CLA	25	0
20	2	1215	CLA	24	0
20	A	1785	CLA	17	0
20	A	1801	CLA	15	0
22	B	1774	BCR	8	0
20	A	1767	CLA	23	0
20	F	1156	CLA	13	0
20	3	1214	CLA	3	0
21	A	7031	LMU	4	0
20	B	1743	CLA	29	0
20	B	1746	CLA	23	0
21	A	7043	LMU	16	0
20	4	1196	CLA	34	0
22	3	1220	BCR	21	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	F	1155	CLA	1	0
21	1	1202	LMU	5	0
20	4	1207	CLA	5	0
21	2	1225	LMU	1	1
20	B	1741	CLA	6	0
20	A	1763	CLA	31	0
20	3	1215	CLA	17	0
20	A	1783	CLA	61	0
20	R	1055	CLA	6	0
22	A	1808	BCR	43	0
20	1	1189	CLA	11	0
20	A	1791	CLA	24	1
20	3	1218	CLA	25	0
20	B	1738	CLA	19	0
20	R	1054	CLA	11	0
20	B	1763	CLA	13	0
20	1	1200	CLA	11	0
21	A	7030	LMU	12	0
20	A	1760	CLA	29	0
20	B	1747	CLA	23	0
20	1	1196	CLA	6	0
20	A	1777	CLA	13	0
22	A	1807	BCR	62	0
21	B	1782	LMU	1	0
20	B	1758	CLA	34	0
20	B	1755	CLA	62	0
21	A	7040	LMU	4	0
20	A	1788	CLA	40	0
20	A	1769	CLA	22	0
20	B	1759	CLA	34	0
20	B	1770	CLA	24	0
21	R	1057	LMU	5	0
20	G	1099	CLA	6	0
22	A	1804	BCR	22	0
20	3	1217	CLA	8	0
20	A	1811	CLA	20	0
20	A	1813	CLA	33	0
20	4	1206	CLA	2	0
20	B	1753	CLA	40	0
20	1	1198	CLA	20	0
20	B	1787	CLA	50	0
20	A	1759	CLA	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	7041	LMU	9	0
21	K	1086	LMU	6	0
20	K	1146	CLA	11	0
20	L	1505	CLA	3	0
20	A	1789	CLA	20	0
20	1	1199	CLA	2	0
20	4	1200	CLA	3	0
20	4	1198	CLA	25	0
20	1	1188	CLA	7	0
20	2	1218	CLA	7	0
20	B	1751	CLA	16	0
21	A	7032	LMU	28	0
22	A	1803	BCR	41	0
22	I	1032	BCR	47	0
20	2	1223	CLA	4	0
20	H	1079	CLA	19	0
20	B	1754	CLA	23	0
22	A	1805	BCR	48	0
20	B	1766	CLA	3	0
22	B	1778	BCR	30	0
20	B	1771	CLA	24	0
21	A	7017	LMU	3	0
22	A	1806	BCR	36	0
20	A	1796	CLA	63	0
20	B	1785	CLA	22	0
20	L	1167	CLA	18	0
21	A	7034	LMU	1	0
21	A	7019	LMU	2	0
20	A	1762	CLA	18	0
20	J	1044	CLA	41	0
21	2	7003	LMU	3	0
20	A	1798	CLA	29	0
21	A	7028	LMU	4	0
20	4	1209	CLA	5	0
21	A	7016	LMU	42	0
23	B	1773	PQN	33	0
20	L	1166	CLA	7	0
20	3	1216	CLA	7	0
20	4	1204	CLA	8	0
20	J	1043	CLA	29	0
21	A	7027	LMU	6	0
20	1	1193	CLA	6	2

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	1208	CLA	8	0
20	A	1776	CLA	47	0
20	B	1757	CLA	21	0
20	A	1765	CLA	25	0
20	F	1157	CLA	13	0
20	4	1205	CLA	3	0
20	2	1217	CLA	9	0
20	B	1762	CLA	28	0
22	B	1777	BCR	31	0
20	A	1793	CLA	35	0
25	C	1082	SF4	5	0
20	4	1202	CLA	4	0
21	R	1056	LMU	19	0
20	4	1197	CLA	2	0
21	A	7039	LMU	19	0
20	4	1201	CLA	25	0
20	B	1772	CLA	2	0
20	A	1773	CLA	11	0
20	3	3008	CLA	17	0
20	B	1767	CLA	15	0
20	B	1742	CLA	9	0
20	A	1816	CLA	35	0
20	A	1774	CLA	31	0
20	B	1749	CLA	18	0
20	2	1220	CLA	74	0
22	L	1170	BCR	13	0
20	B	1756	CLA	46	0
20	A	1792	CLA	22	0
20	A	1768	CLA	4	0
20	A	1781	CLA	85	0
20	A	1786	CLA	9	0
21	A	1809	LMU	4	0
24	B	1783	LMG	30	0
20	K	1142	CLA	20	2
20	2	1222	CLA	14	0
20	4	1199	CLA	22	0
20	B	1739	CLA	22	0
20	B	1740	CLA	20	0
20	K	1085	CLA	26	0
22	B	1780	BCR	53	0
20	1	1194	CLA	5	0
20	A	1764	CLA	26	0

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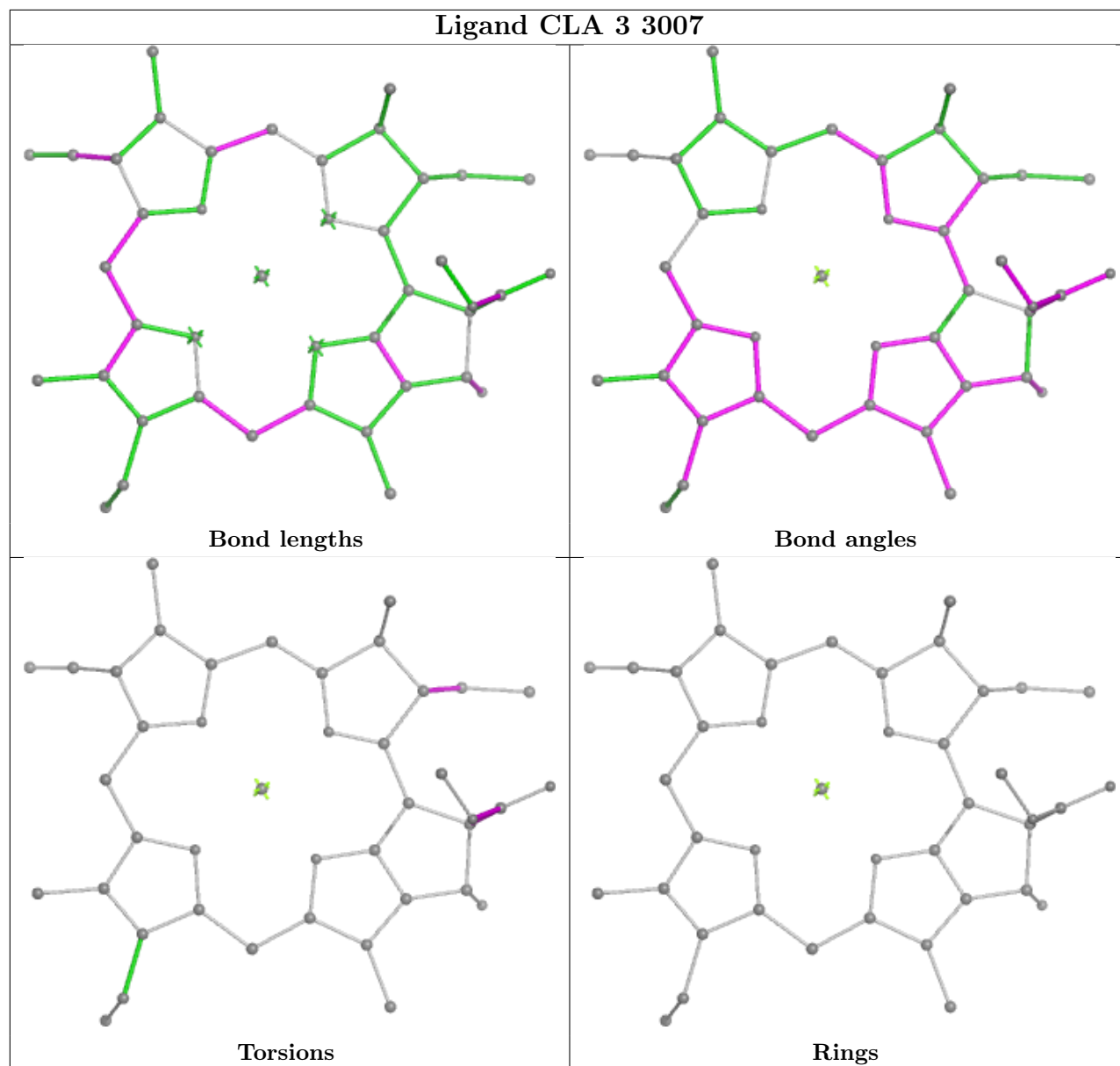
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1765	CLA	20	0
20	A	1771	CLA	13	0
20	A	1770	CLA	27	0
20	A	1779	CLA	35	0
20	A	1815	CLA	19	0
20	A	1794	CLA	21	0
20	B	1760	CLA	10	0
20	B	1768	CLA	48	0
22	B	1775	BCR	20	0
20	L	1168	CLA	12	0
21	A	1810	LMU	4	0
21	A	7023	LMU	26	0
20	J	1045	CLA	45	0
20	A	1784	CLA	18	0
20	B	1752	CLA	14	0
21	A	7033	LMU	19	0
21	A	7037	LMU	24	0
20	A	1761	CLA	32	0
20	A	1817	CLA	9	0
20	B	1744	CLA	20	0
20	A	1772	CLA	35	0
20	1	1197	CLA	20	0
20	2	1213	CLA	13	0
20	A	1780	CLA	17	0
20	K	3009	CLA	3	0
21	A	7042	LMU	35	0
21	A	7013	LMU	9	0
20	B	1761	CLA	12	0
21	A	7020	LMU	21	0
21	A	7036	LMU	19	0
20	A	1778	CLA	11	0
21	1	7004	LMU	10	0
22	B	1781	BCR	17	0
20	1	1190	CLA	5	0
21	A	7026	LMU	21	0
23	A	1802	PQN	12	0
21	A	7022	LMU	11	0
21	A	7025	LMU	1	0
21	A	7021	LMU	24	0
25	B	1784	SF4	18	0
20	A	1795	CLA	40	0
20	A	1797	CLA	35	0

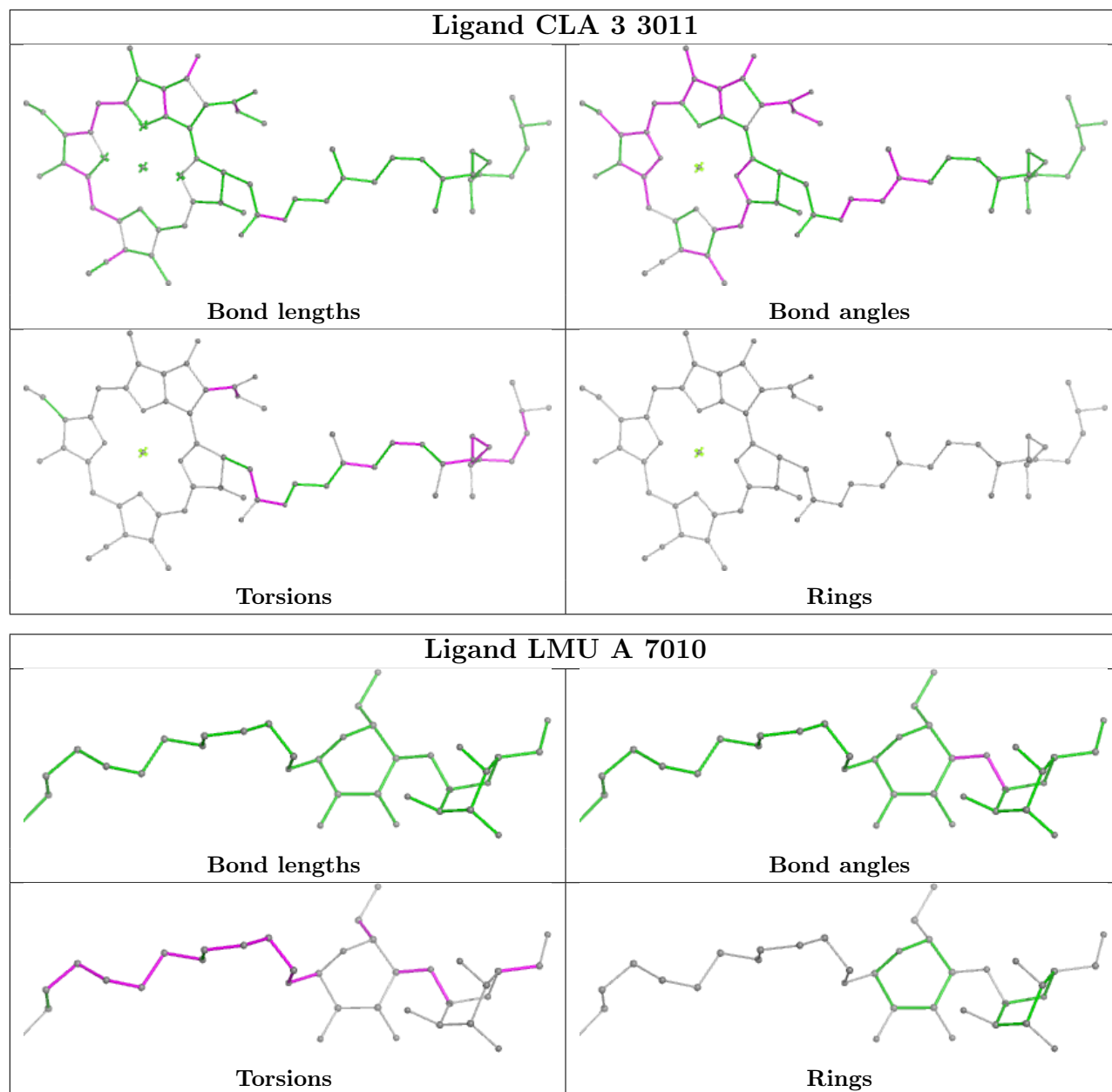
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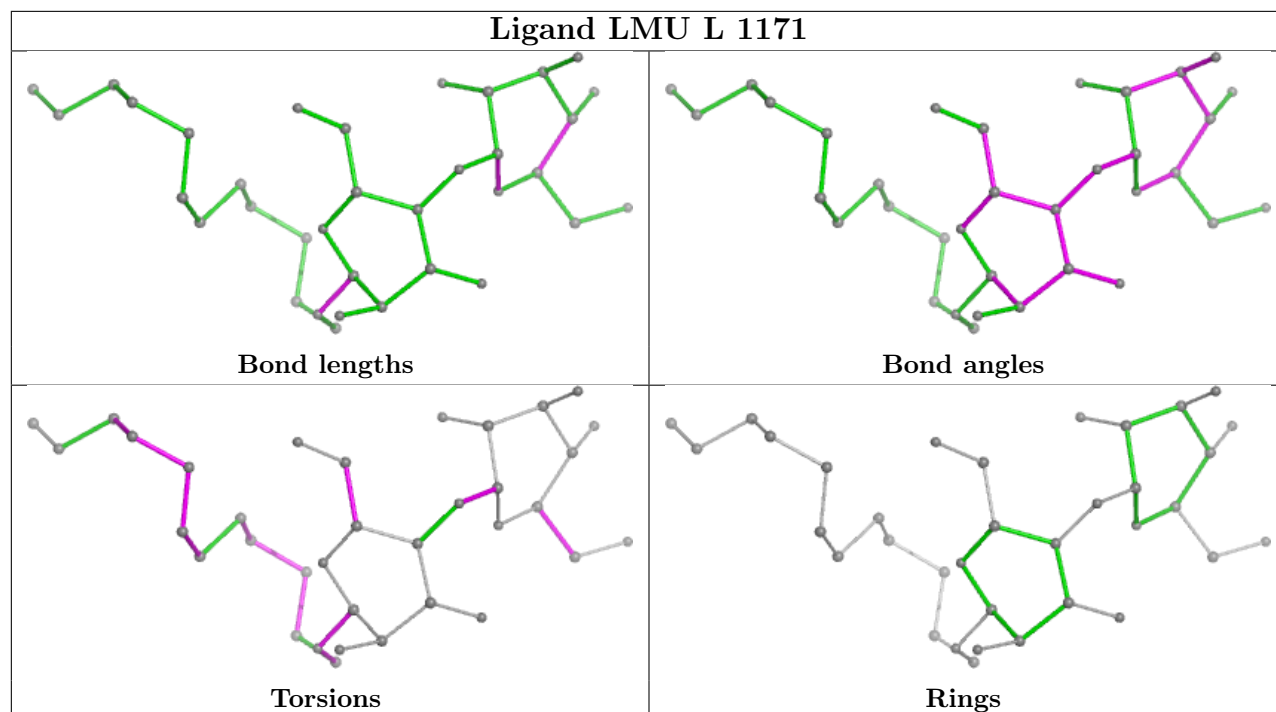
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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20	A	1812	CLA	35	0
21	A	7038	LMU	13	0
20	A	1782	CLA	81	0

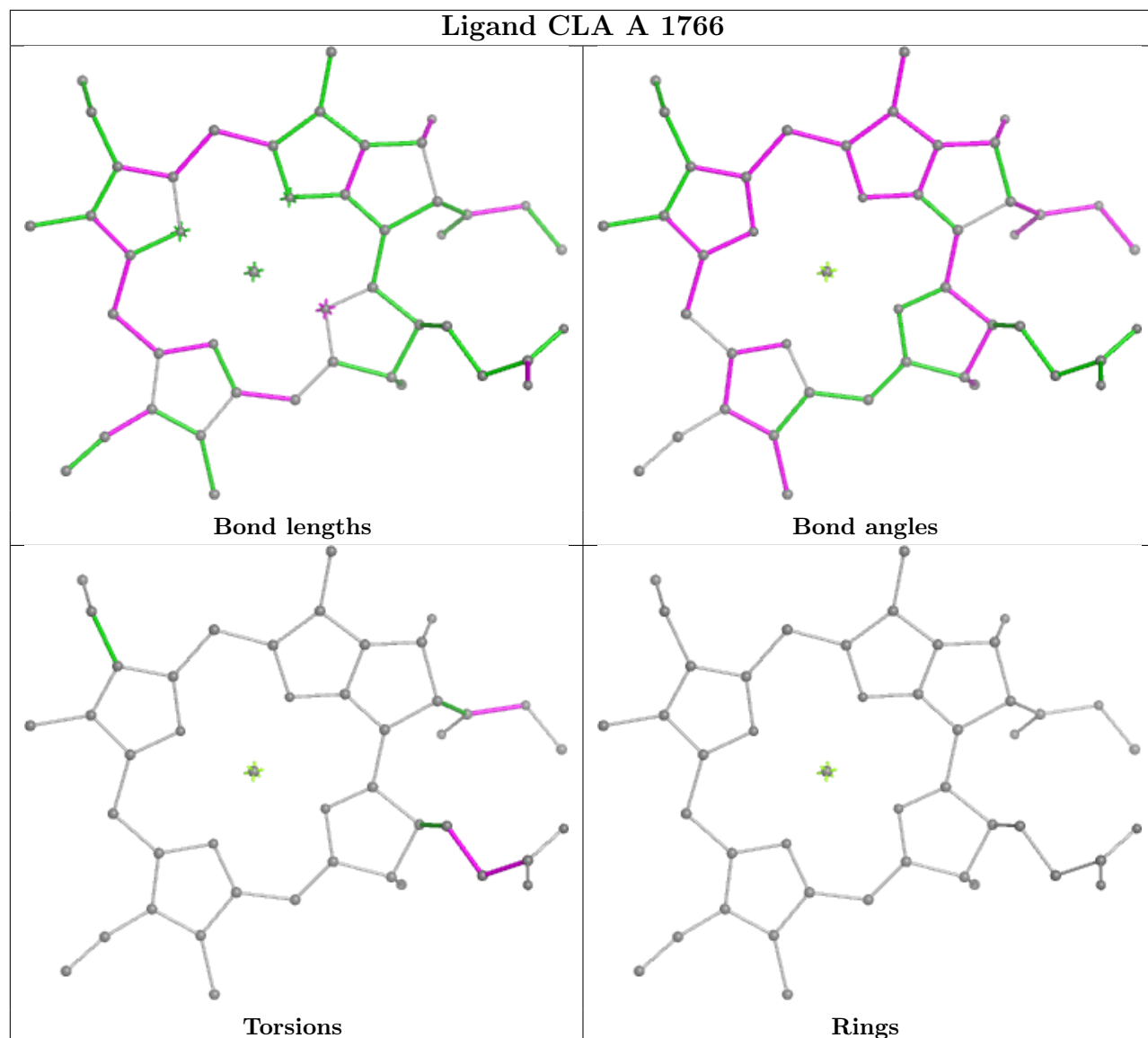
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

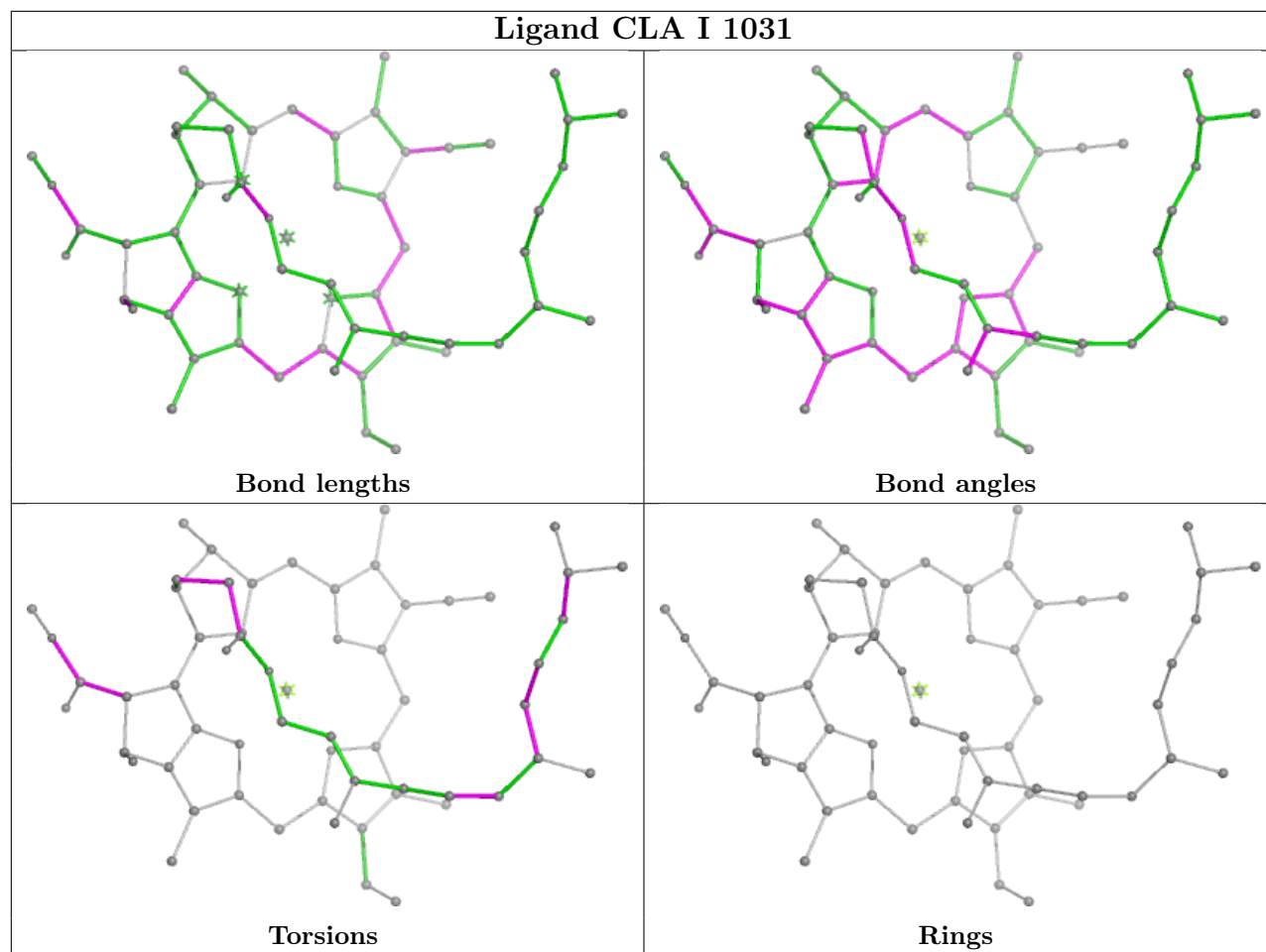






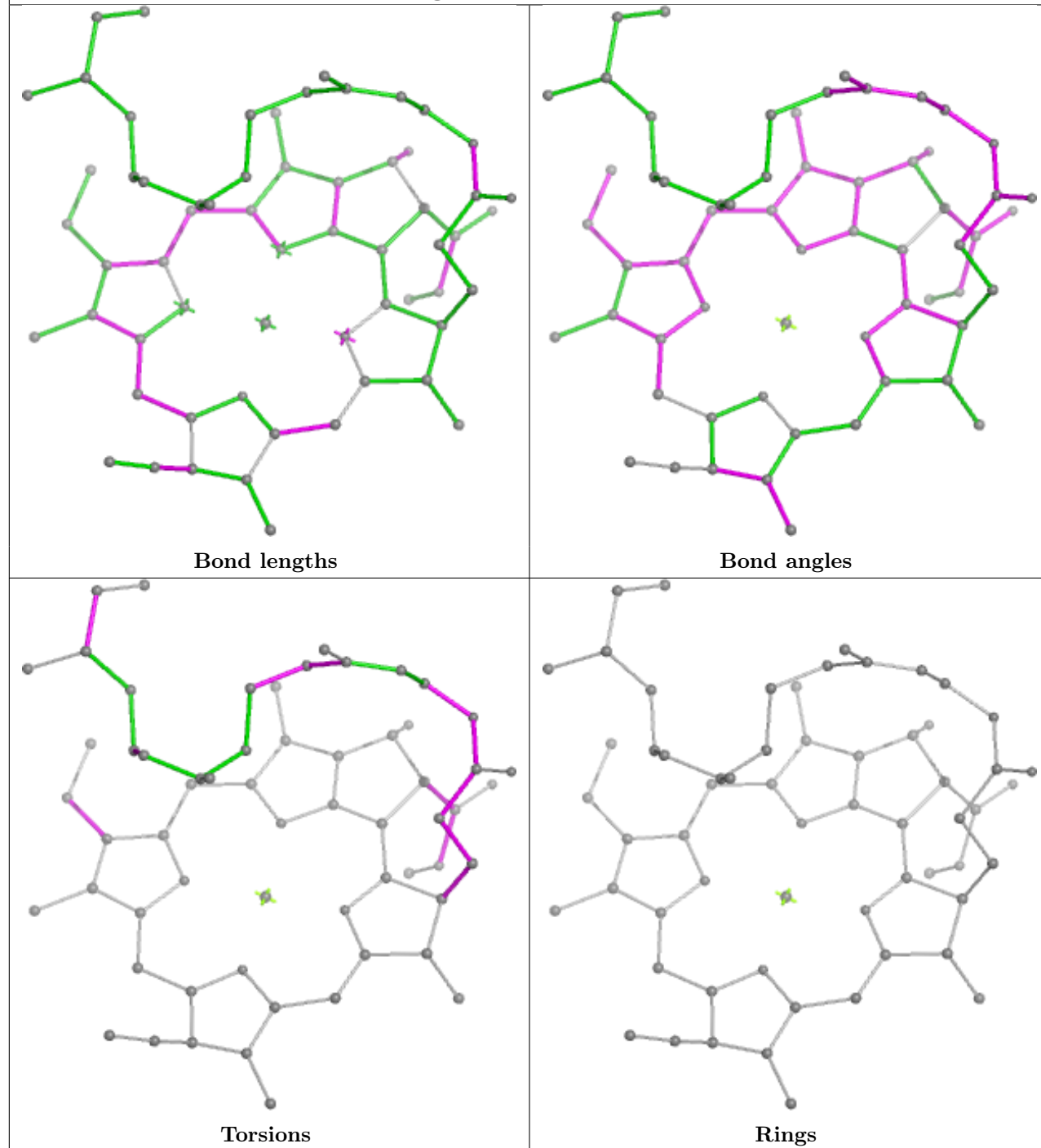
## Ligand CLA A 1766

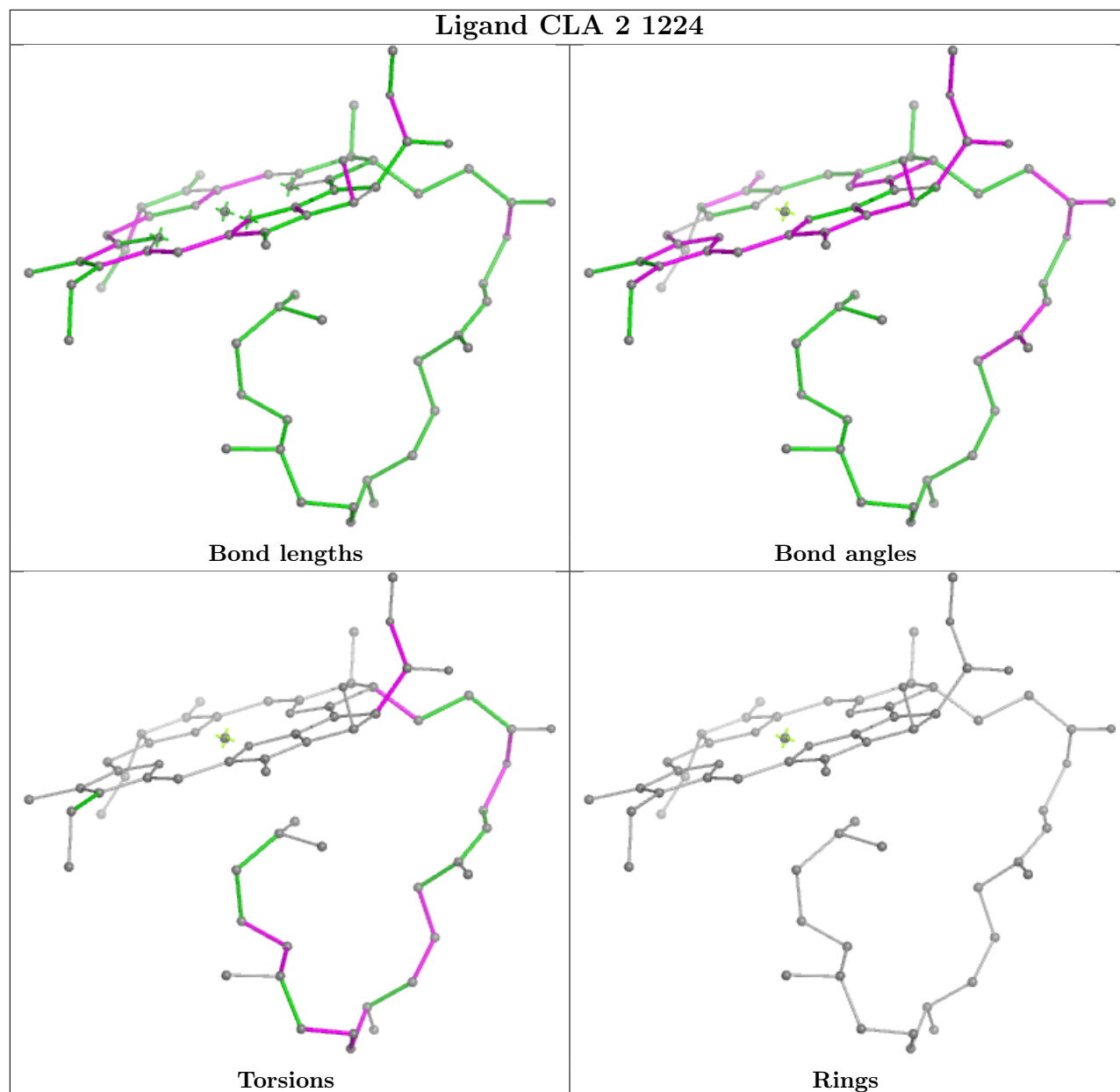


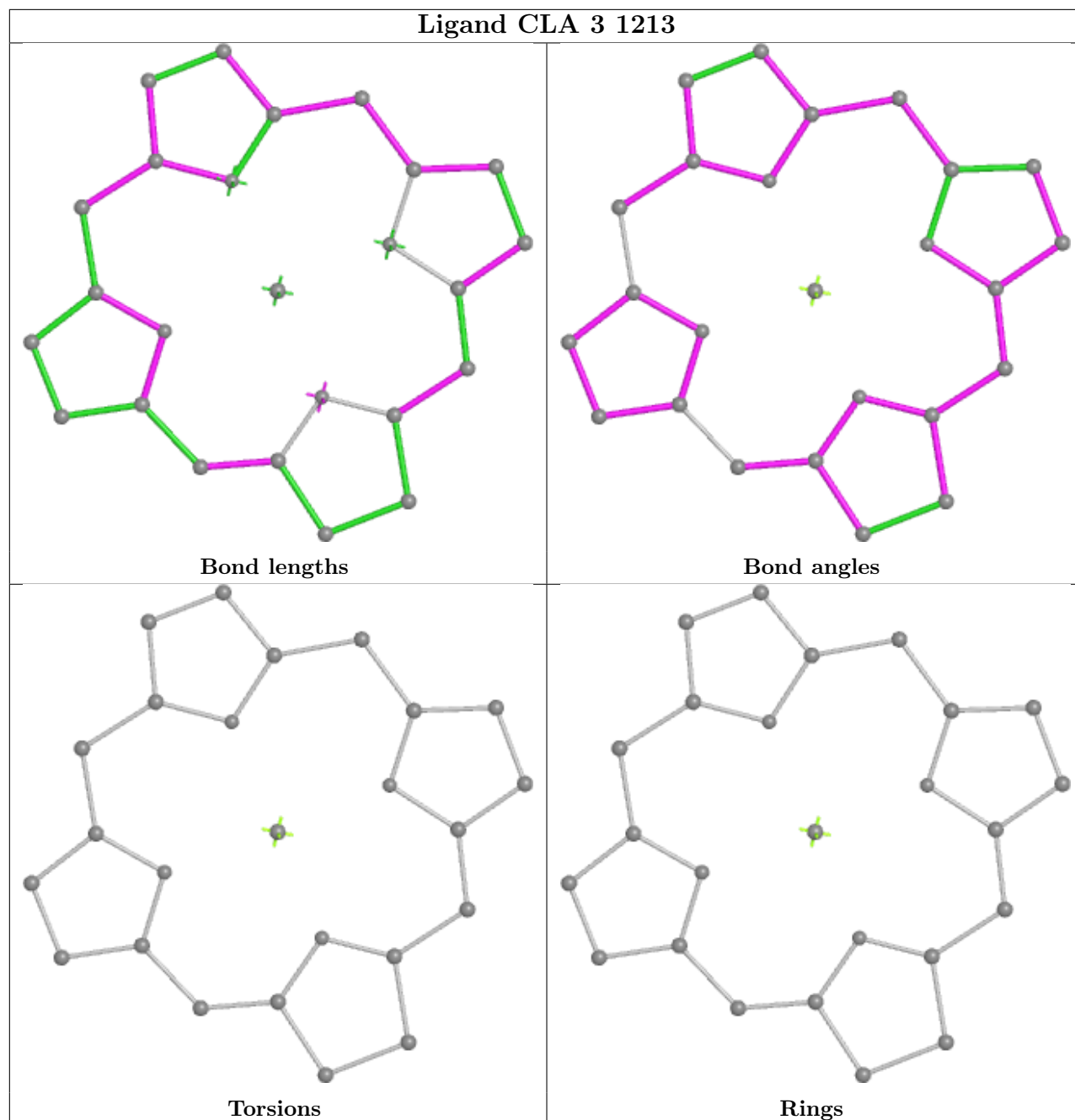


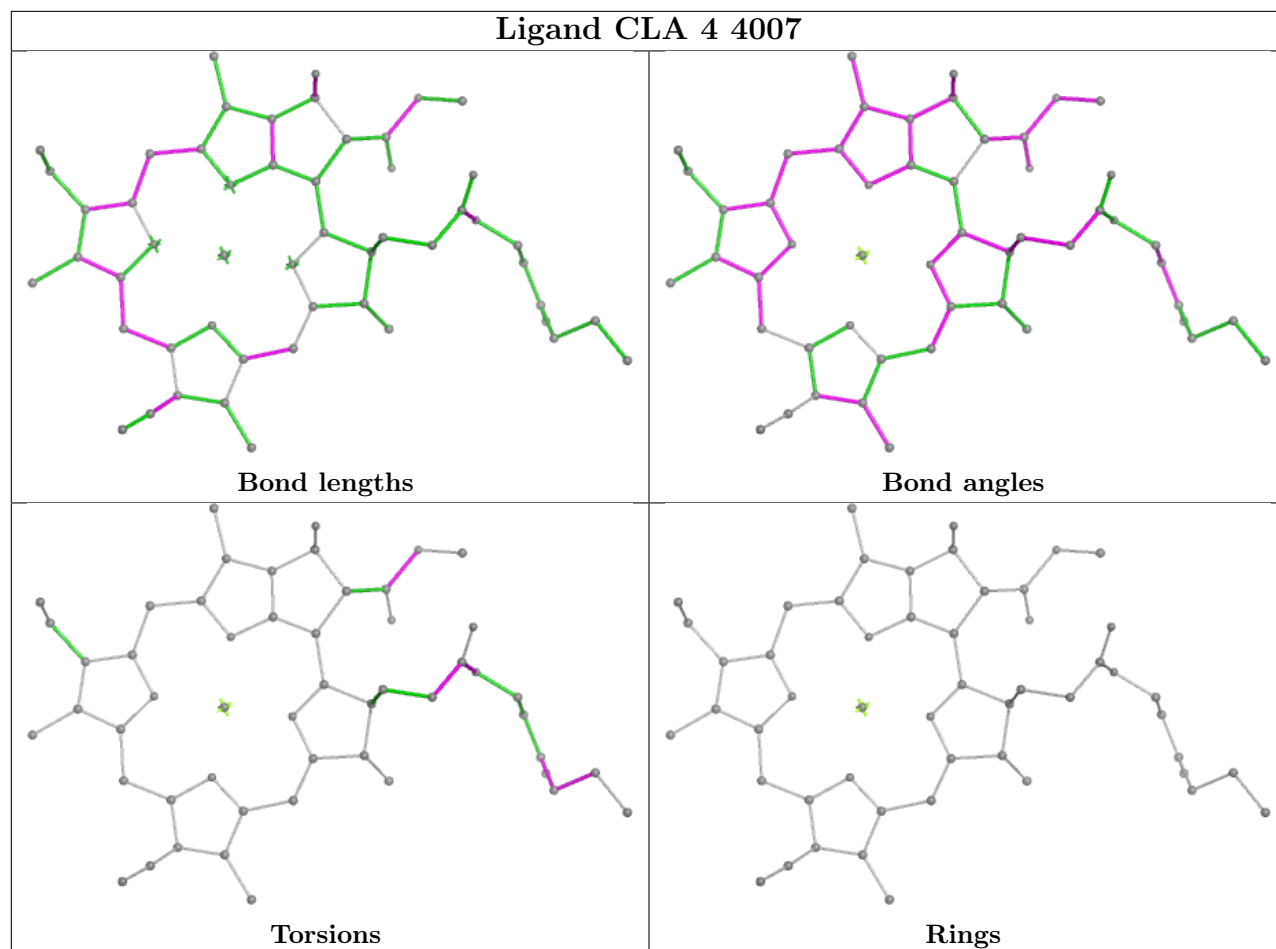


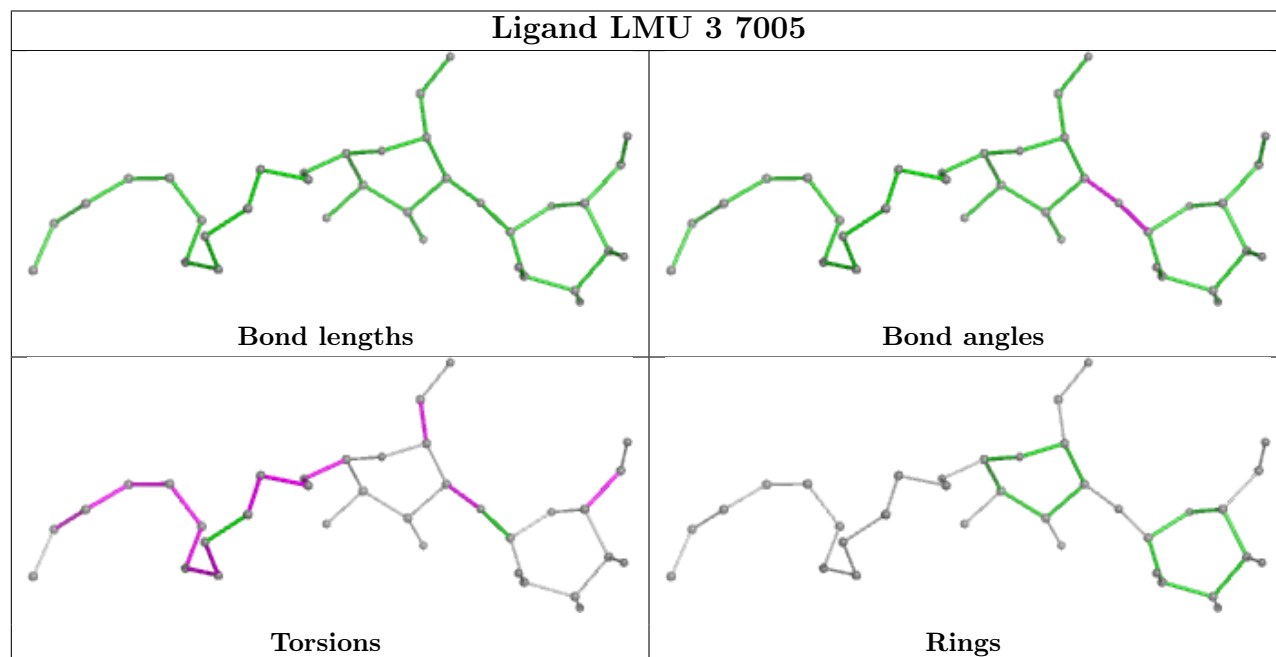
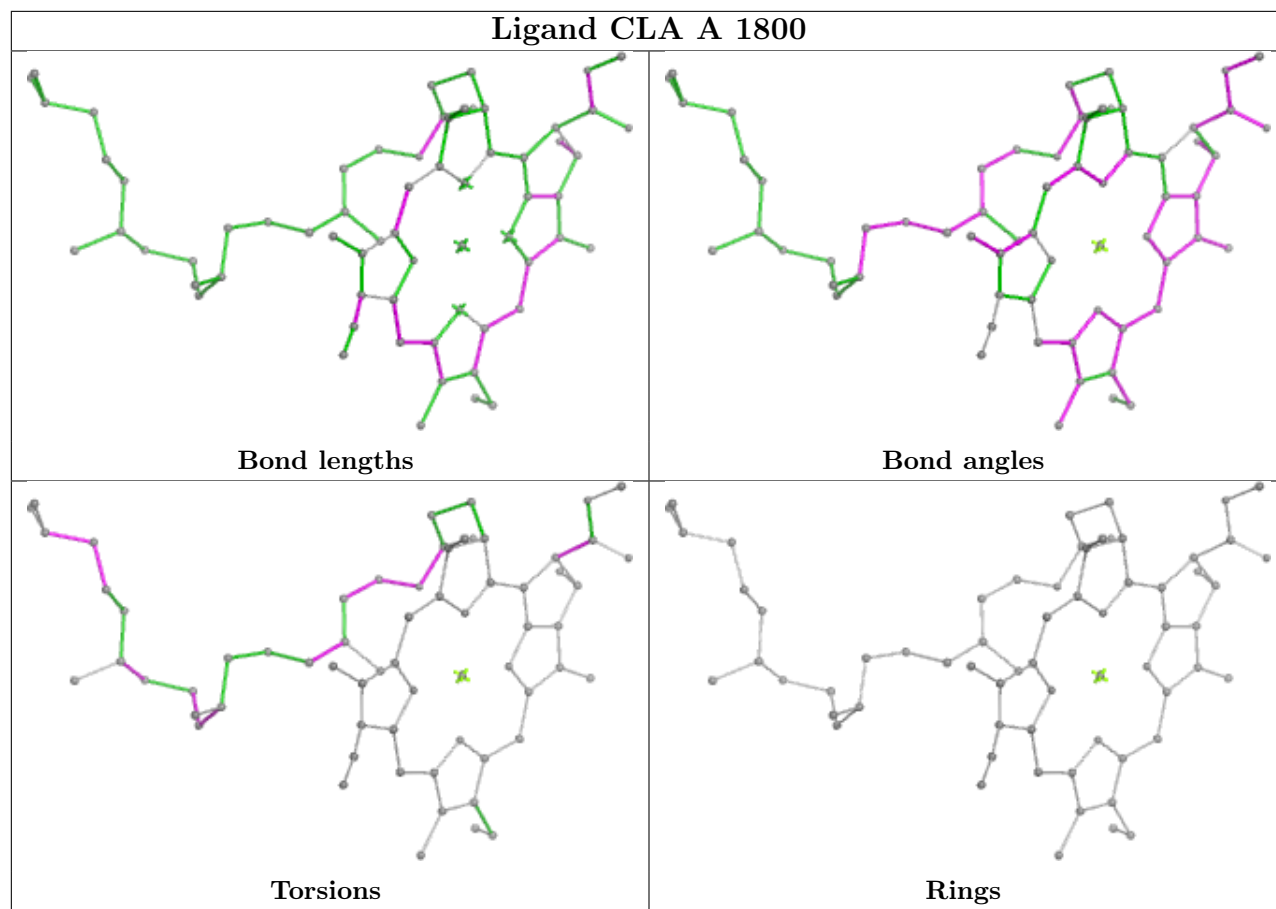
## Ligand CLA 1 1192

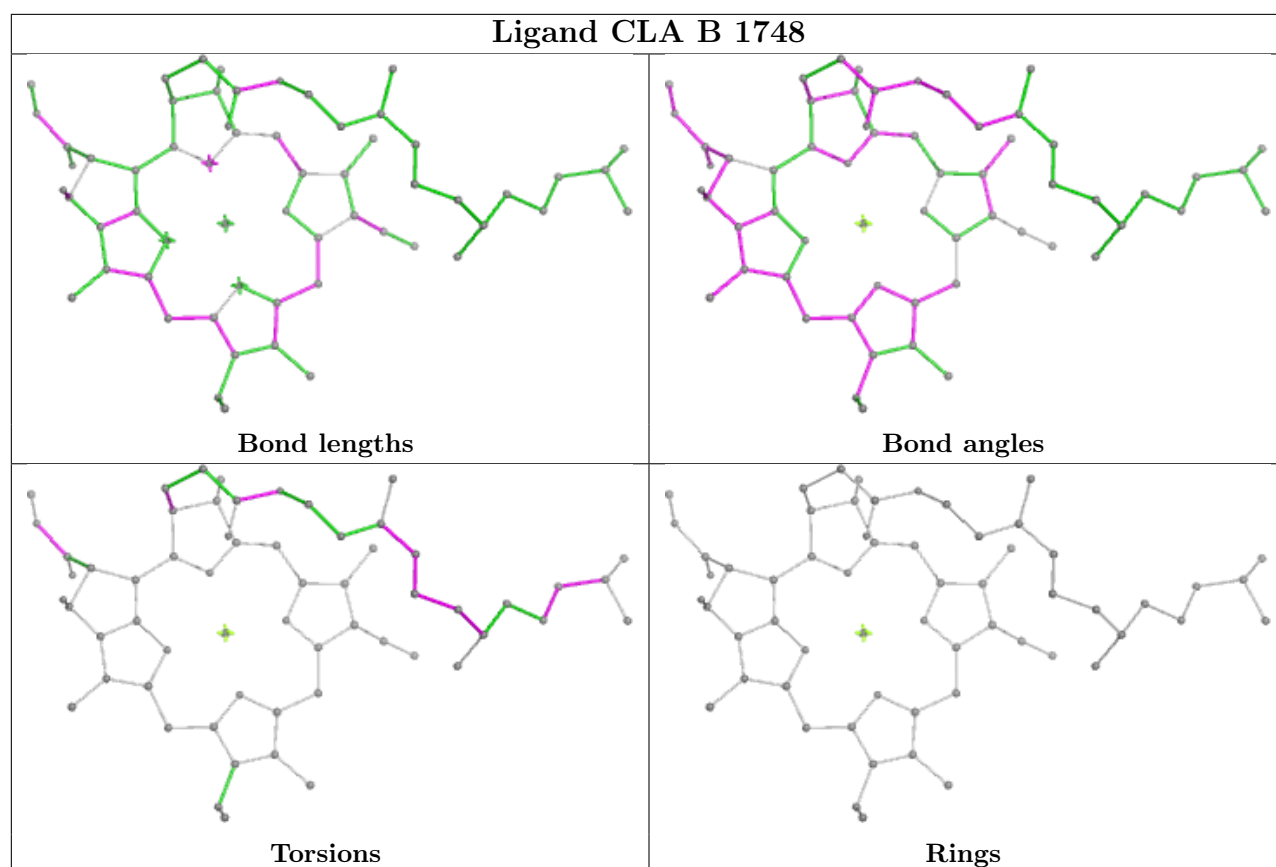




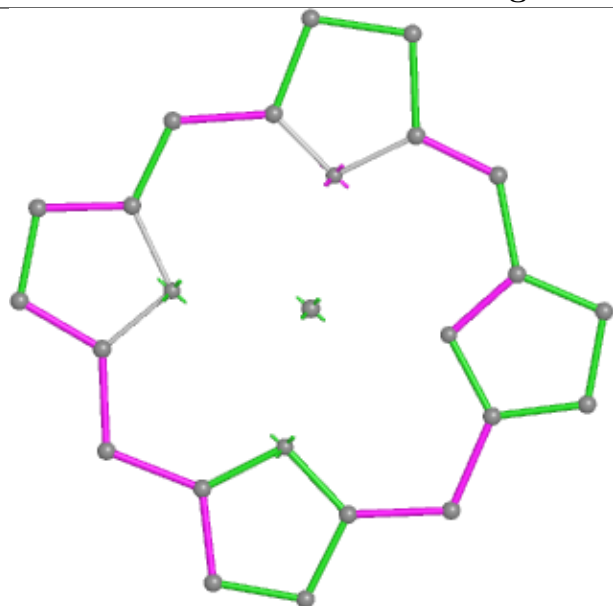




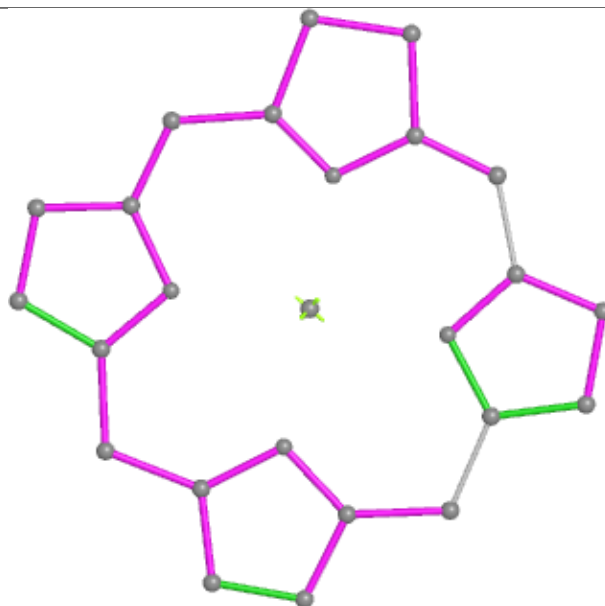




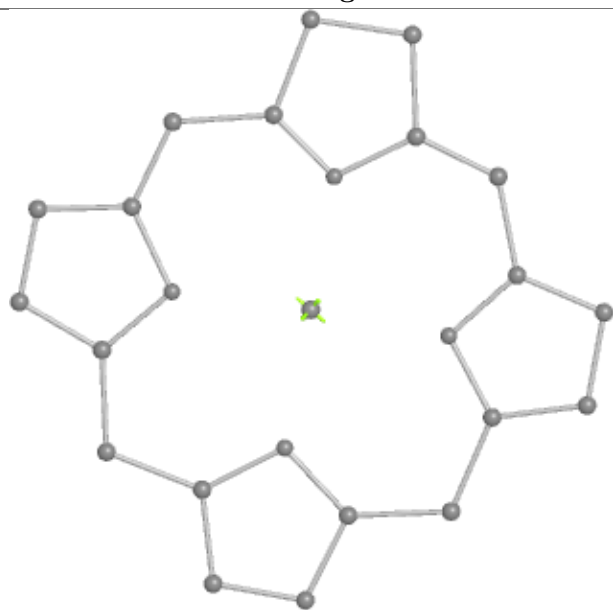
## Ligand CLA 2 1214



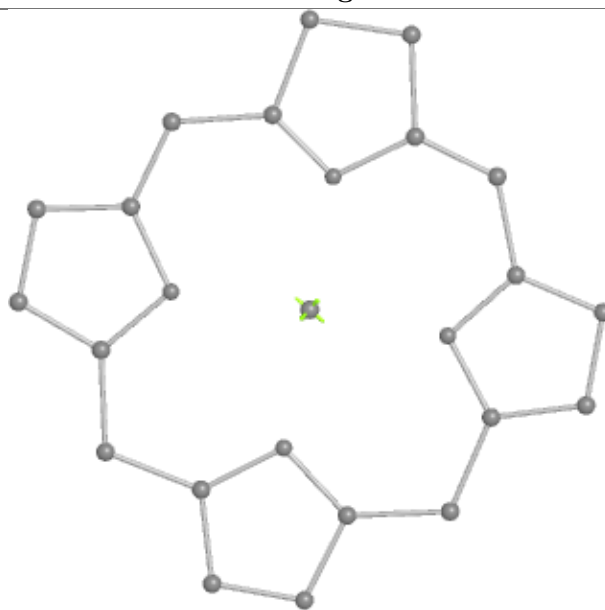
### Bond lengths



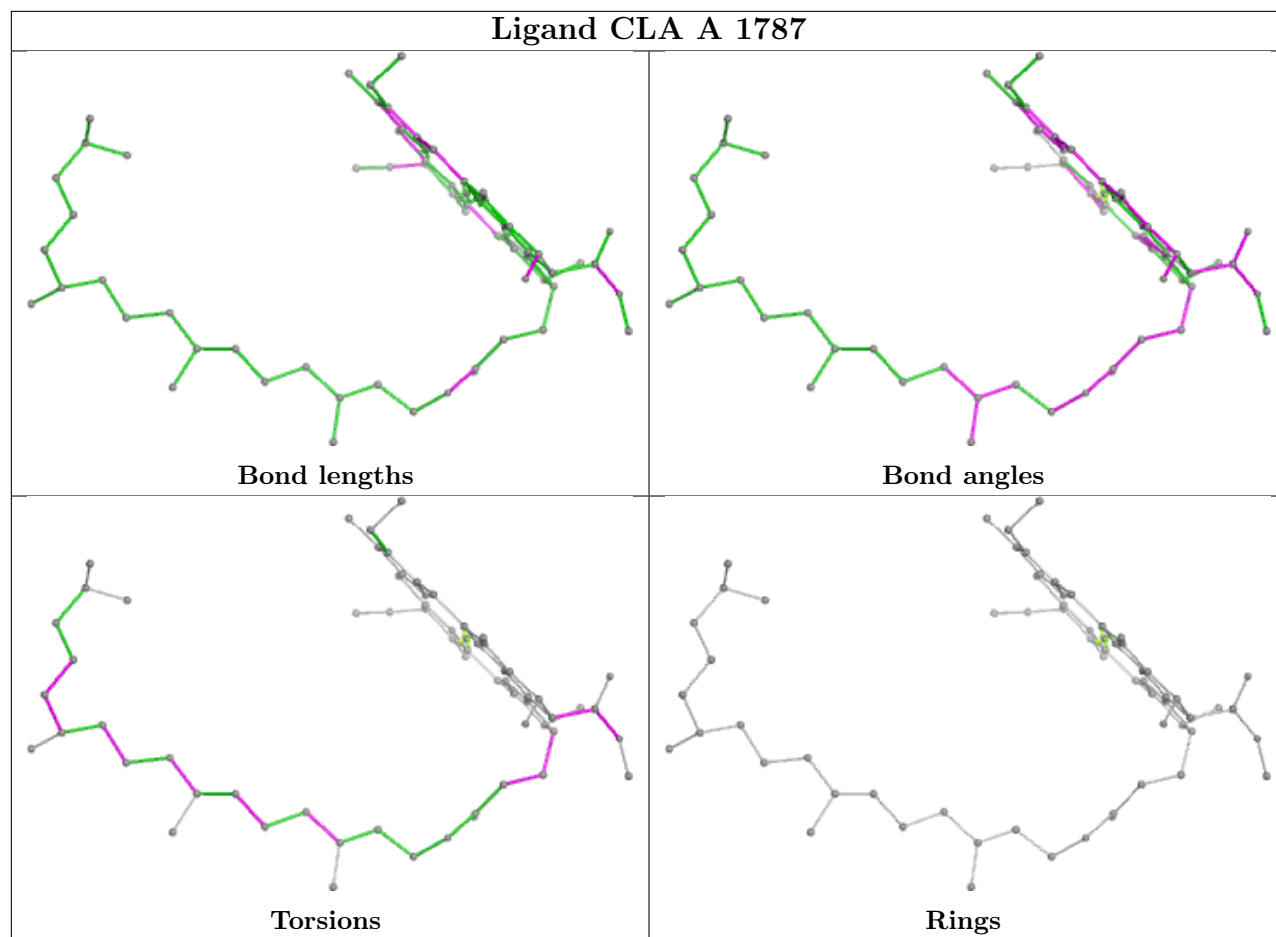
### Bond angles



## Torsions

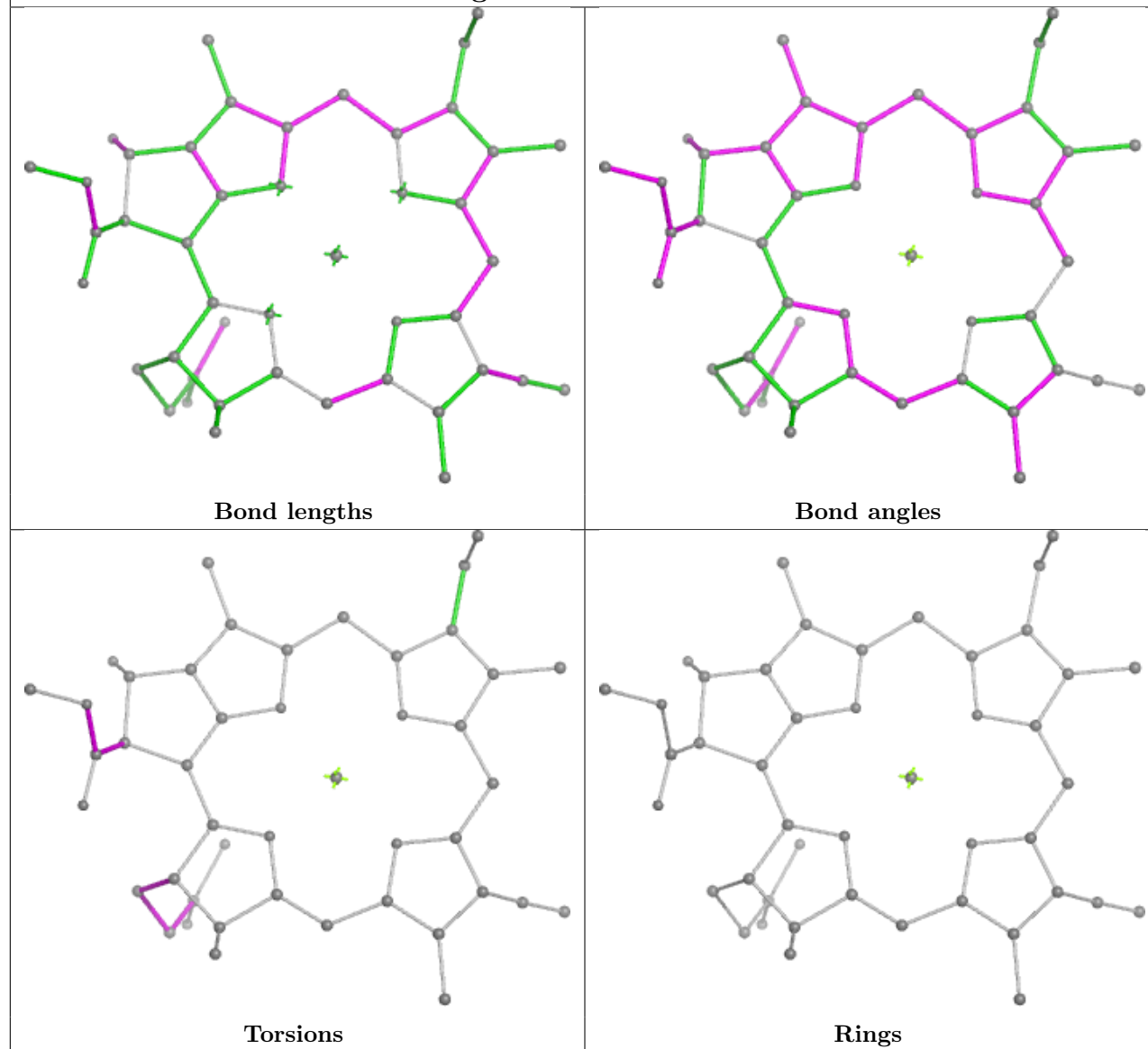


# Rings

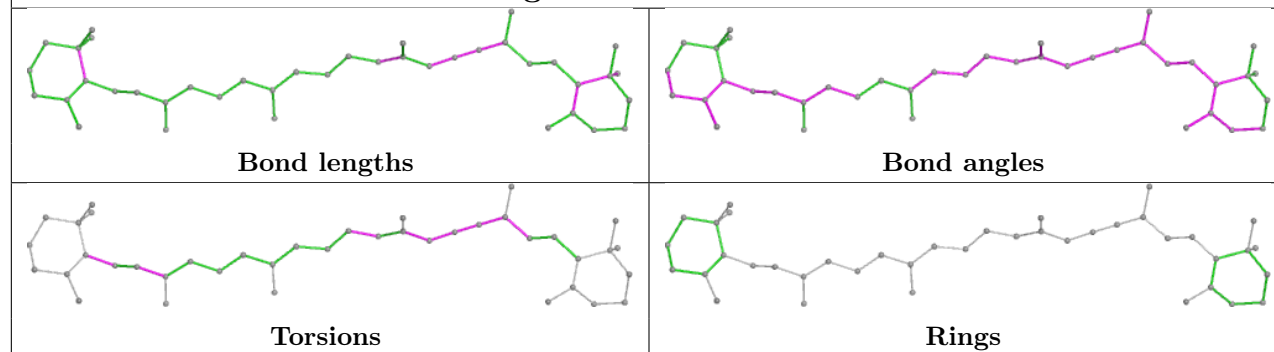


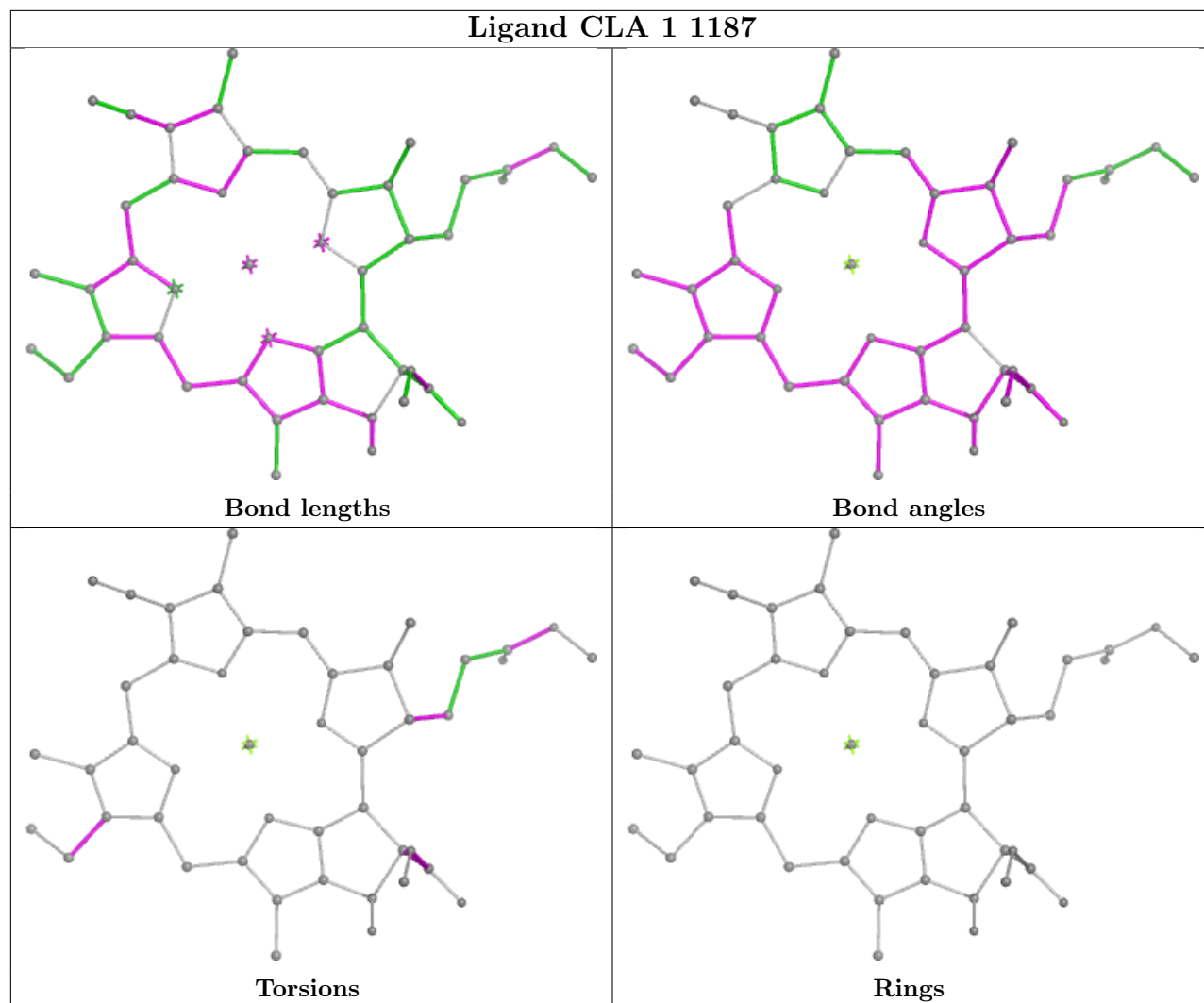


## Ligand CLA B 1764

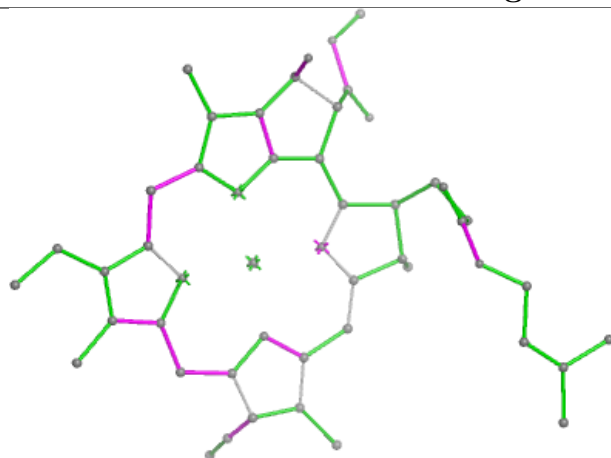


## Ligand BCR L 1169

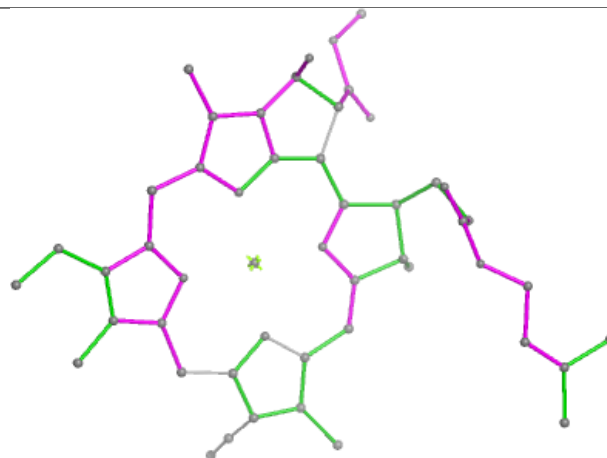




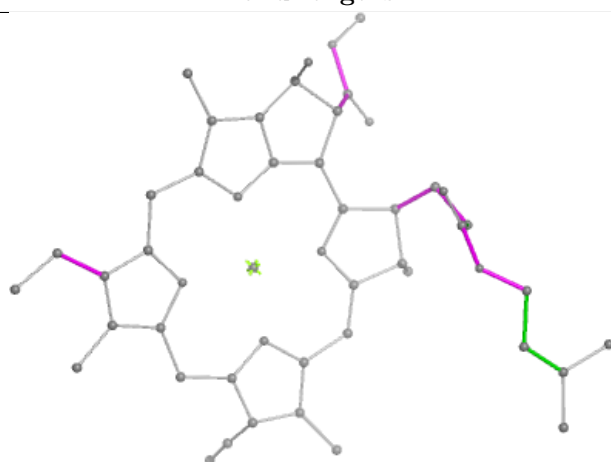
## Ligand CLA A 1790



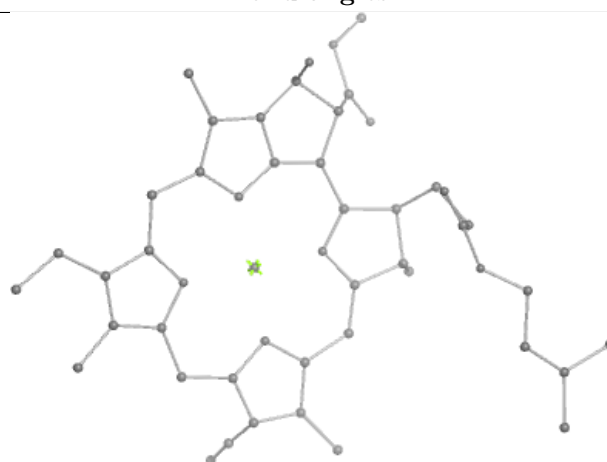
Bond lengths



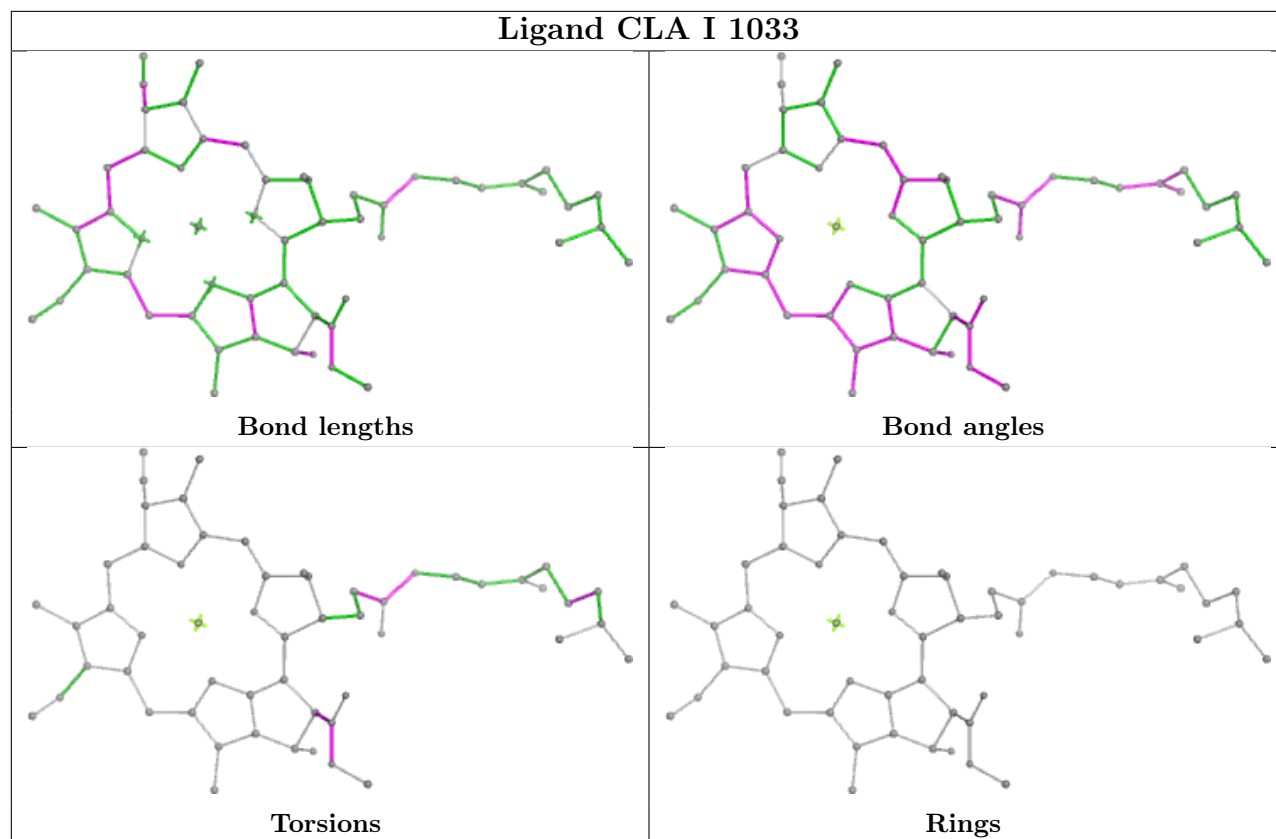
Bond angles

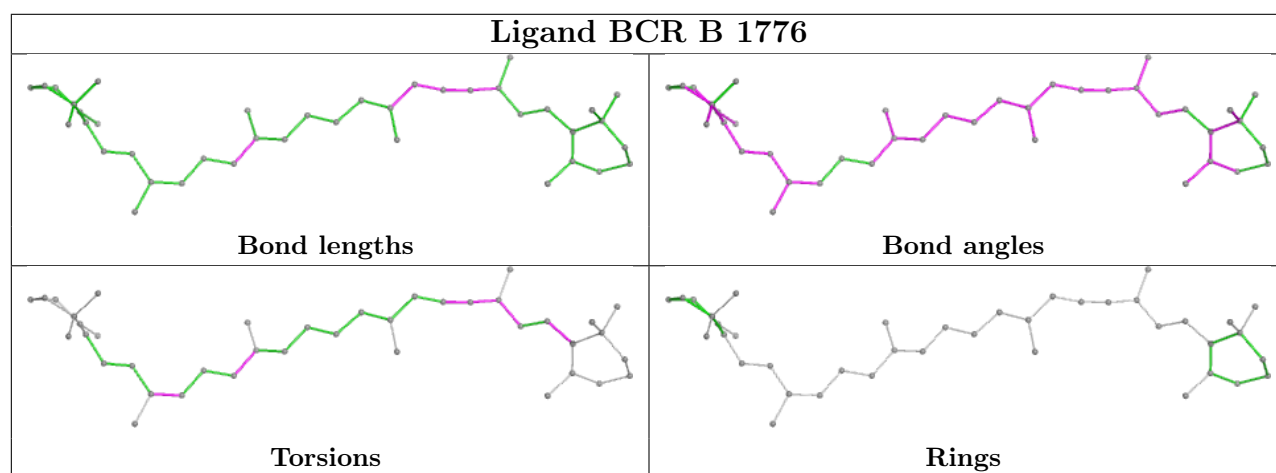
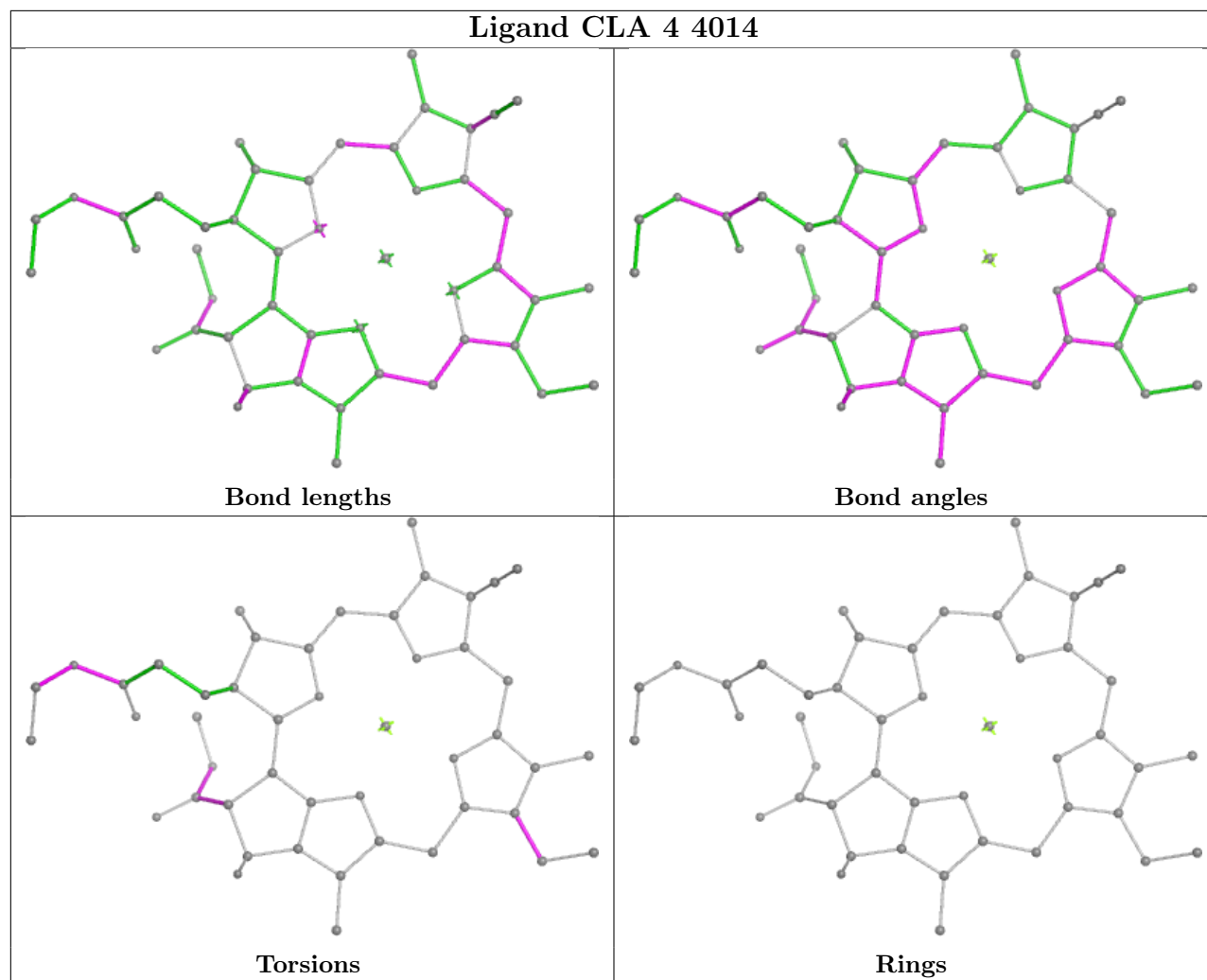


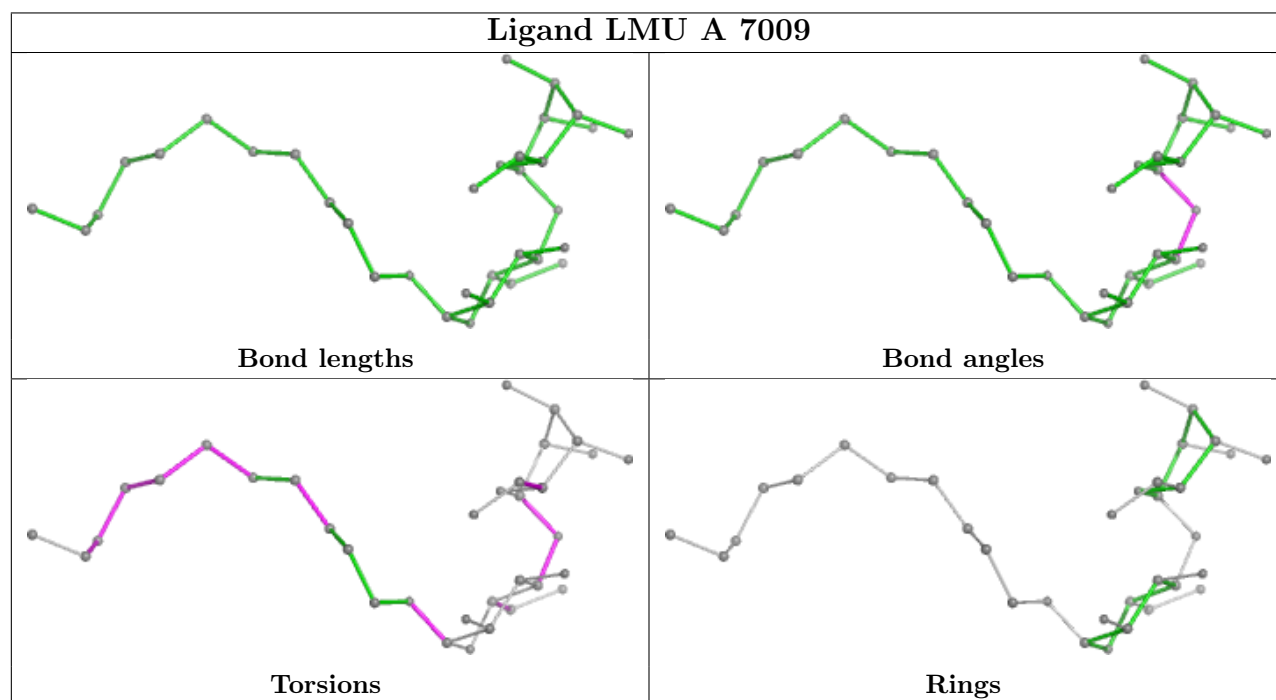
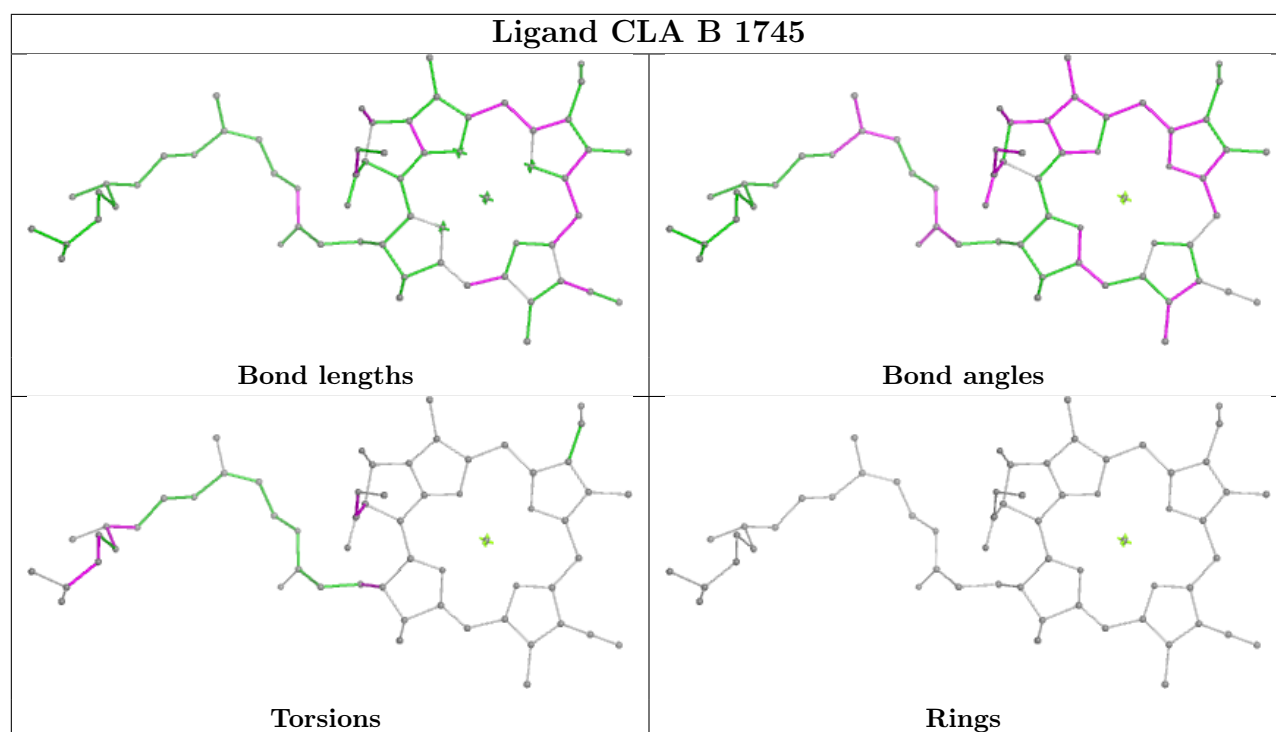
Torsions

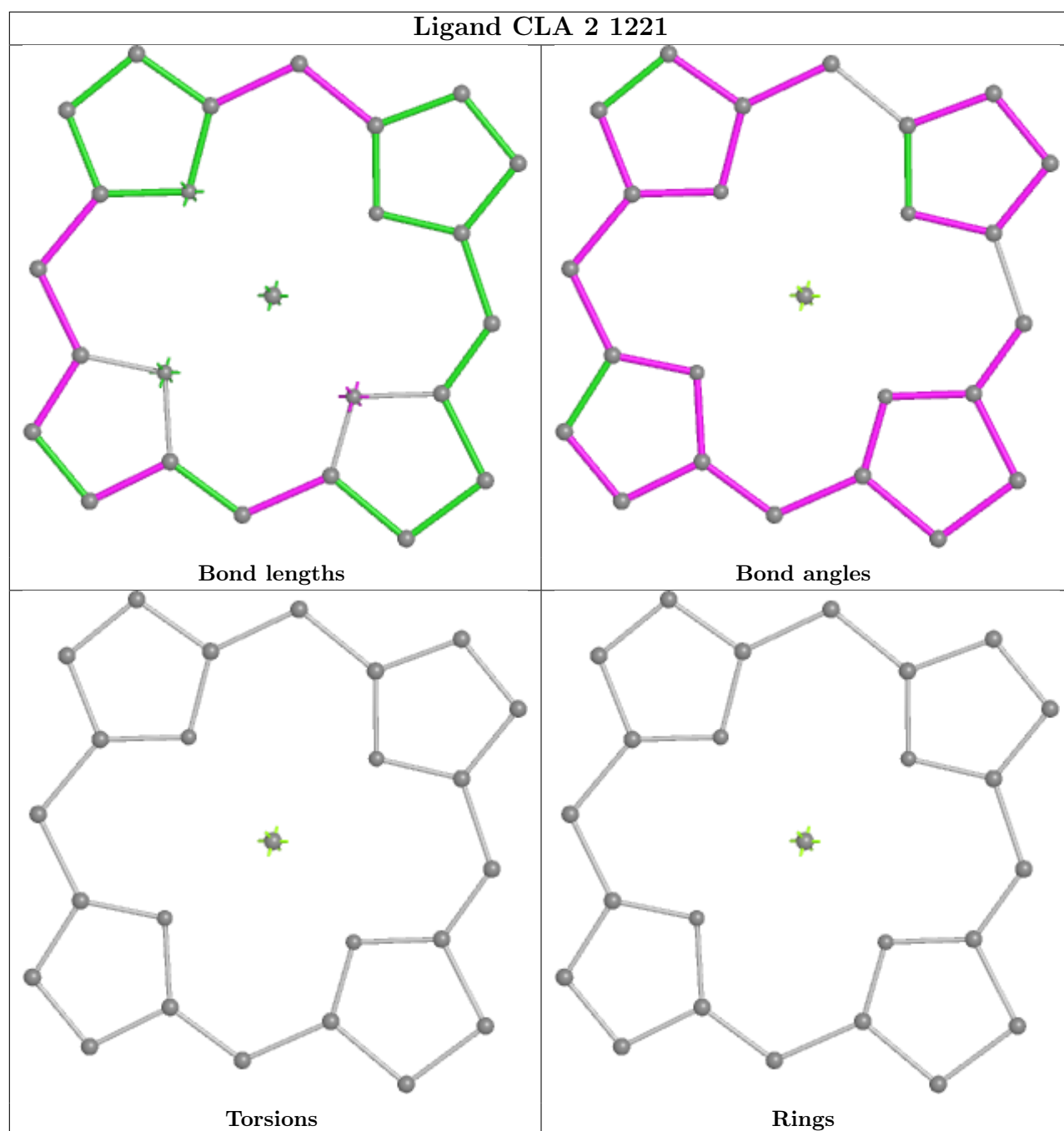


Rings

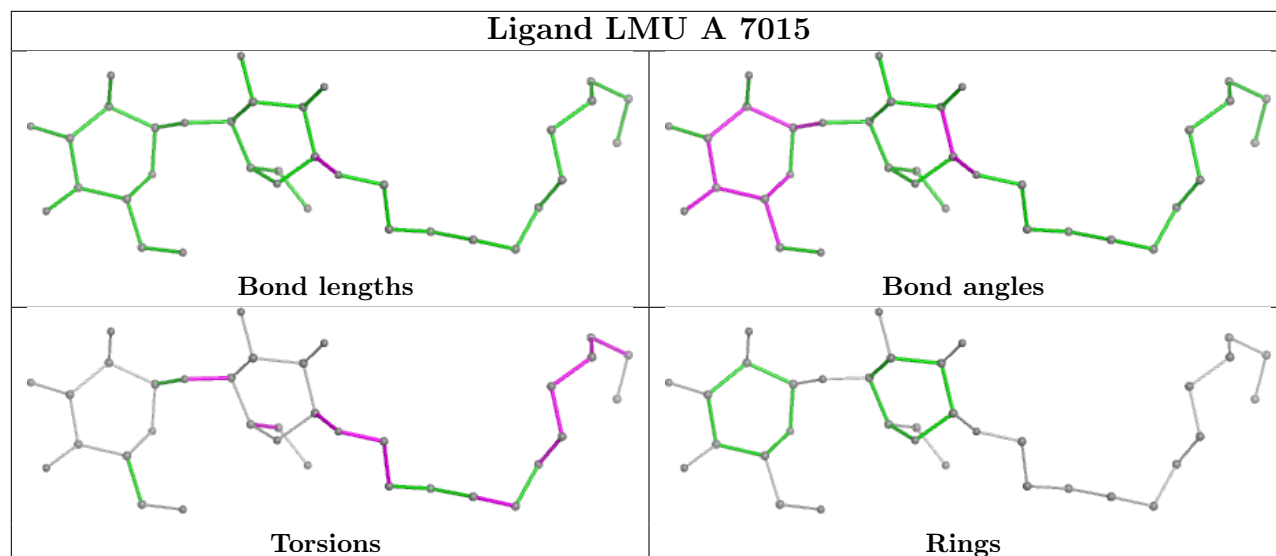




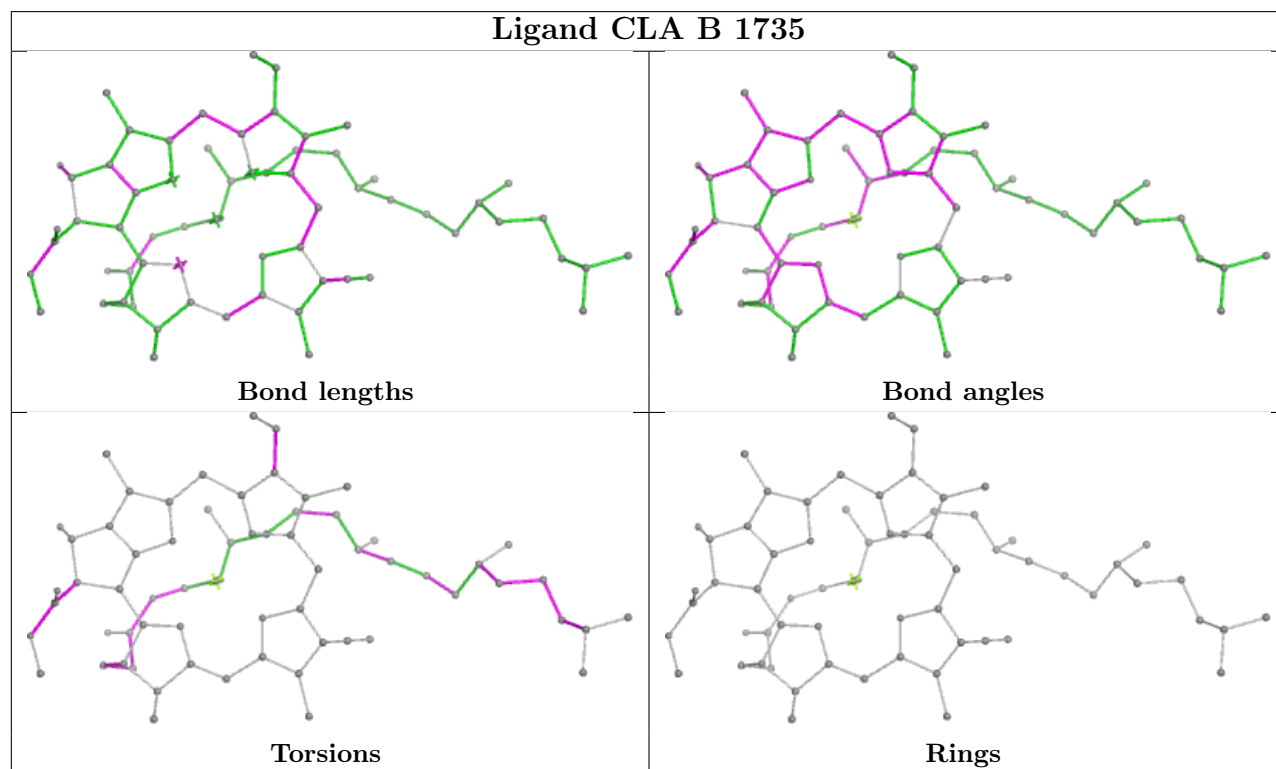




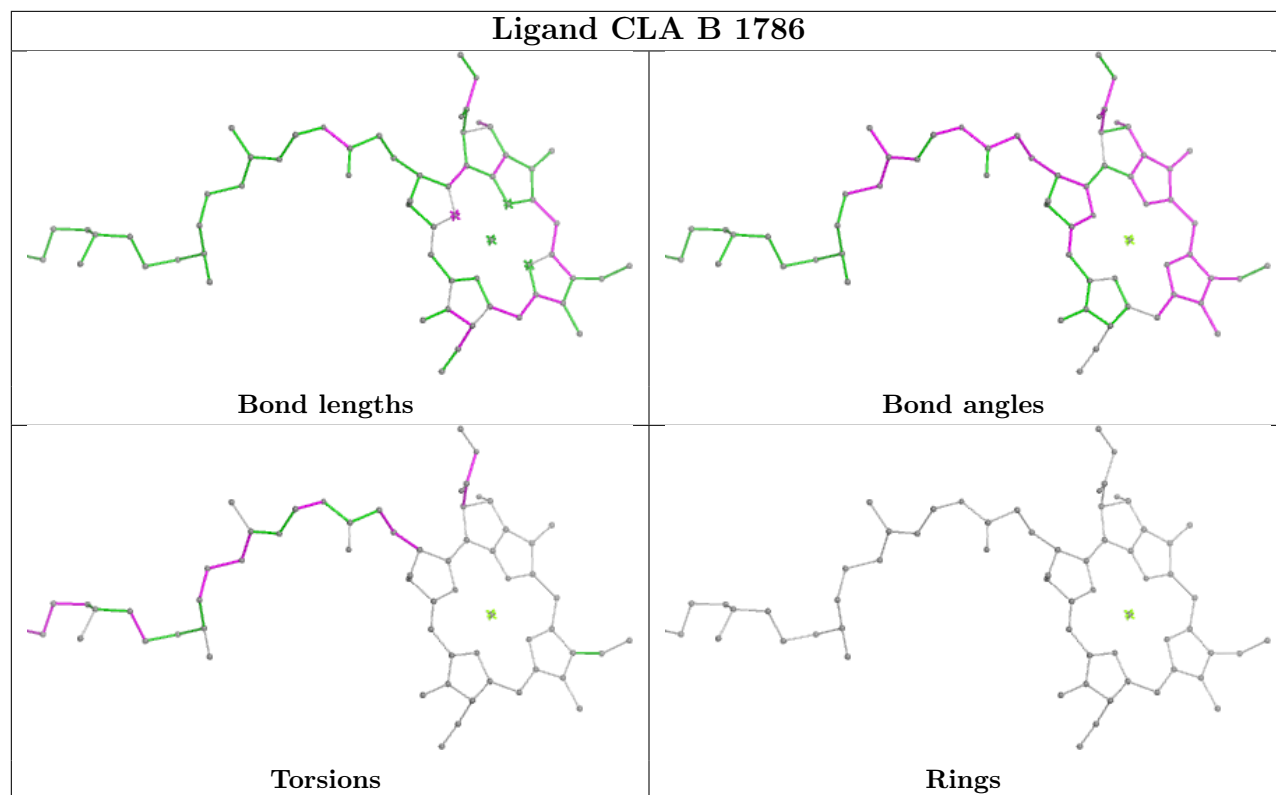
## Ligand LMU A 7015

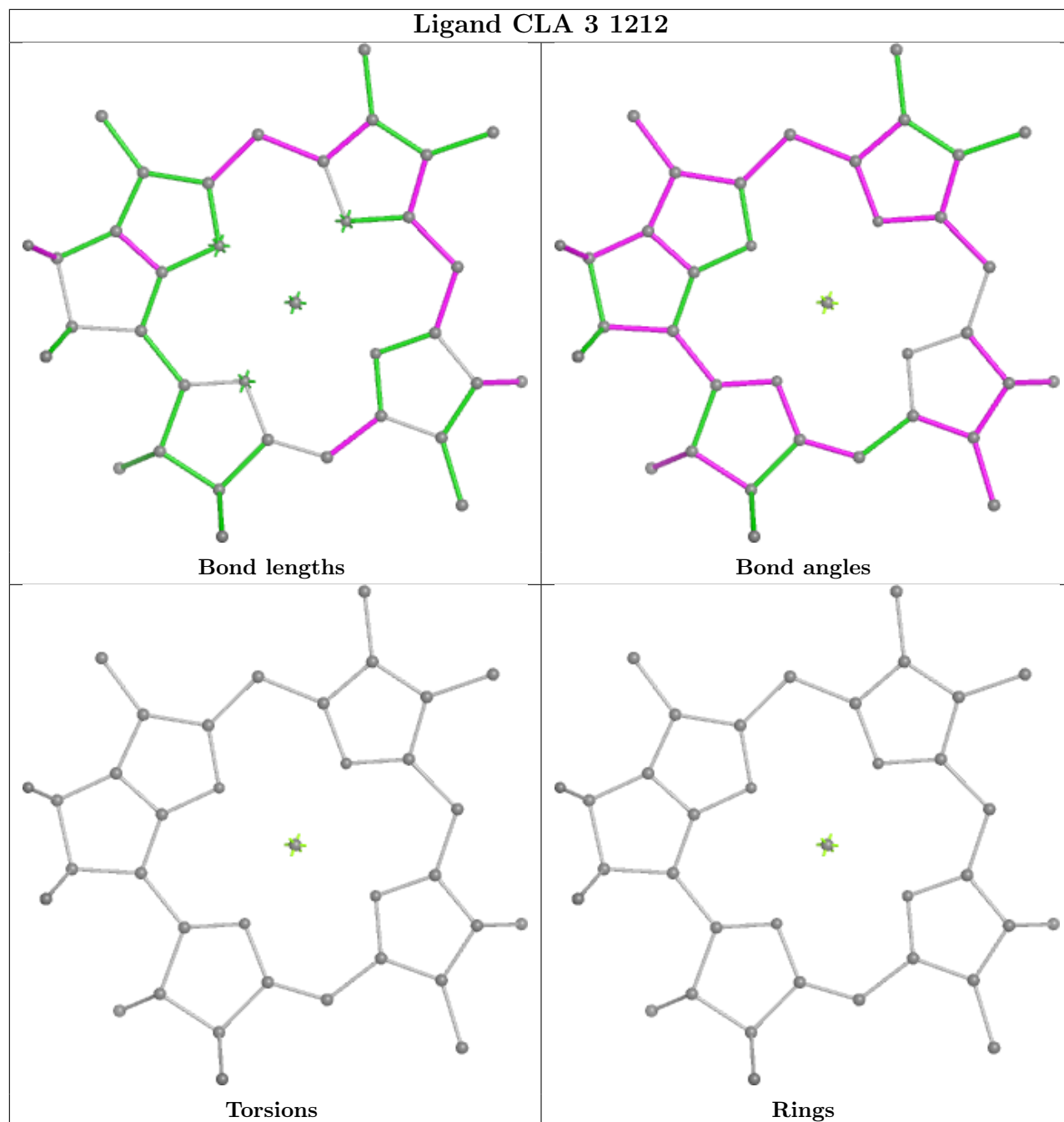


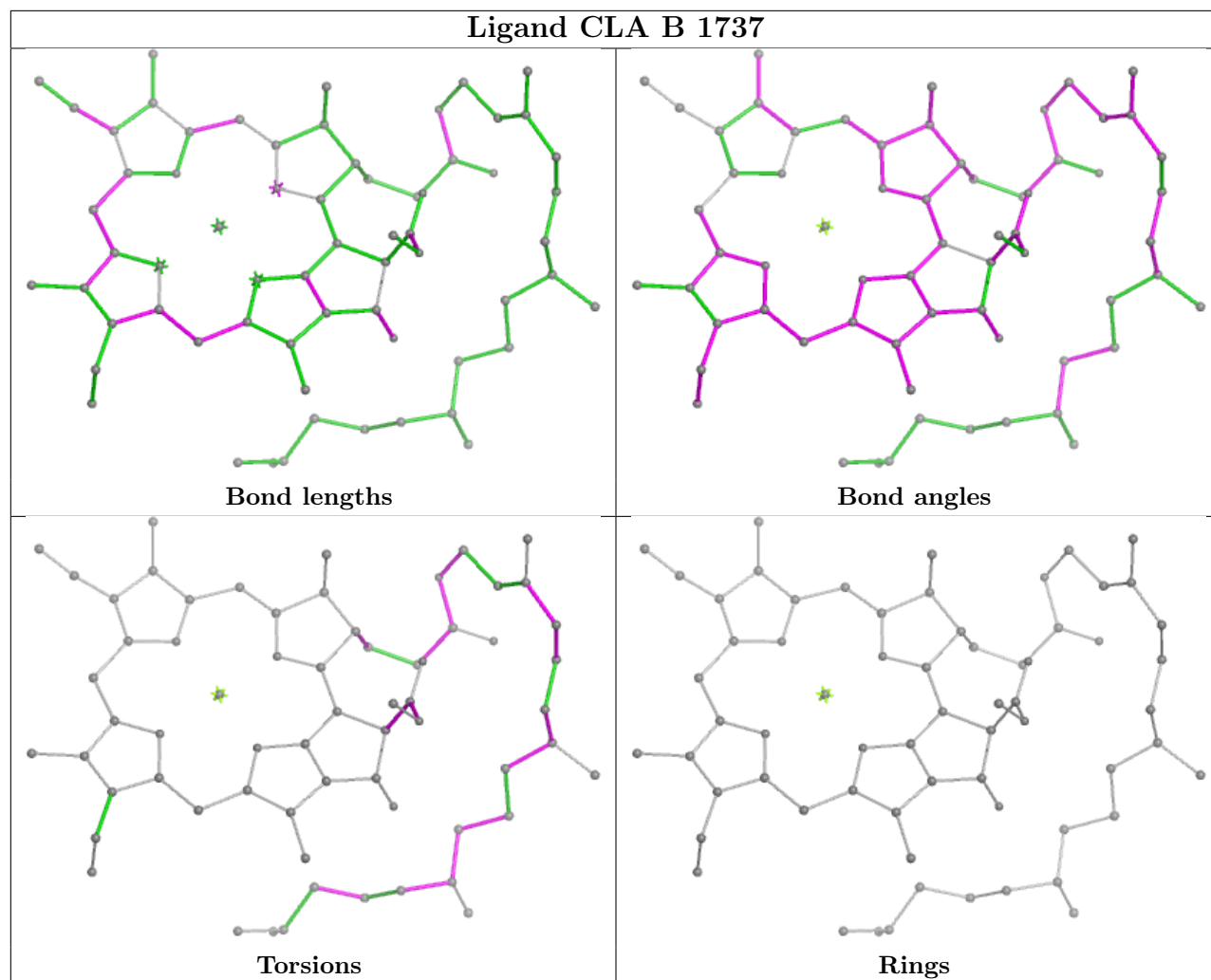
## Ligand CLA B 1735

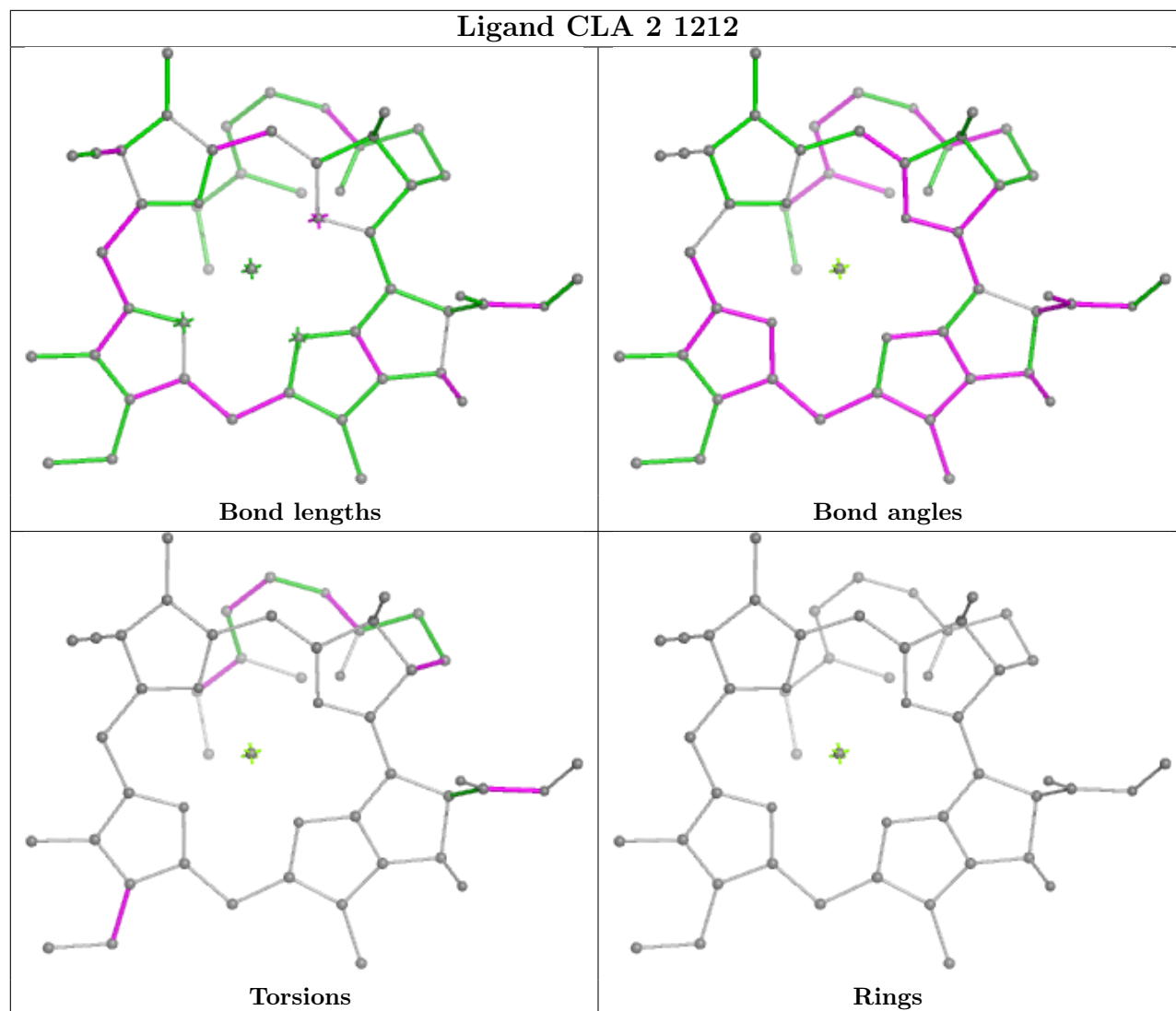


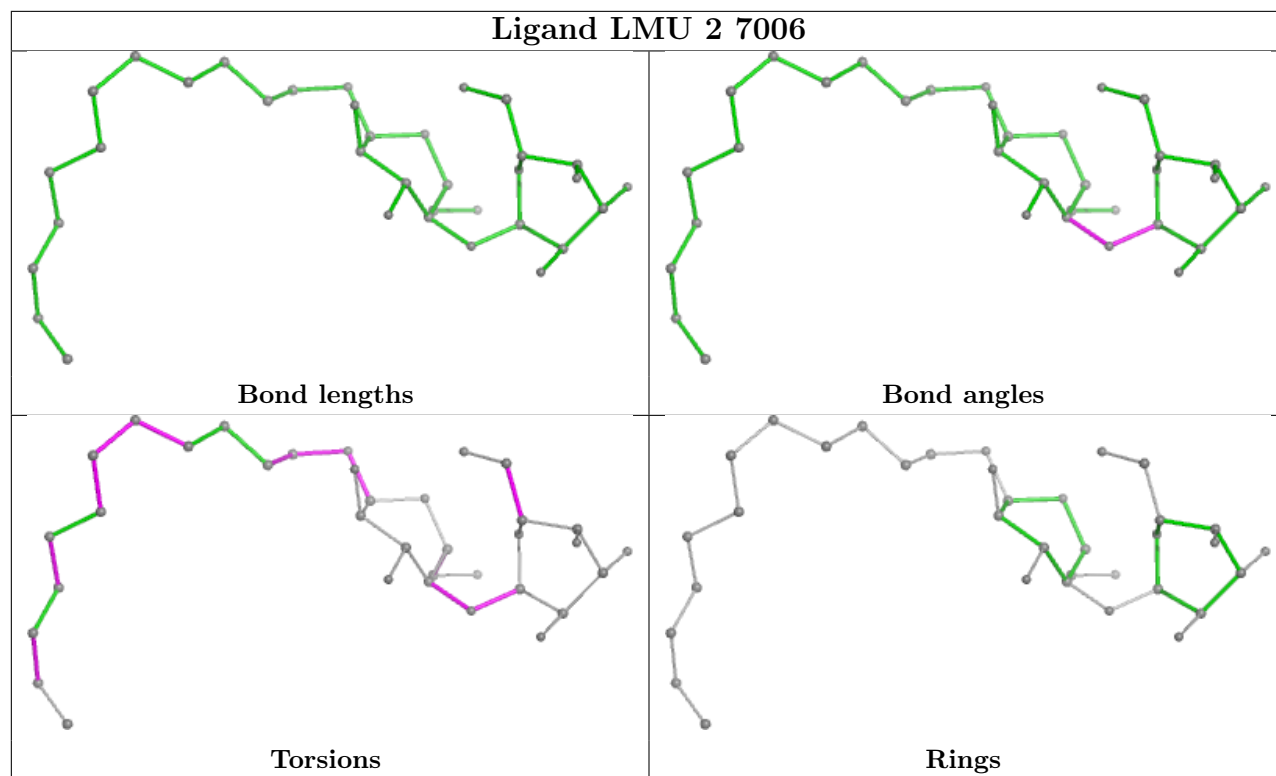




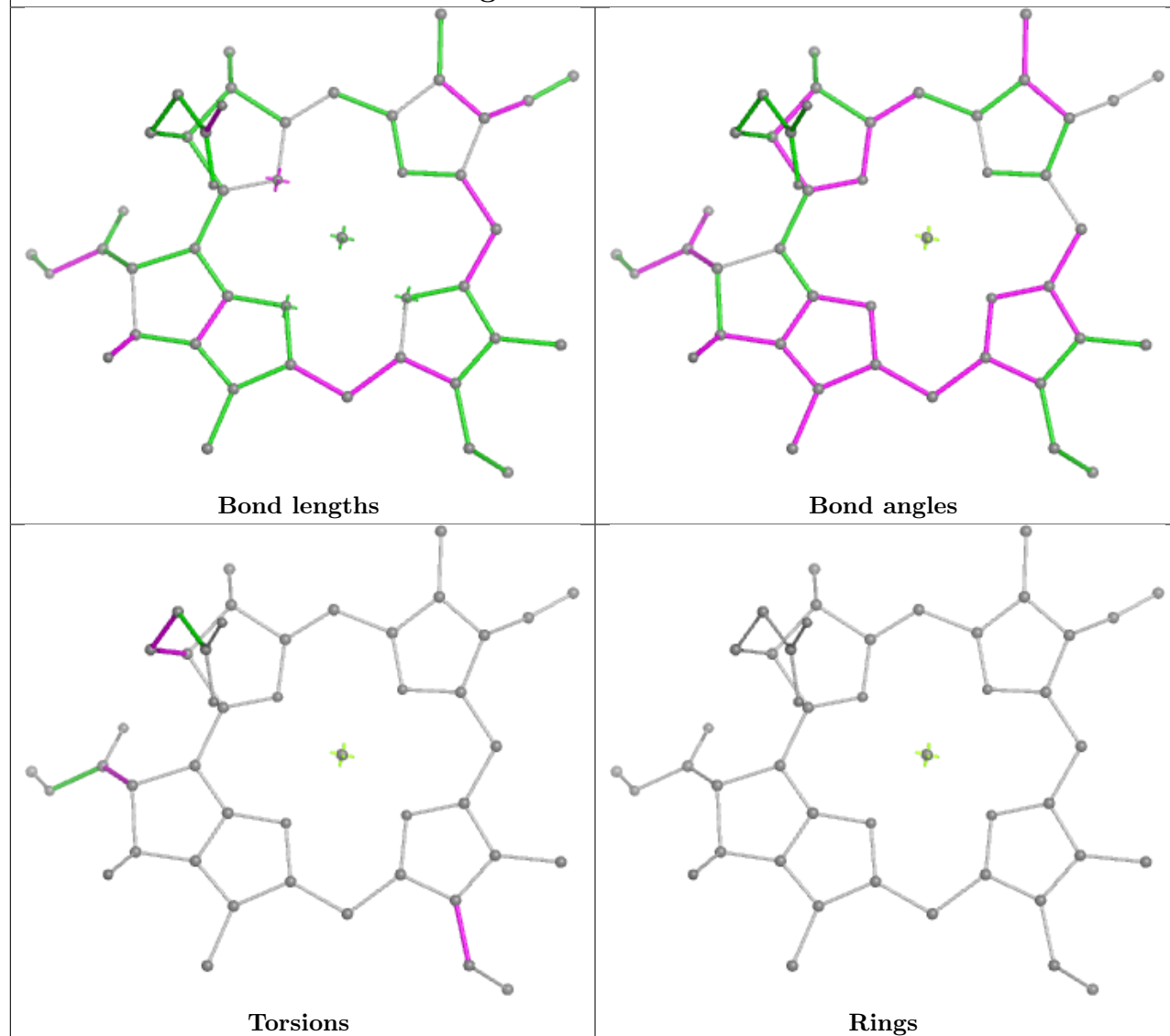




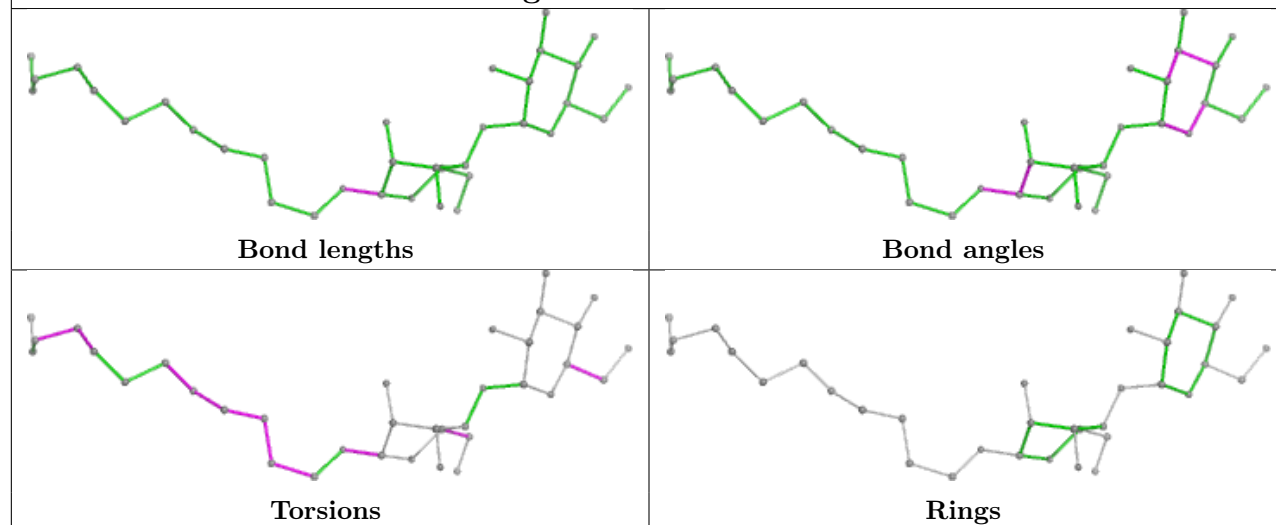


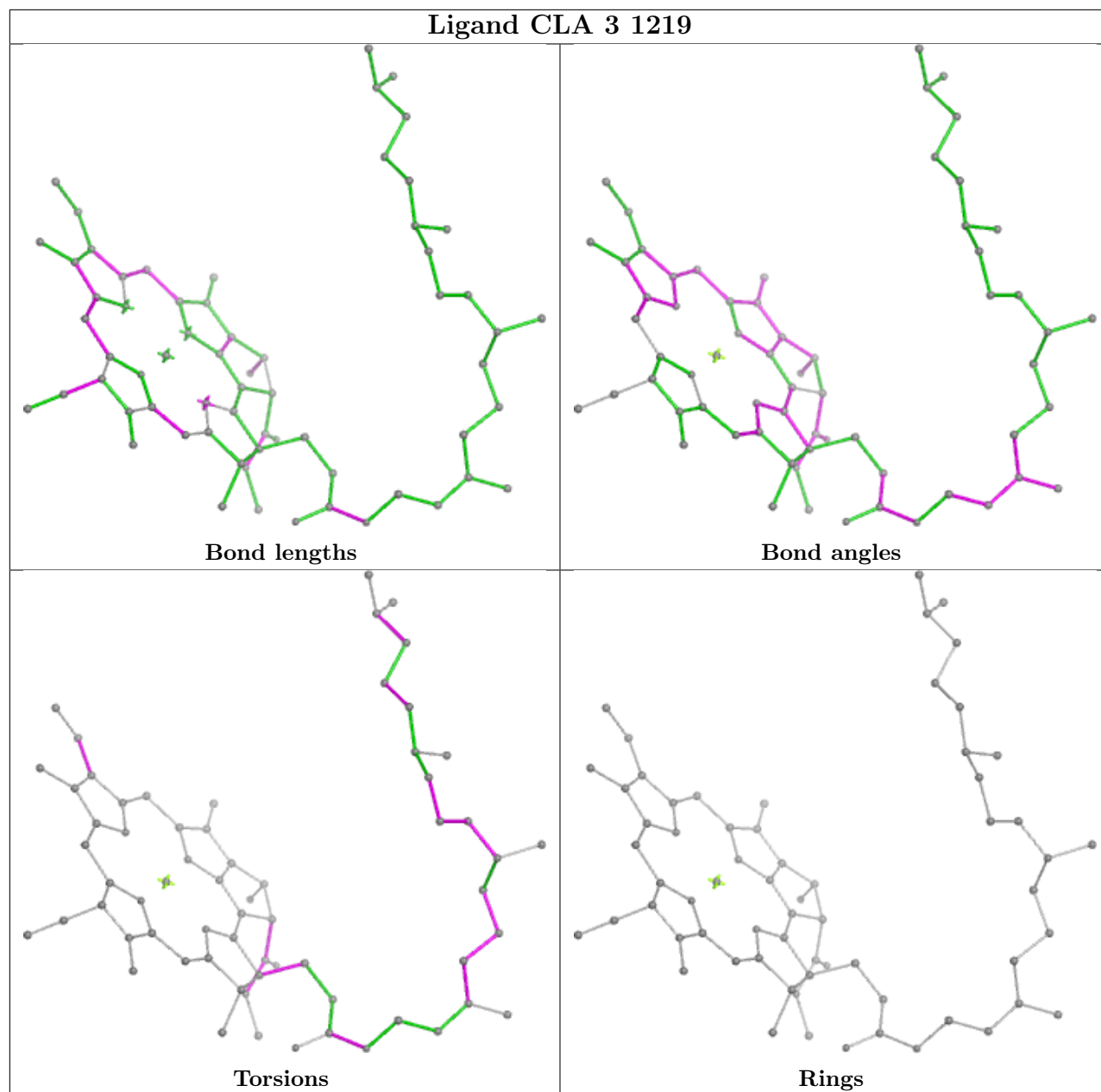


## Ligand CLA B 1736

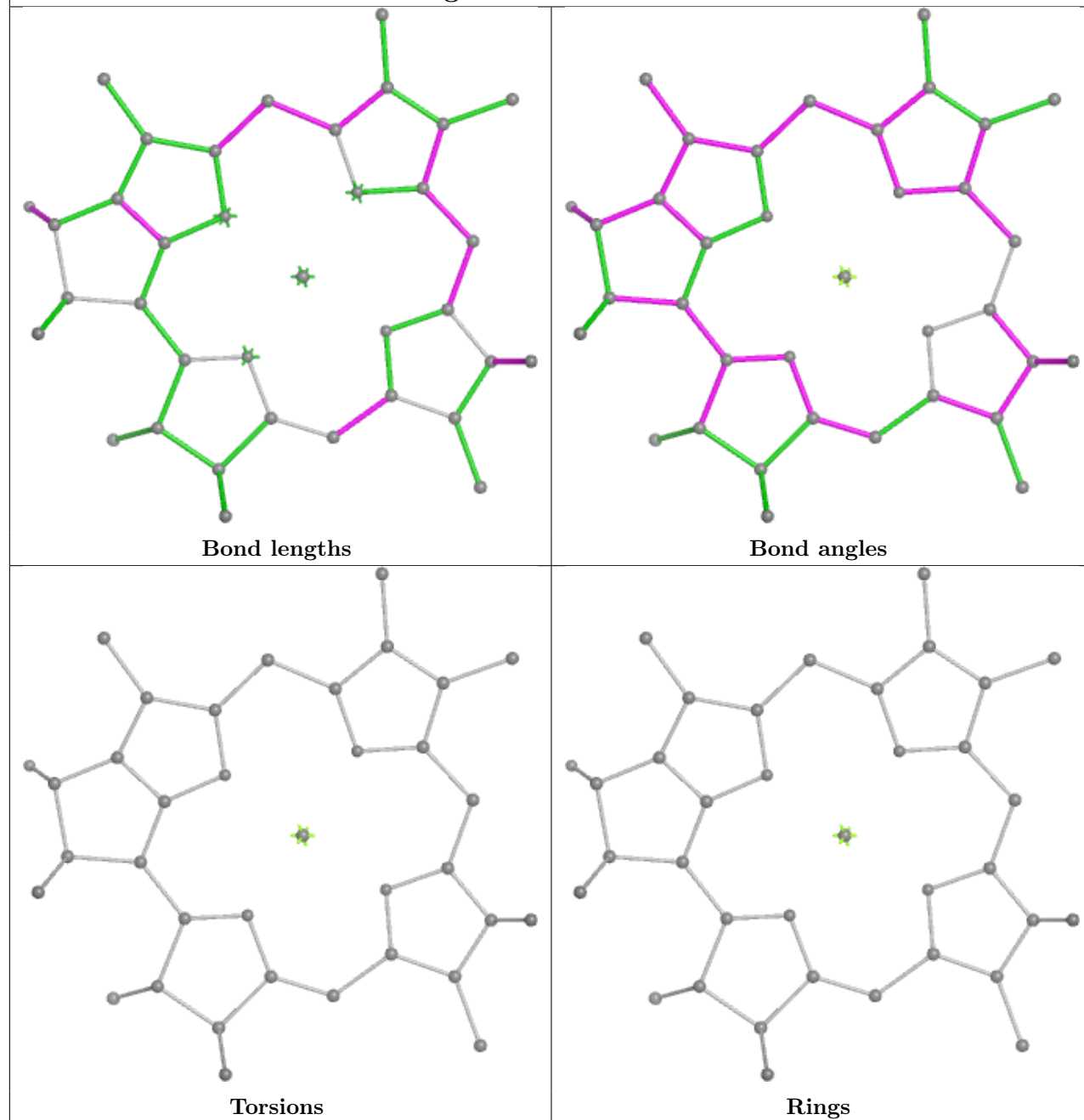


## Ligand LMU 4 1210

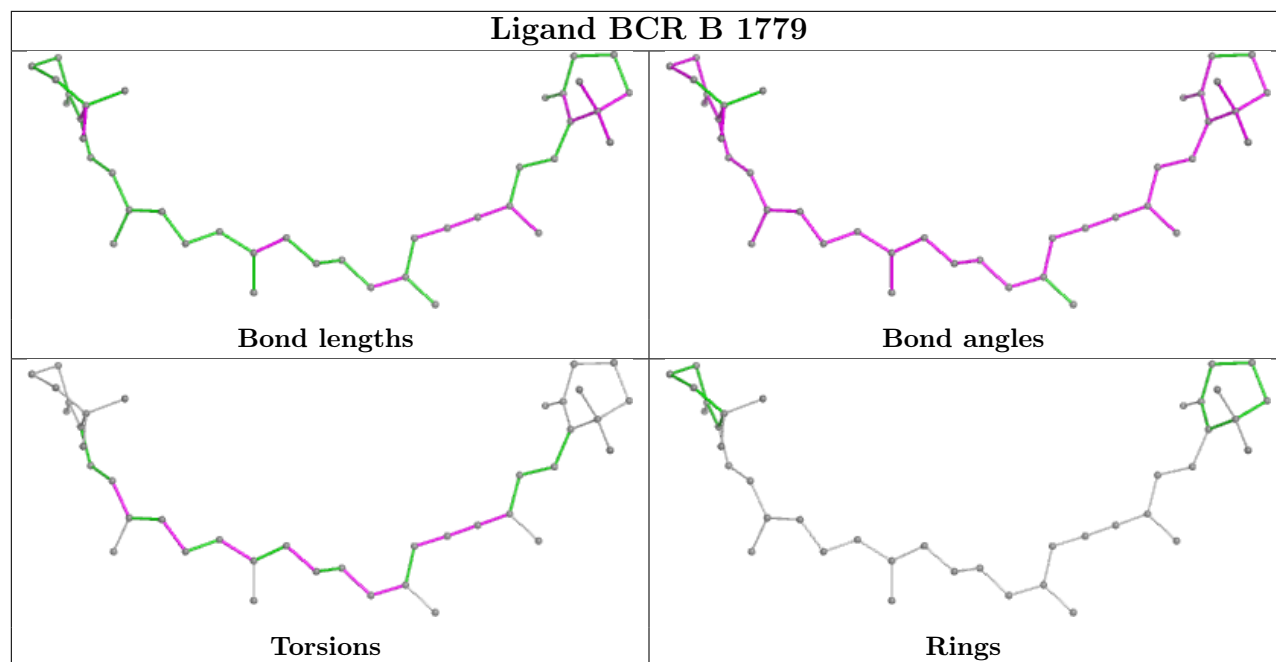




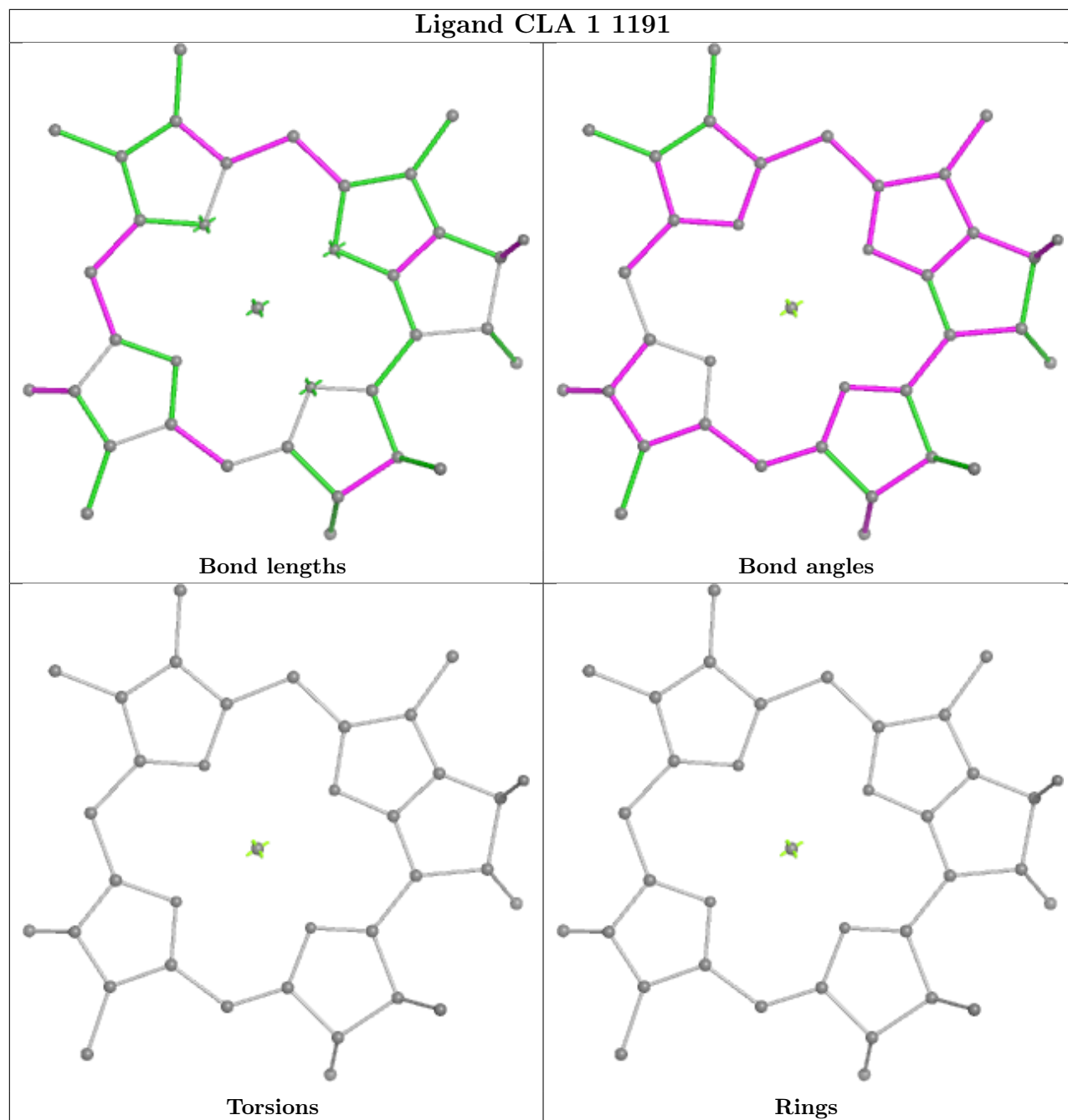
## Ligand CLA A 1775

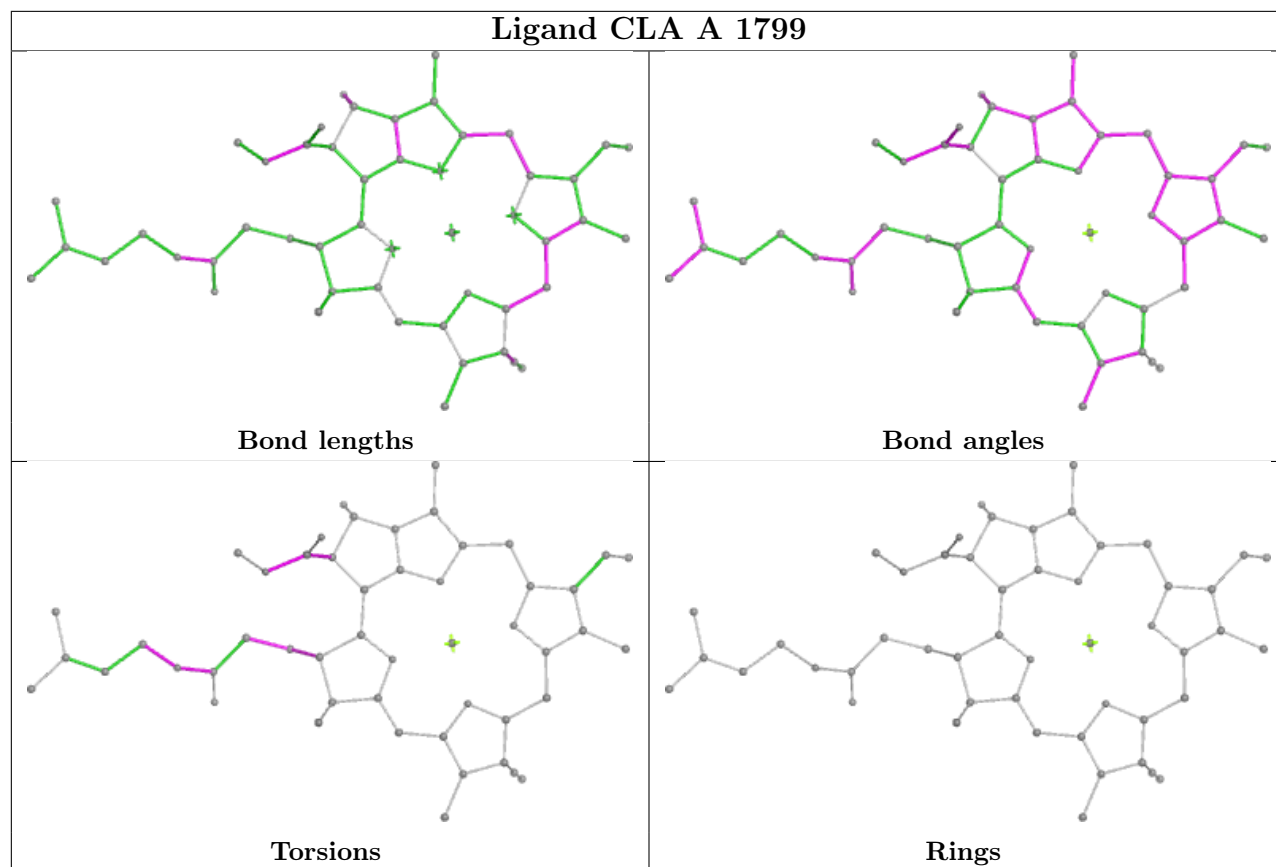




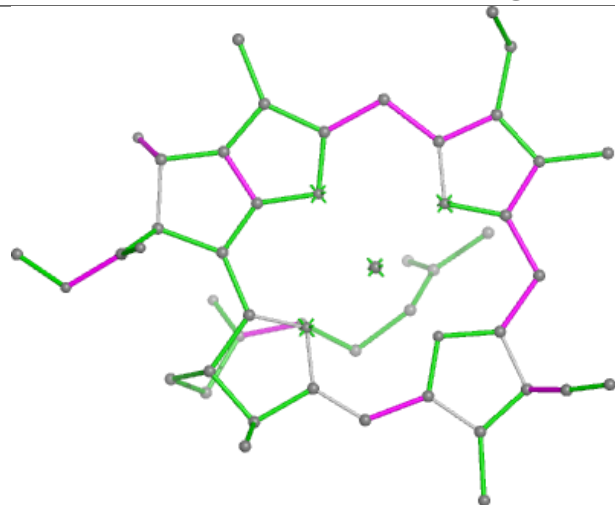


## Ligand CLA 1 1191

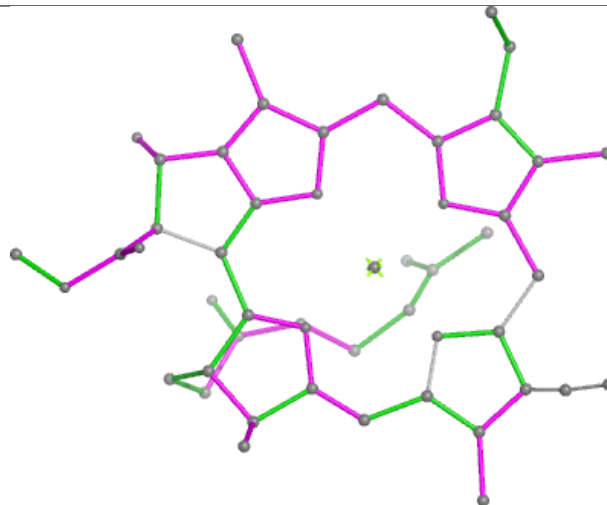




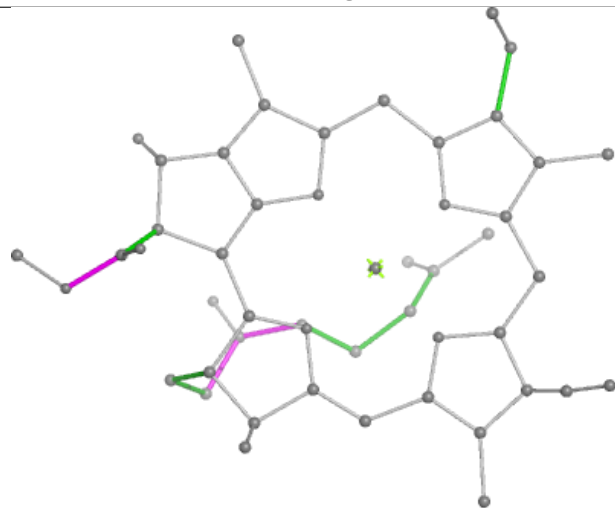
## Ligand CLA B 1750



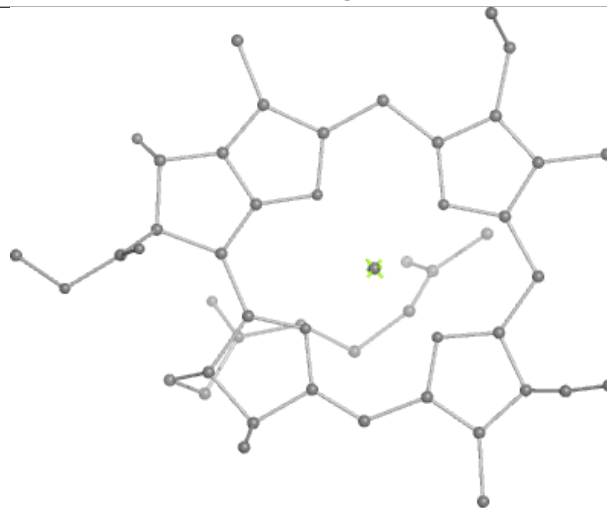
Bond lengths



Bond angles

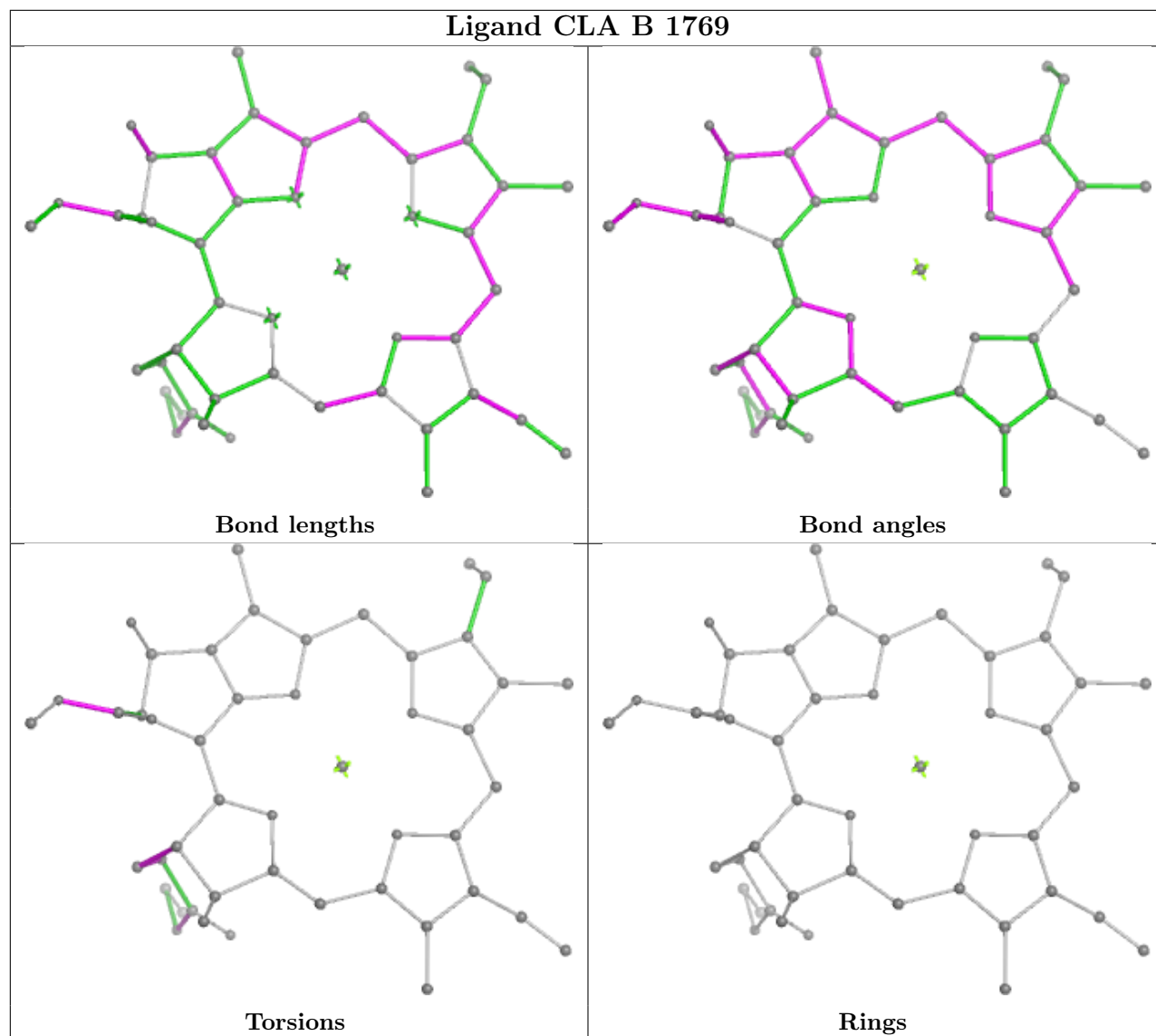


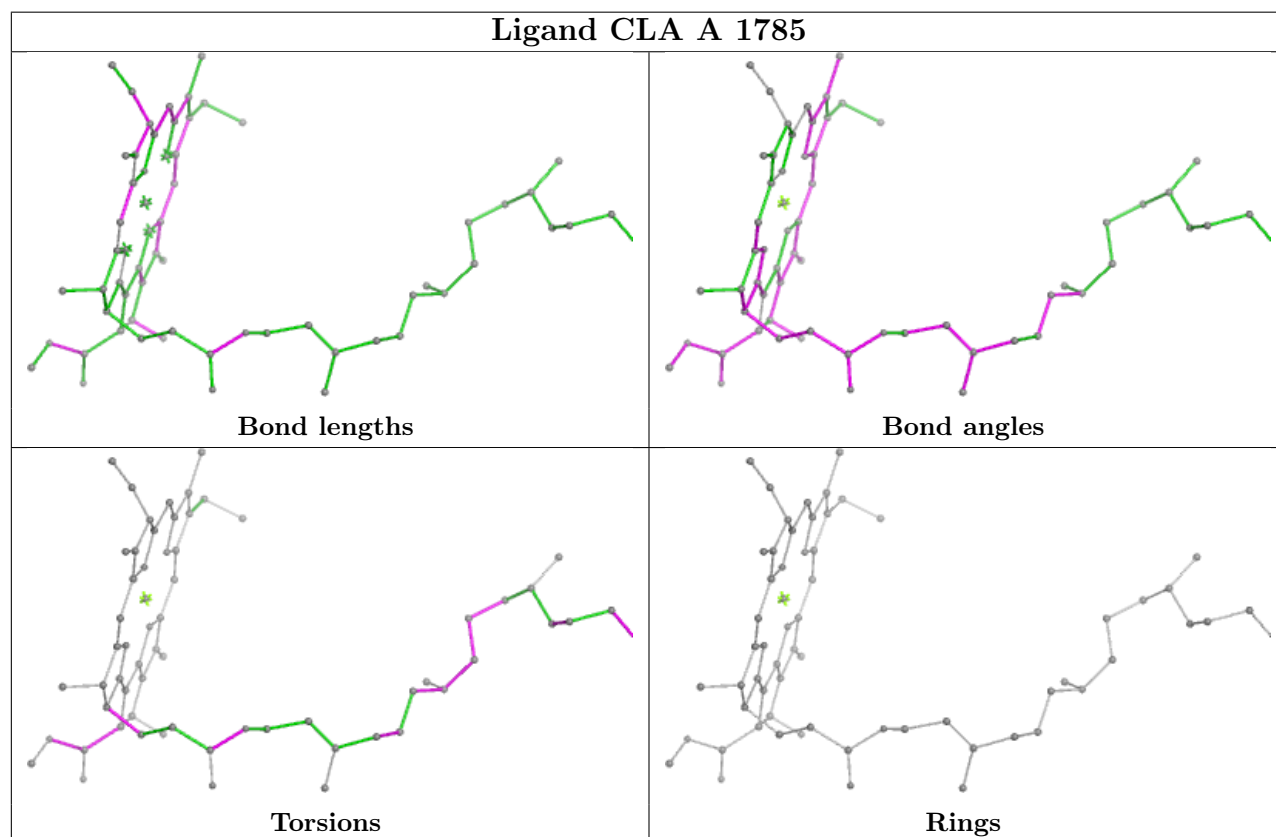
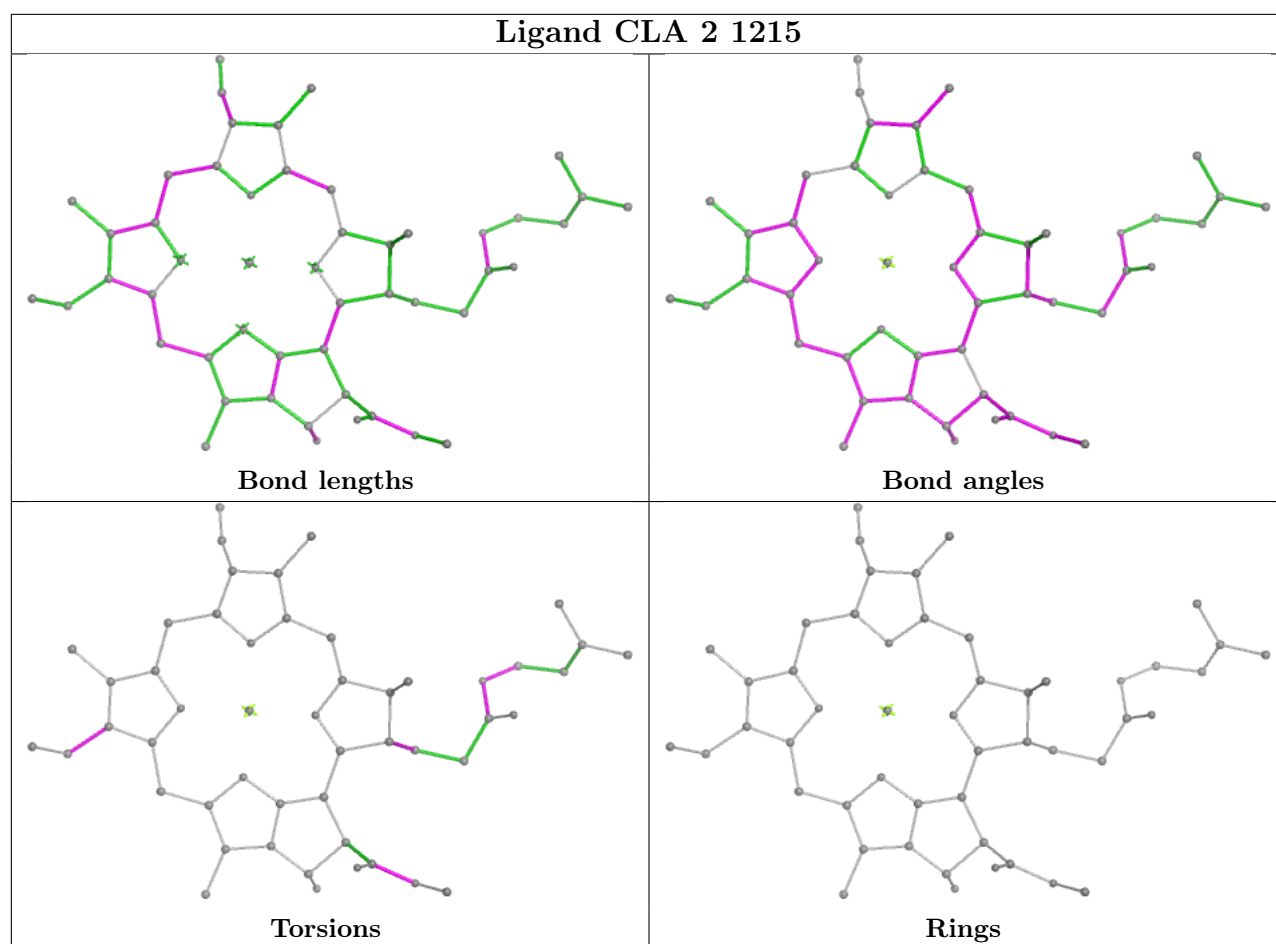
Torsions

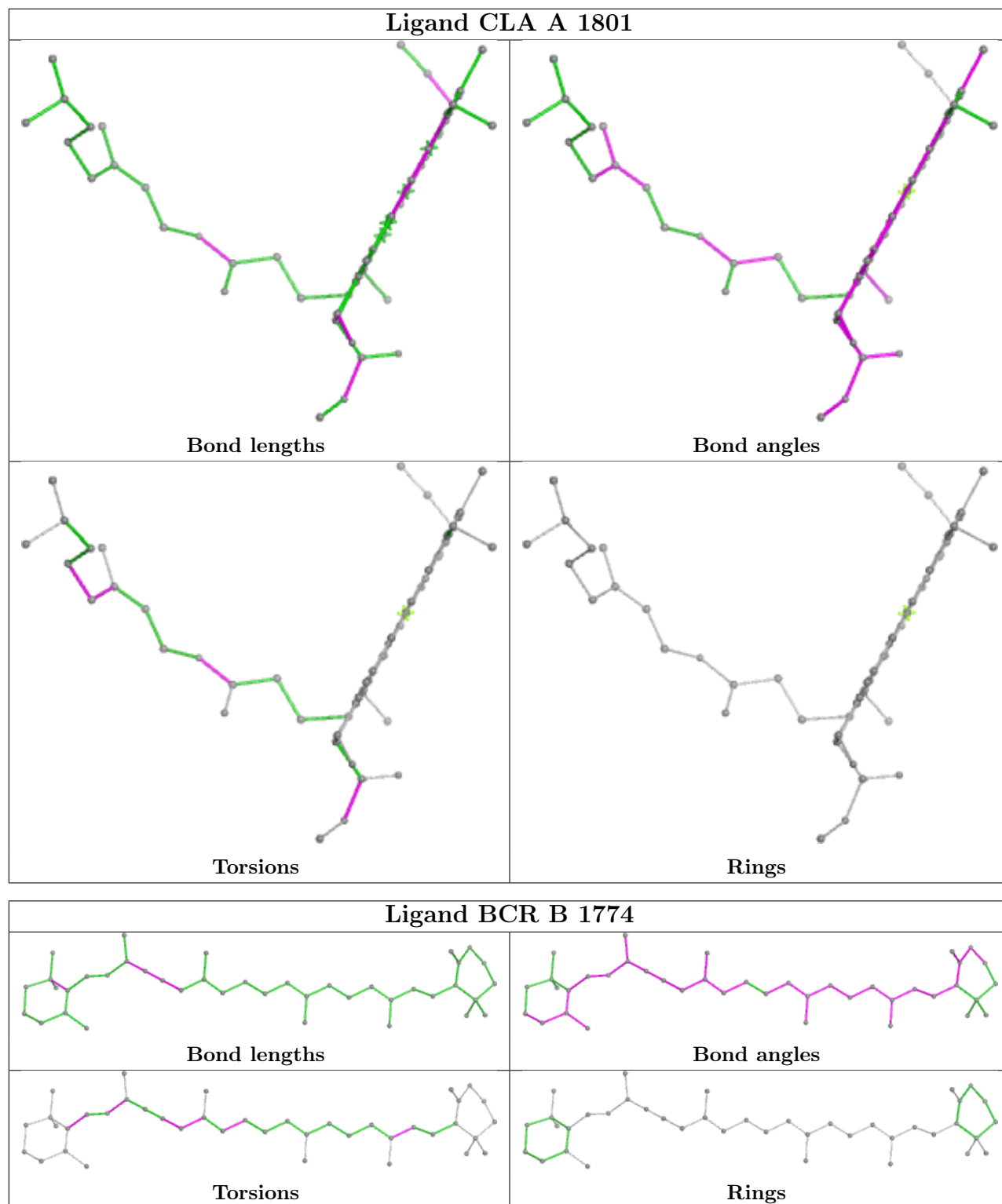


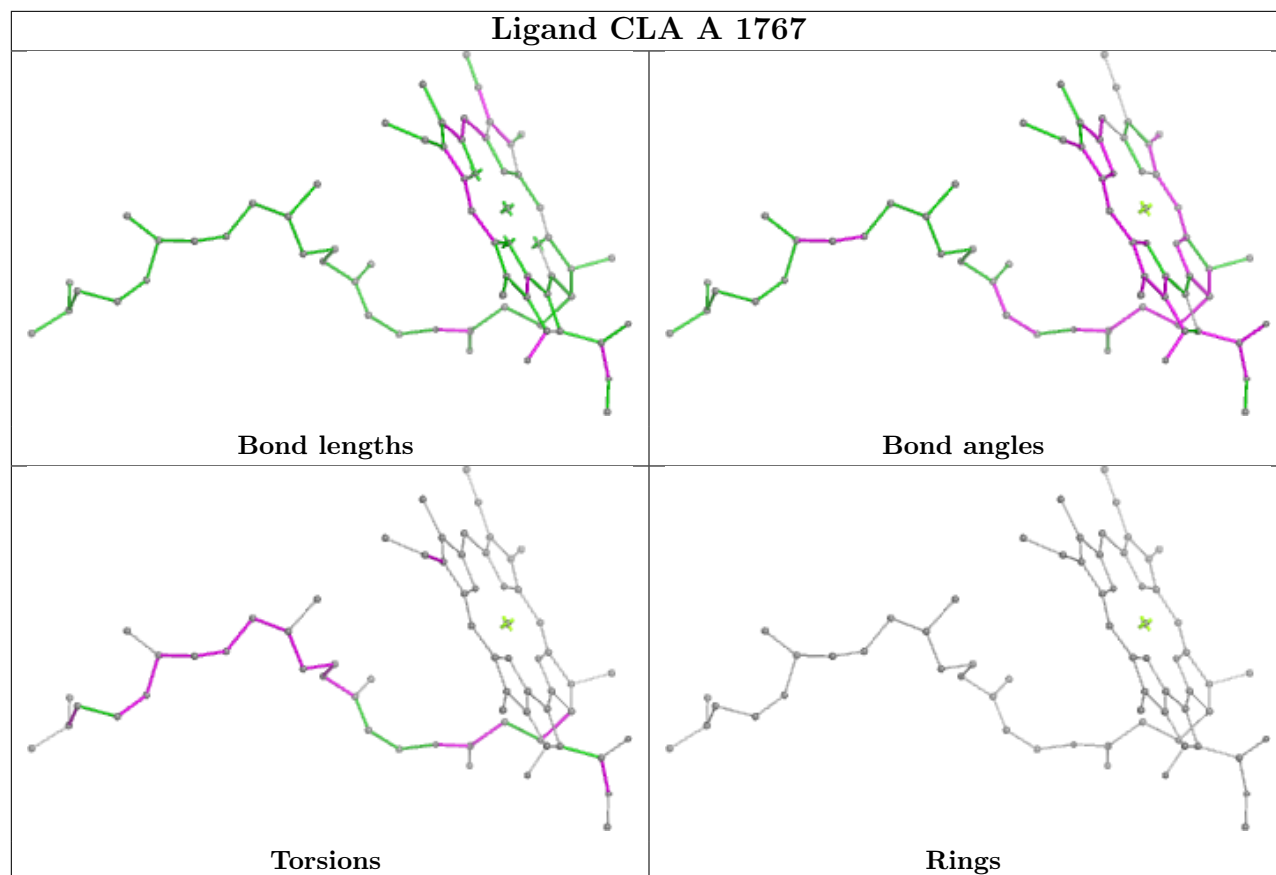
Rings

## Ligand CLA B 1769

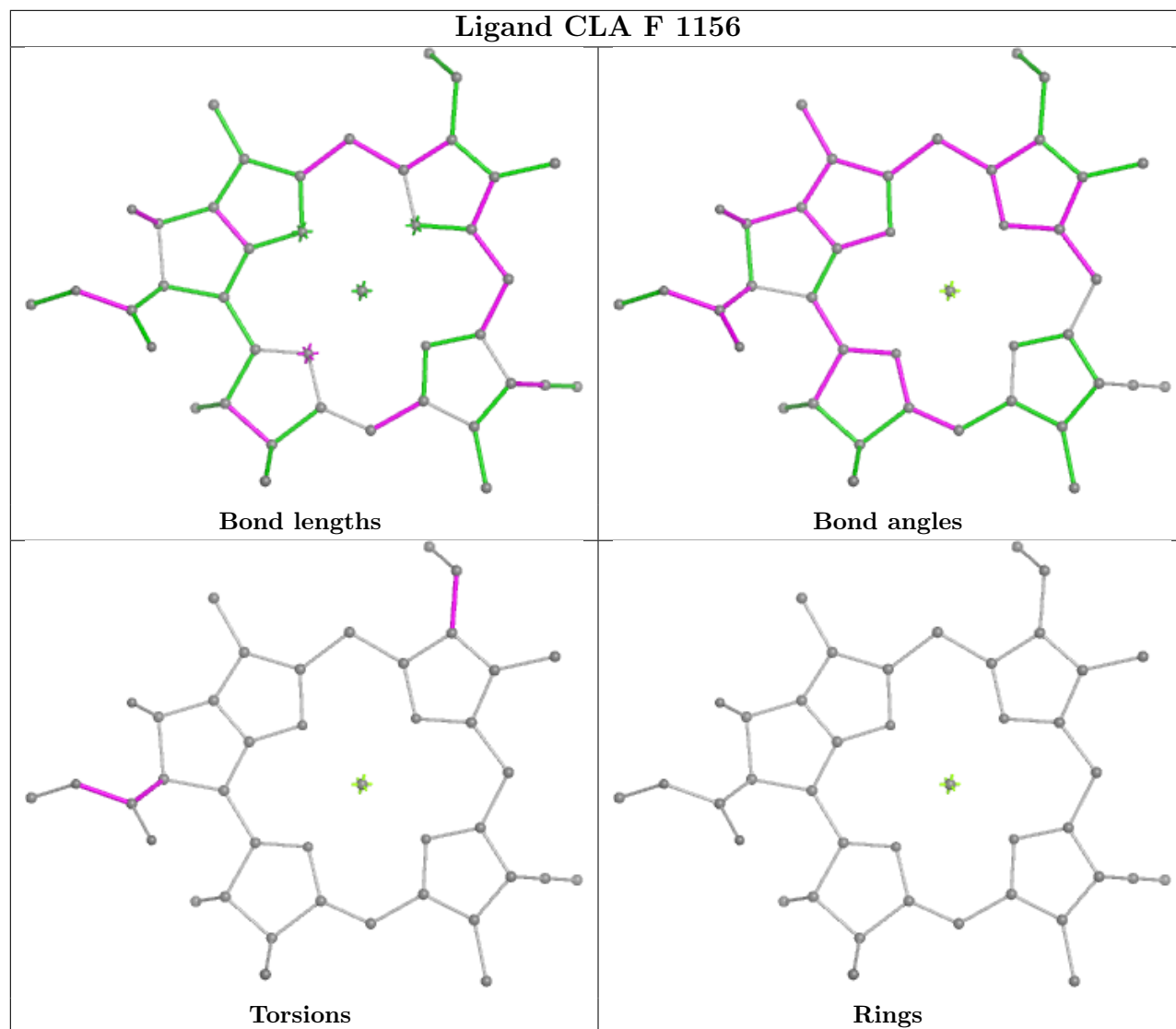


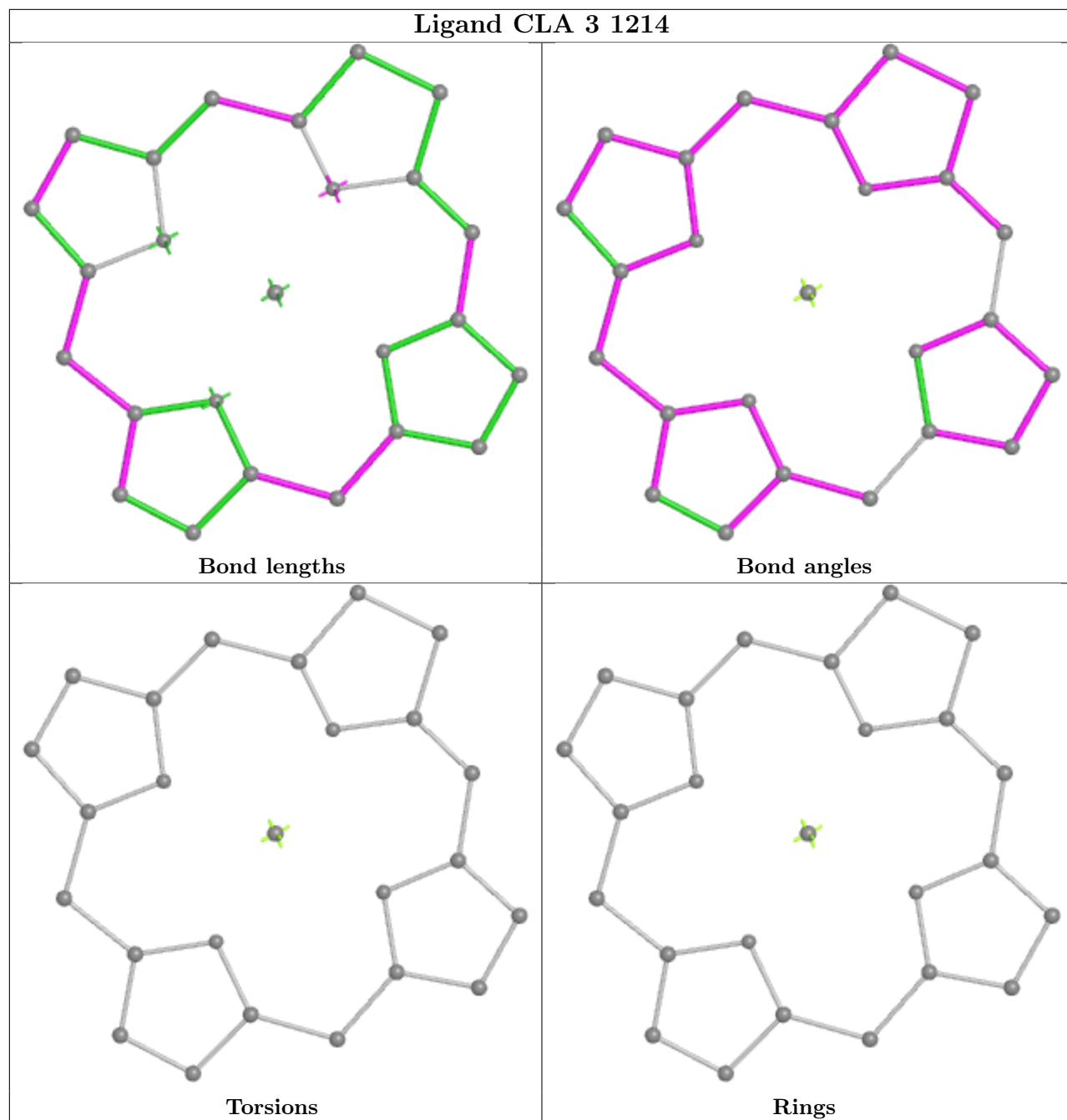




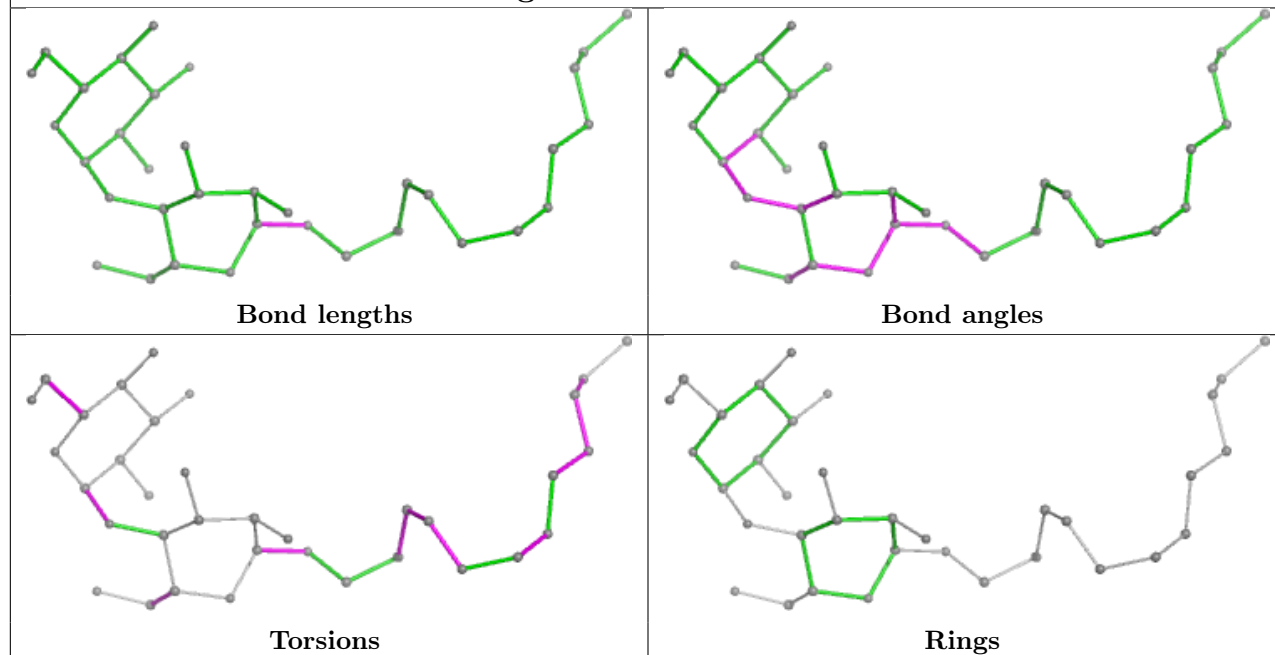




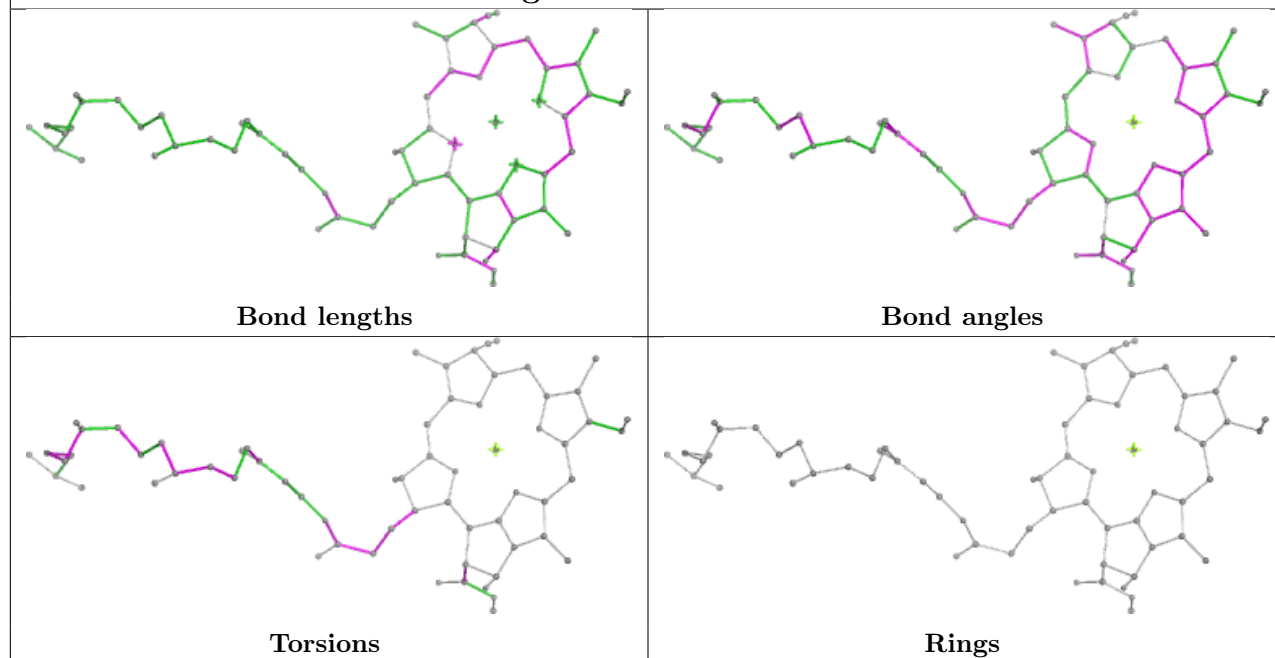




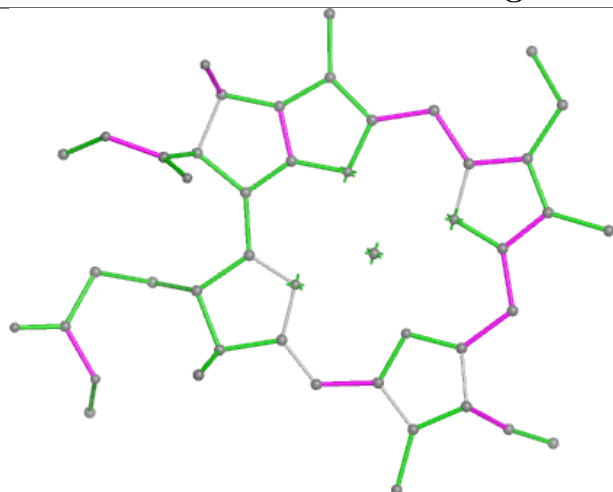
## Ligand LMU A 7031



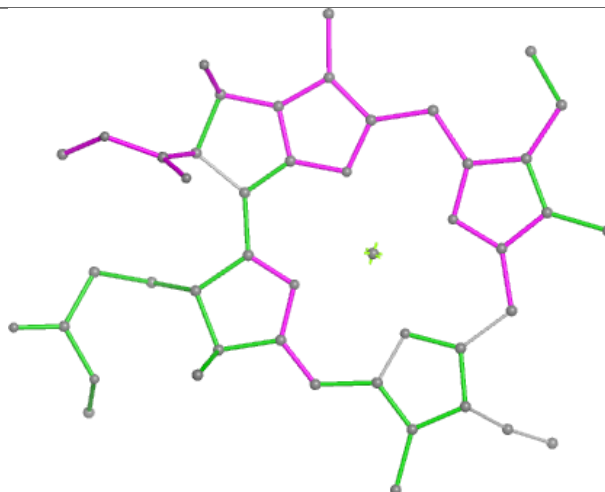
## Ligand CLA B 1743



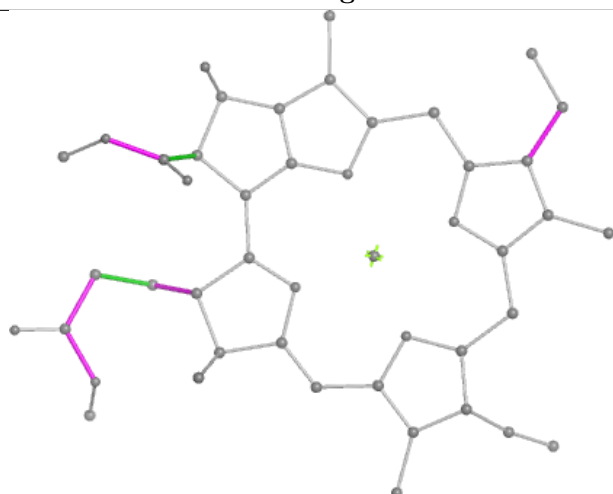
## Ligand CLA B 1746



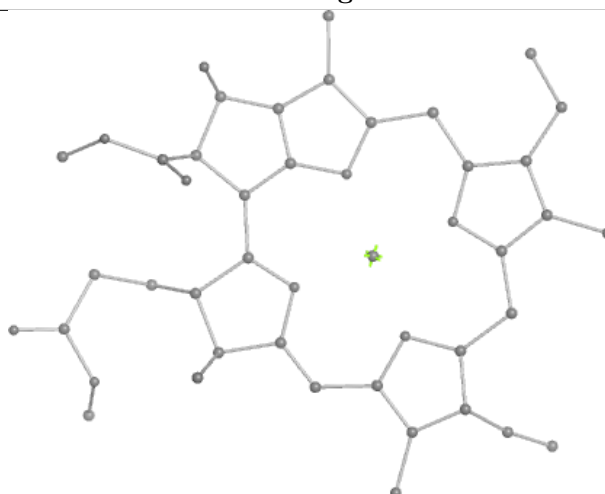
Bond lengths



Bond angles



Torsions

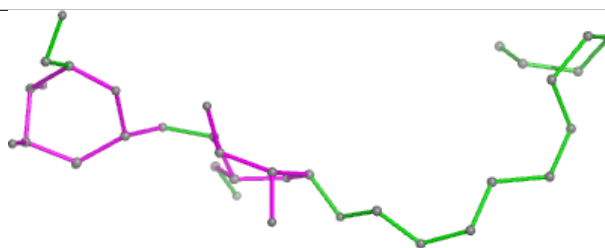


Rings

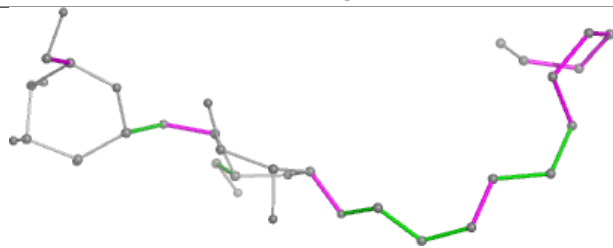
## Ligand LMU A 7043



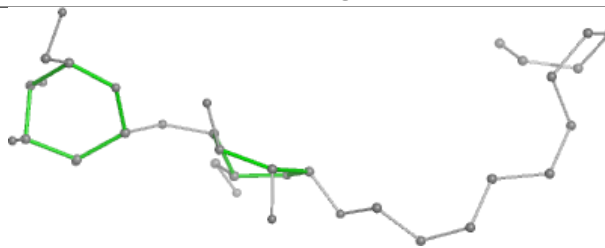
Bond lengths



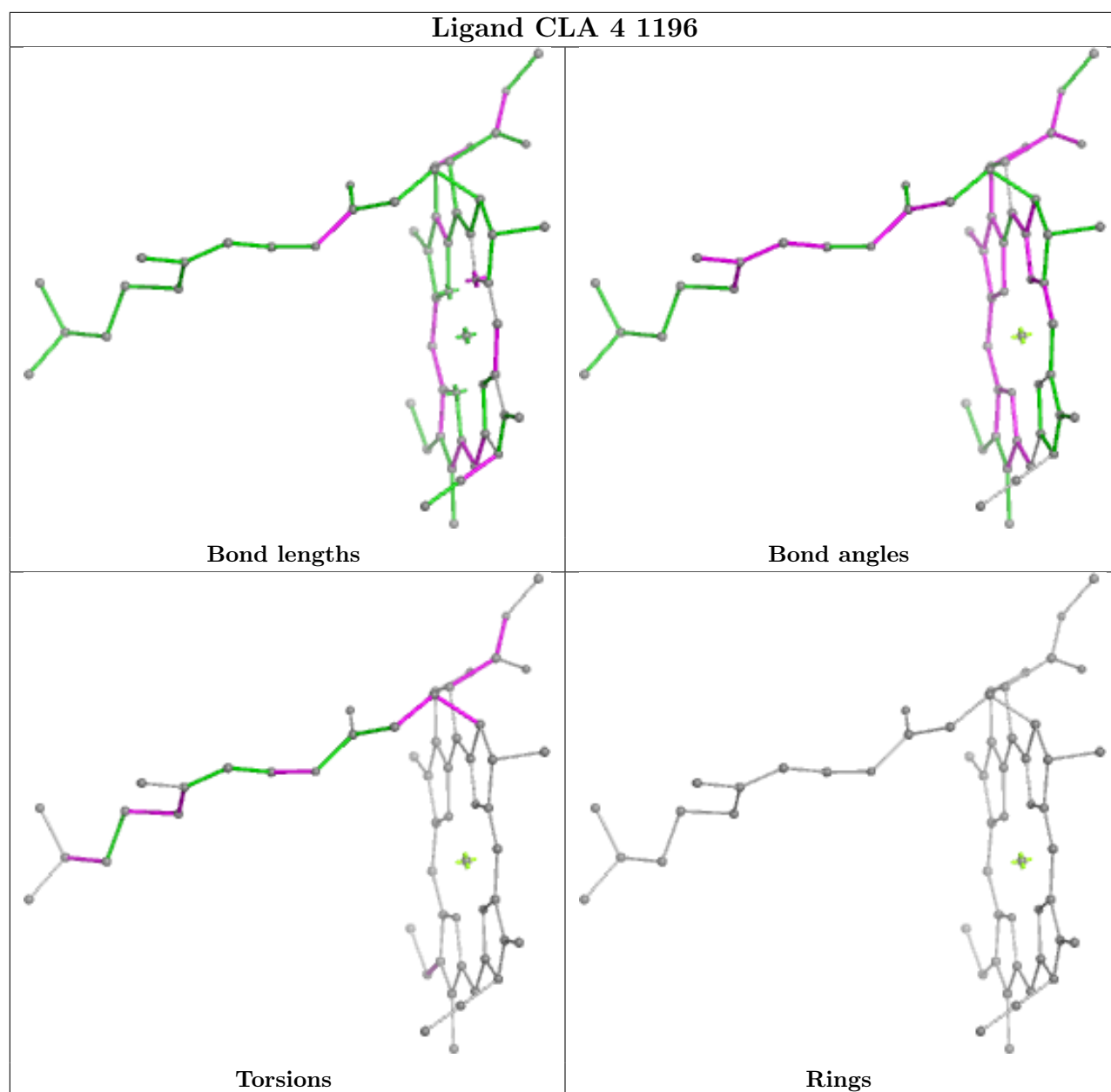
Bond angles

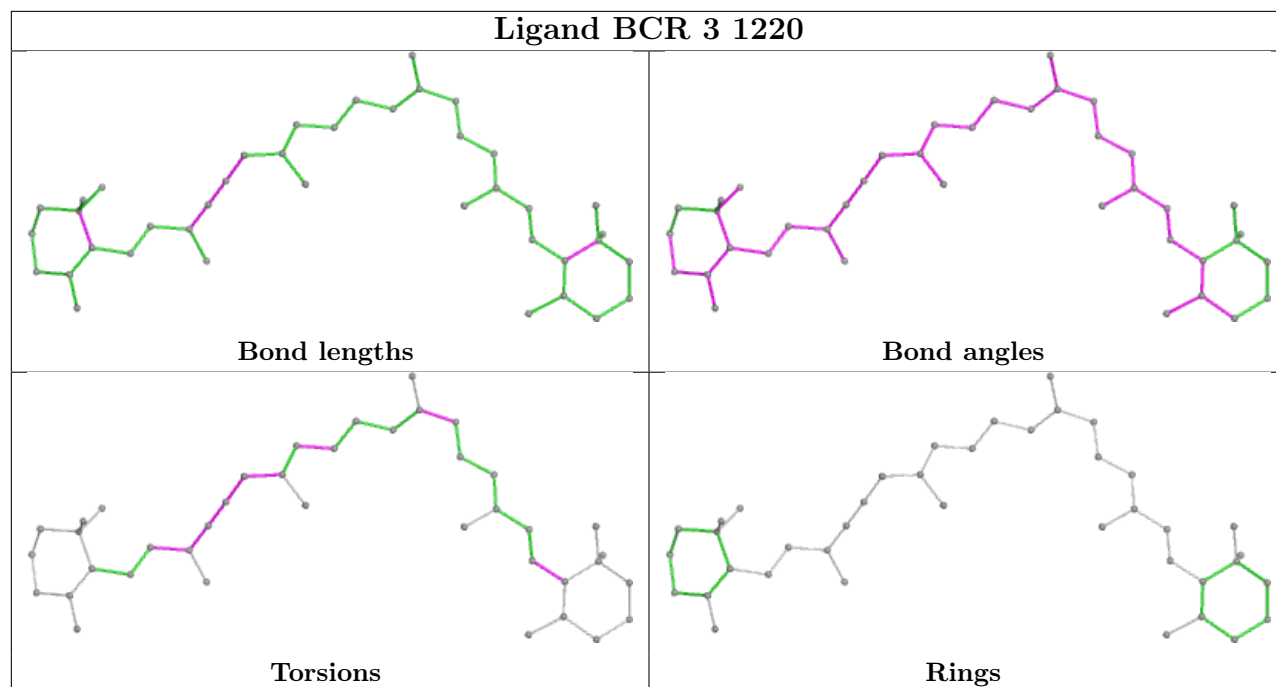


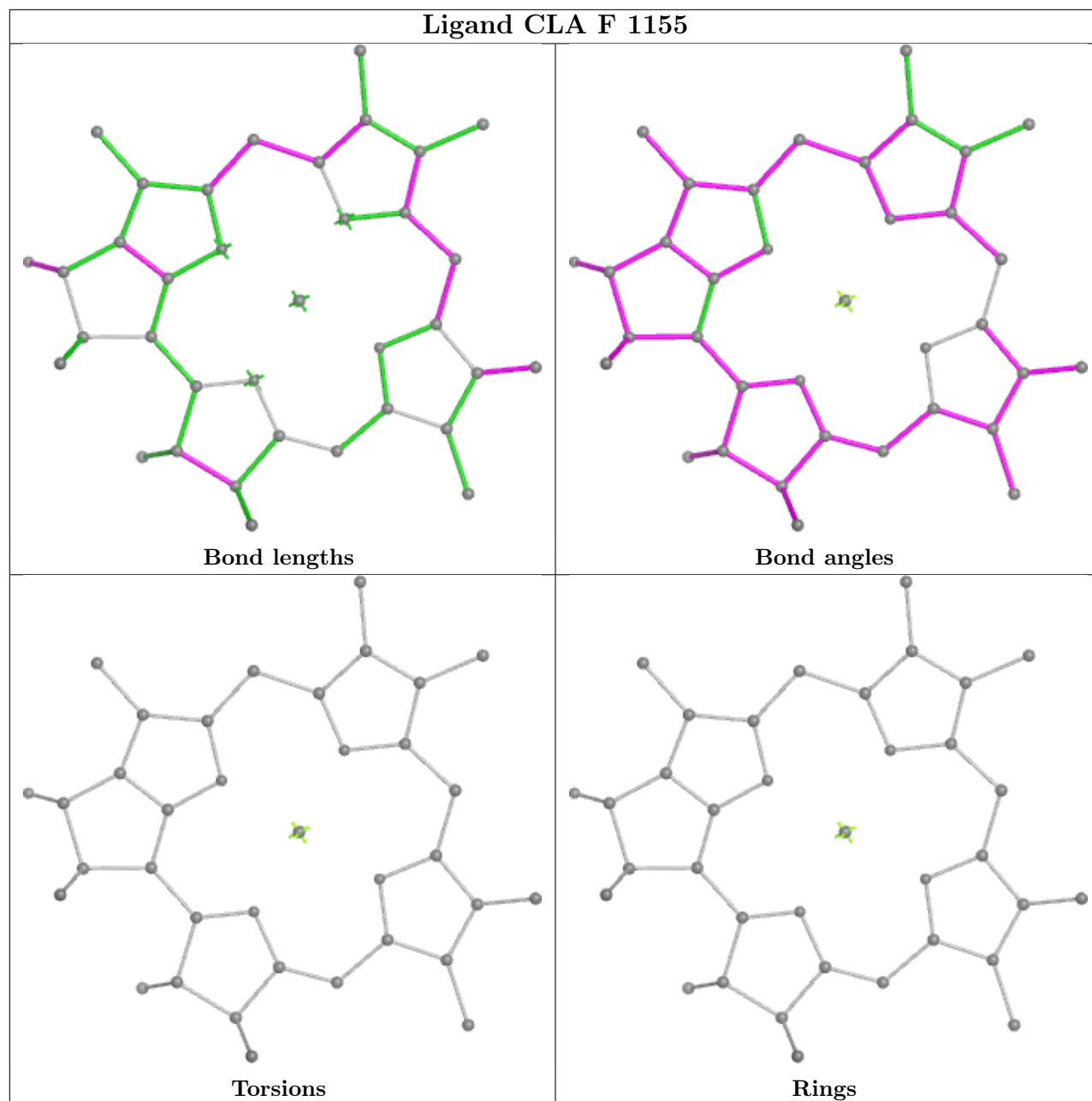
Torsions

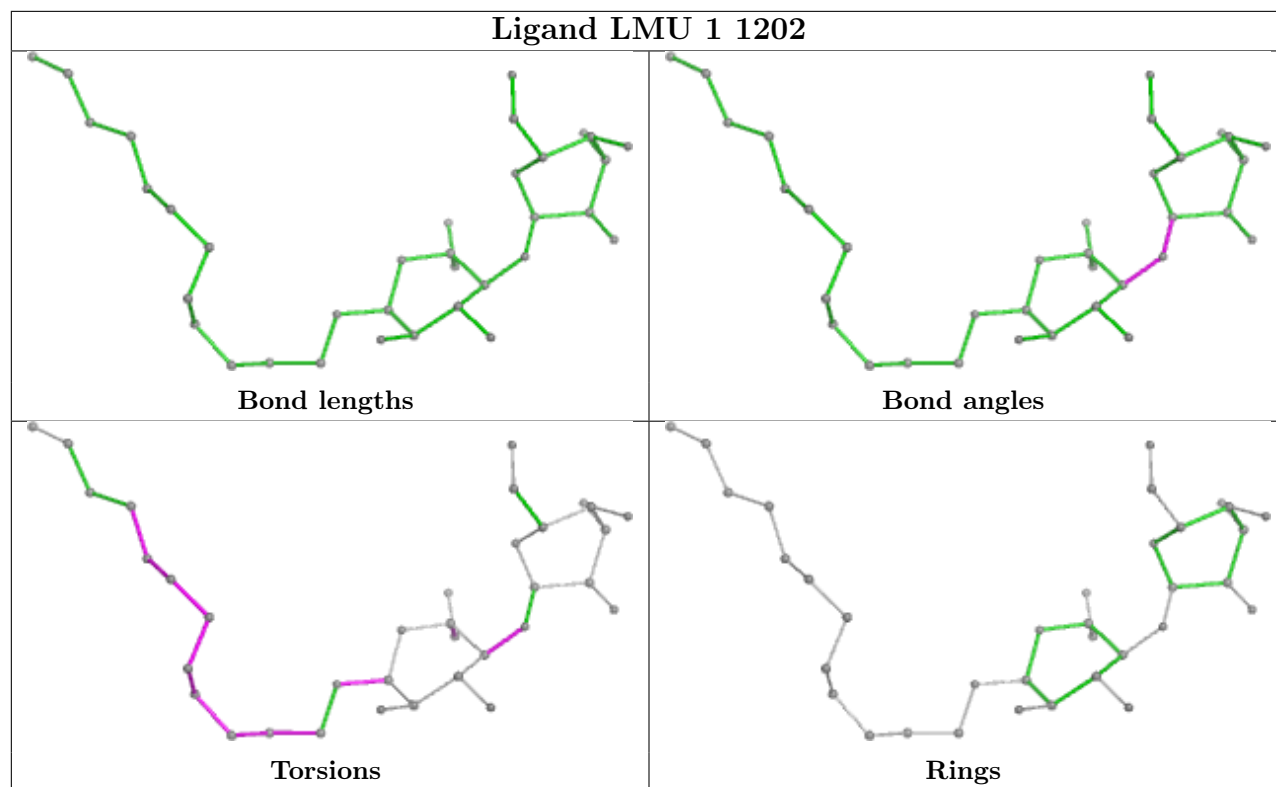


Rings

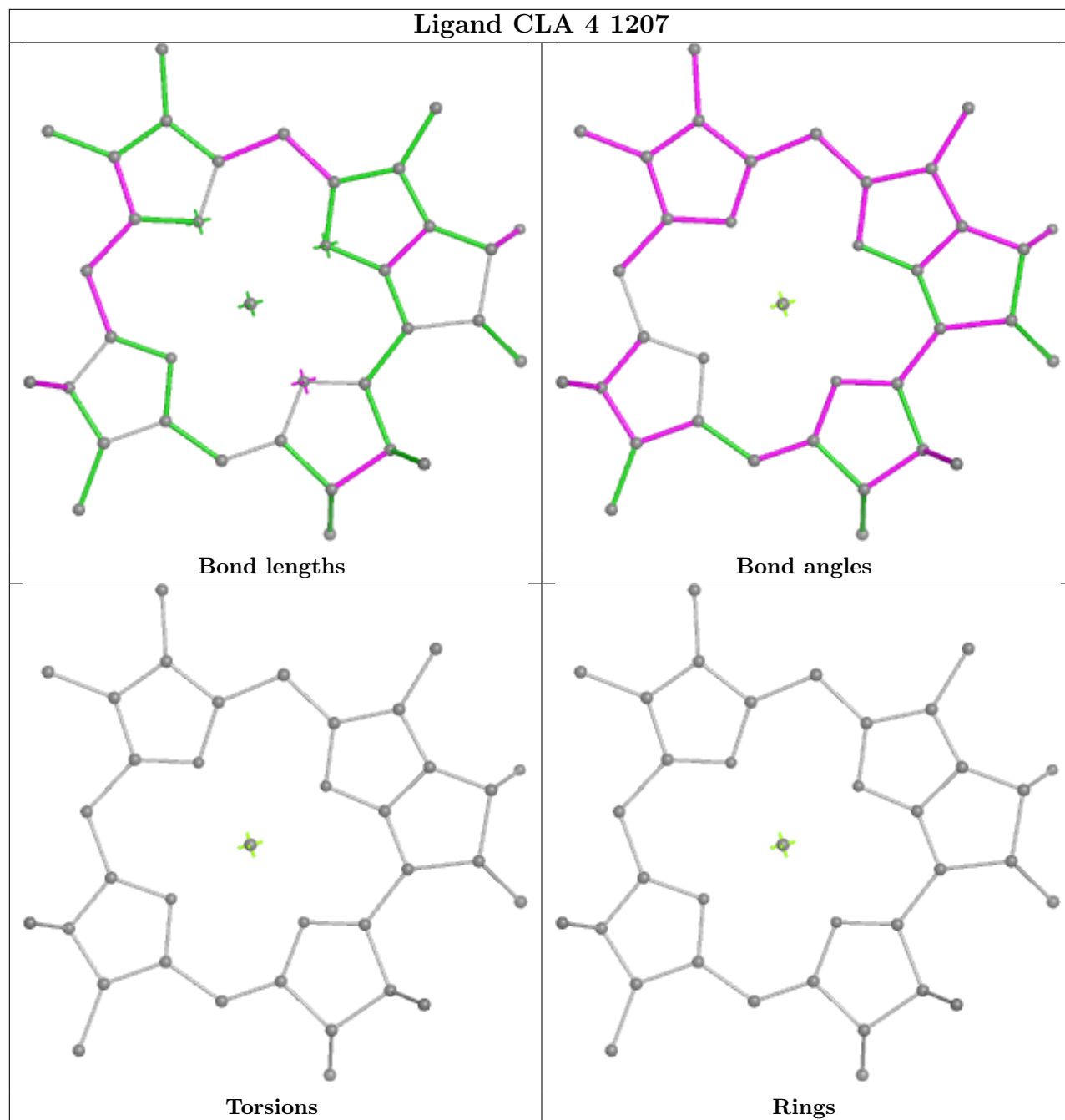


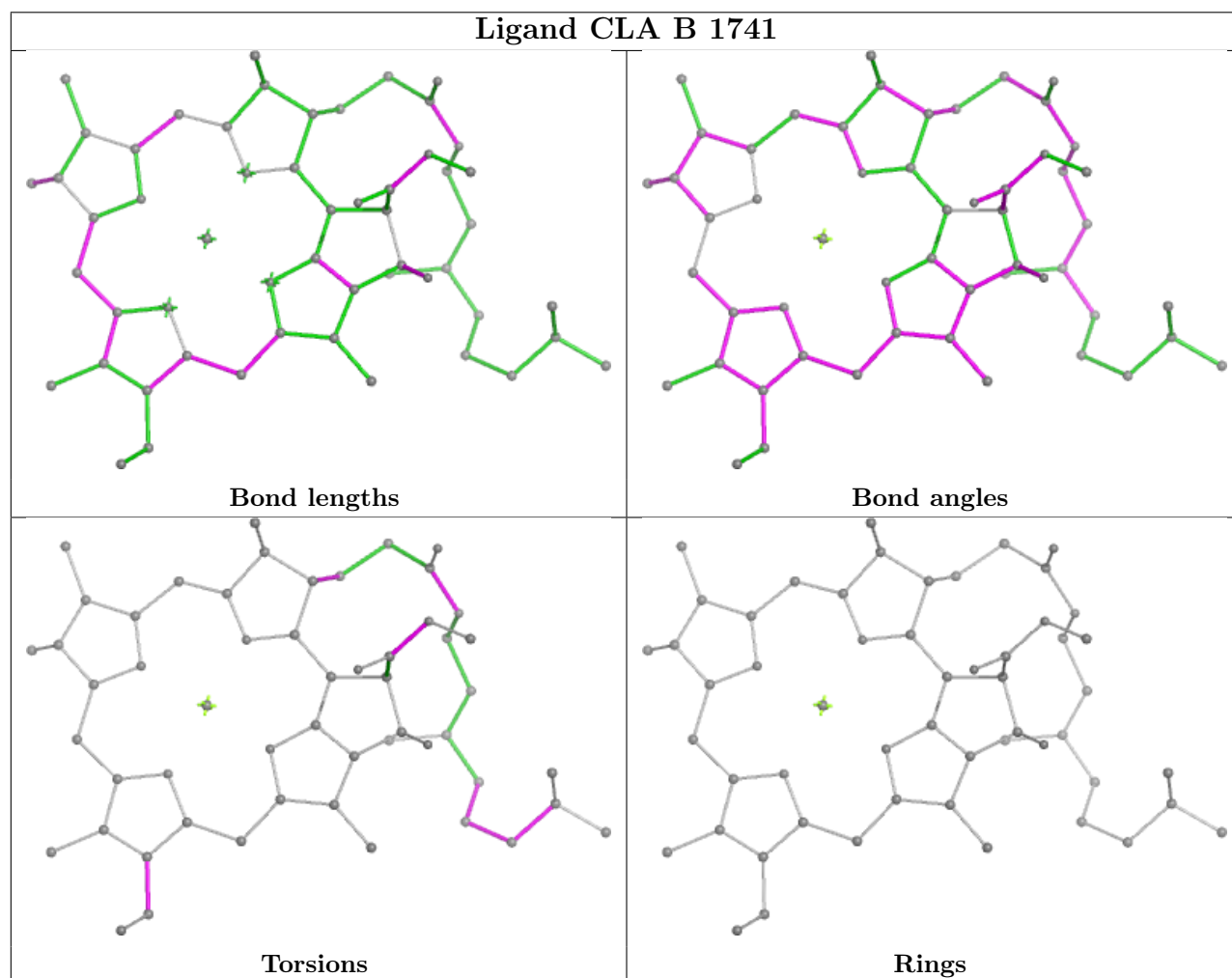
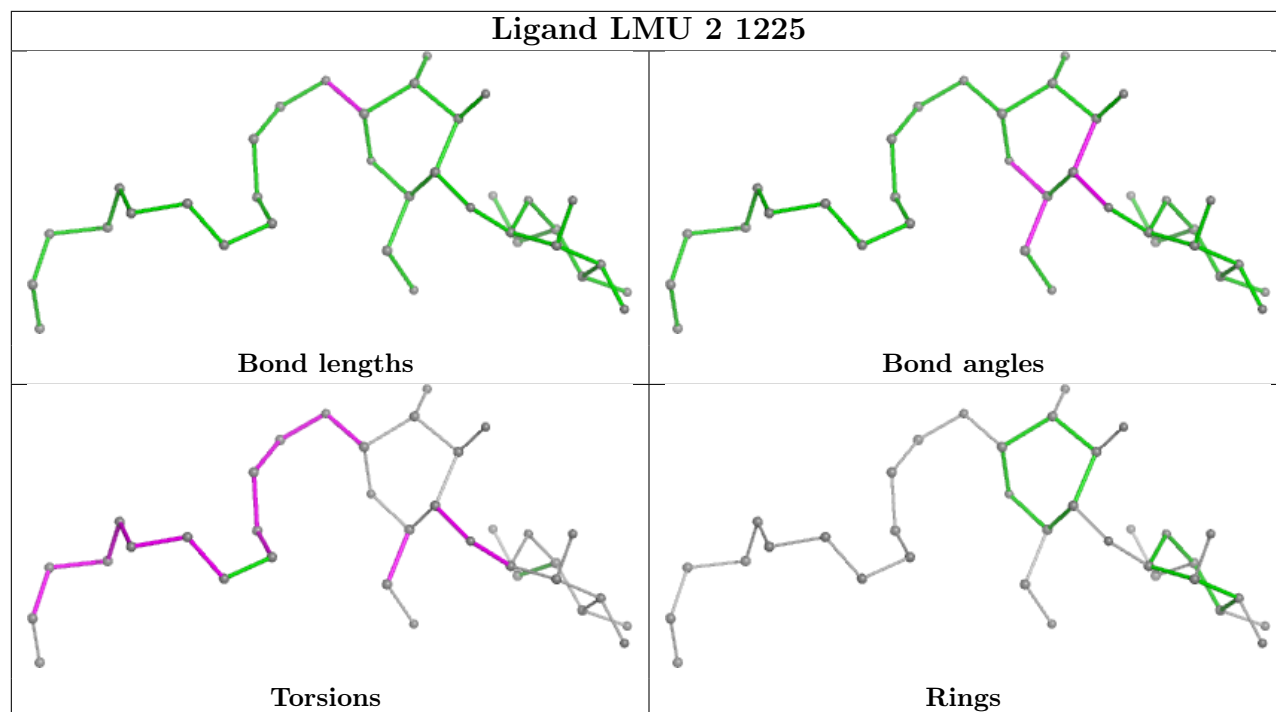




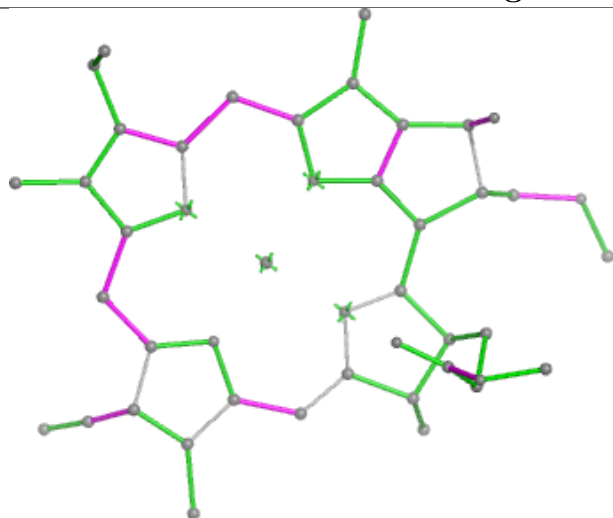




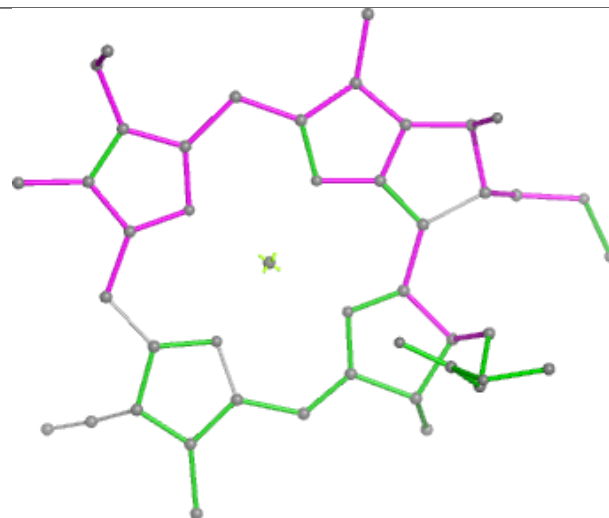




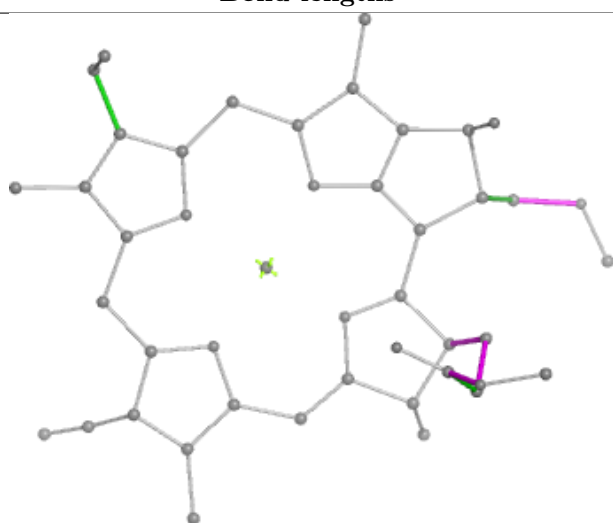
## Ligand CLA A 1763



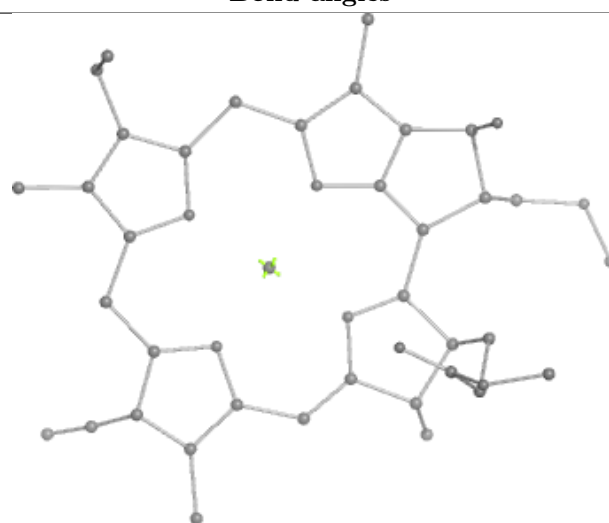
Bond lengths



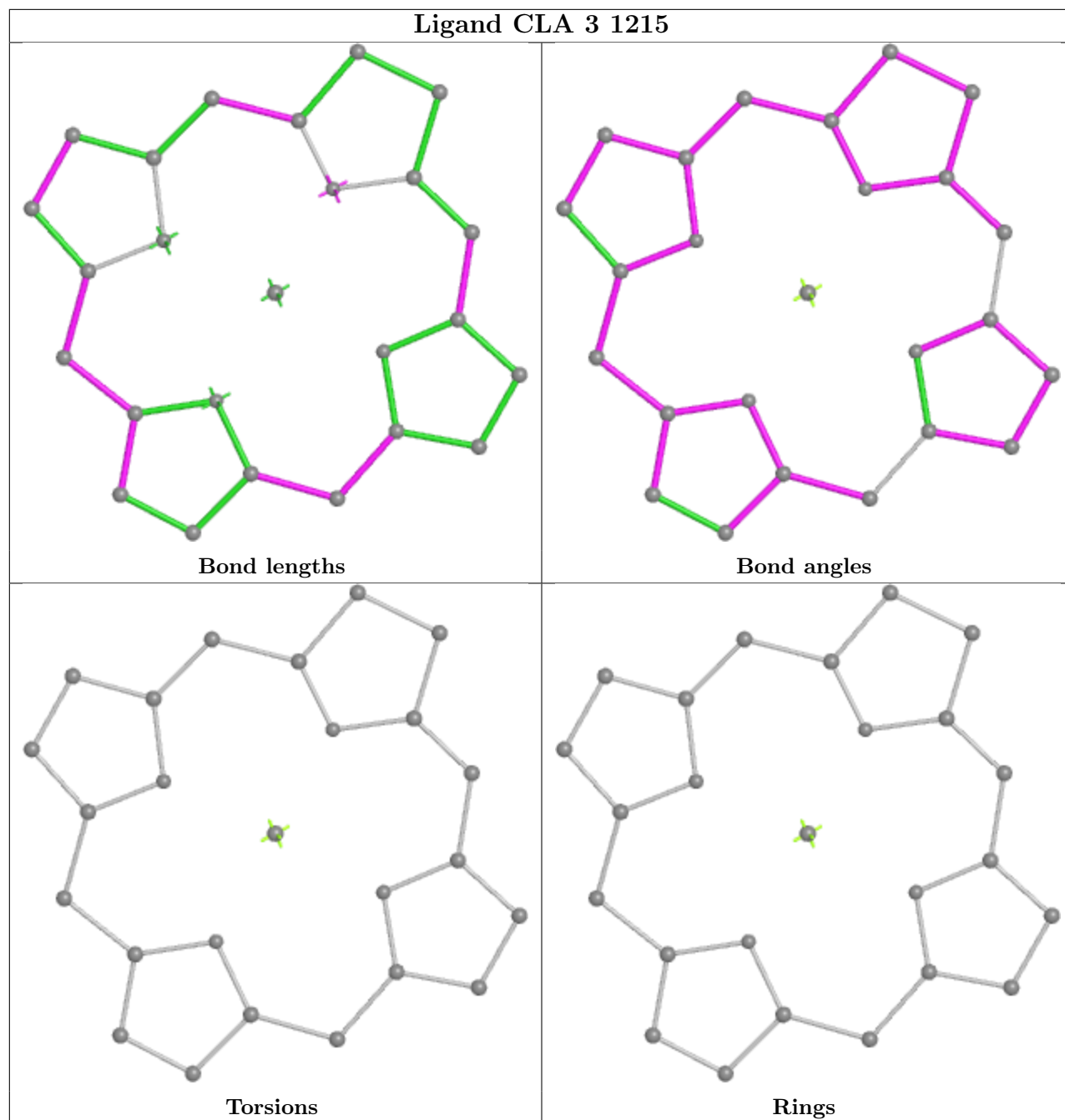
Bond angles

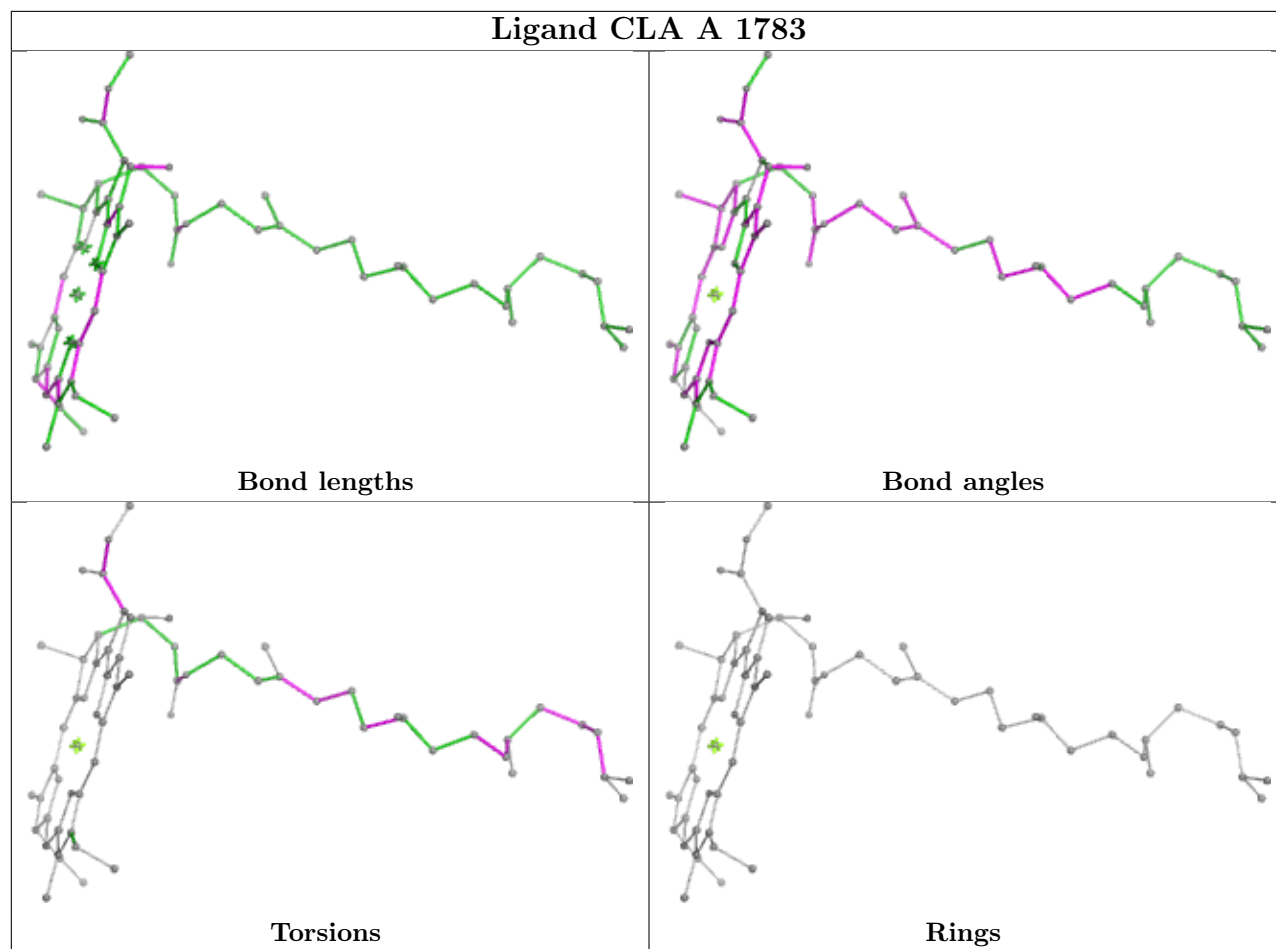


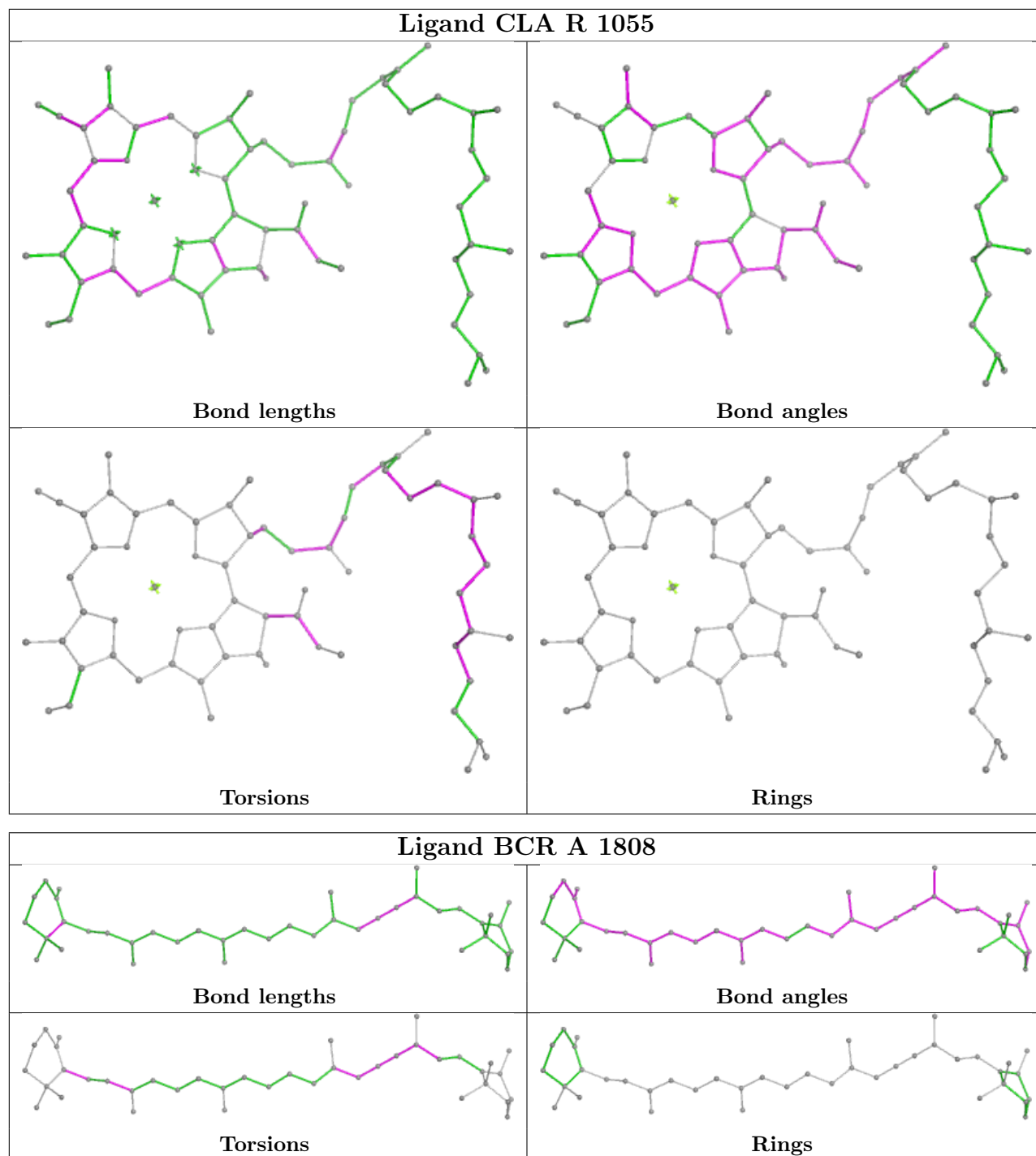
Torsions



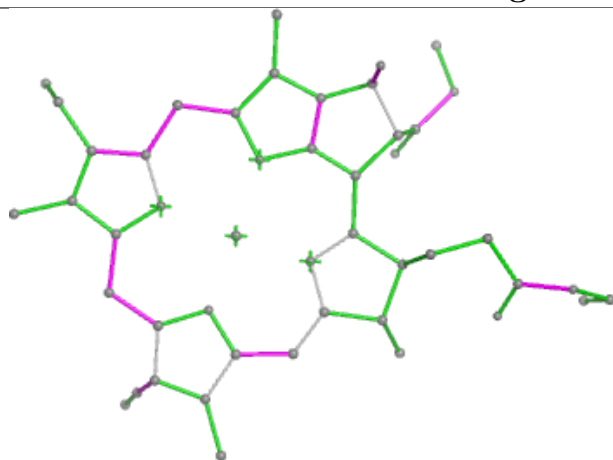
Rings



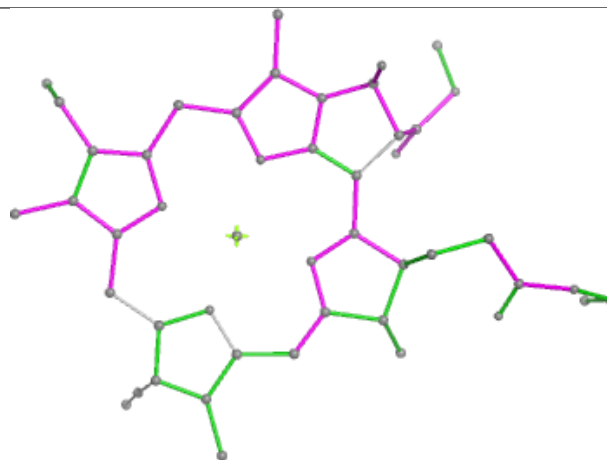




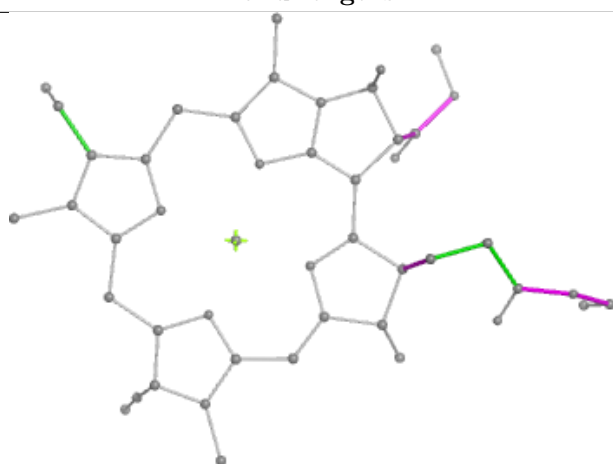
## Ligand CLA 1 1189



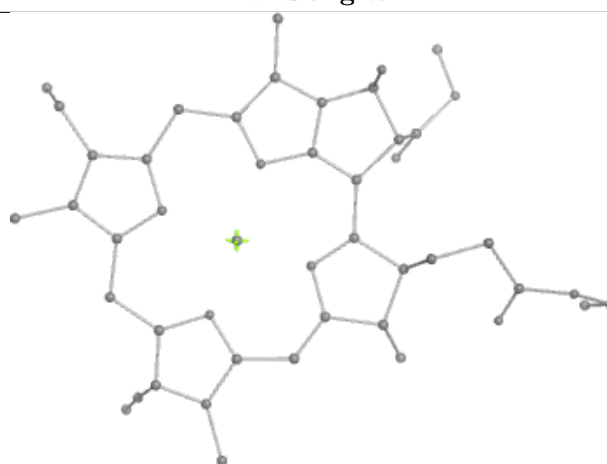
Bond lengths



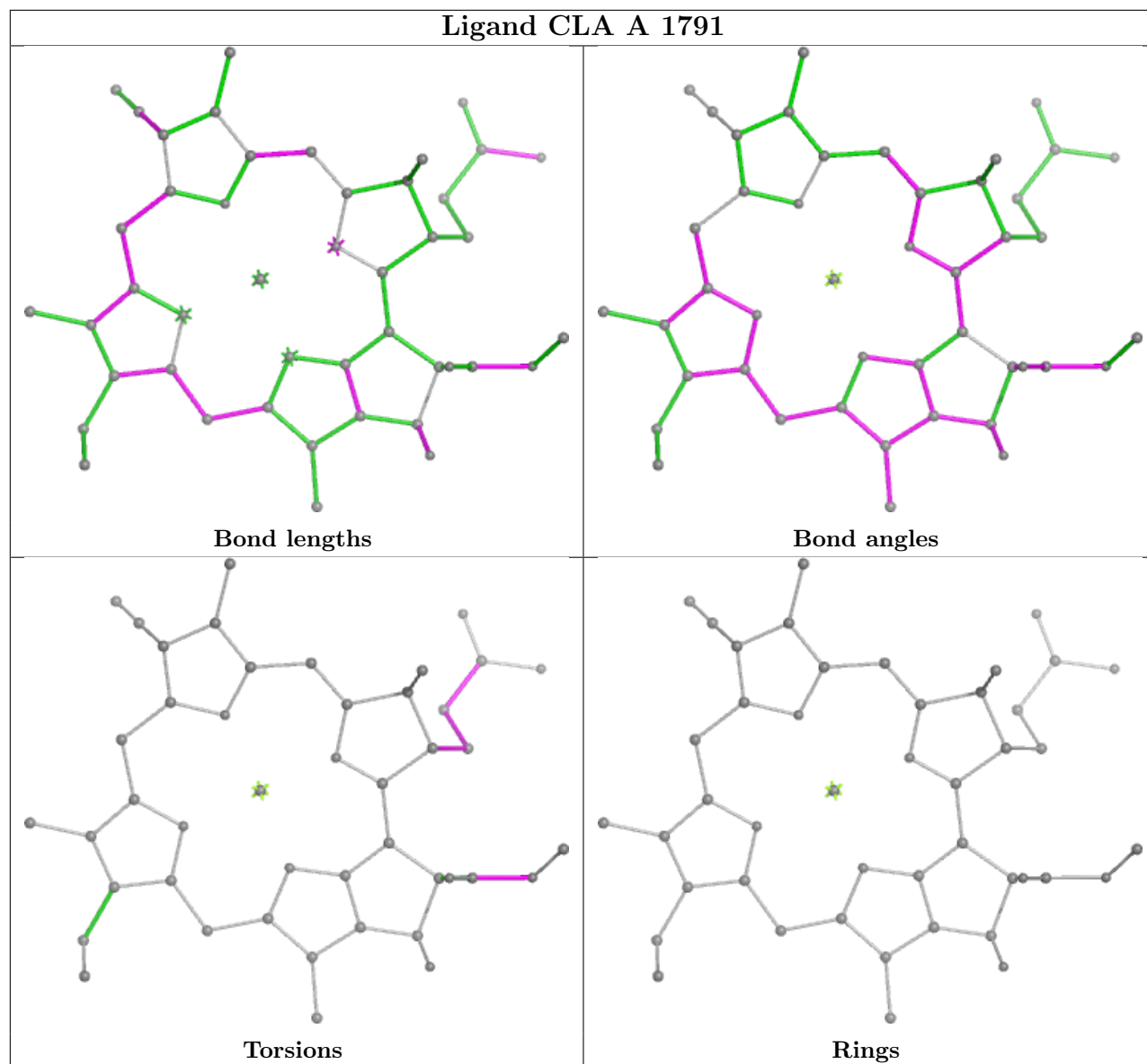
Bond angles



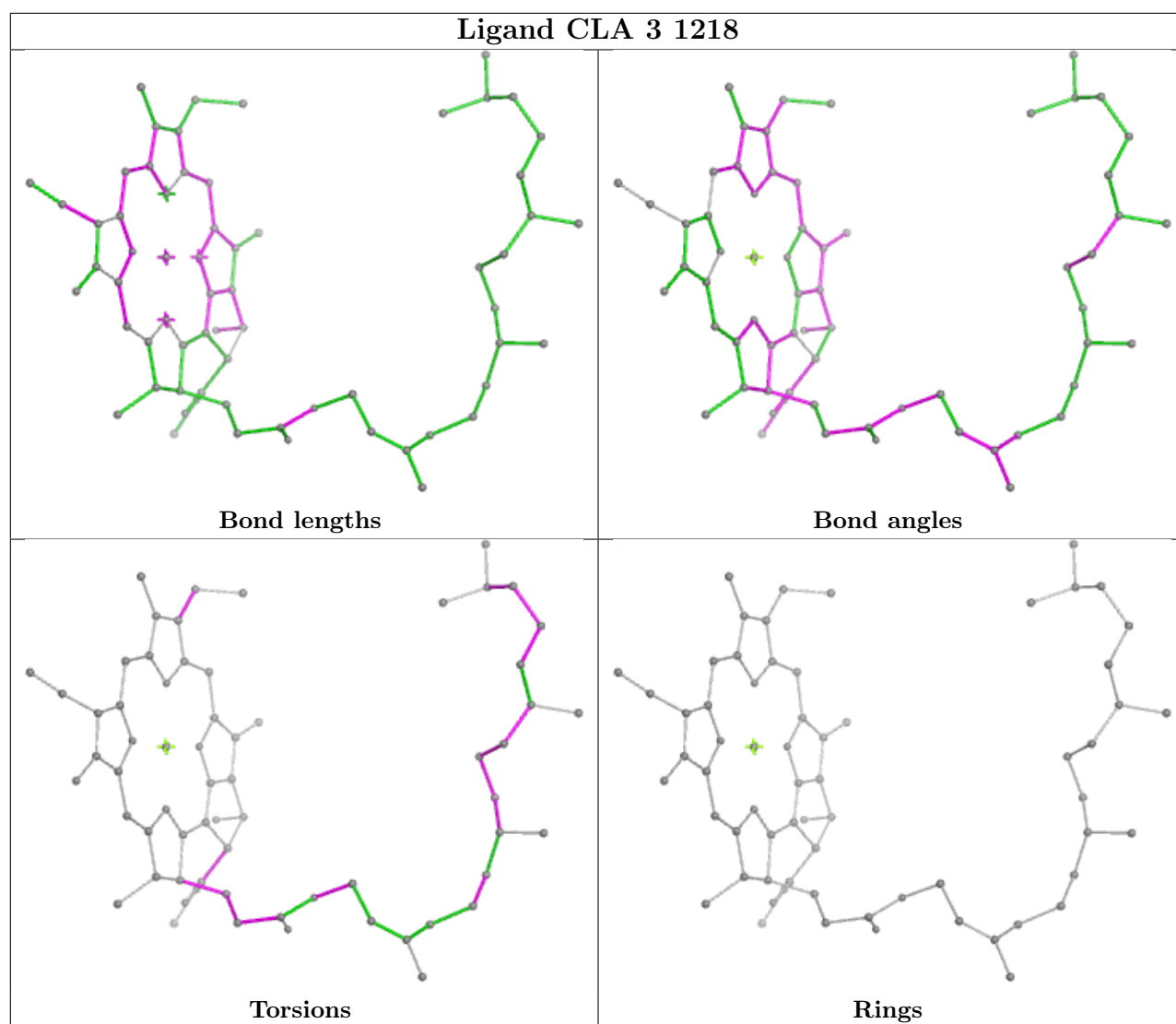
Torsions

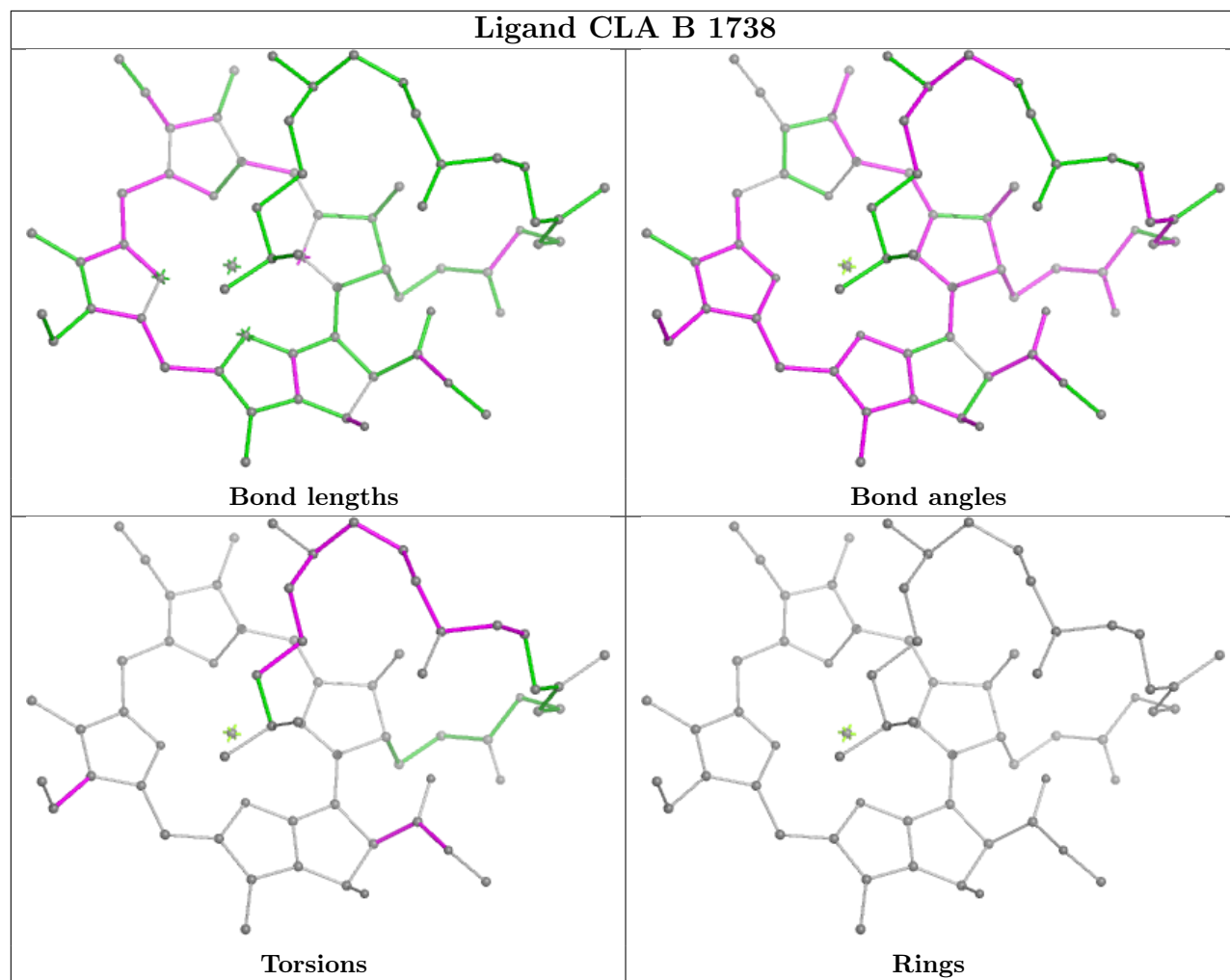


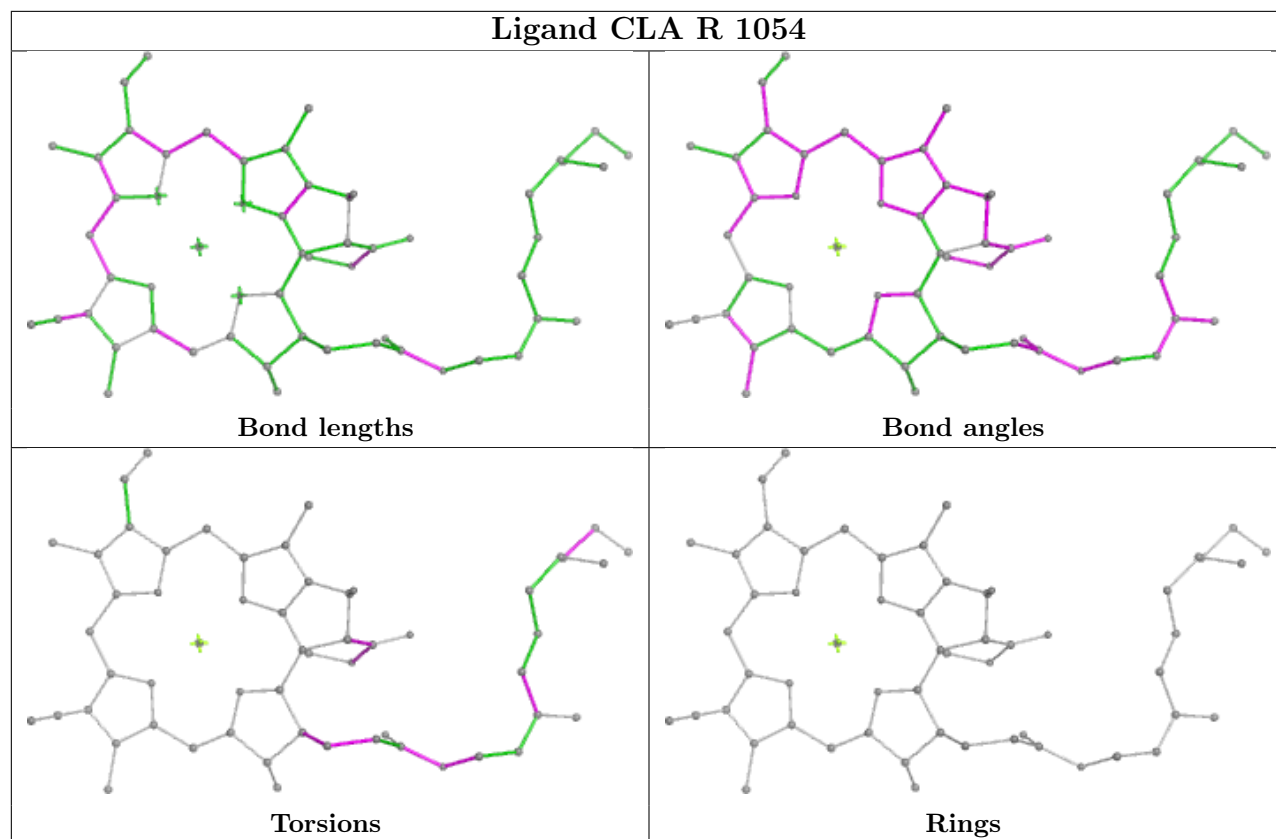
Rings

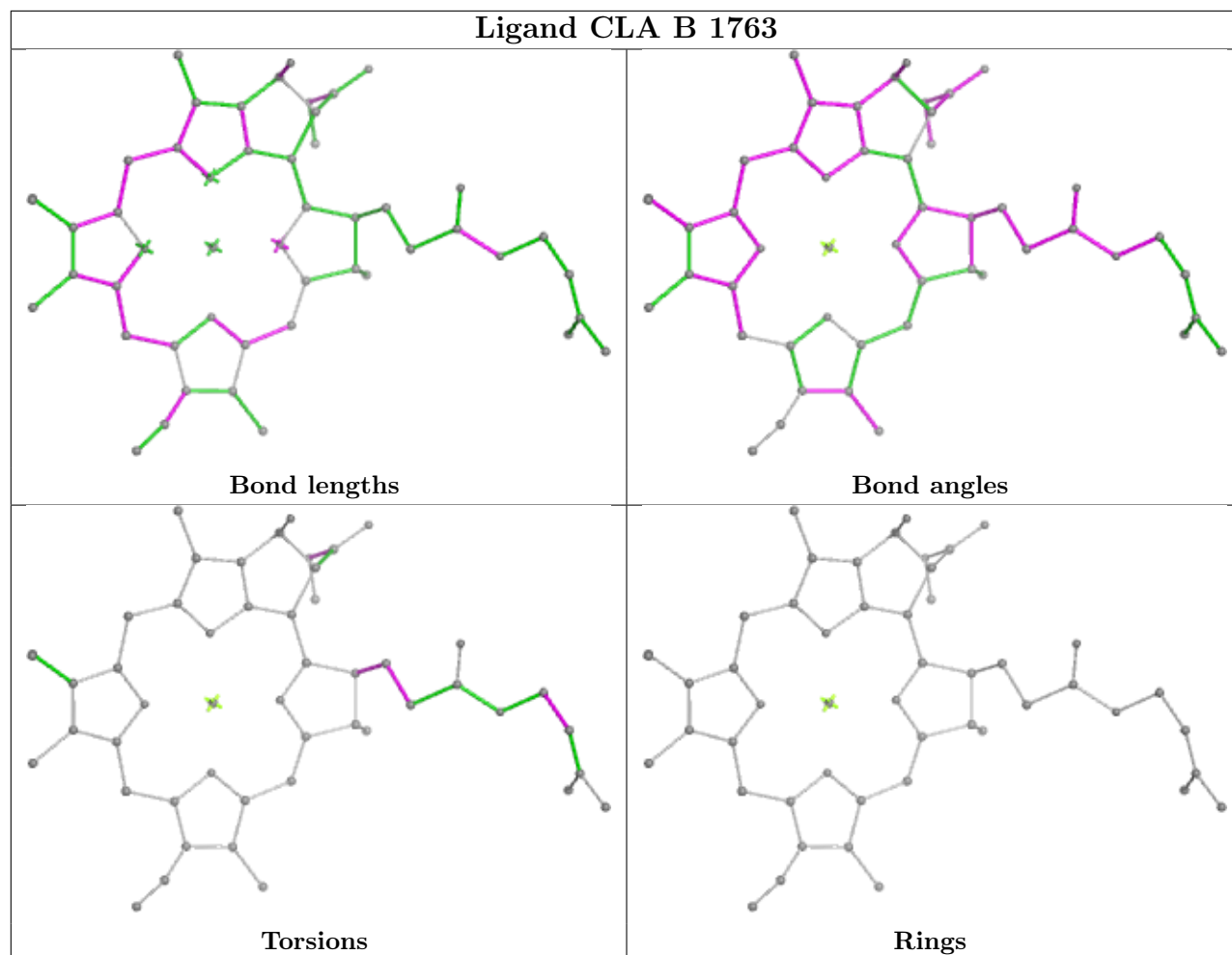


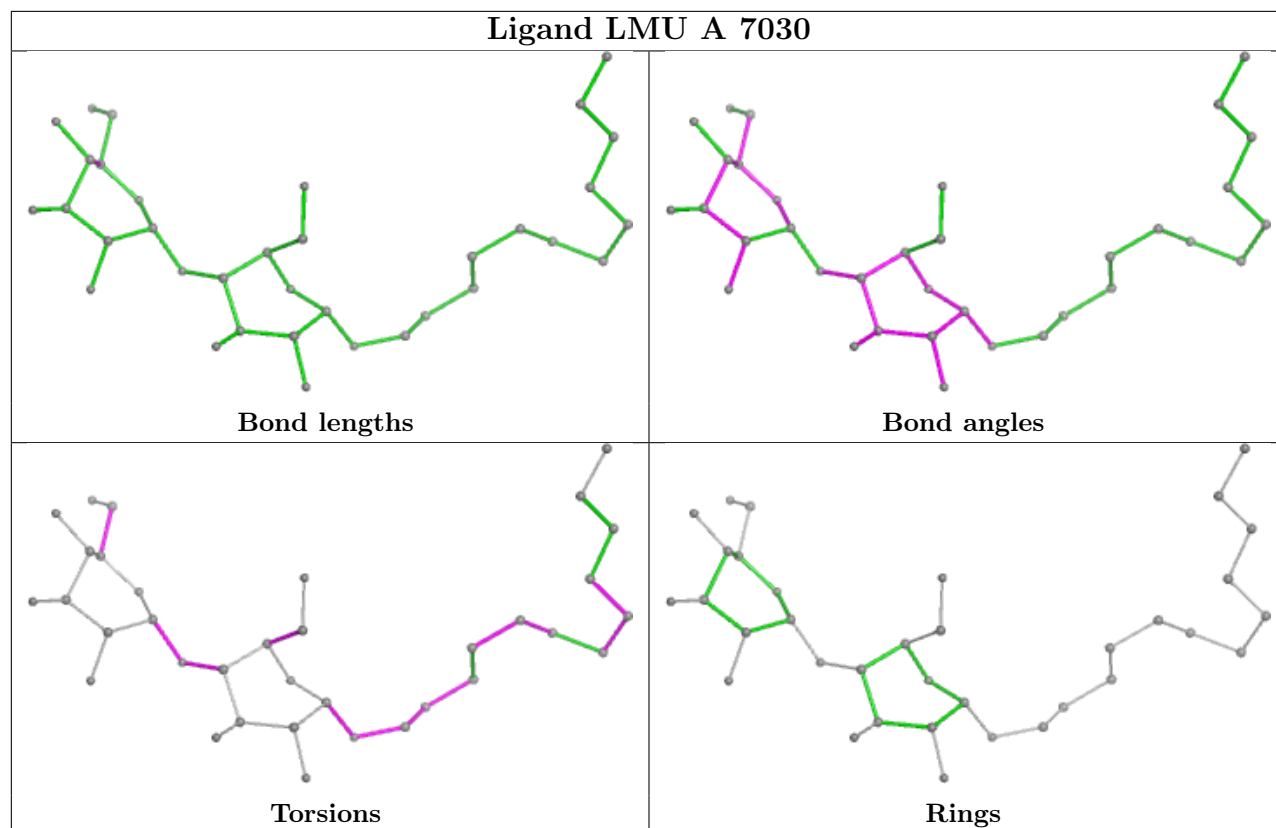
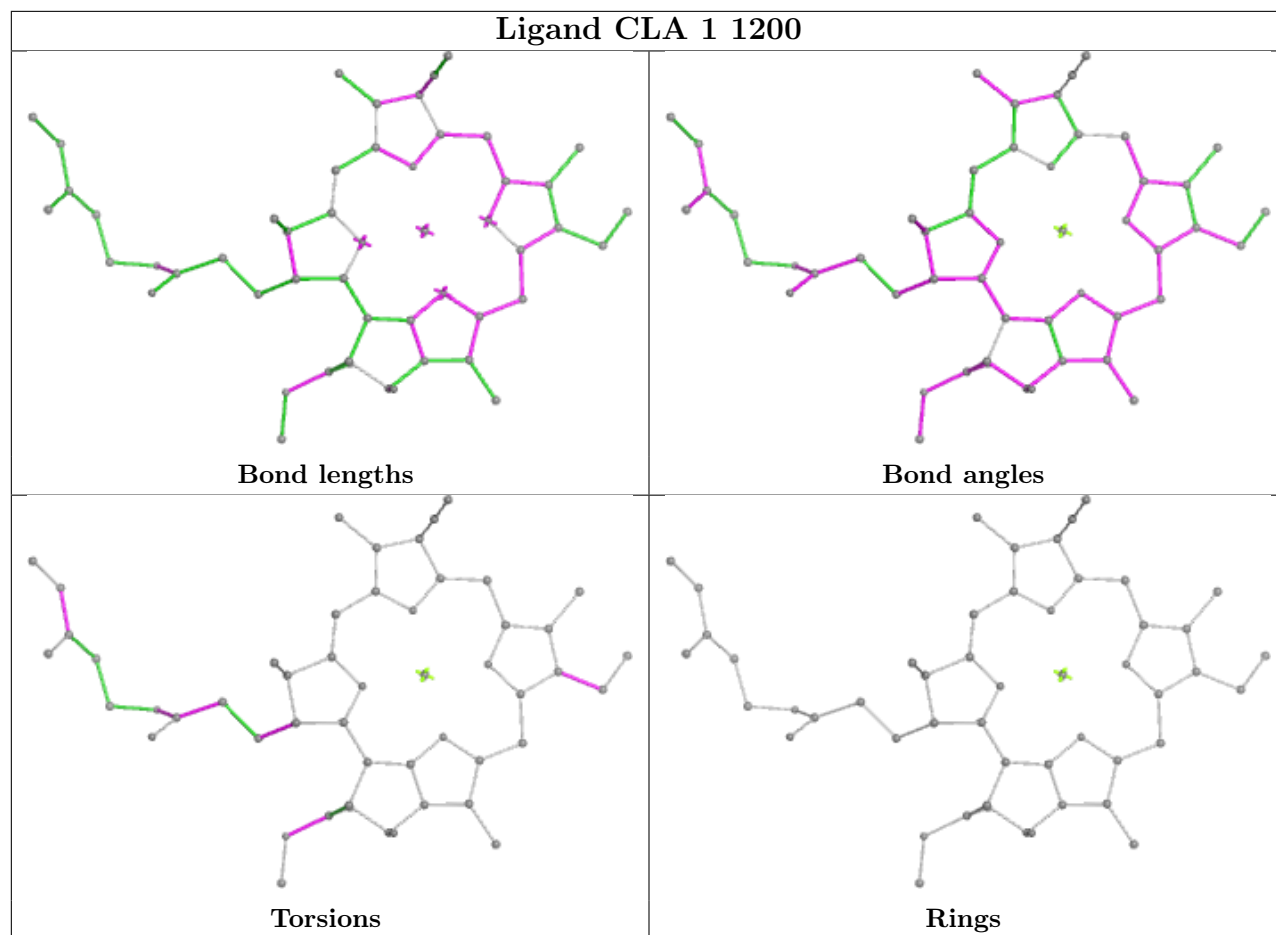




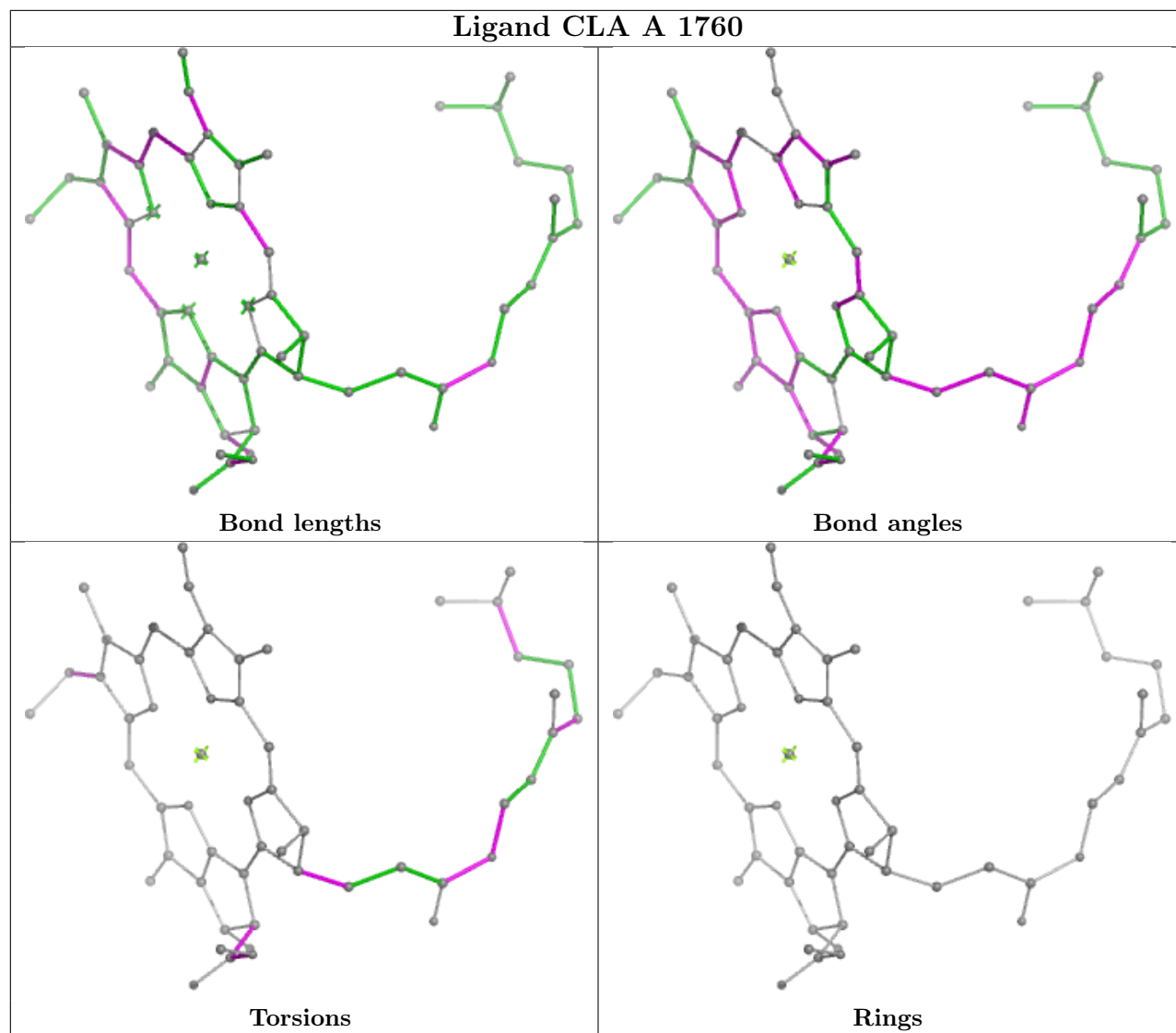


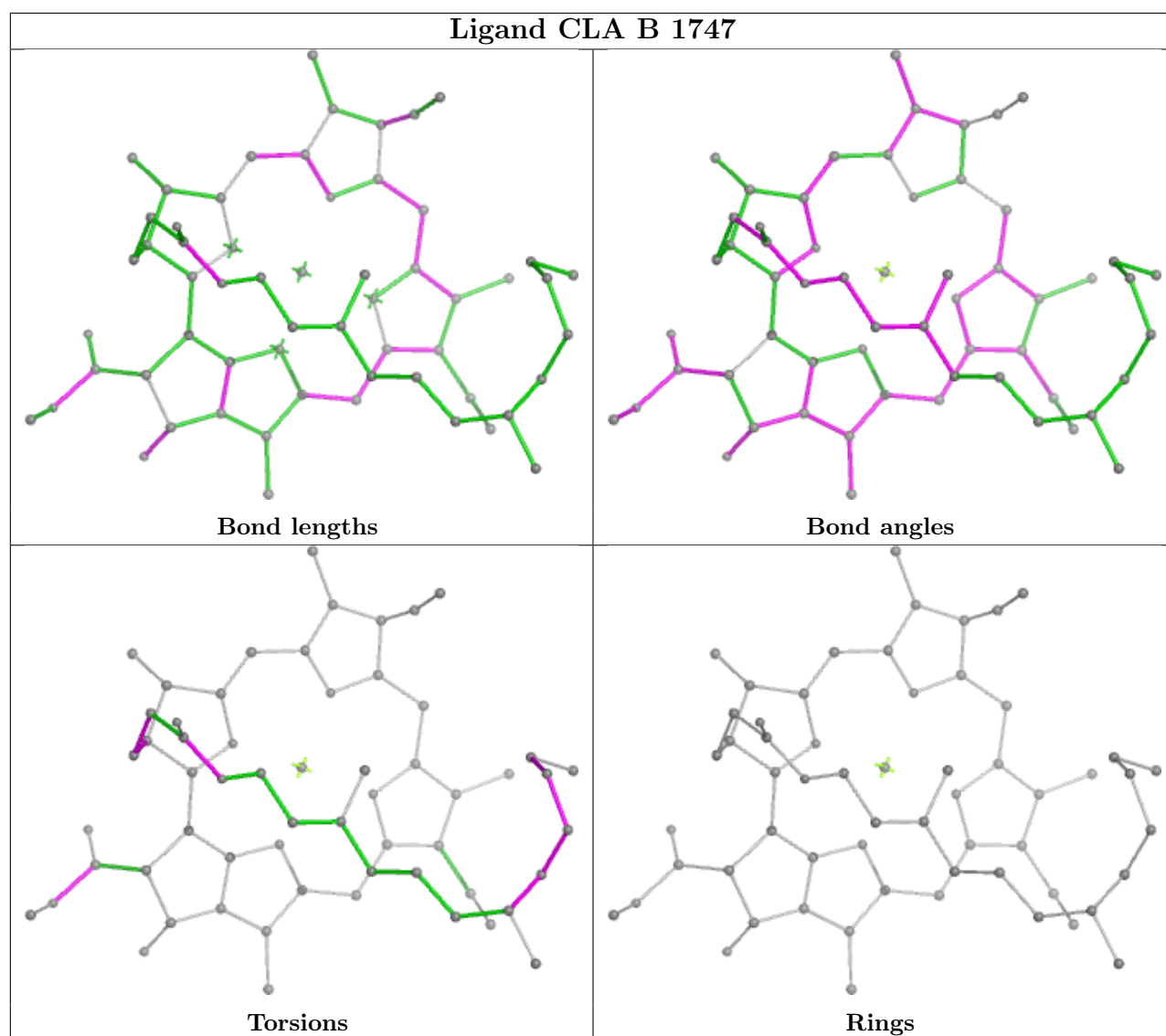




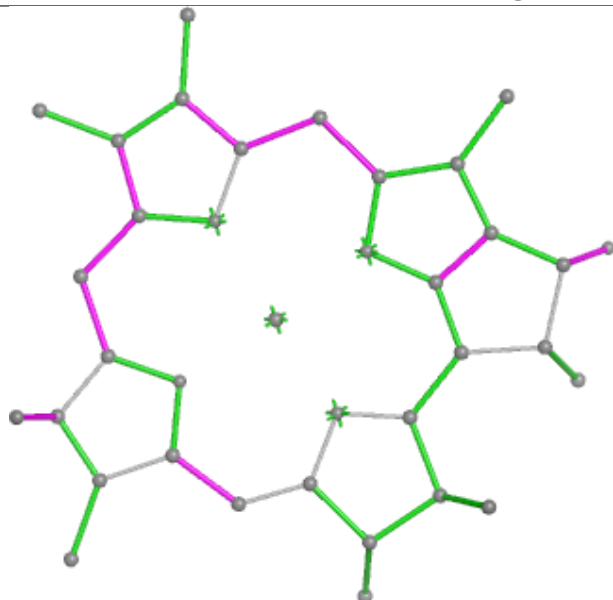


## Ligand CLA A 1760

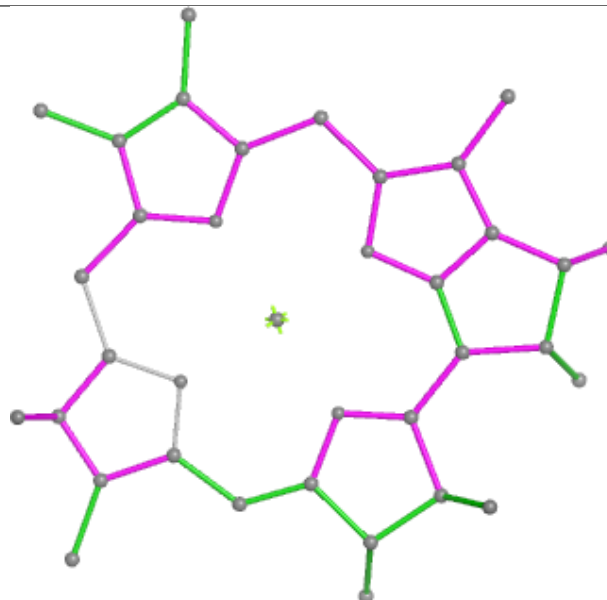




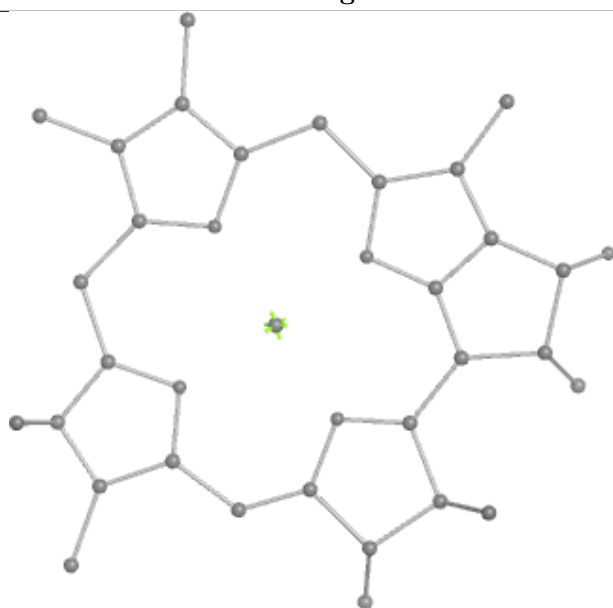
## Ligand CLA 1 1196



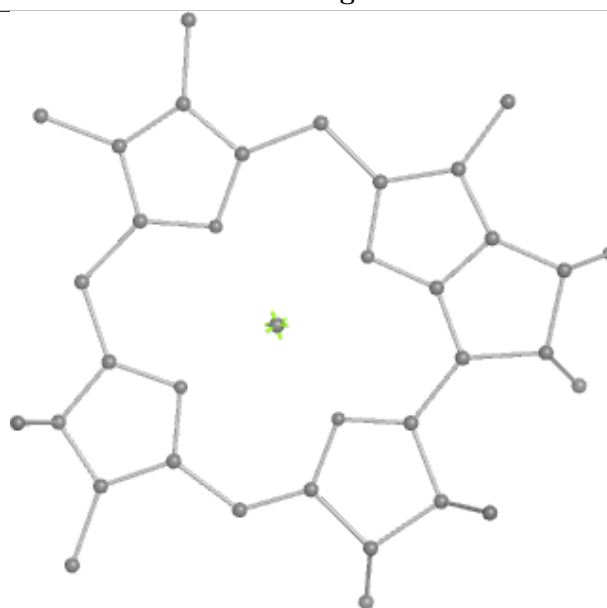
Bond lengths



Bond angles



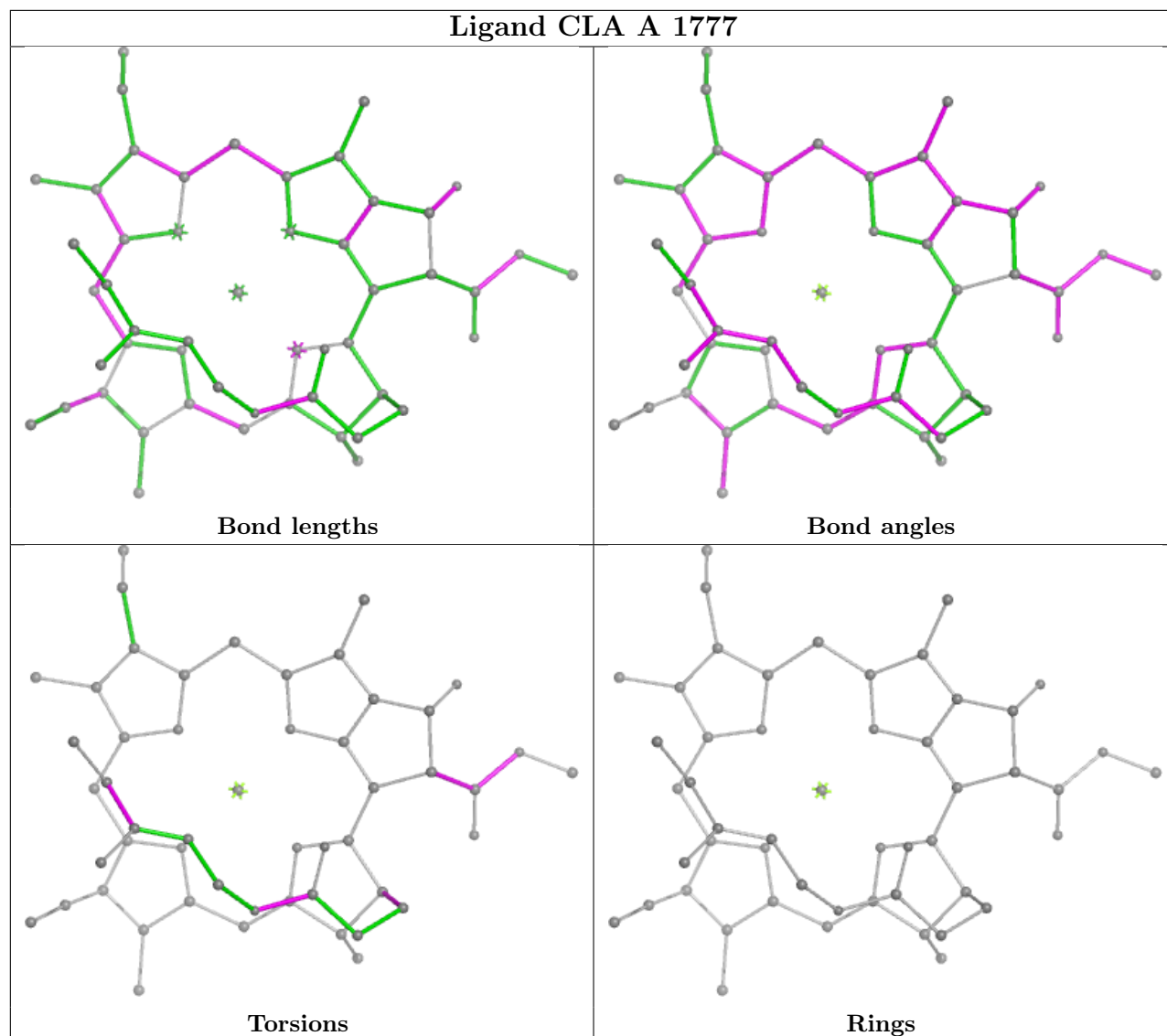
Torsions



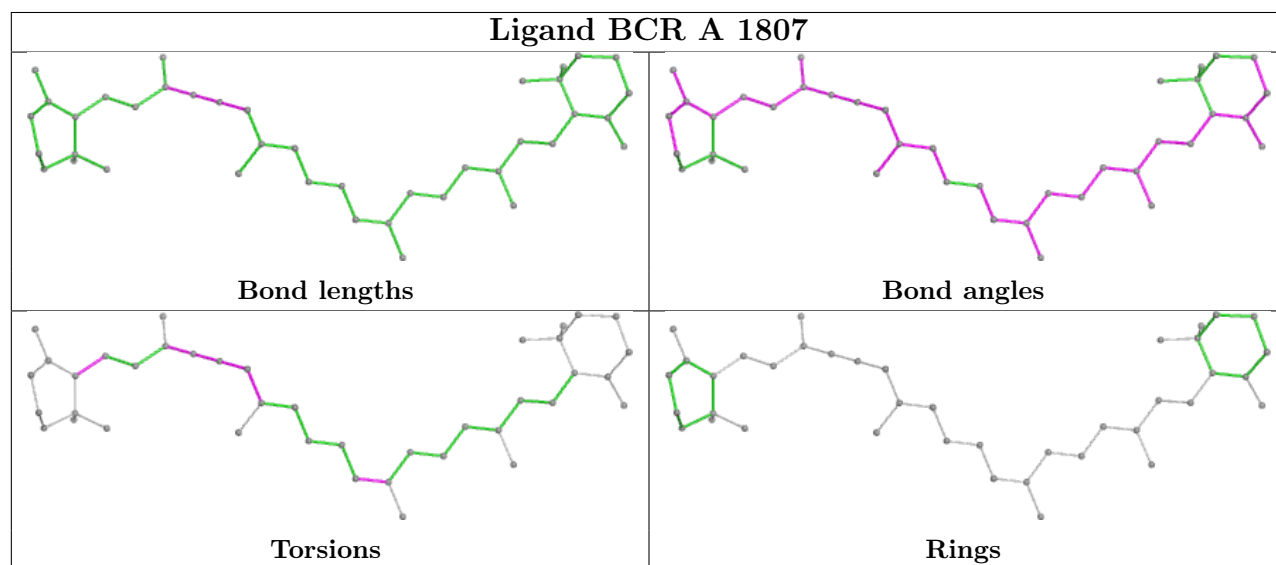
Rings

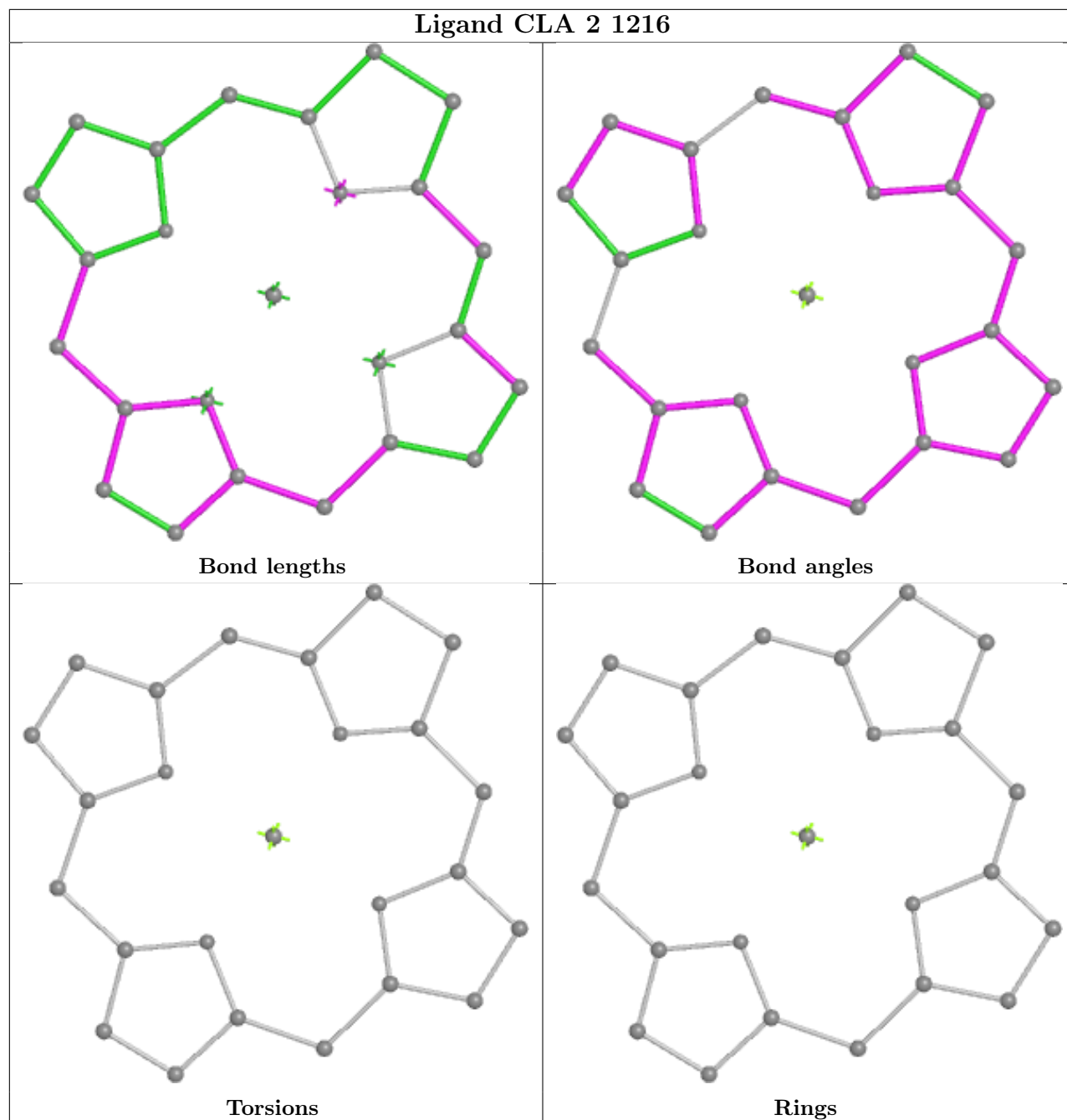


## Ligand CLA A 1777

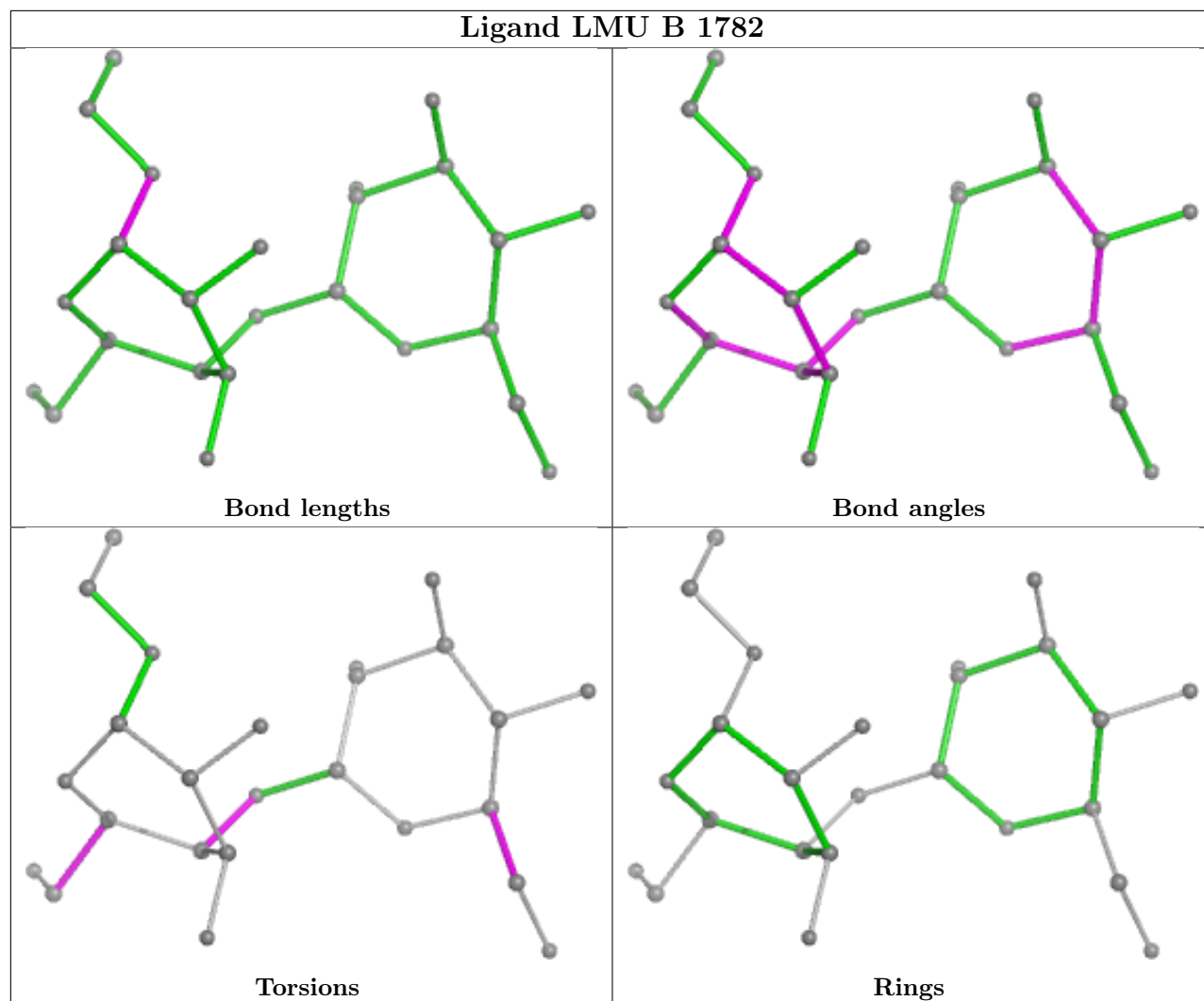


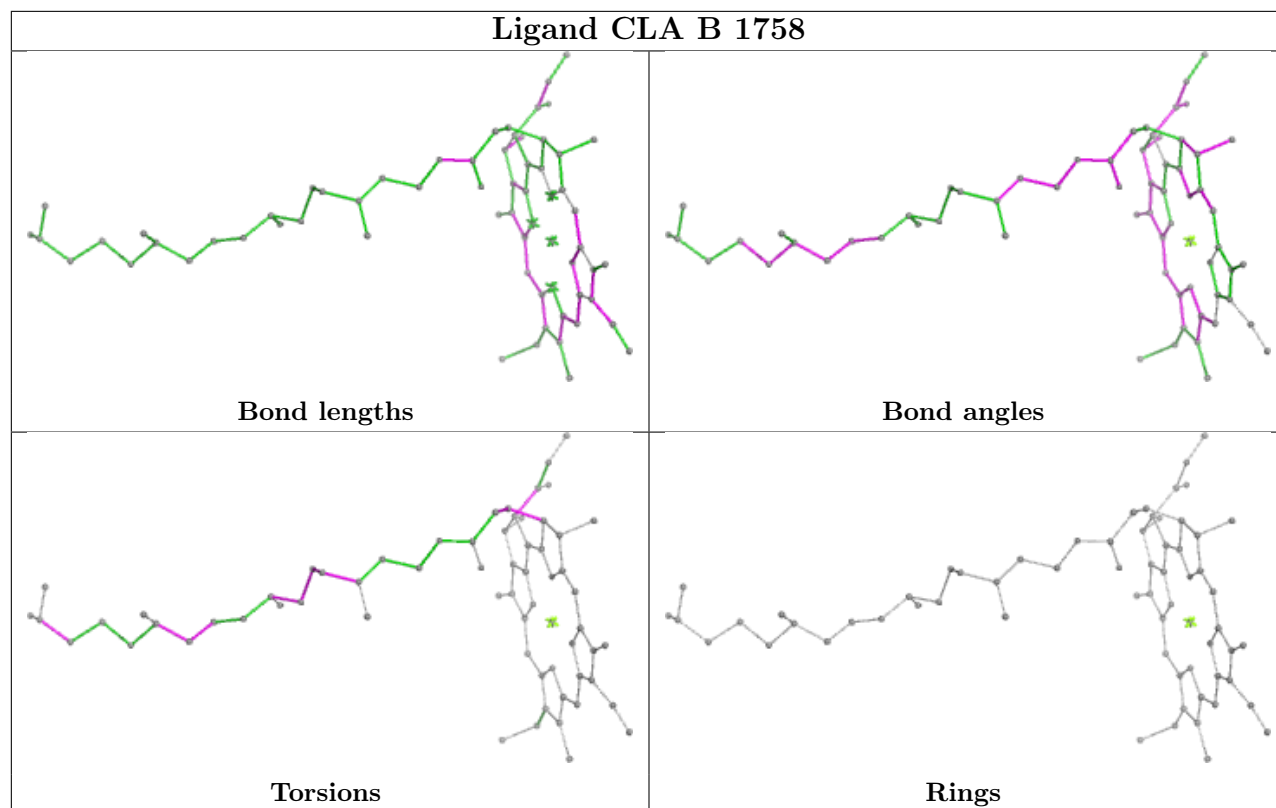
## Ligand BCR A 1807

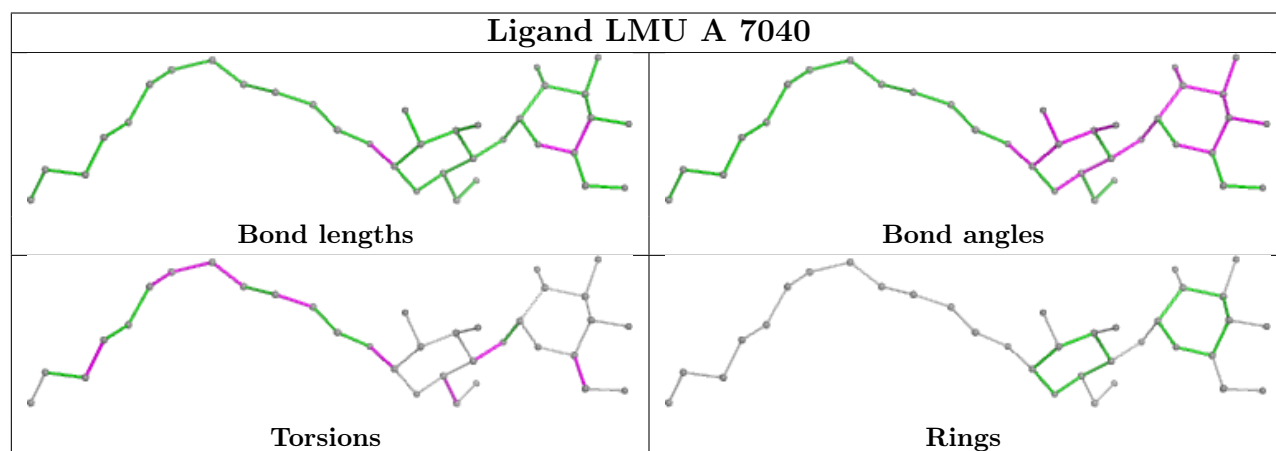
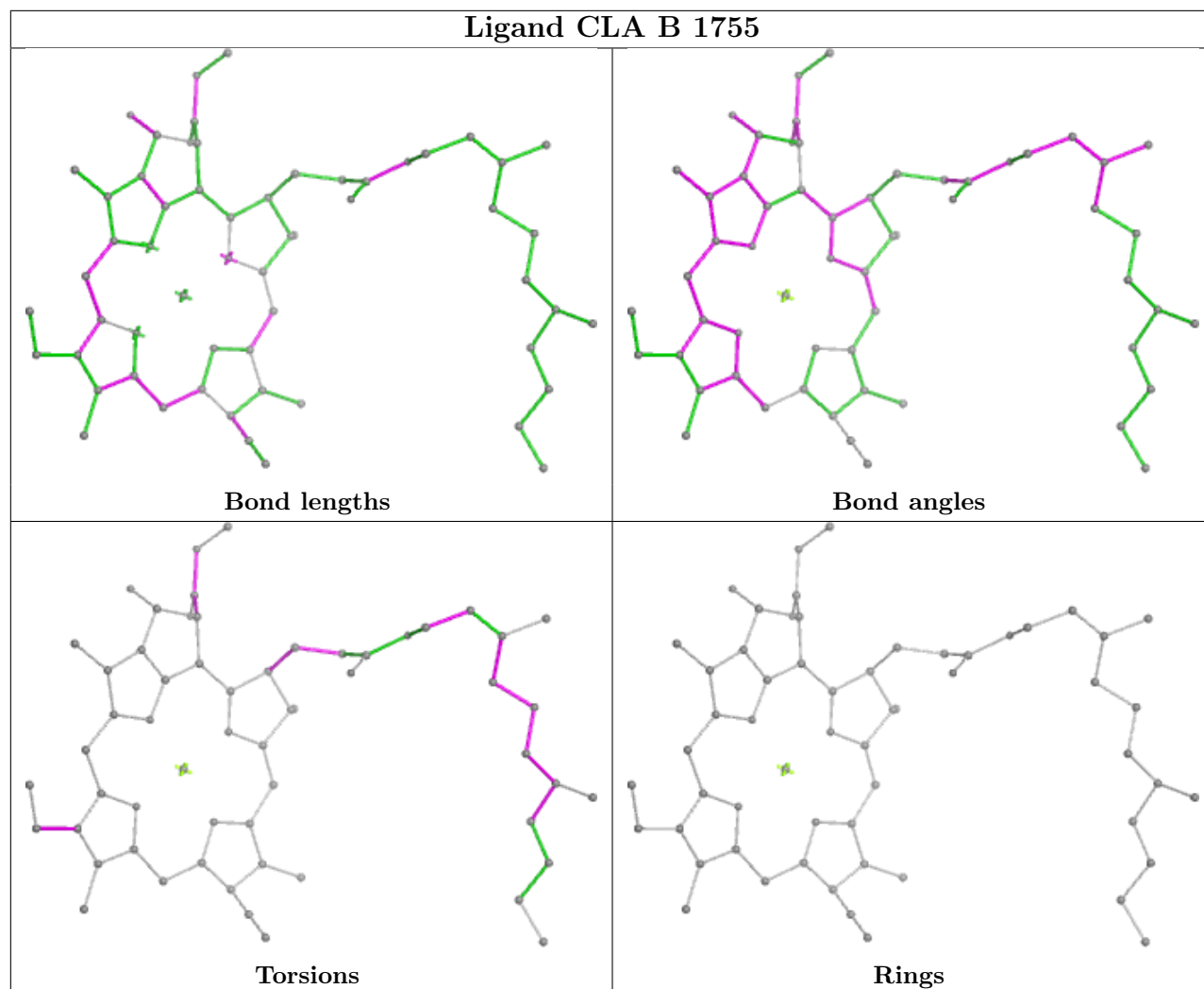


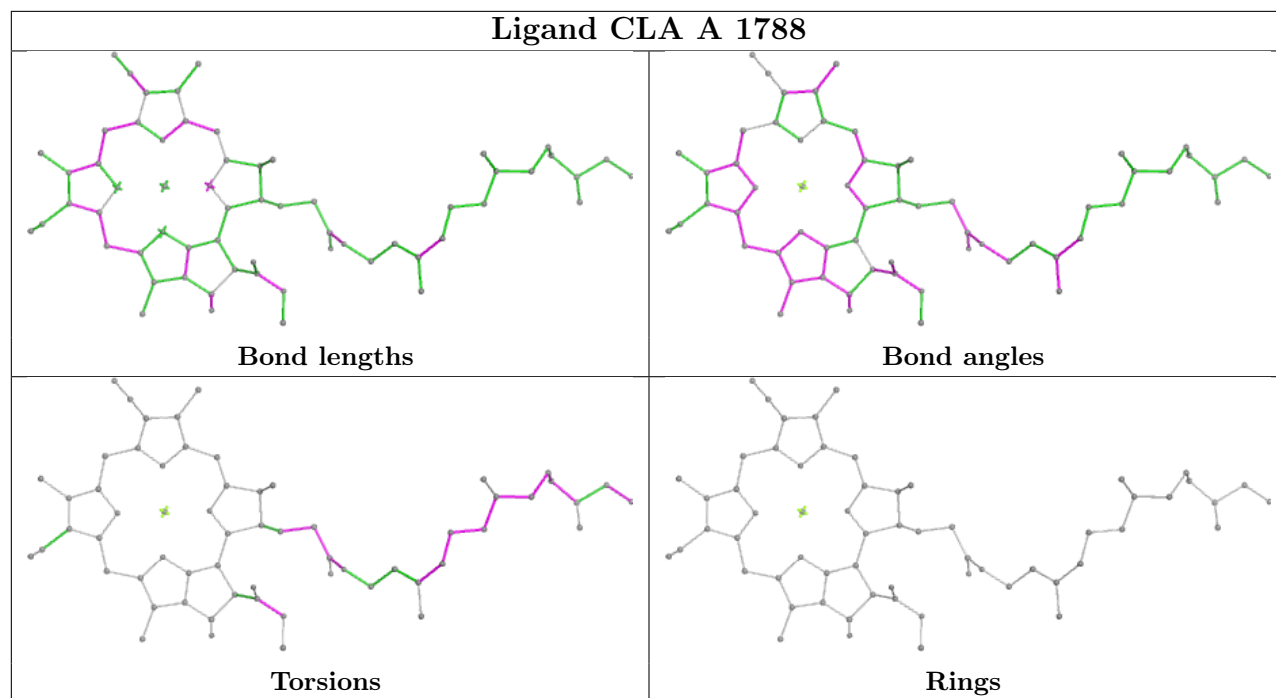


## Ligand LMU B 1782

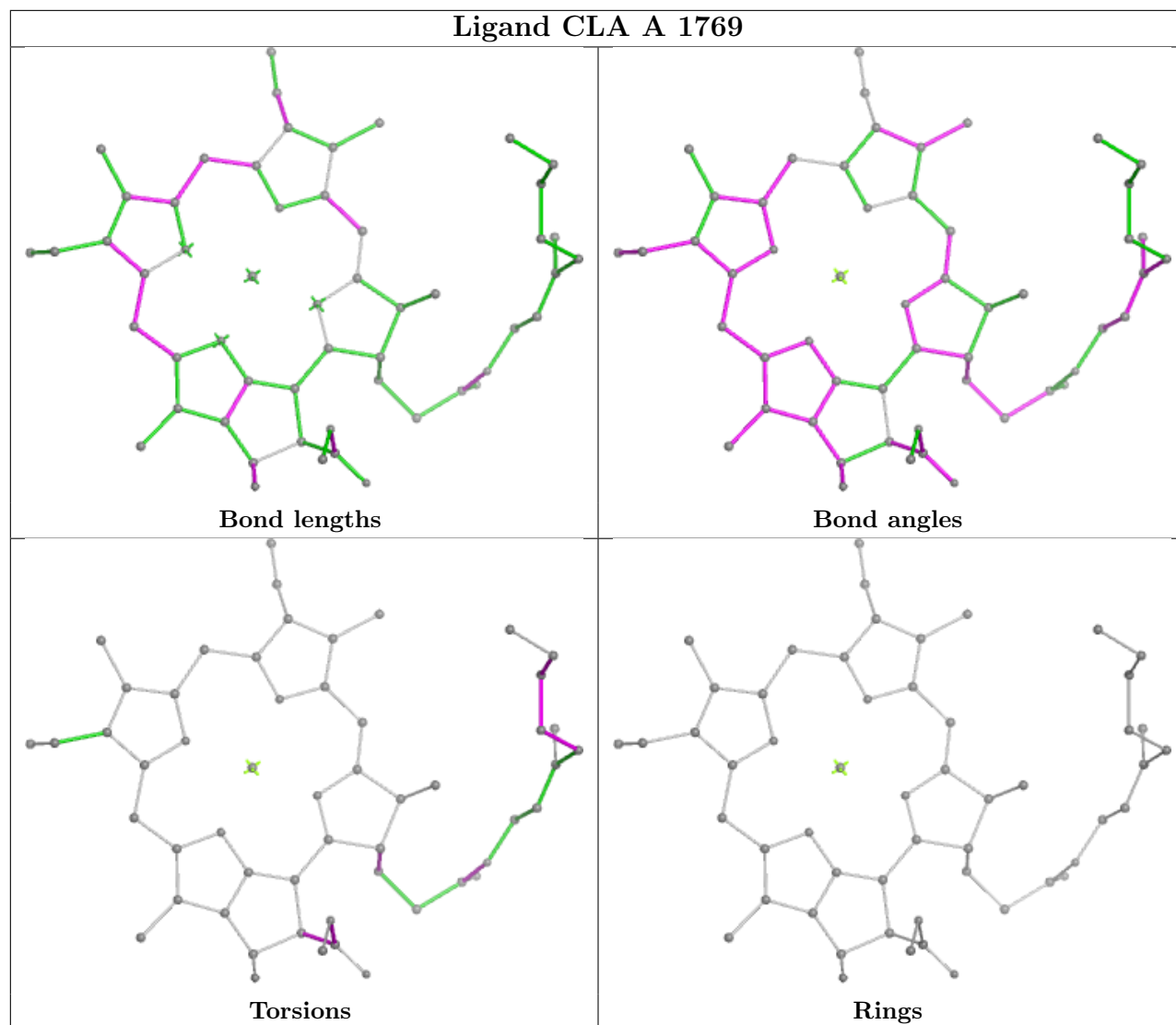


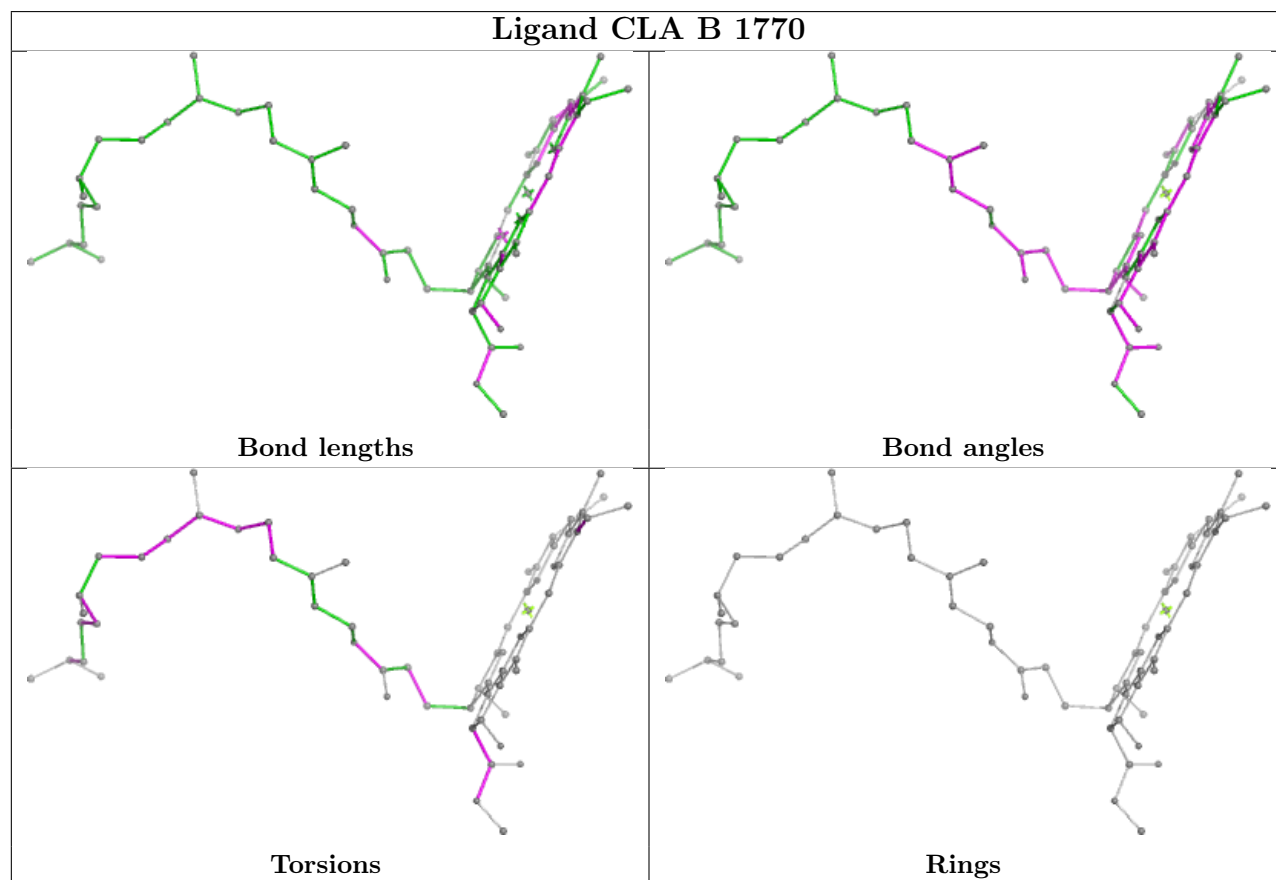
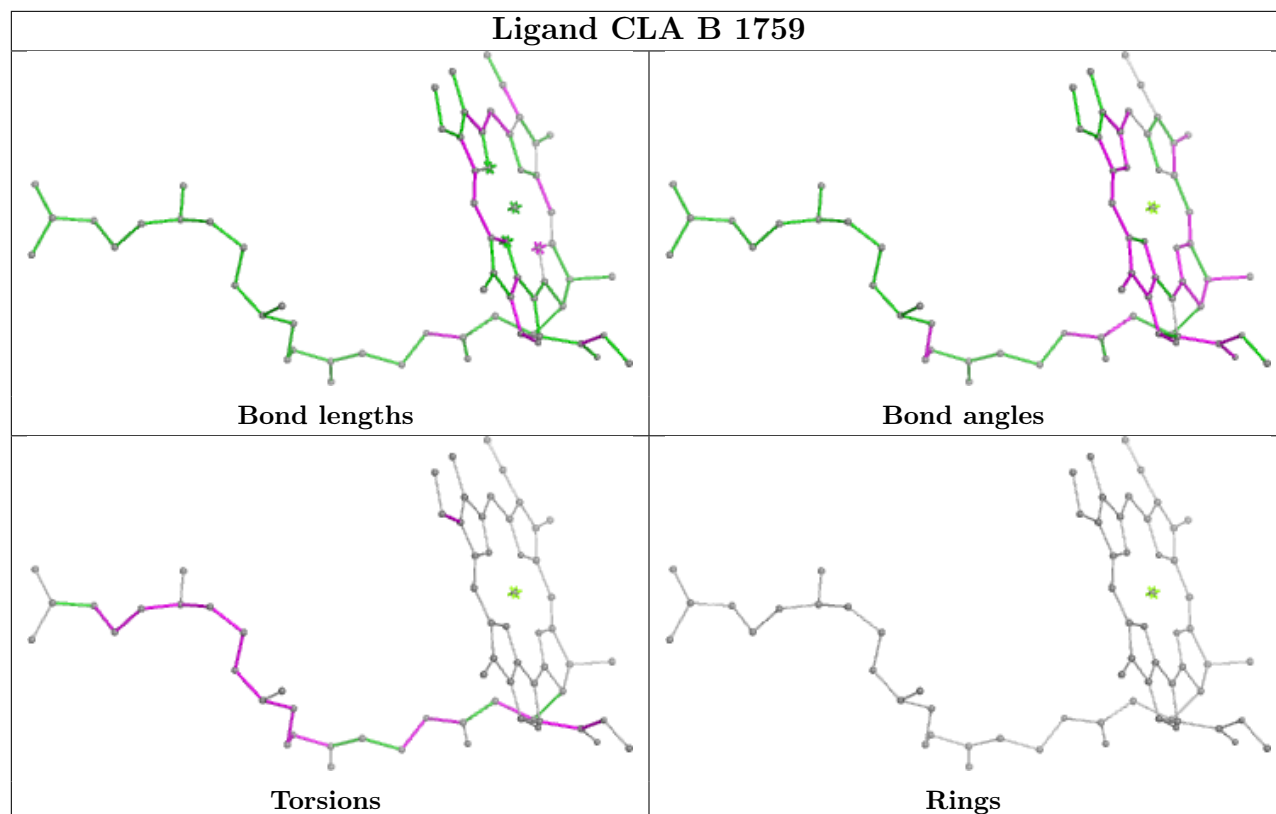






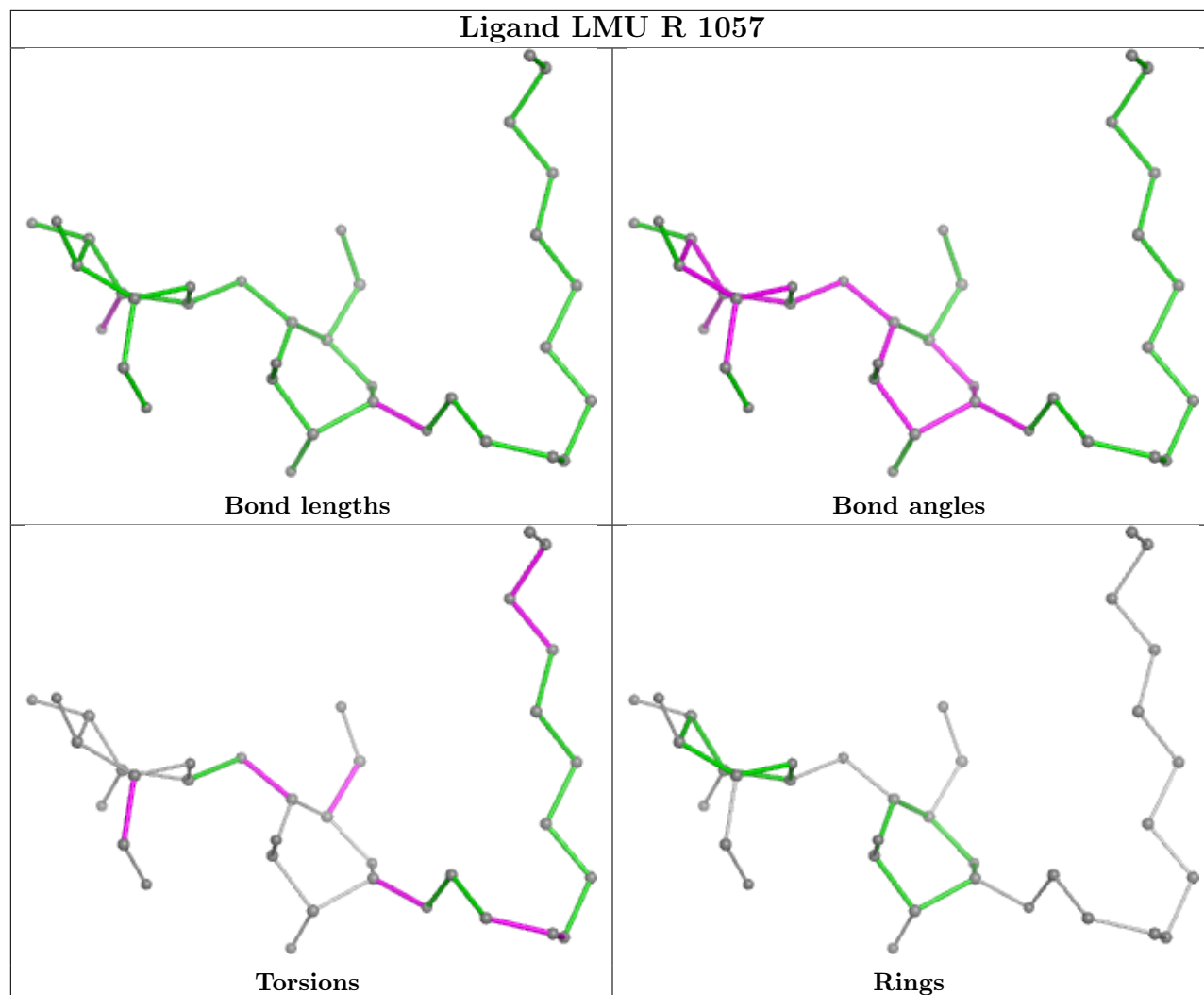
## Ligand CLA A 1769



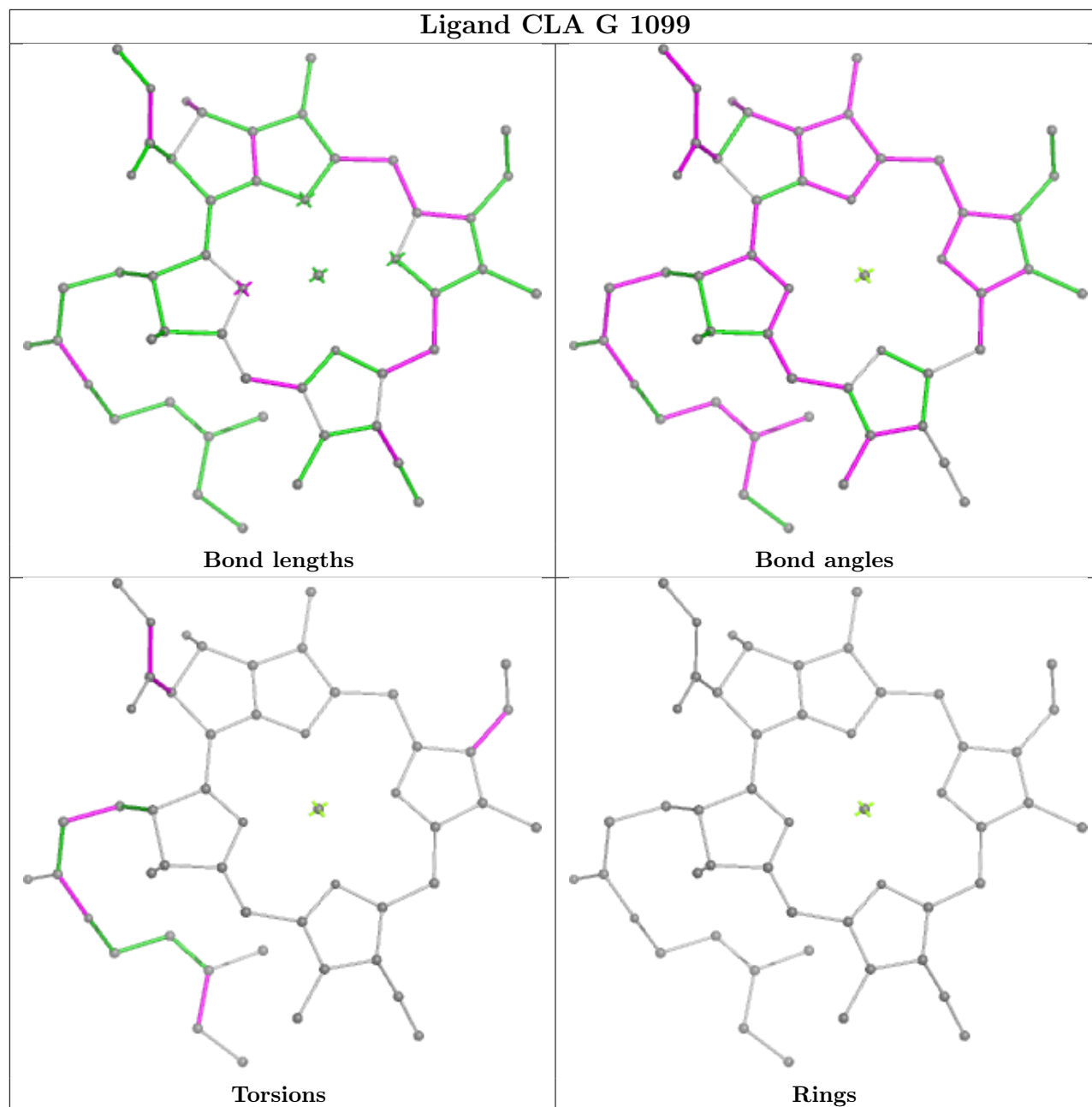


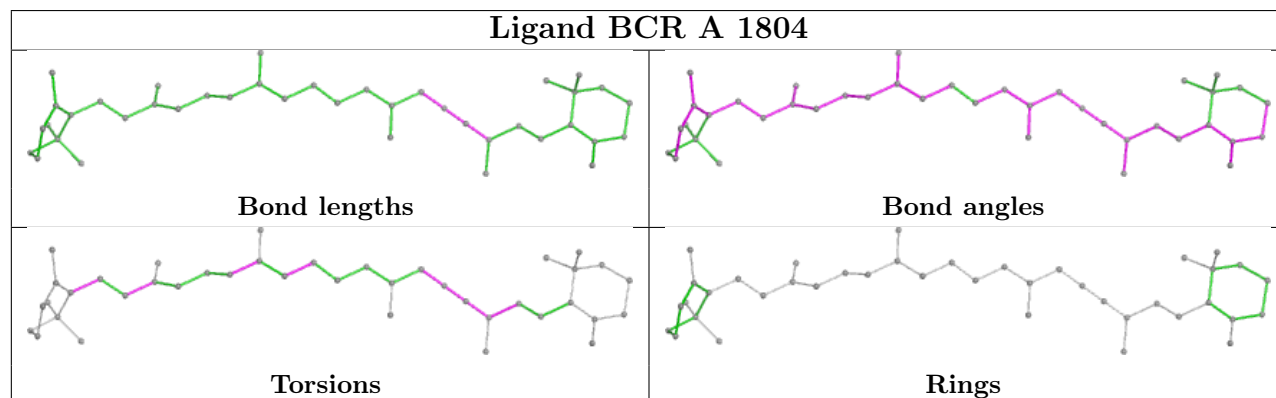
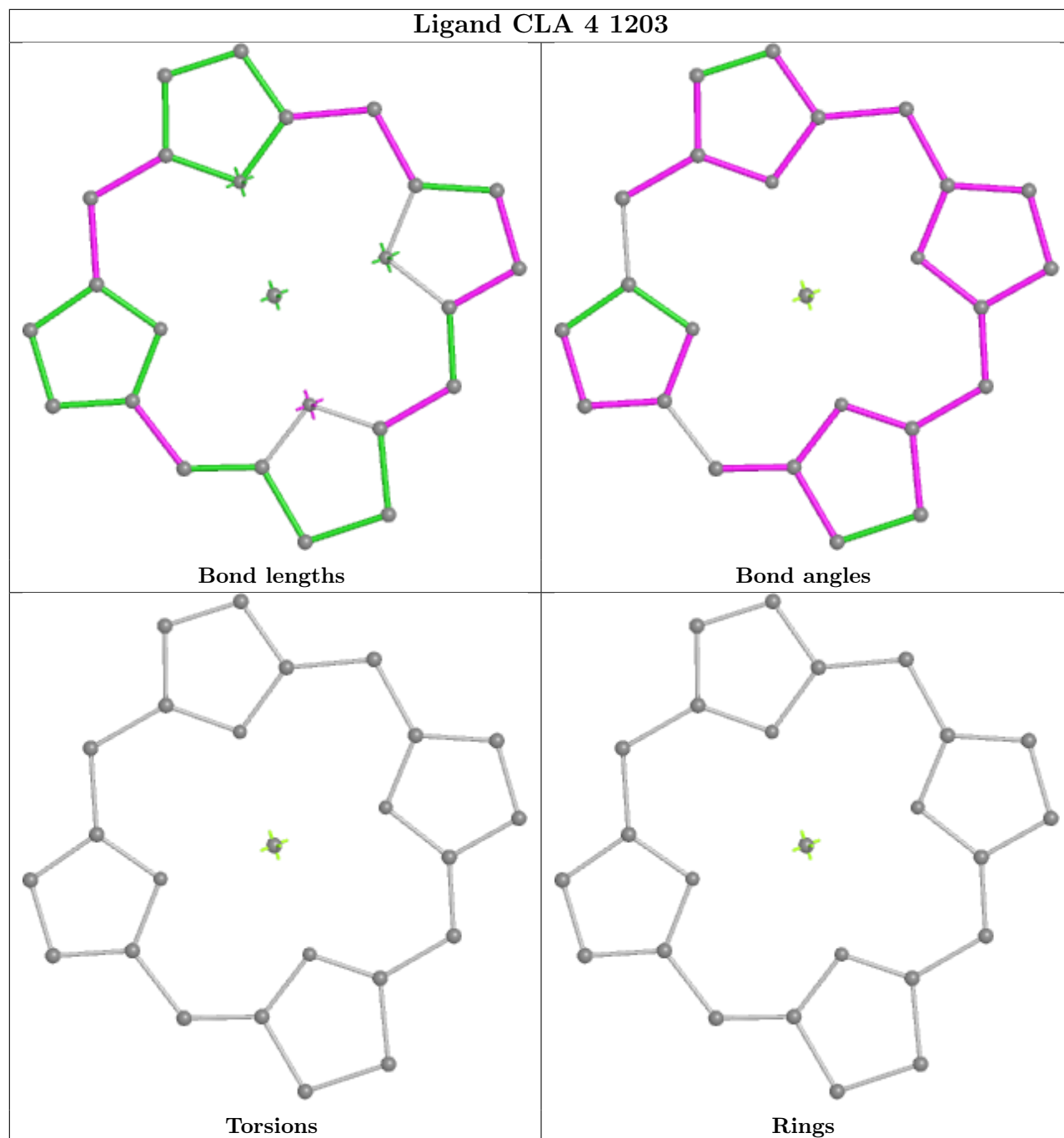


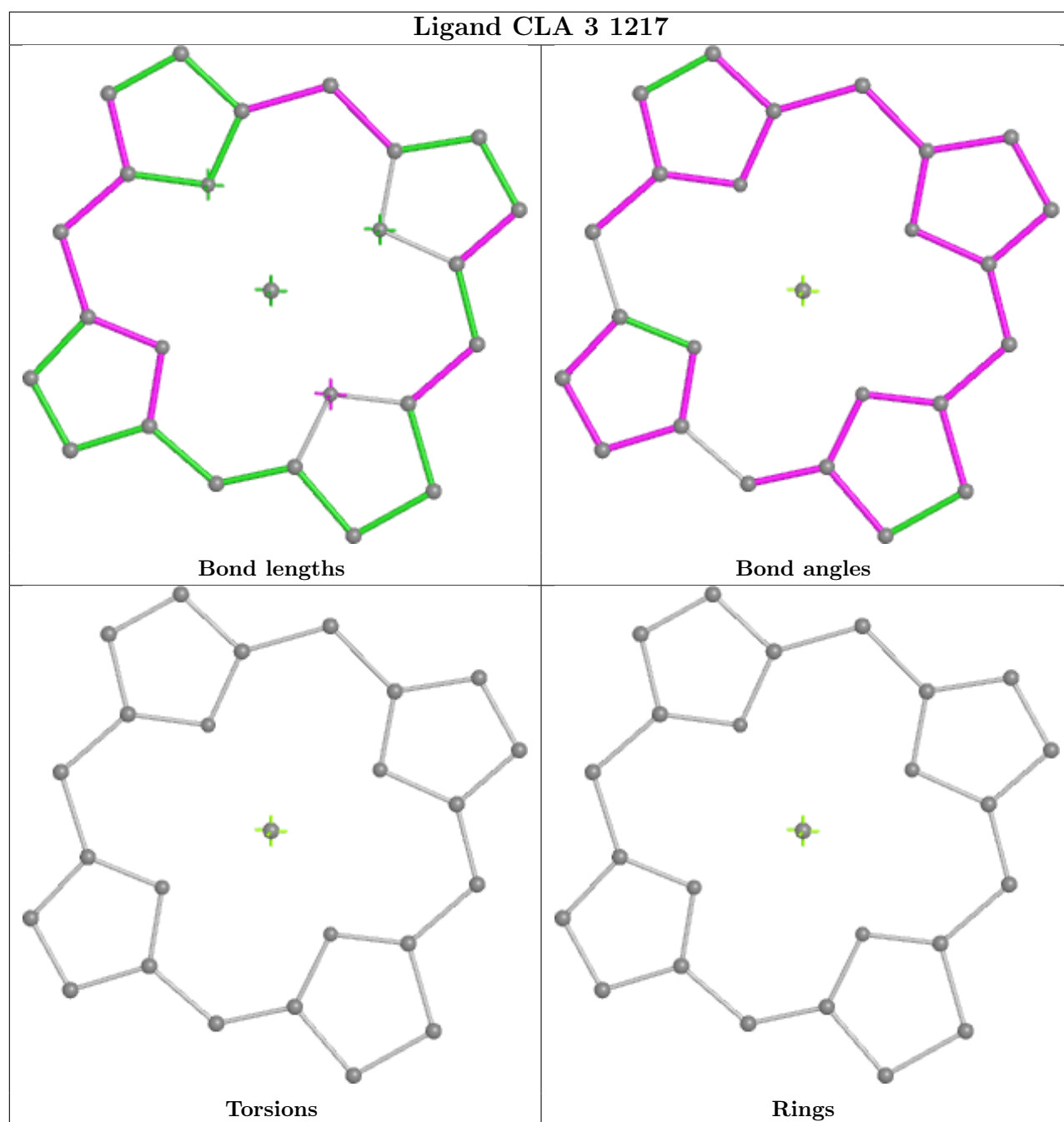
## Ligand LMU R 1057

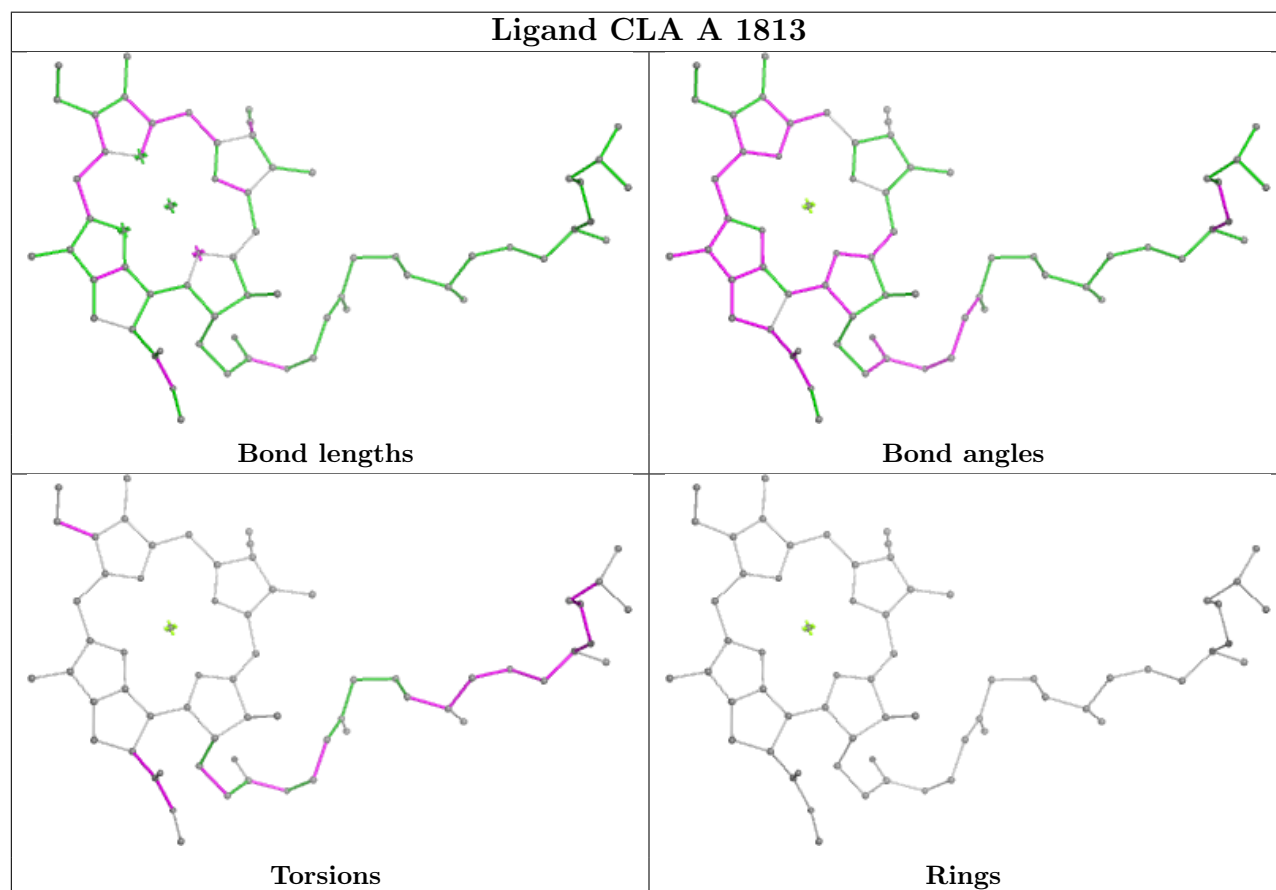
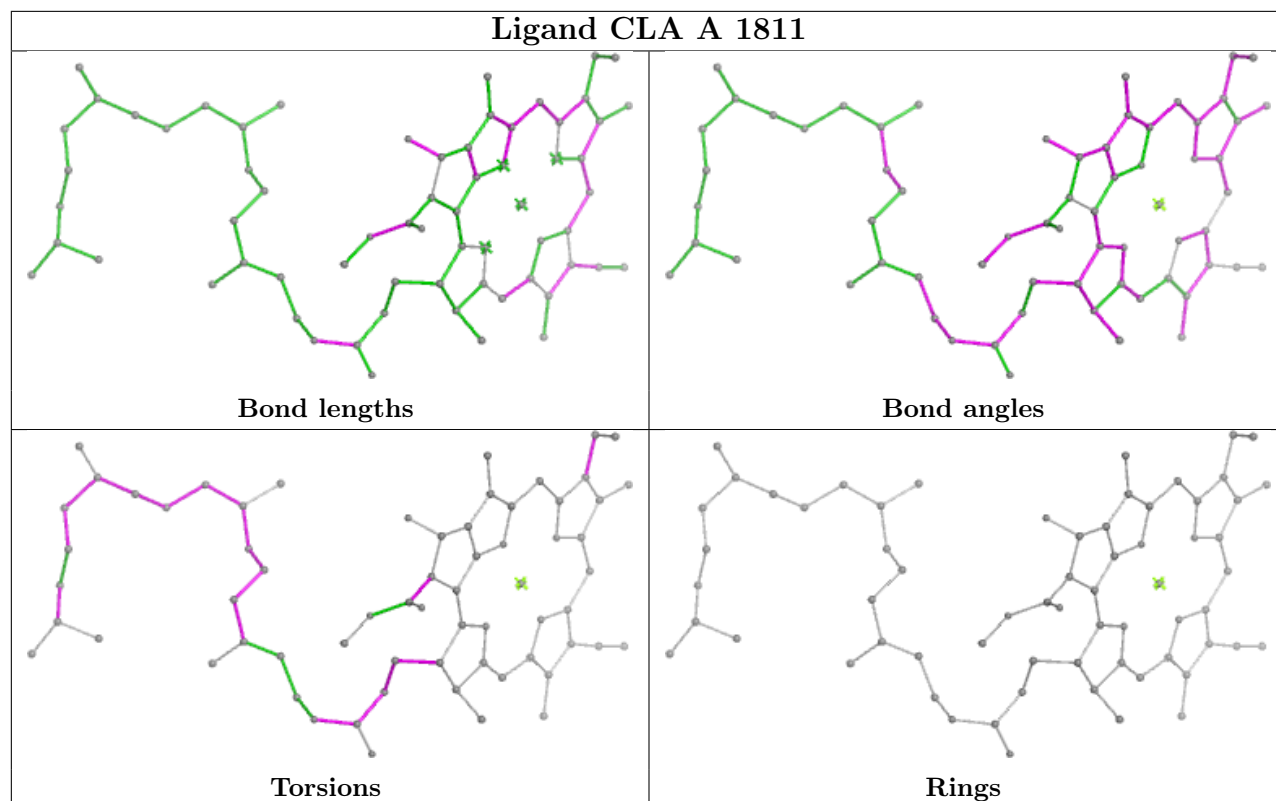


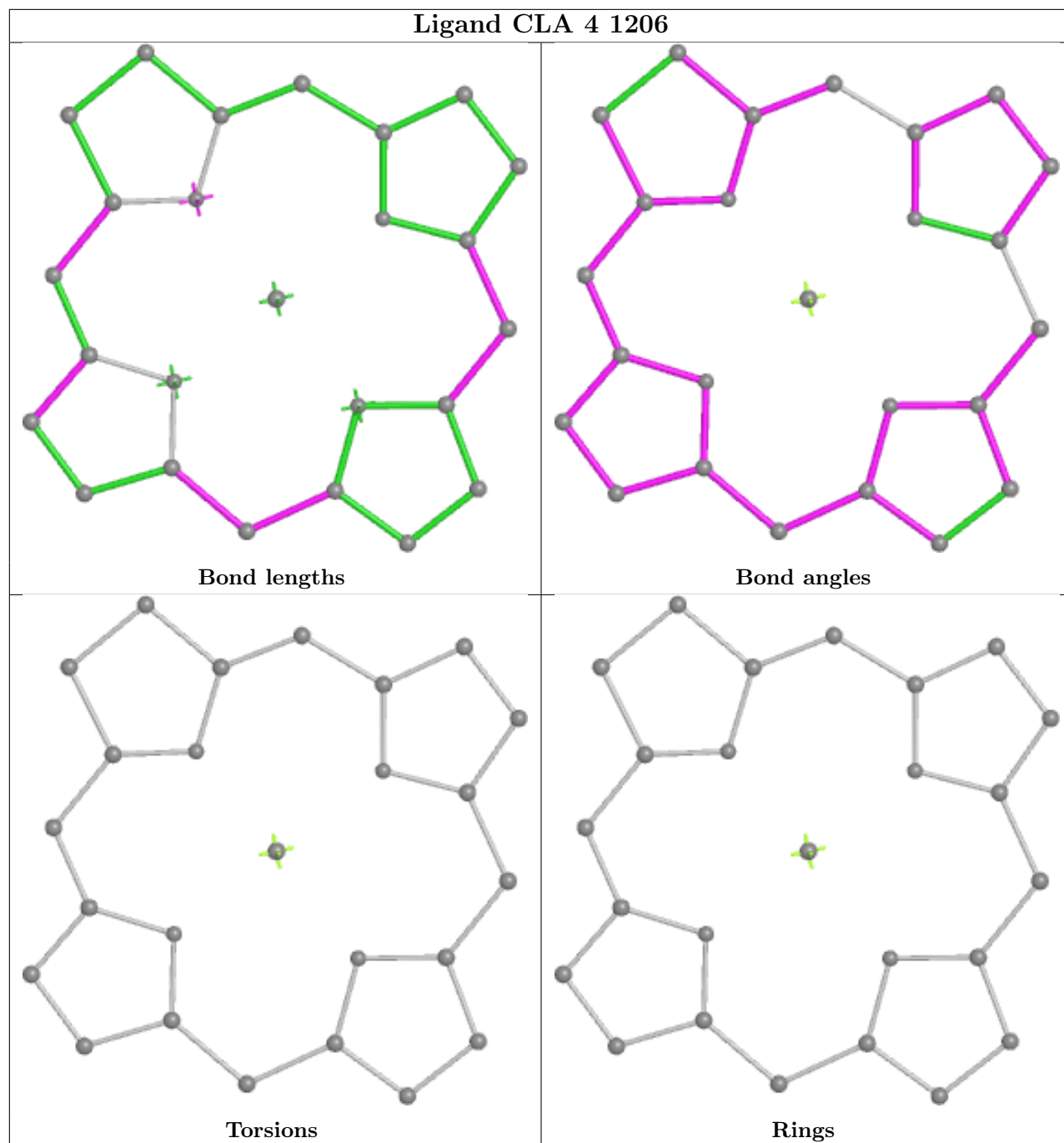
## Ligand CLA G 1099

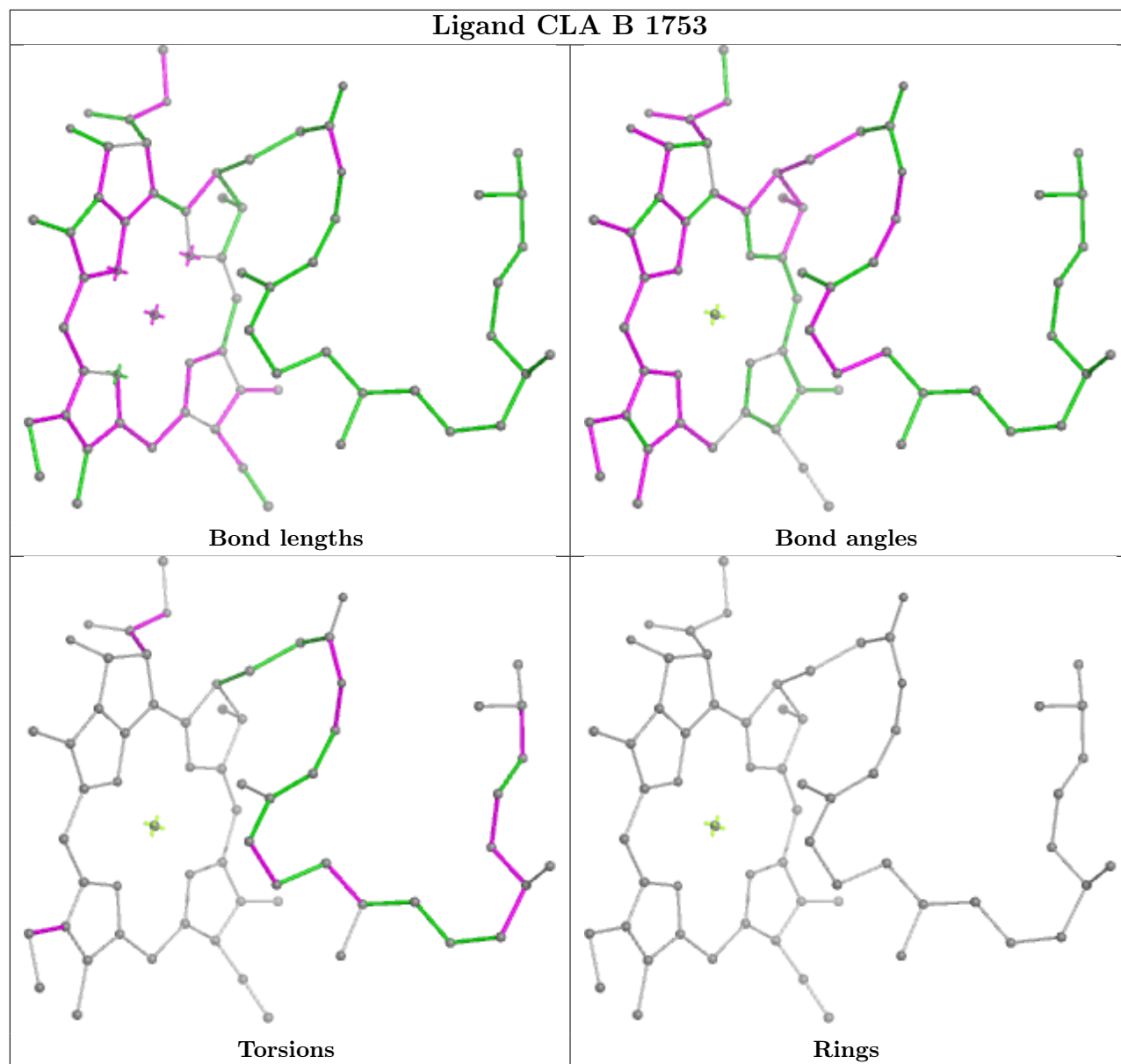


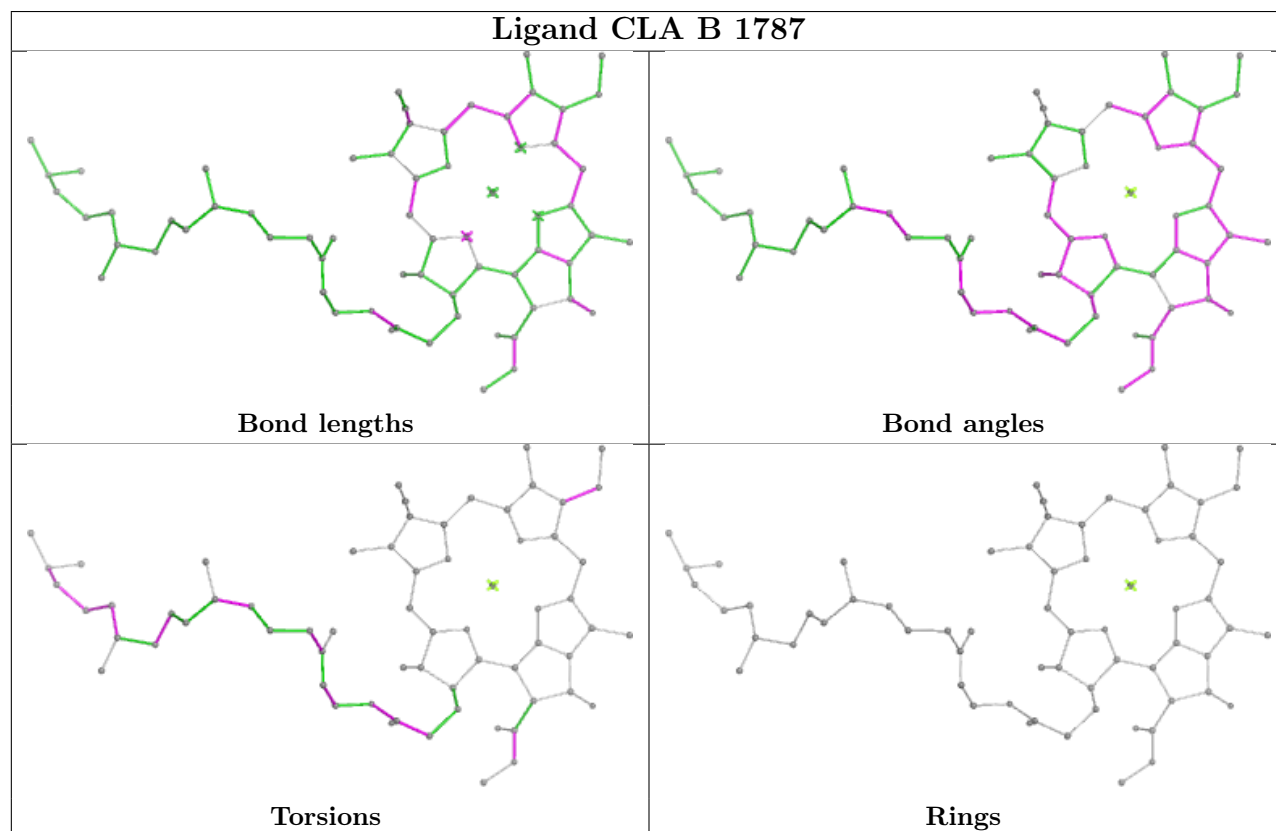
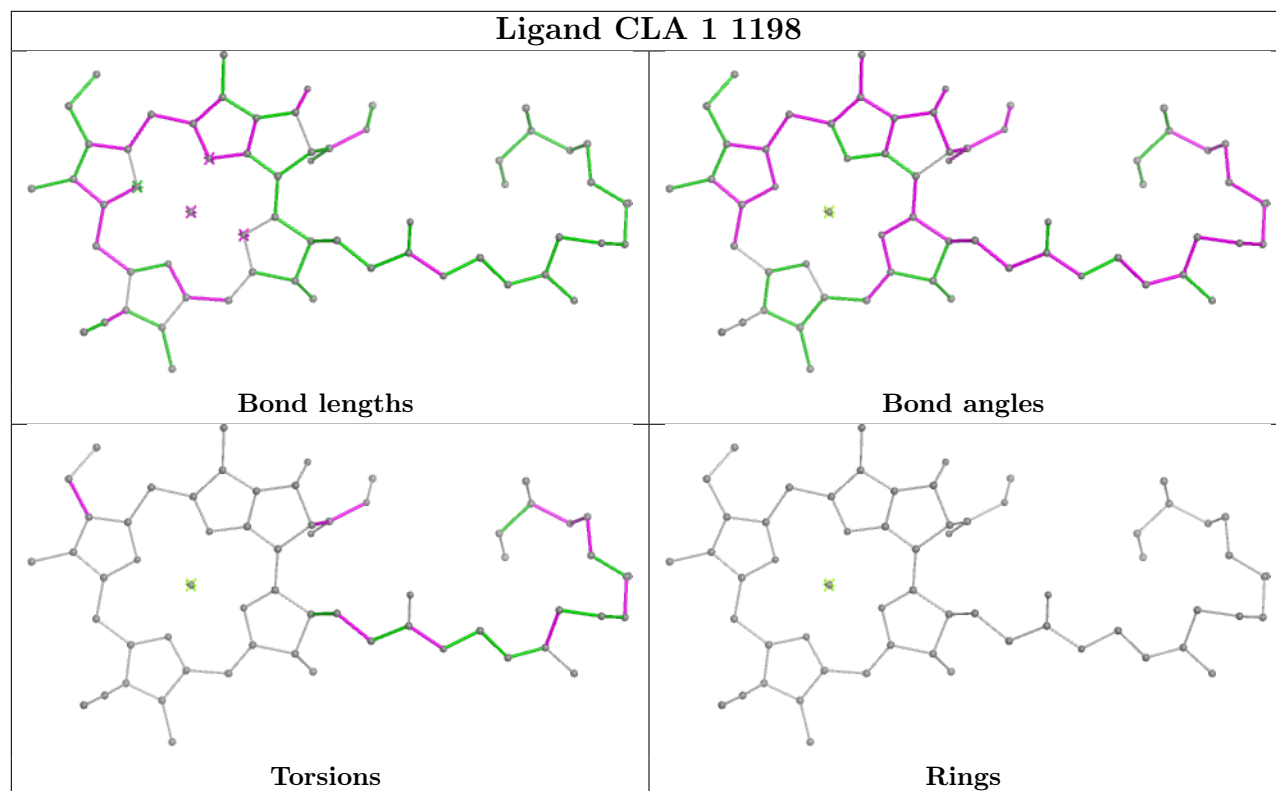




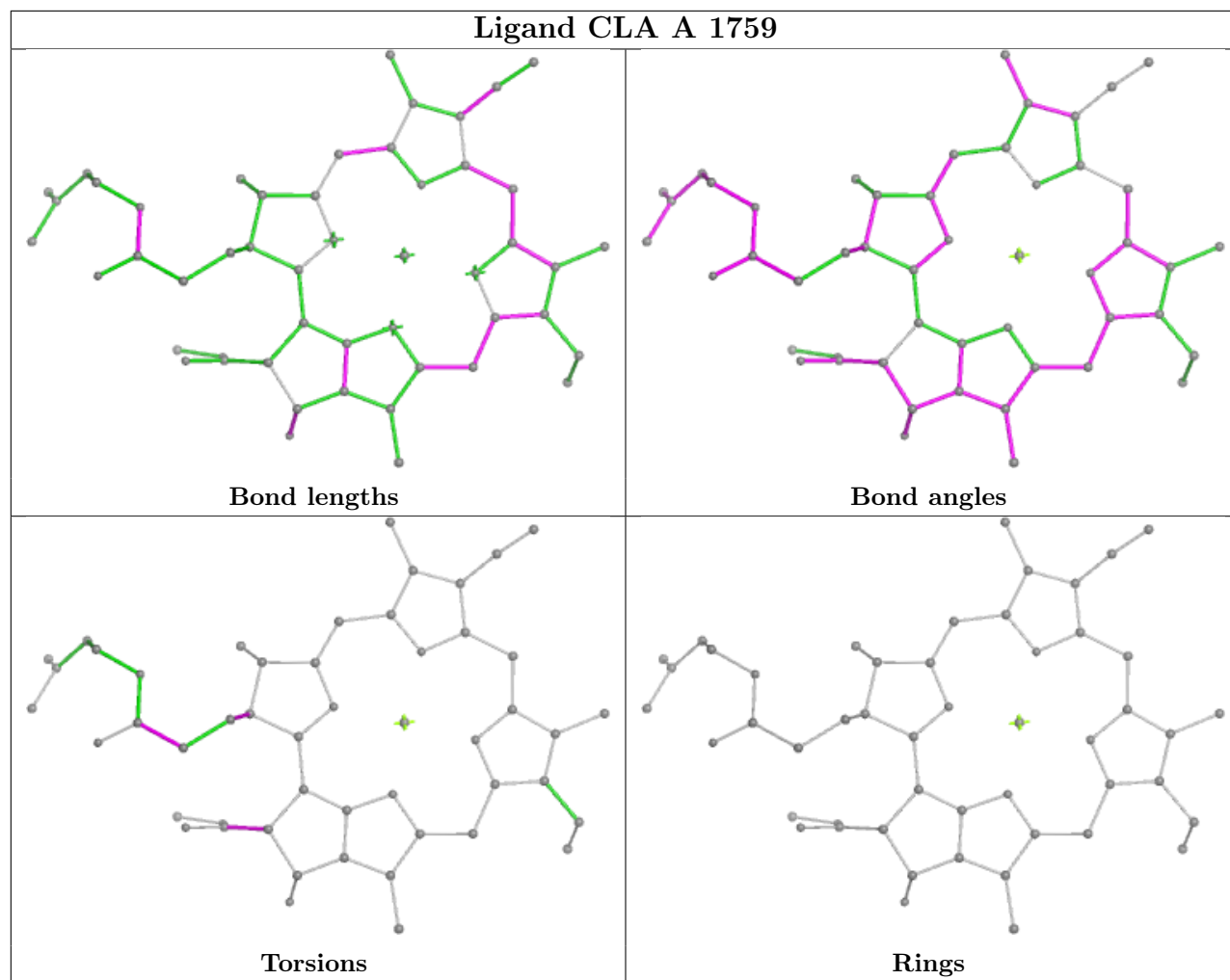




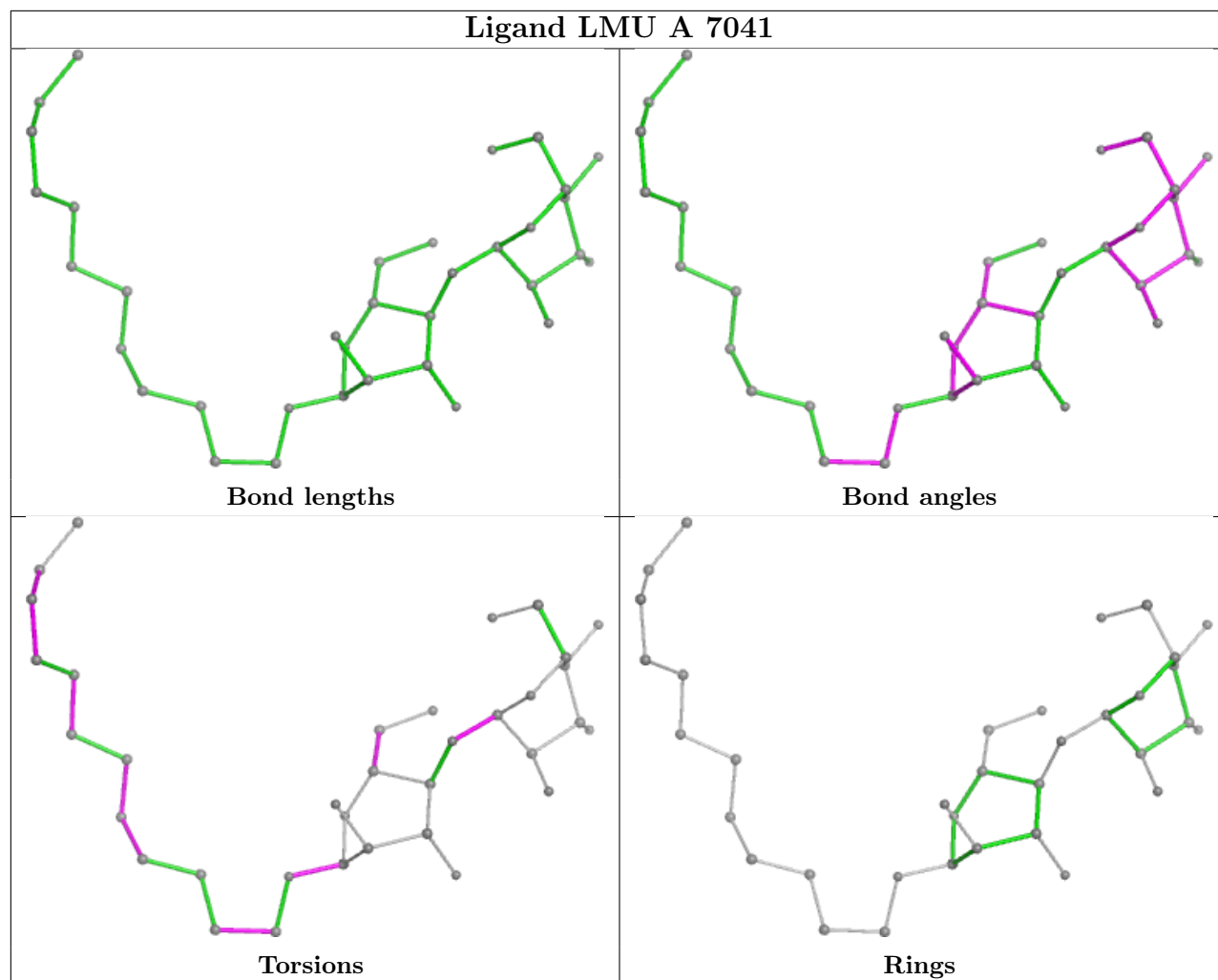


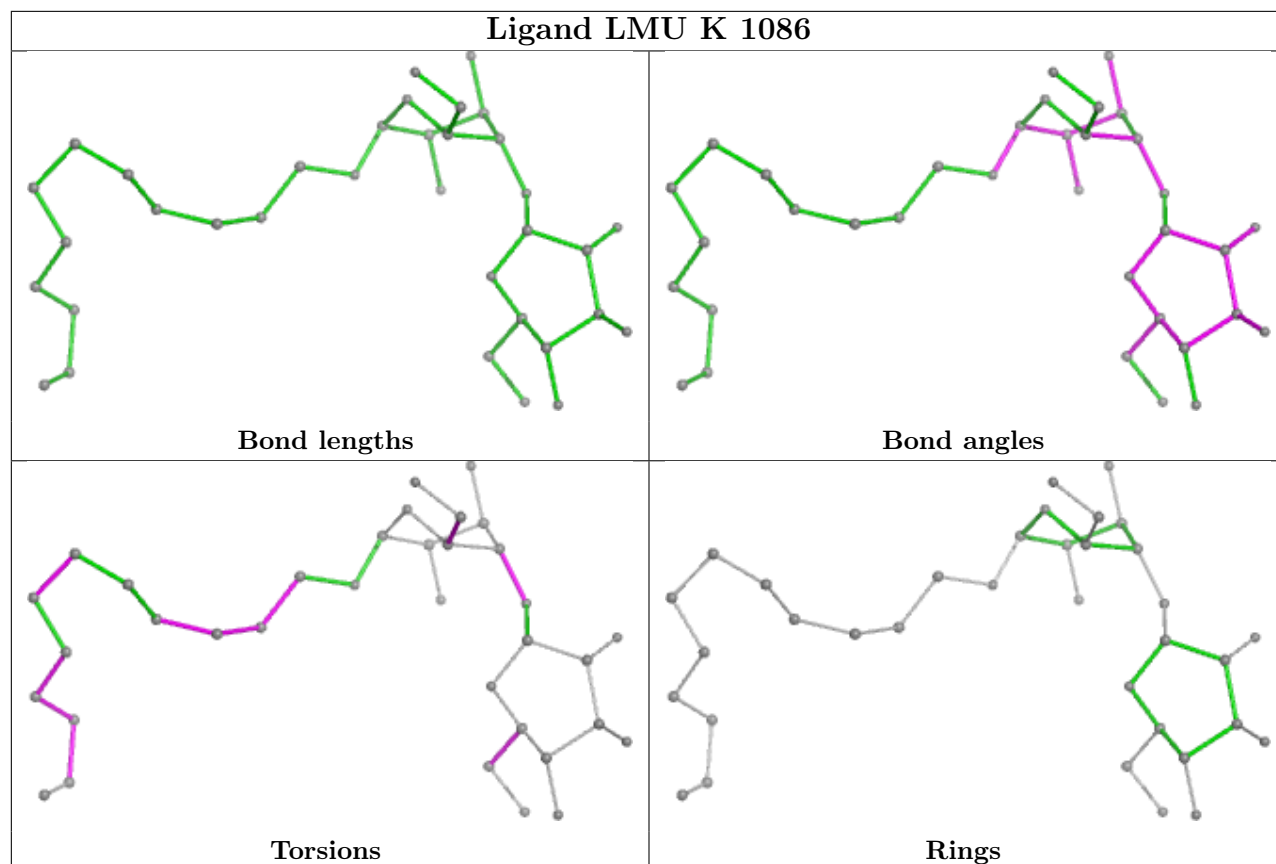


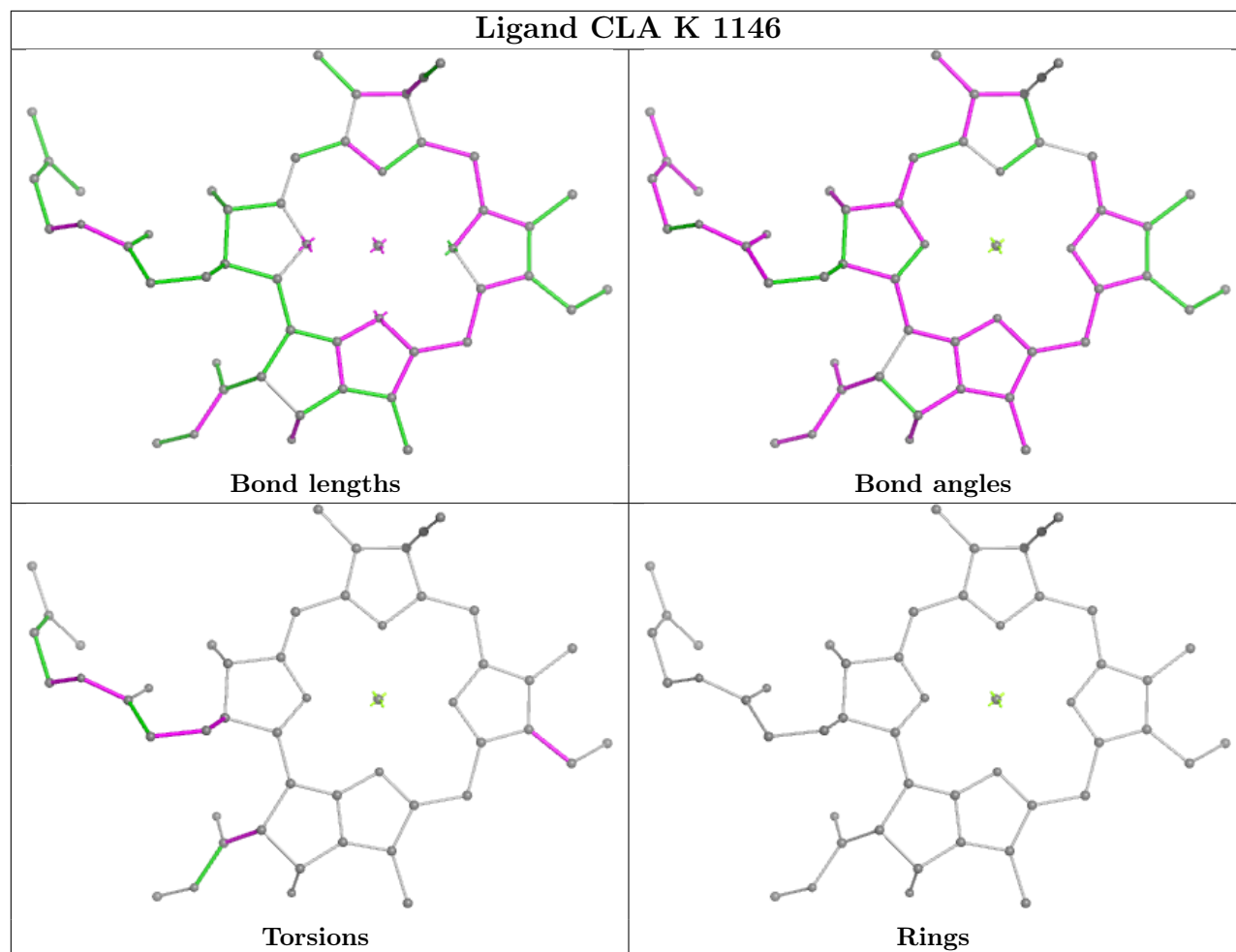


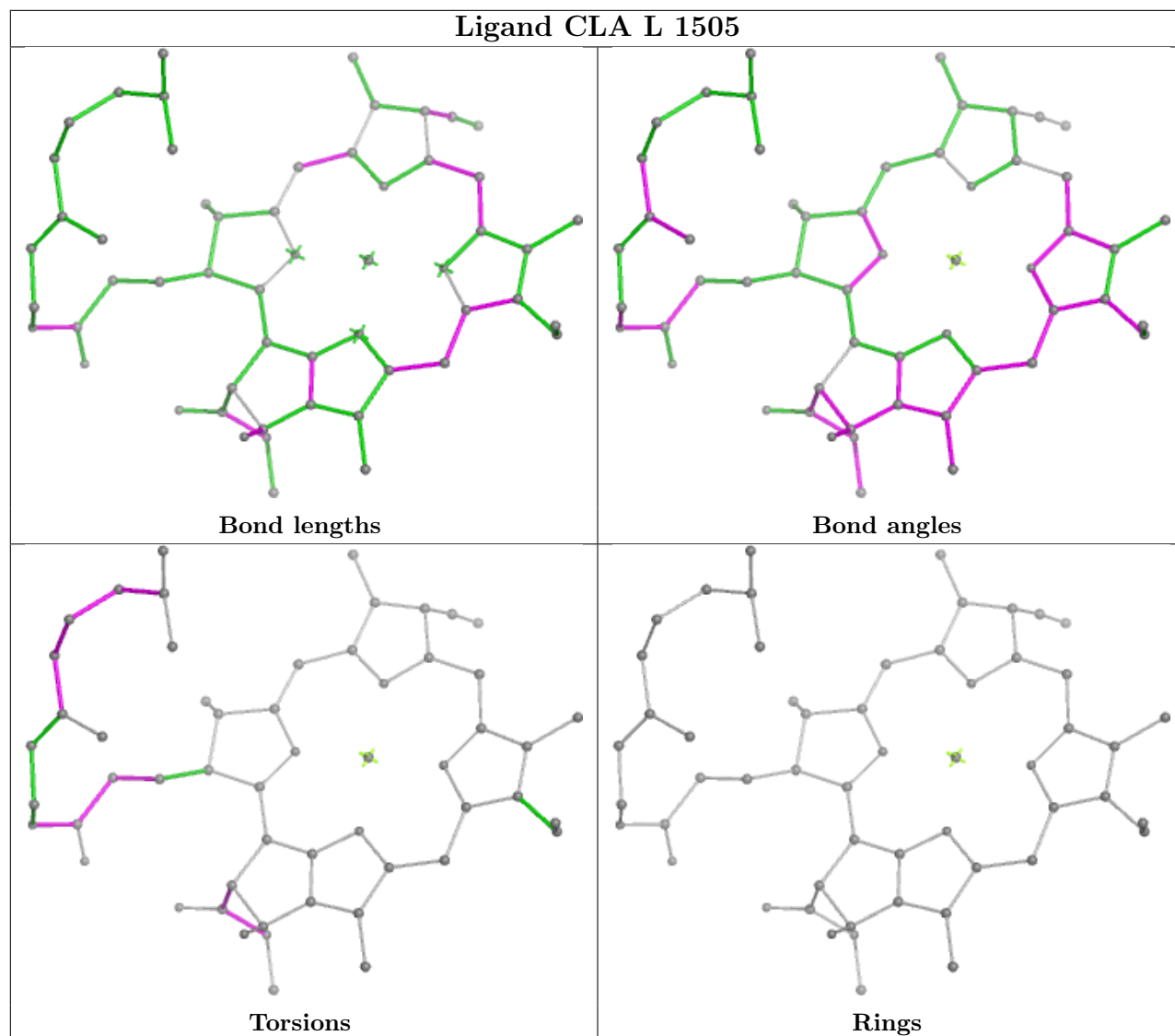


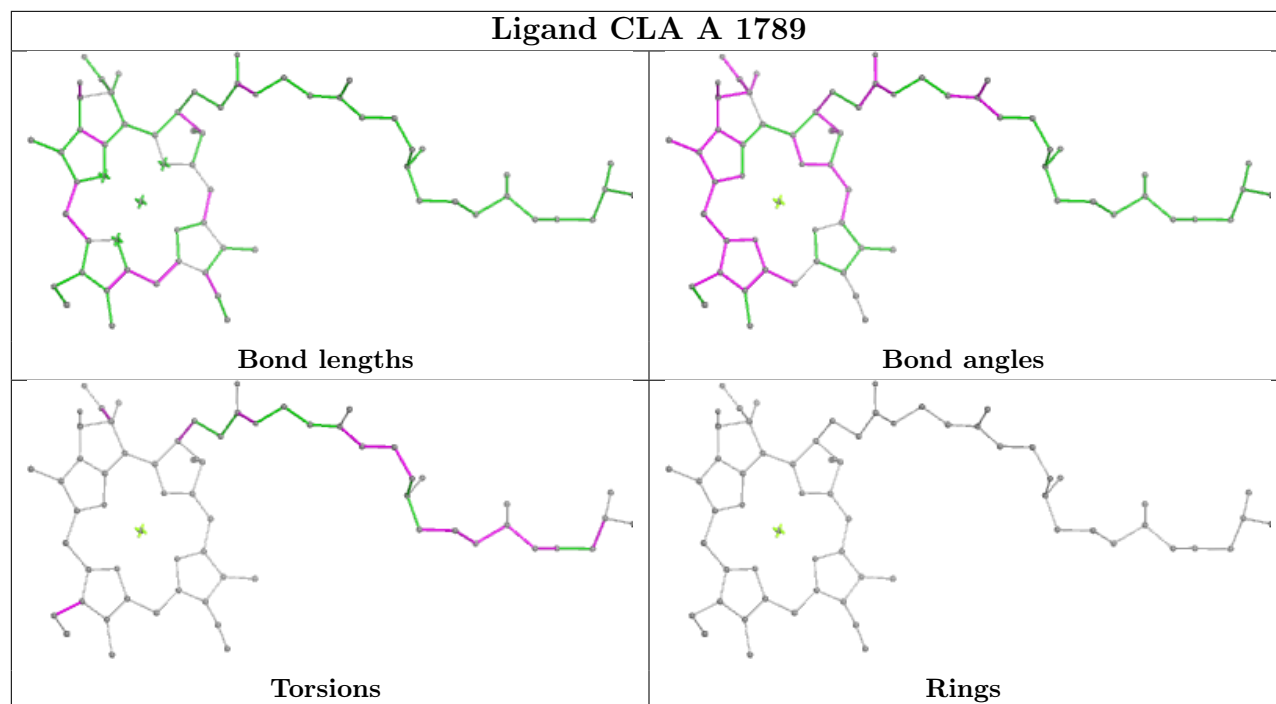
## Ligand LMU A 7041

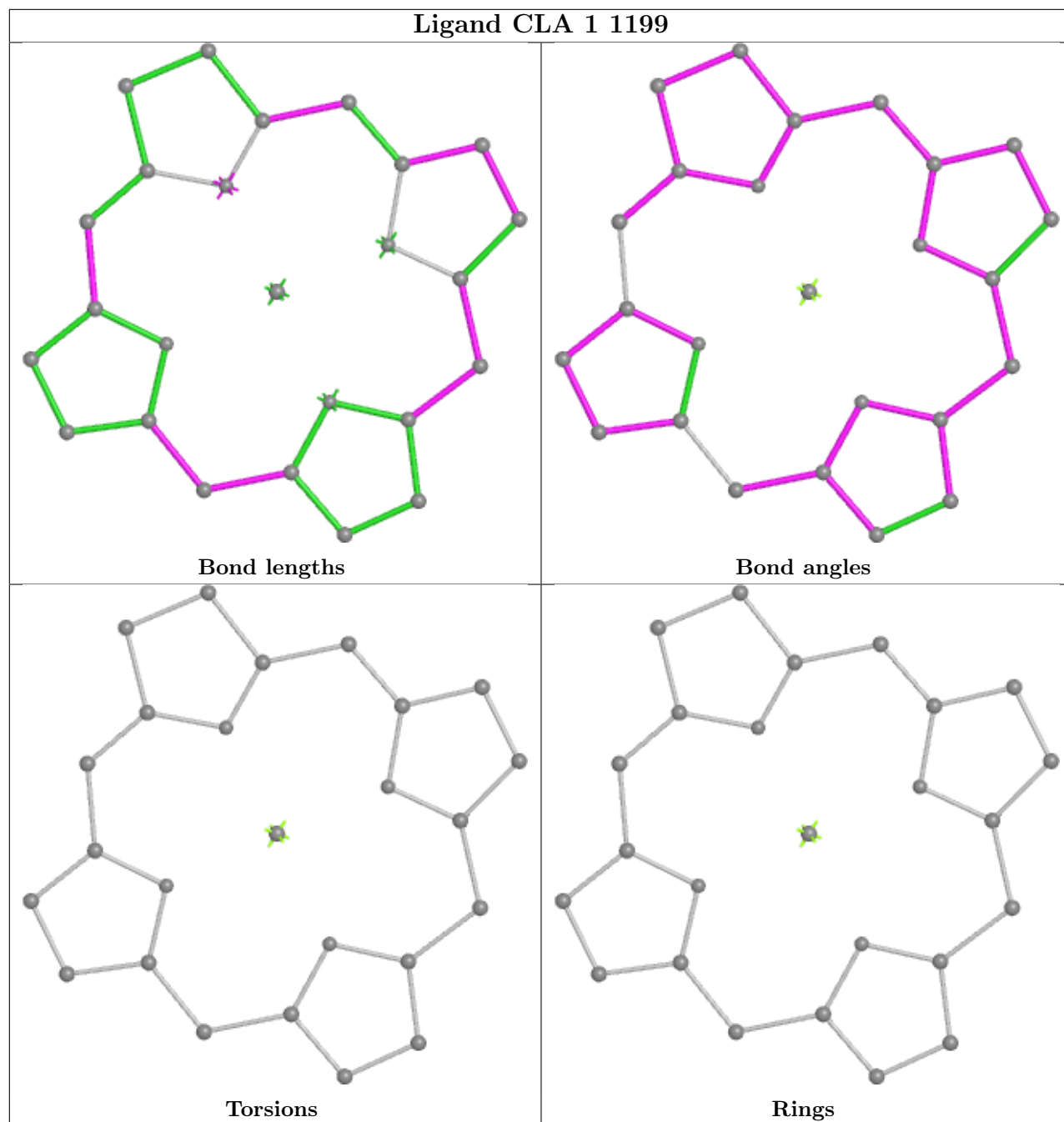


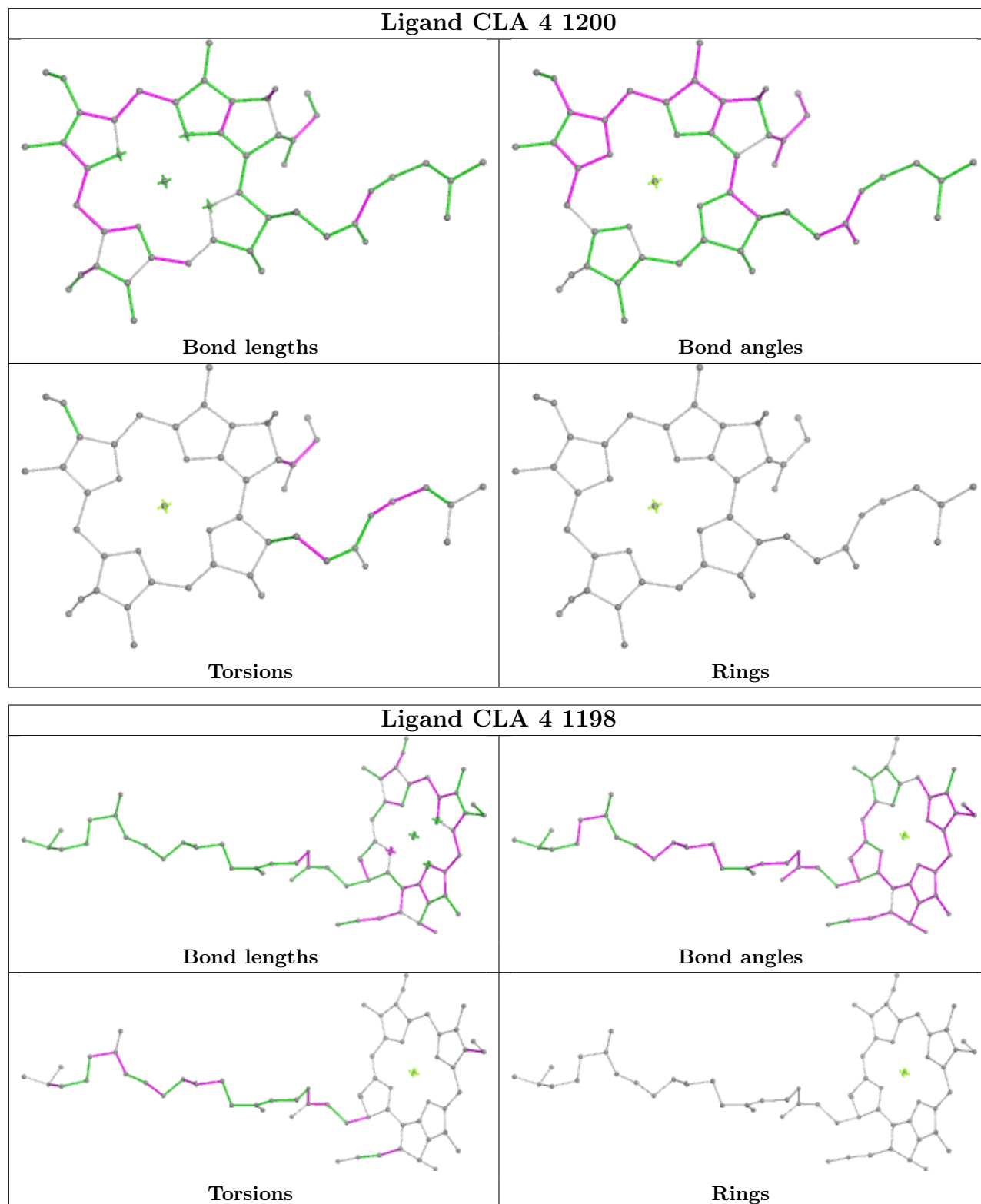




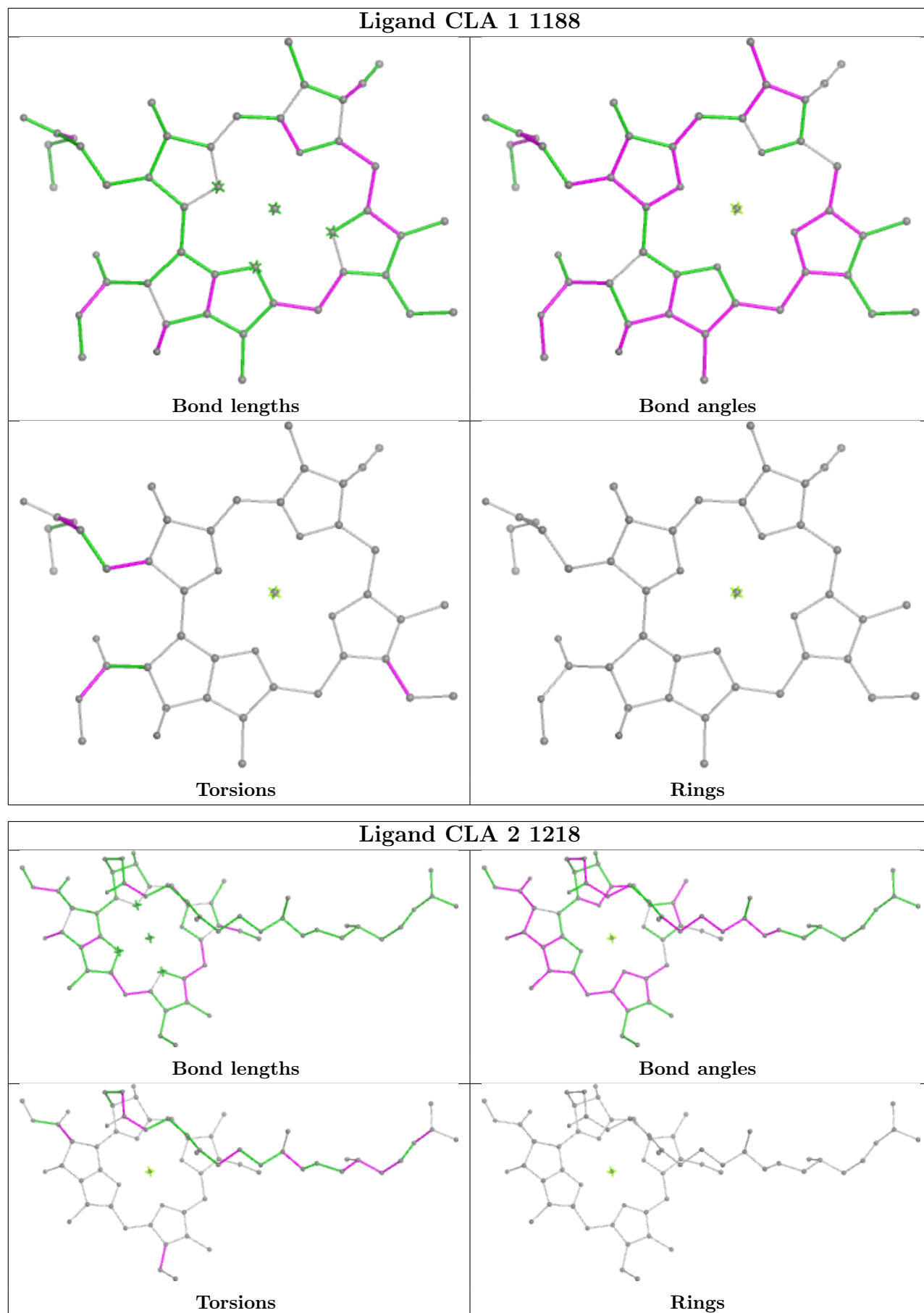


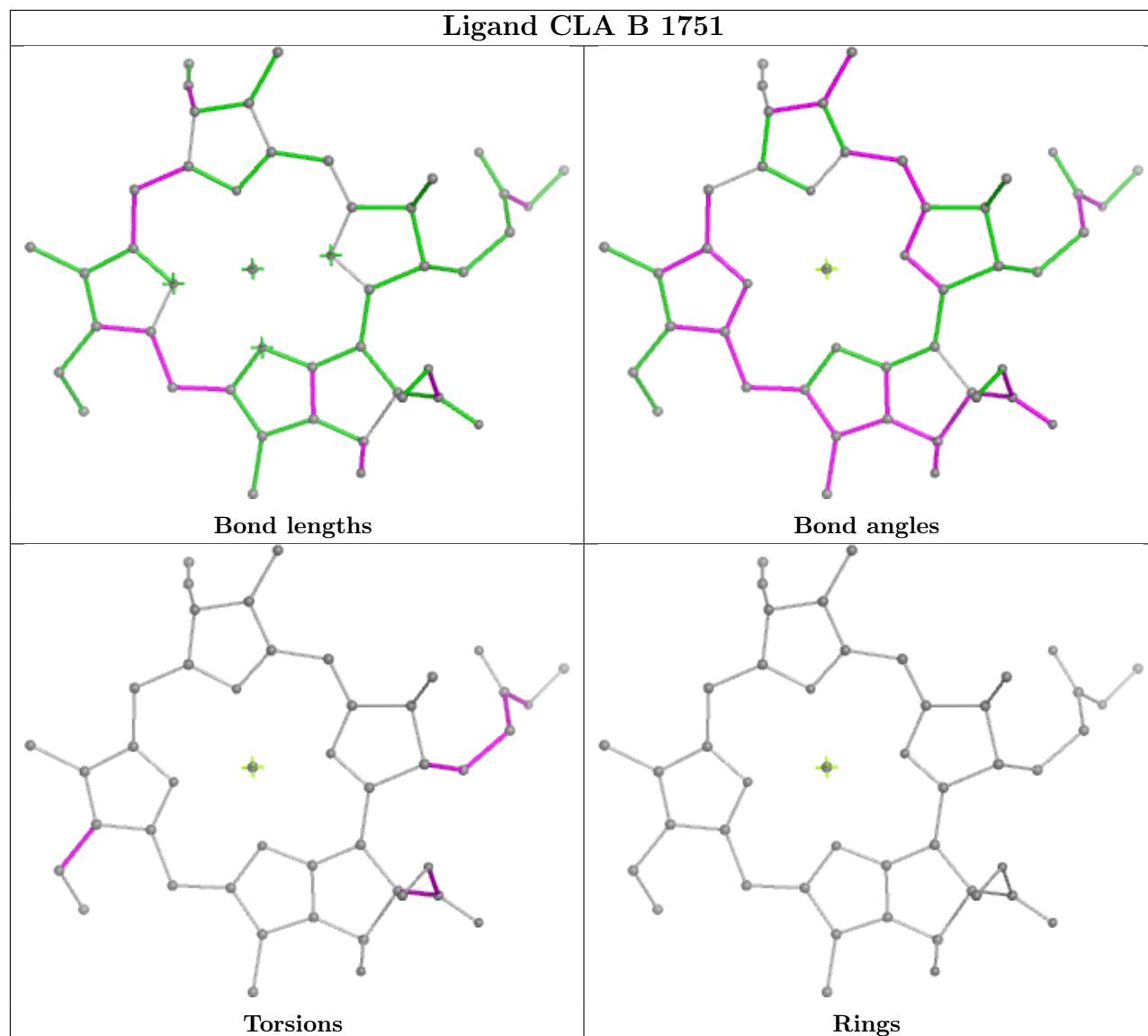




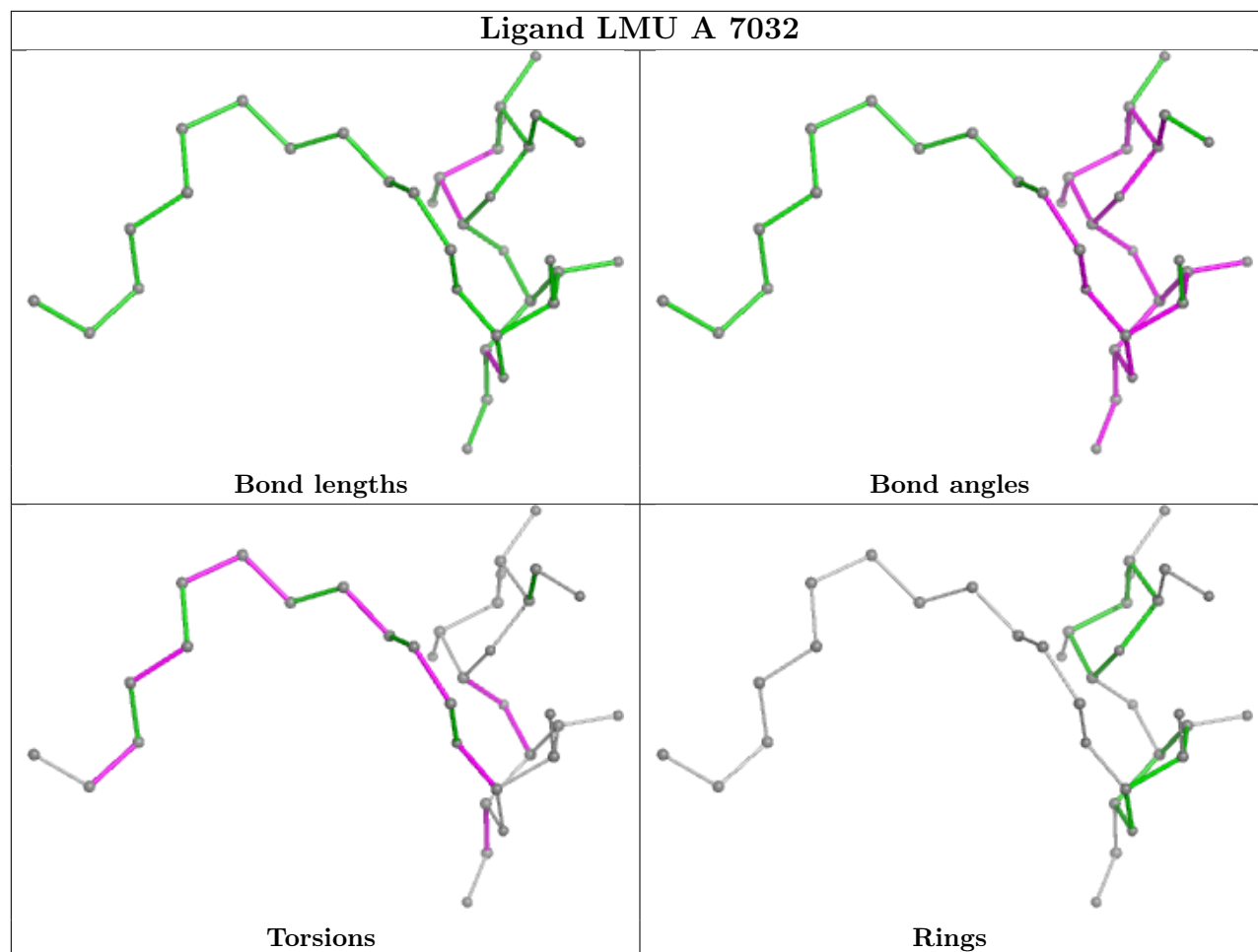




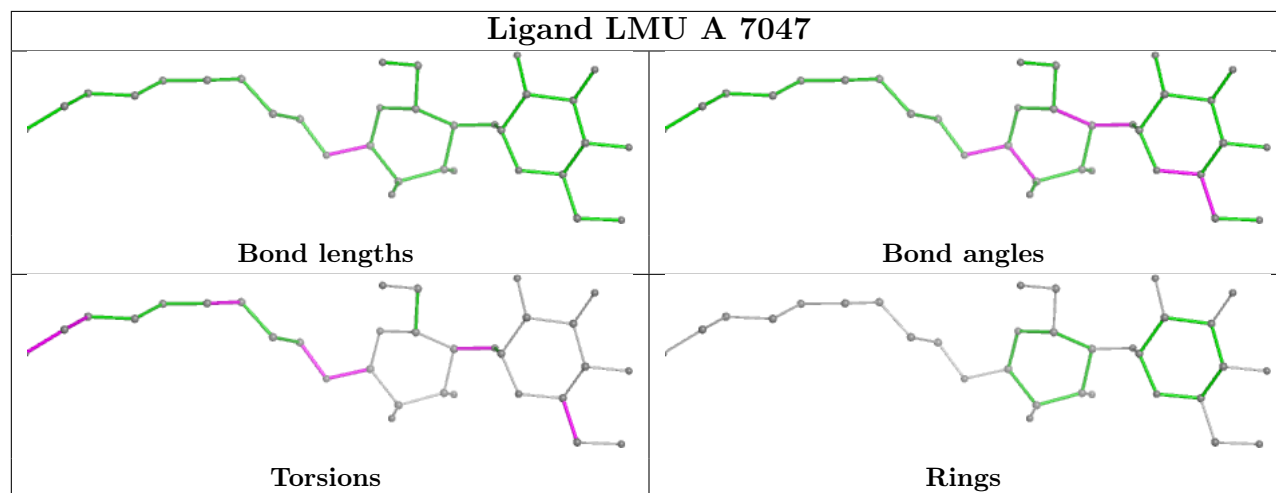


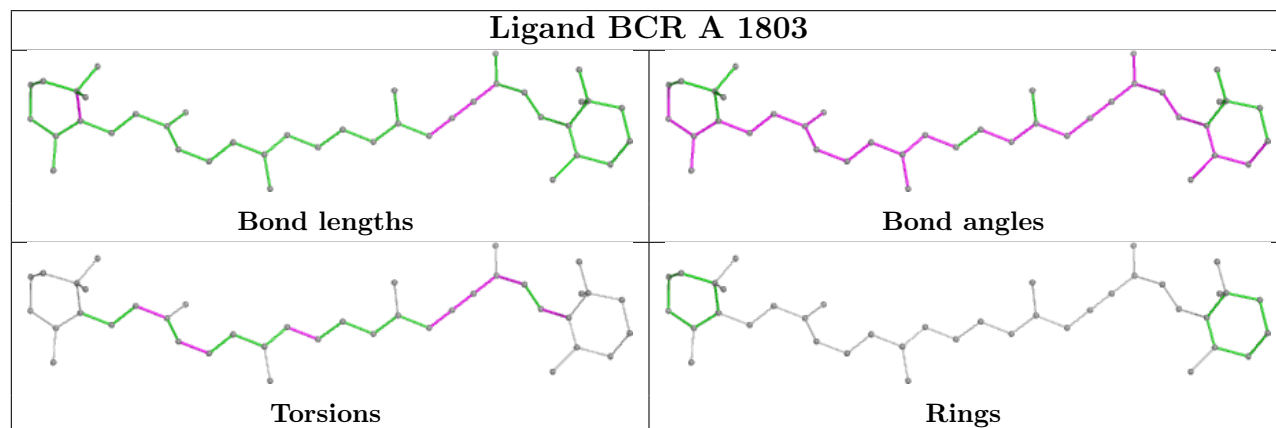
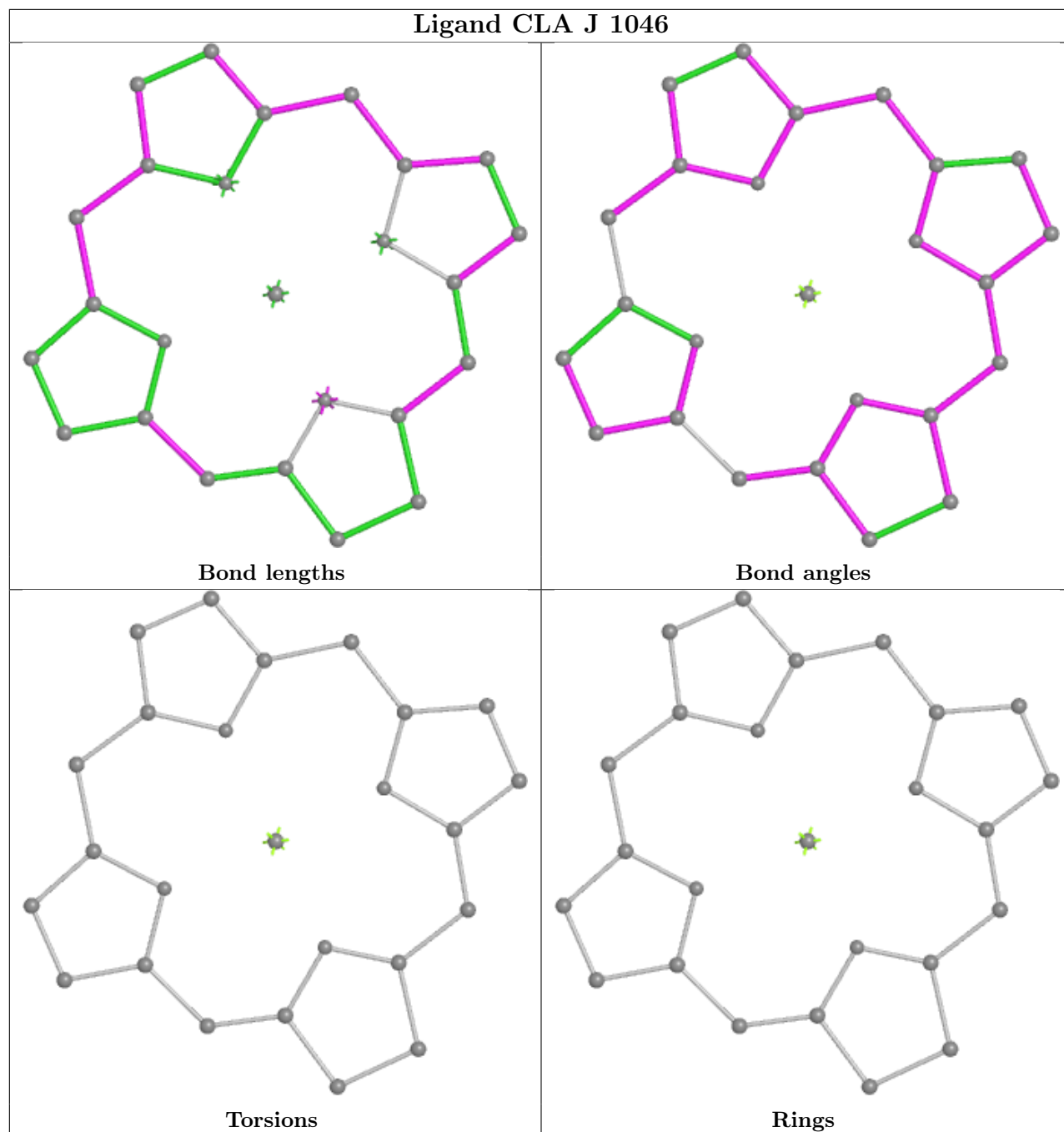


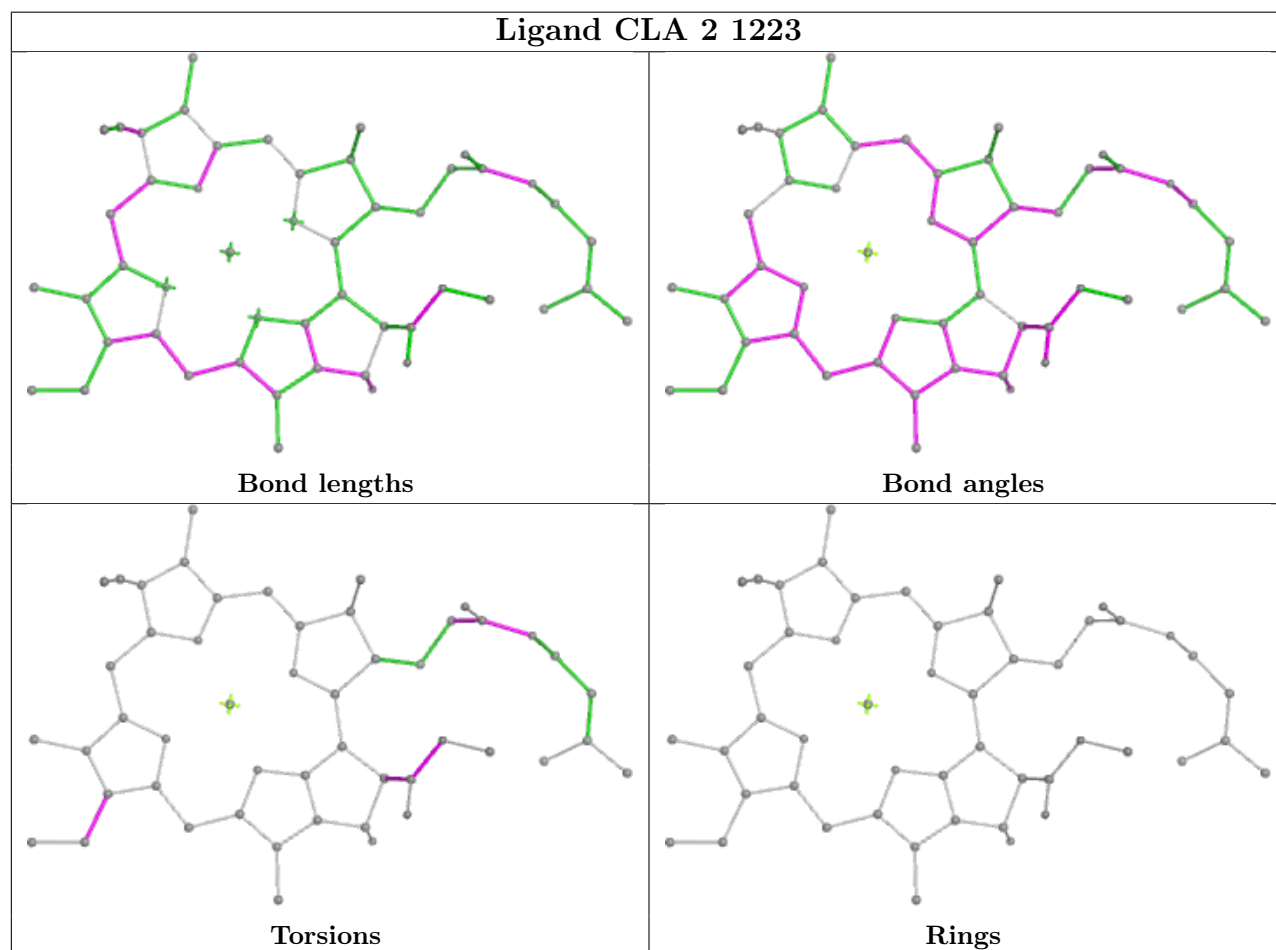
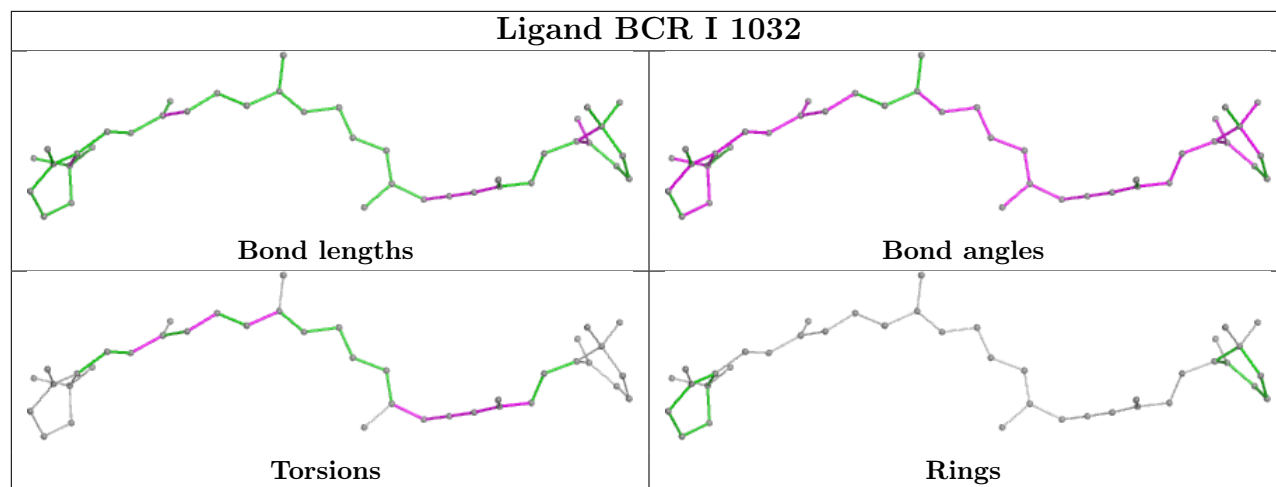
## Ligand LMU A 7032

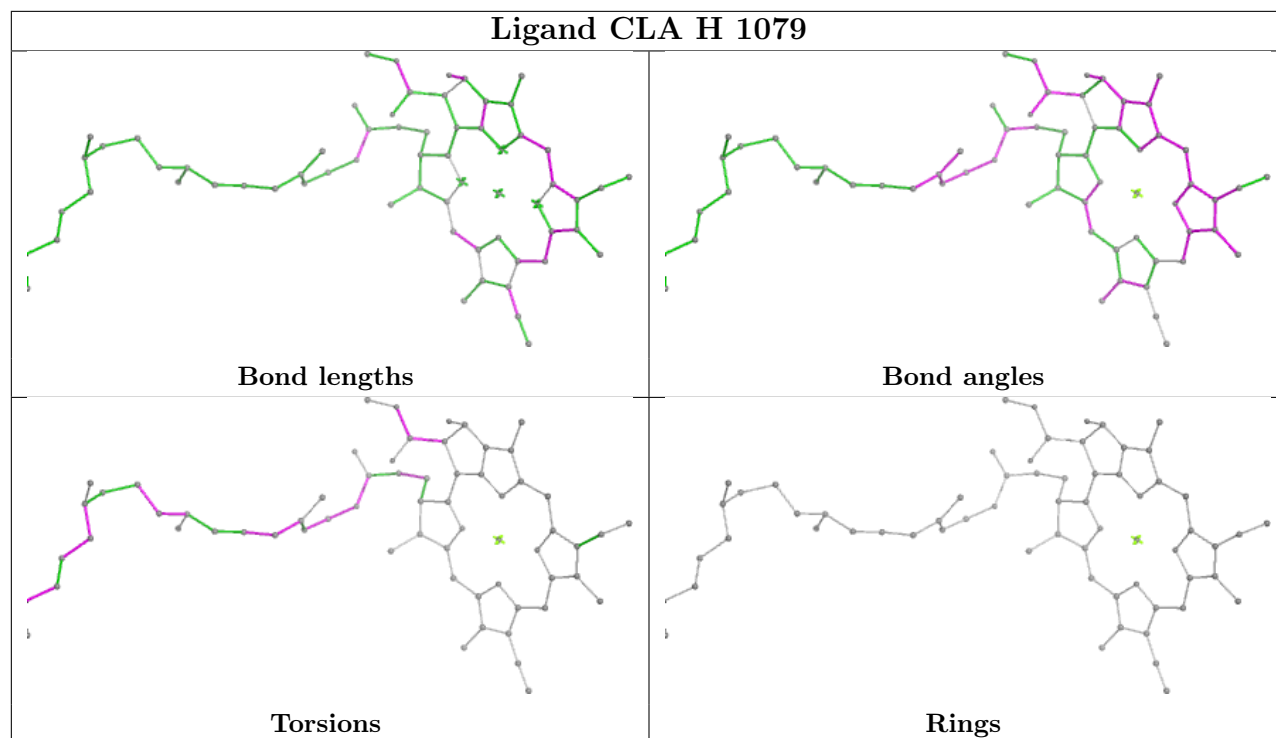


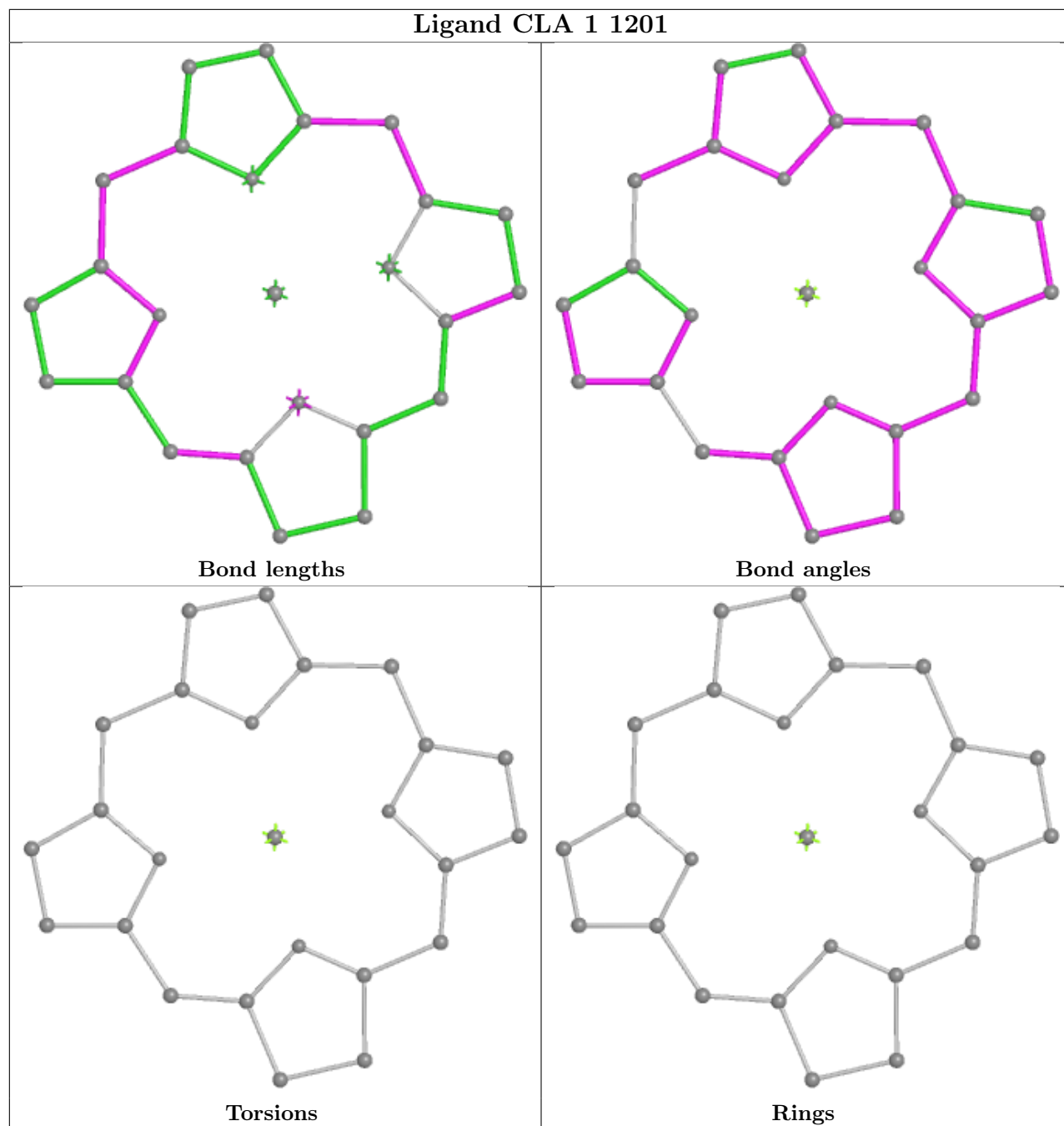
## Ligand LMU A 7047



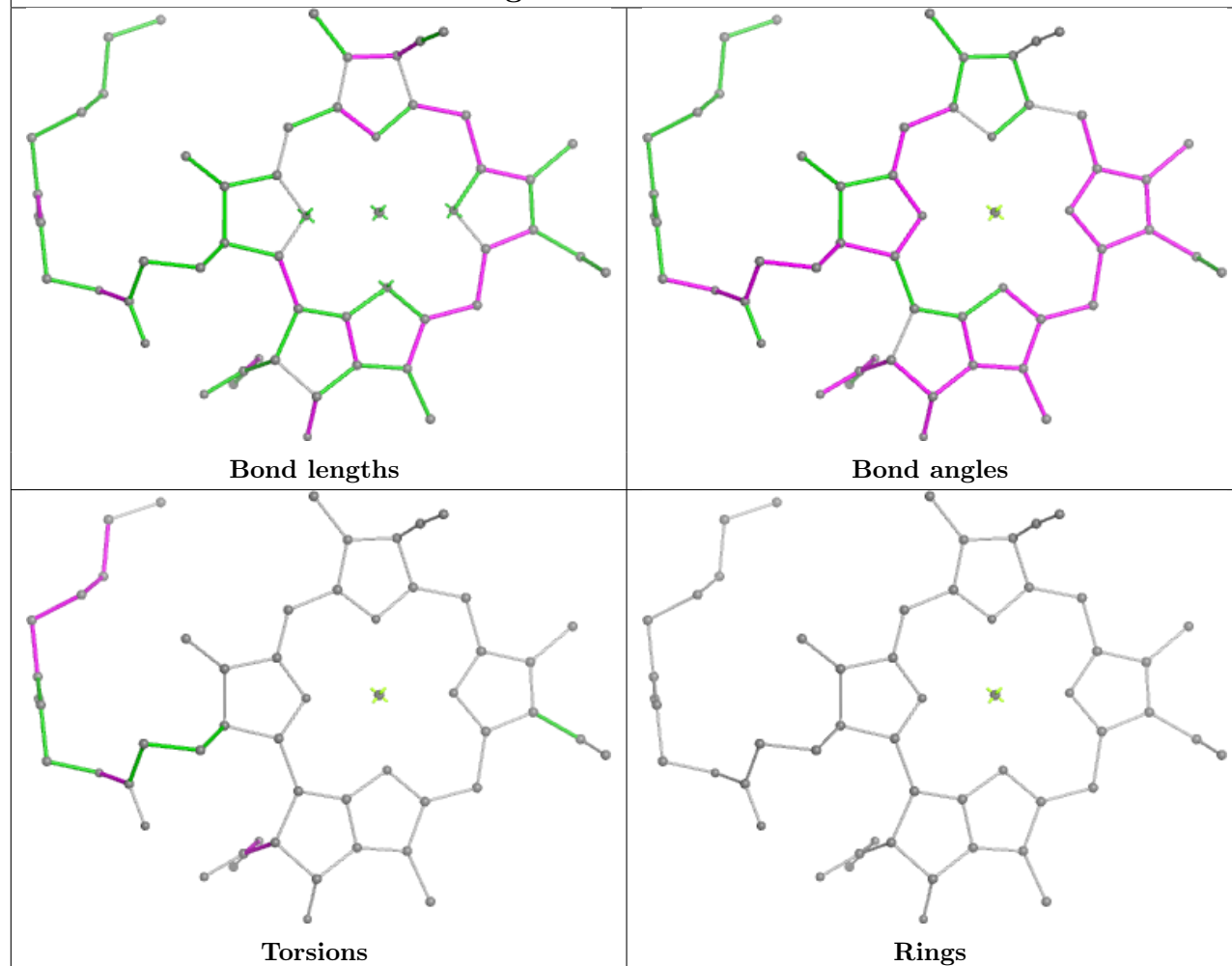




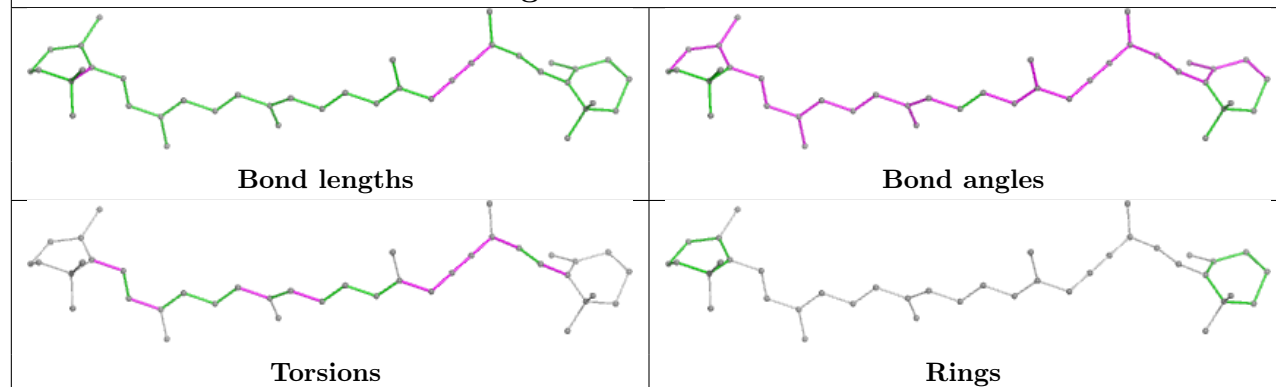




## Ligand CLA B 1754

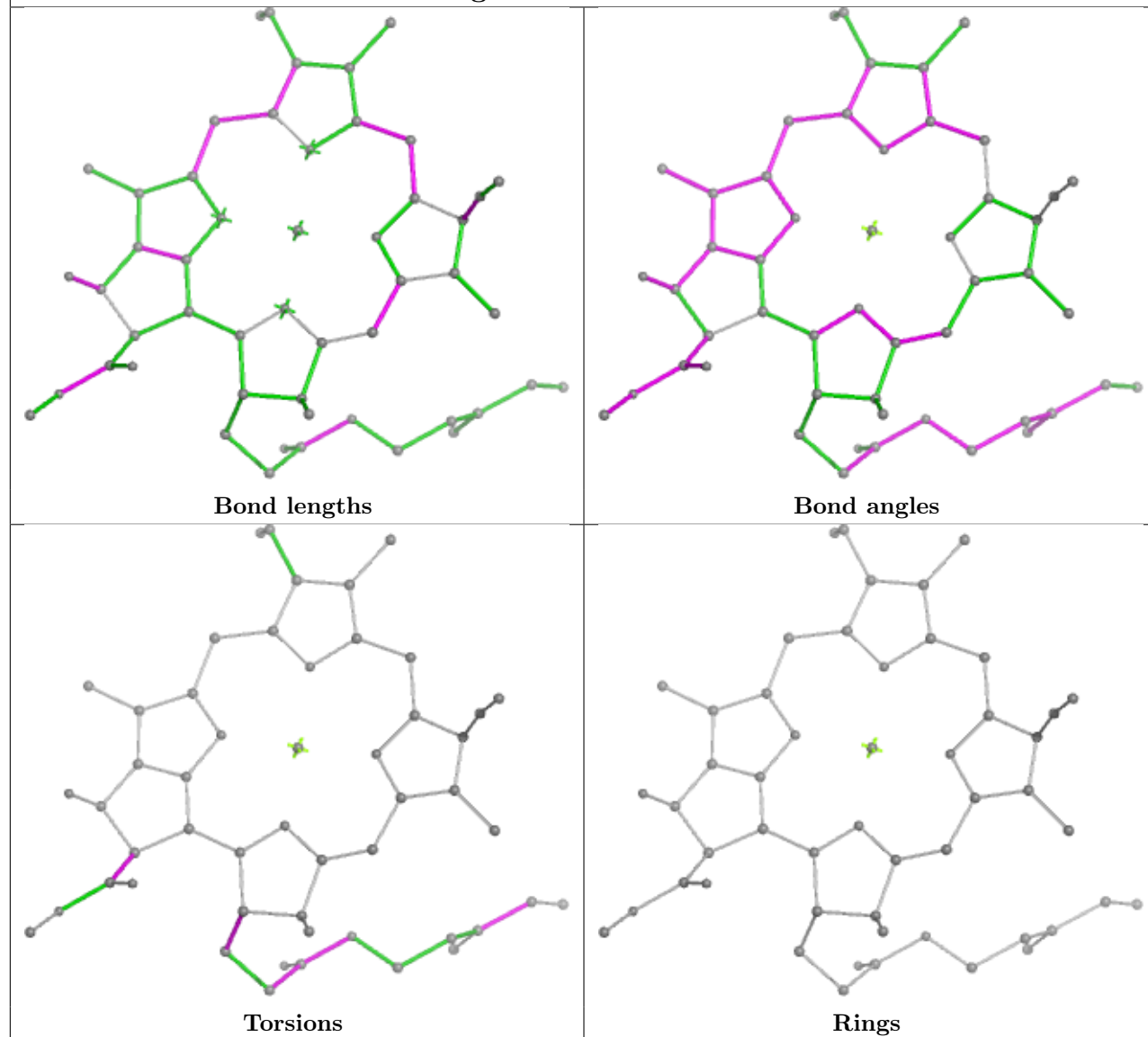


## Ligand BCR A 1805





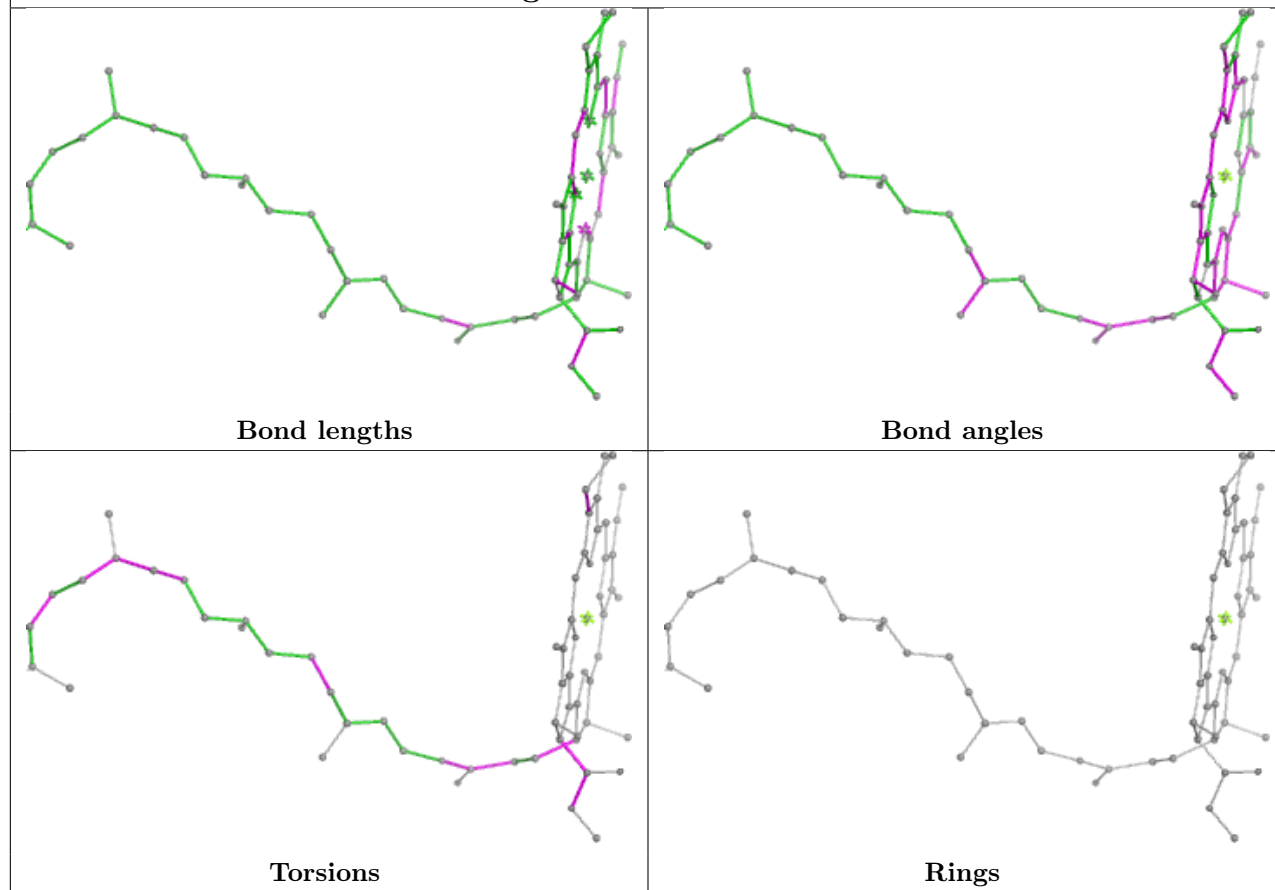
## Ligand CLA B 1766



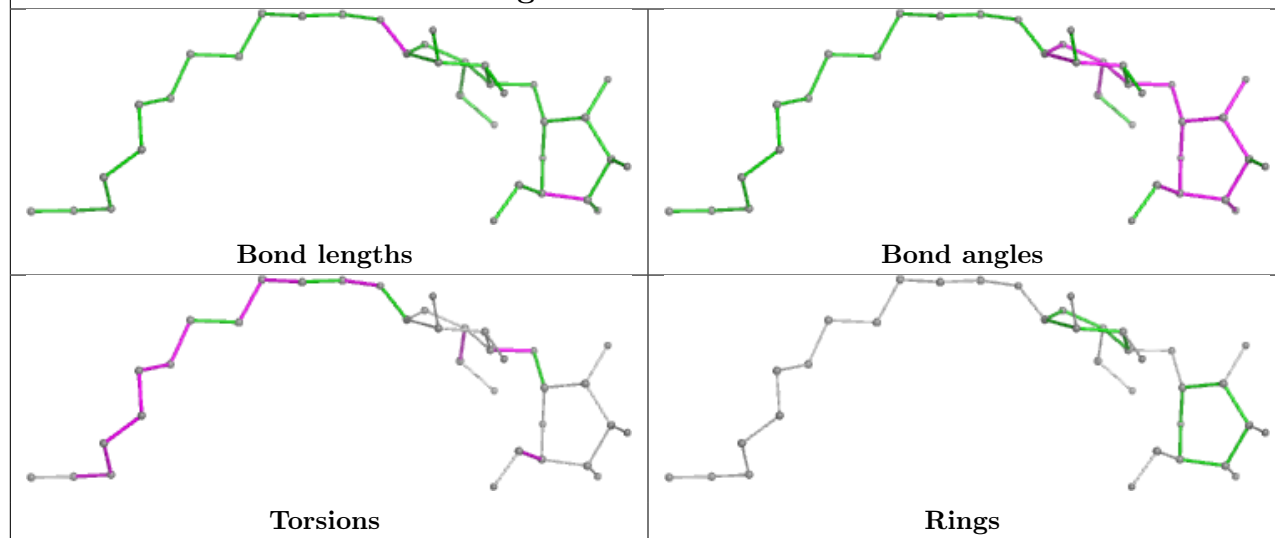
## Ligand BCR B 1778

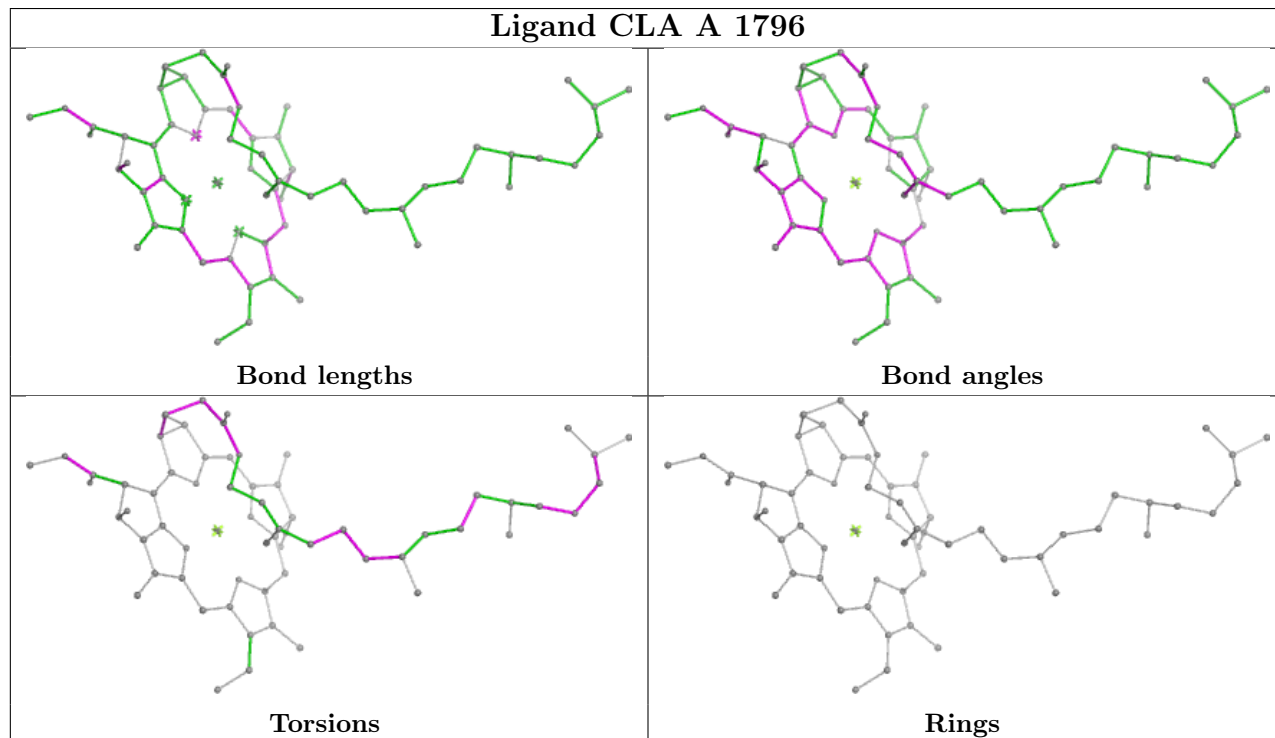
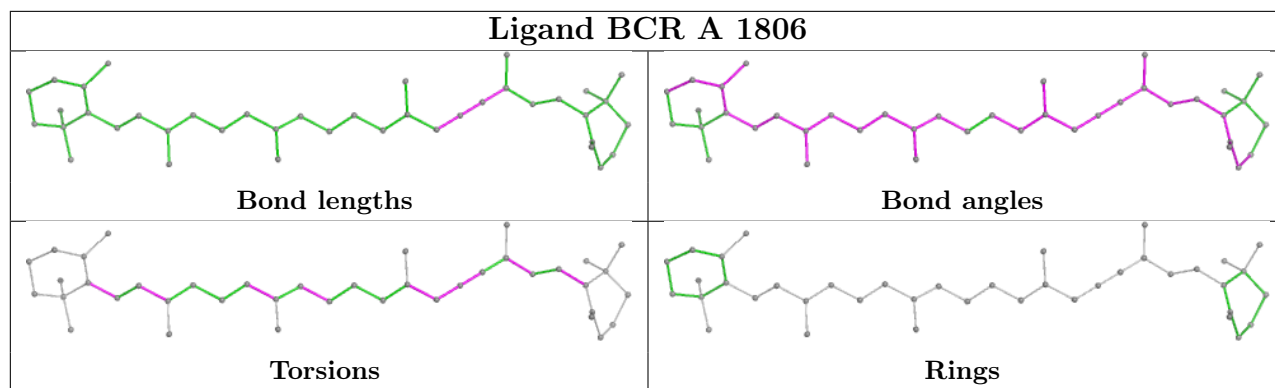


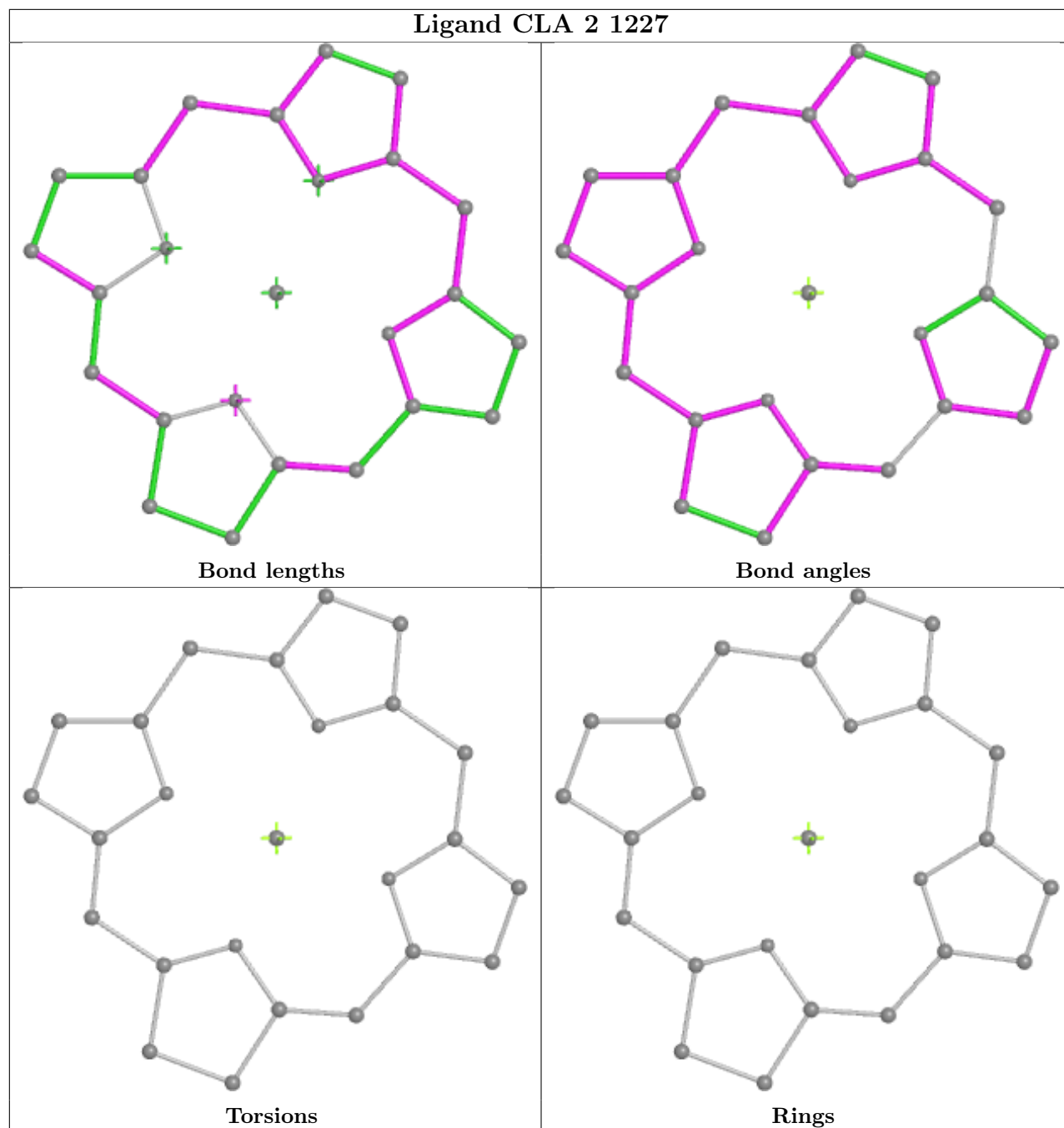
## Ligand CLA B 1771

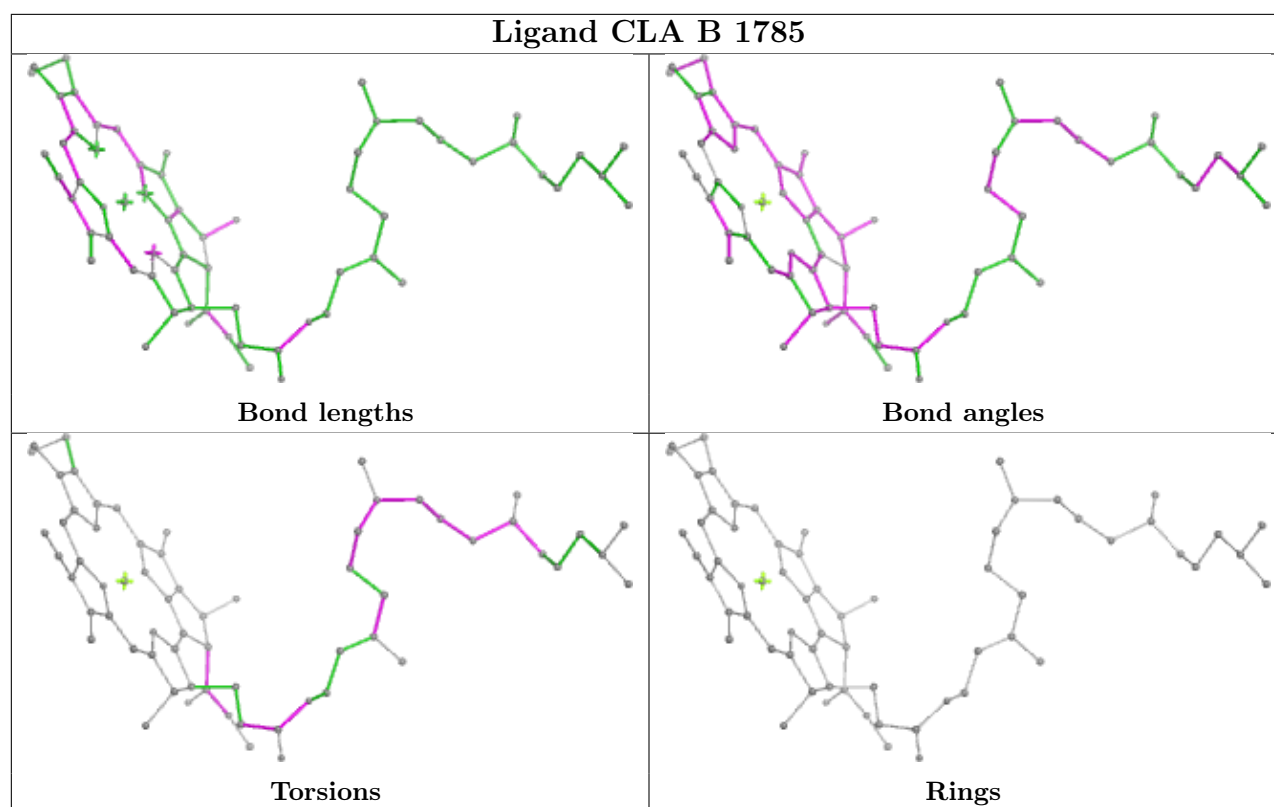


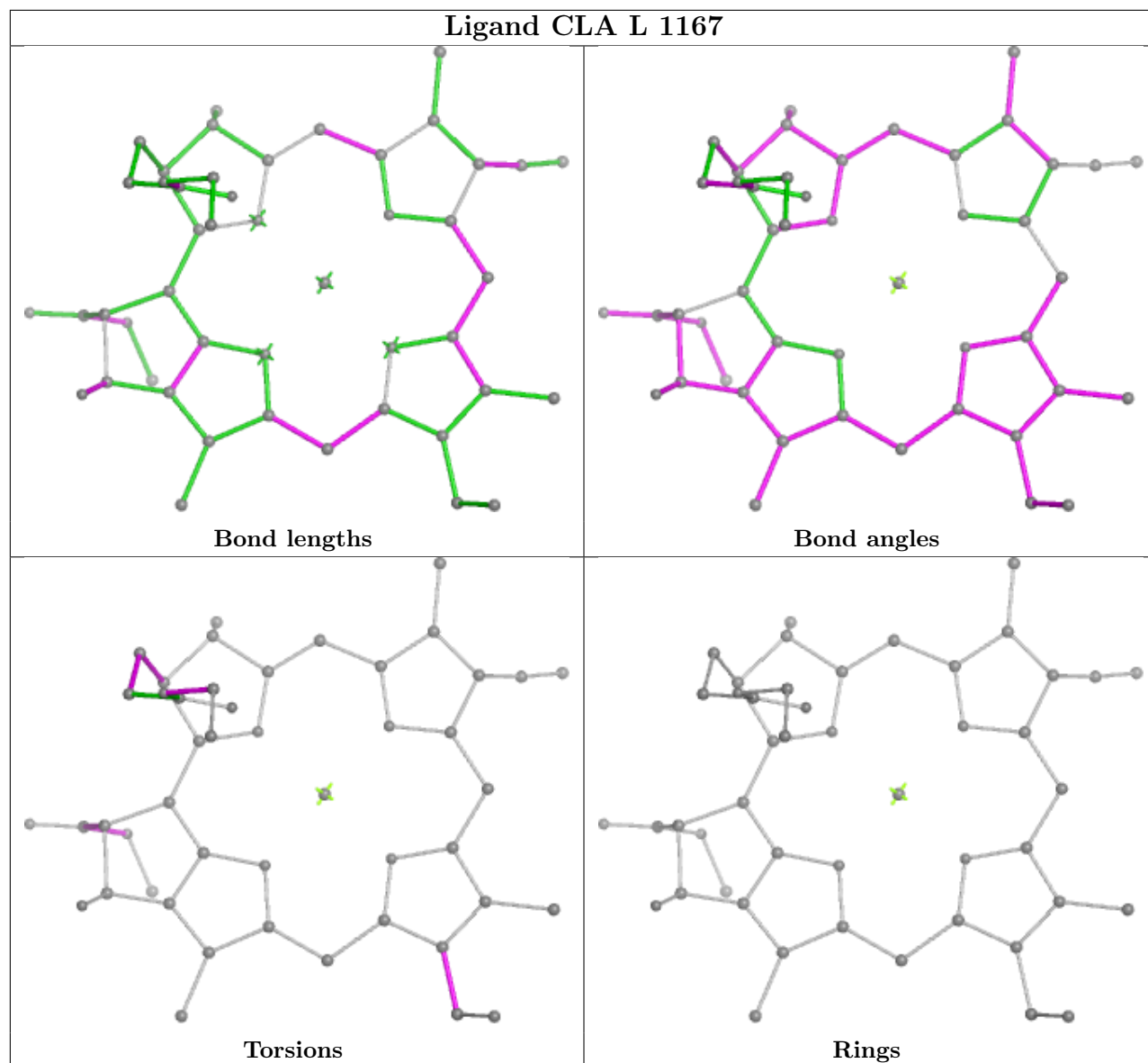
## Ligand LMU A 7017



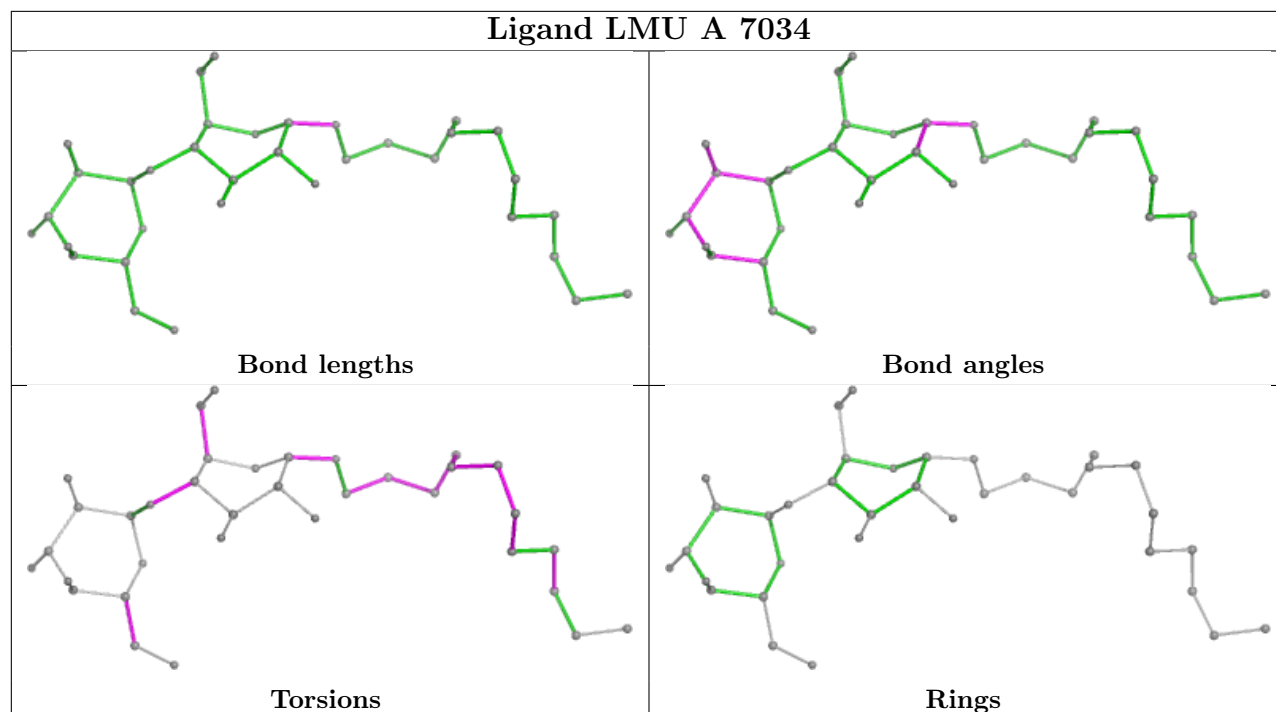




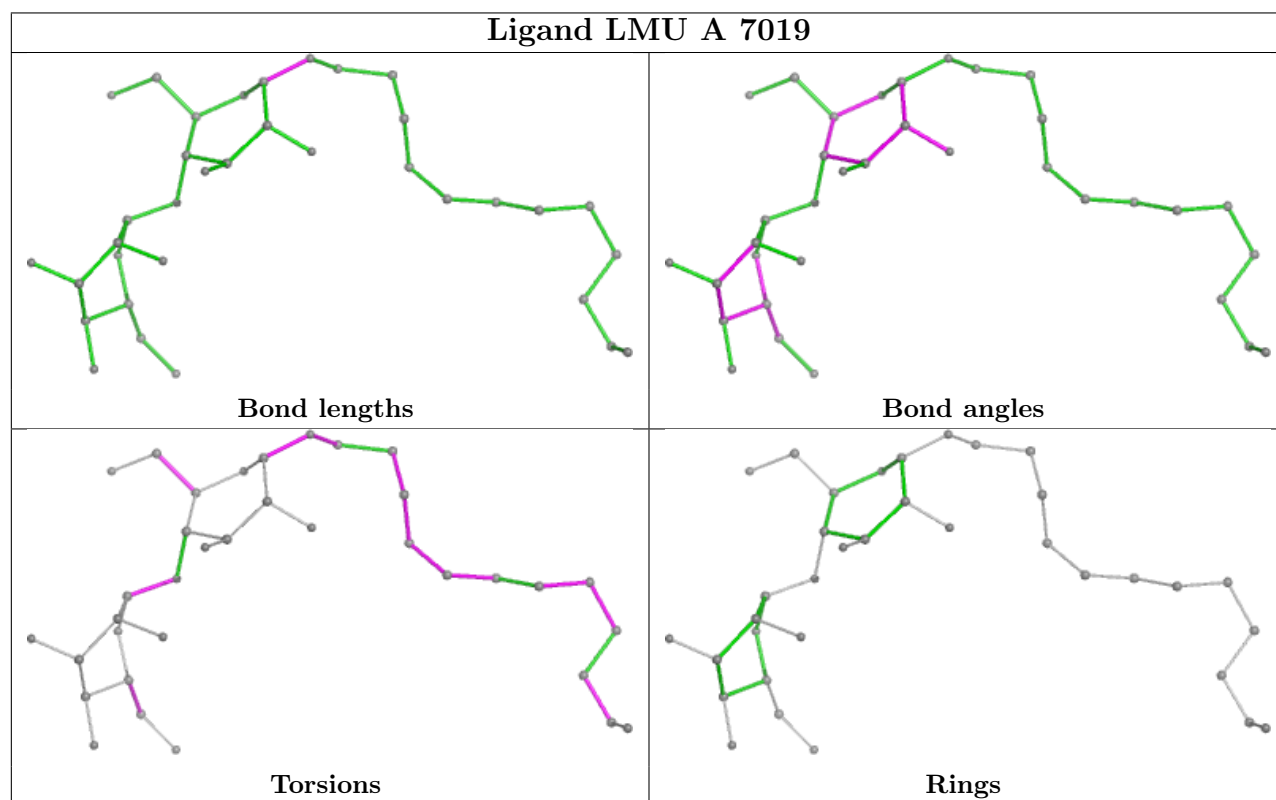




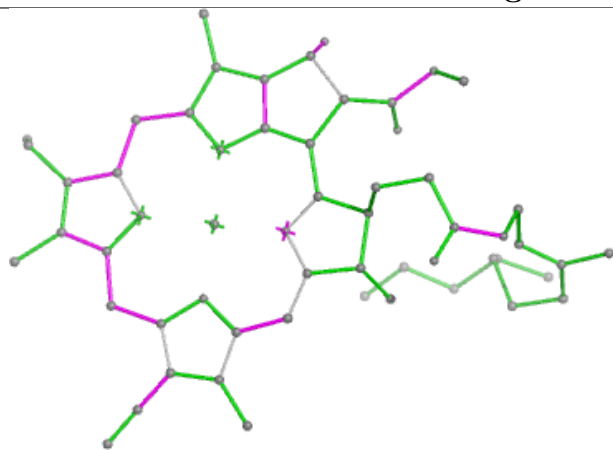
## Ligand LMU A 7034



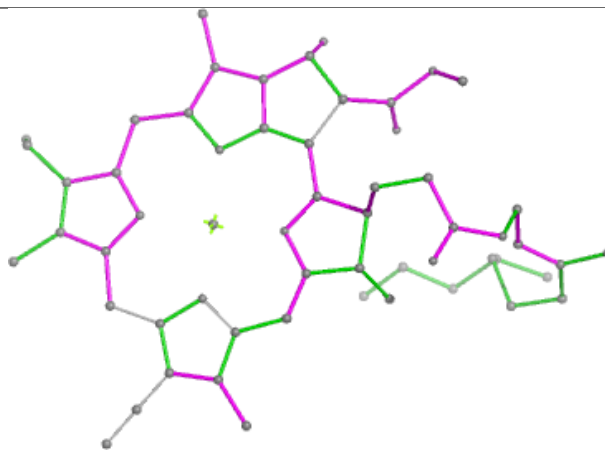
## Ligand LMU A 7019



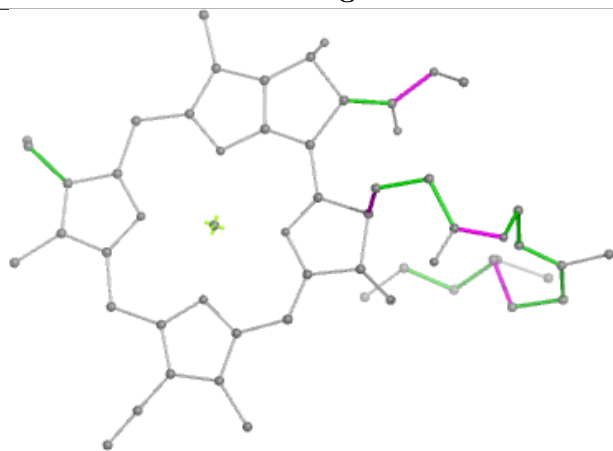
## Ligand CLA A 1762



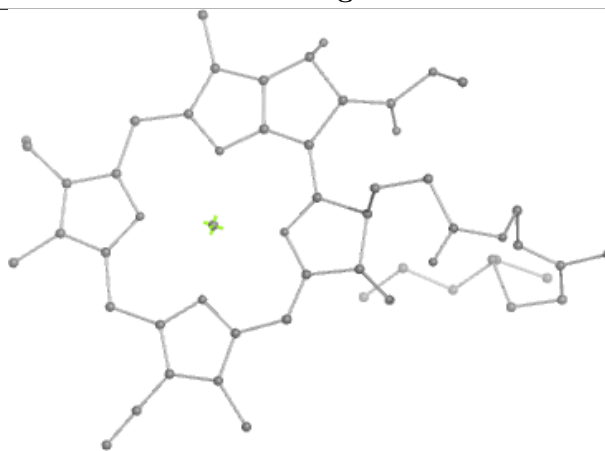
Bond lengths



Bond angles

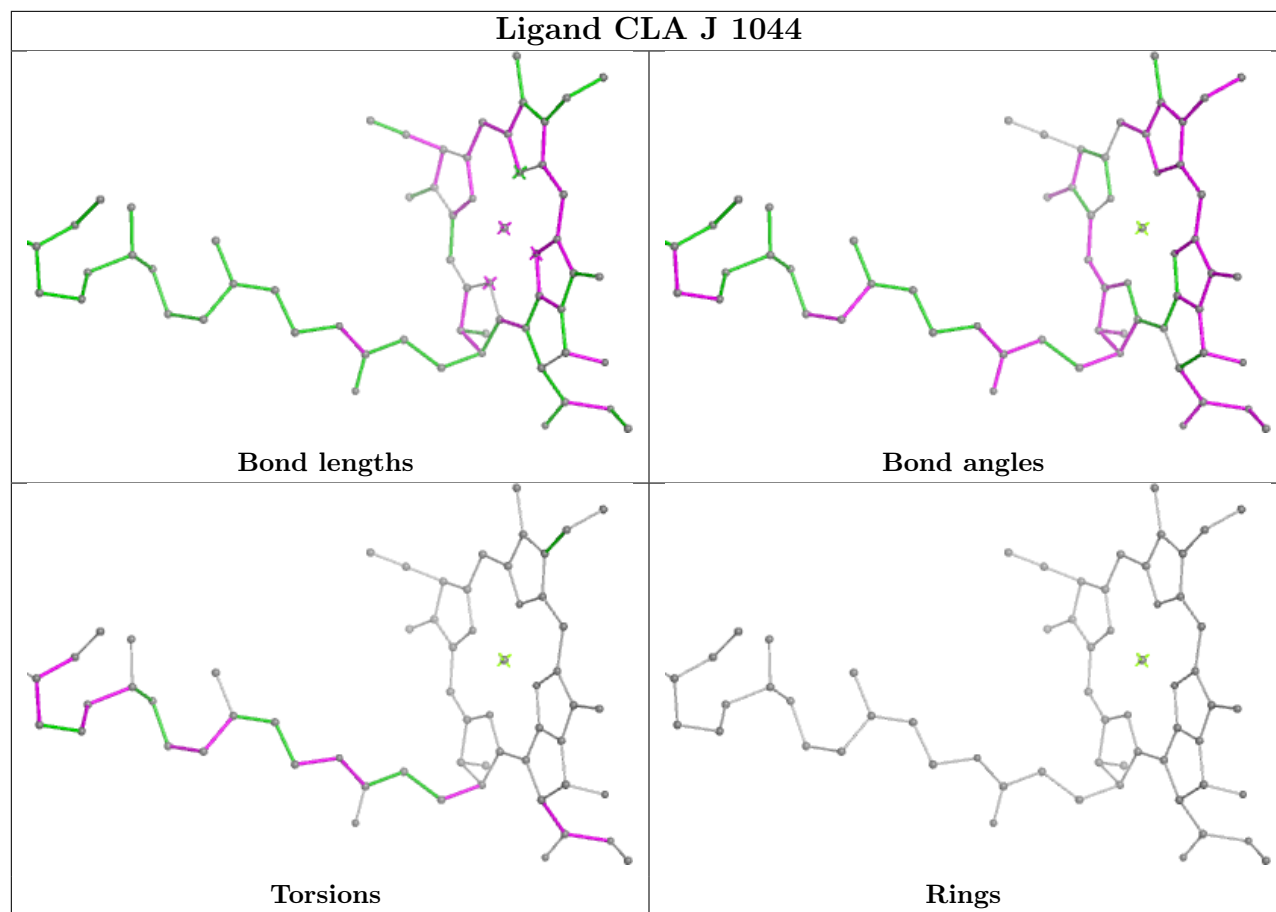


Torsions

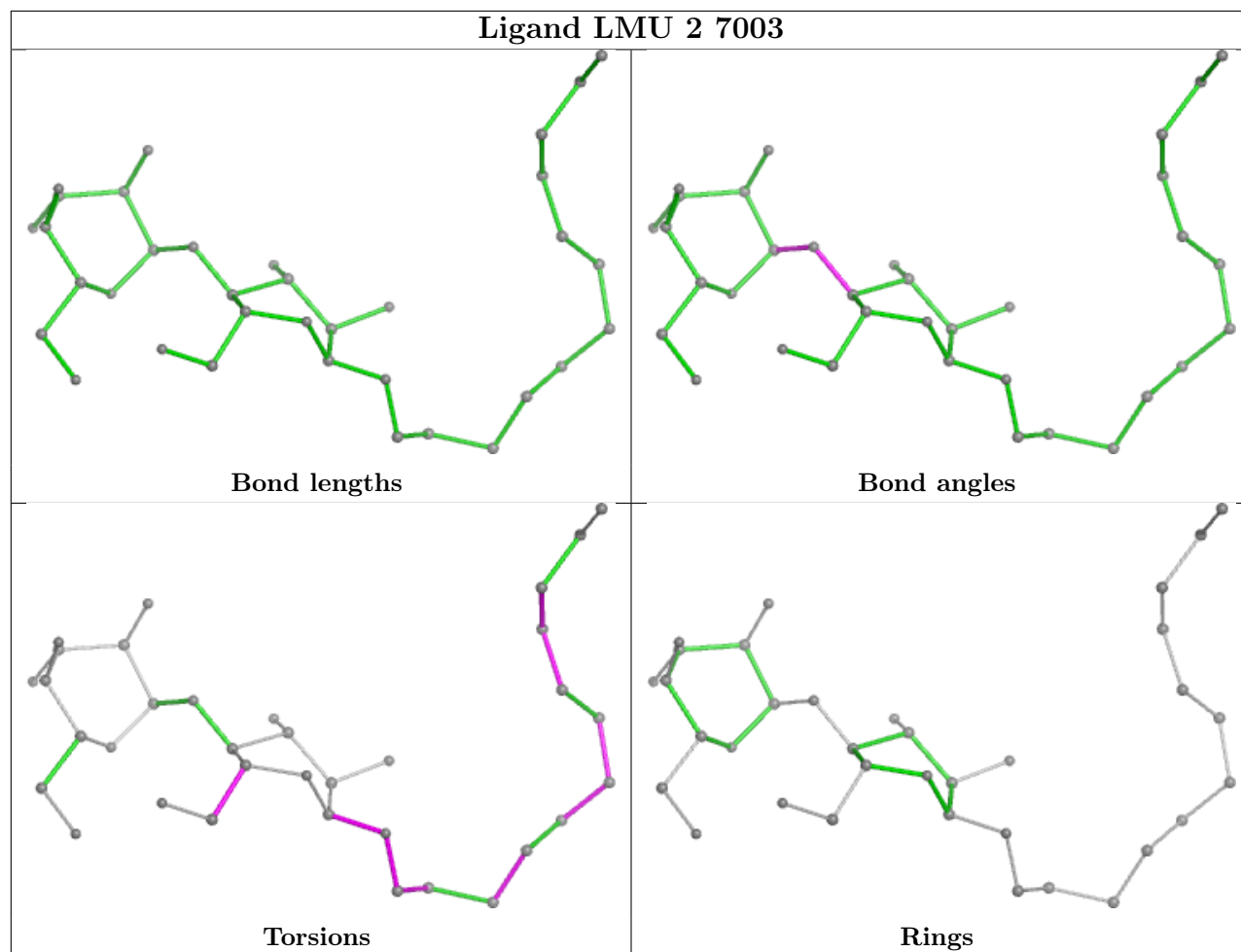


Rings

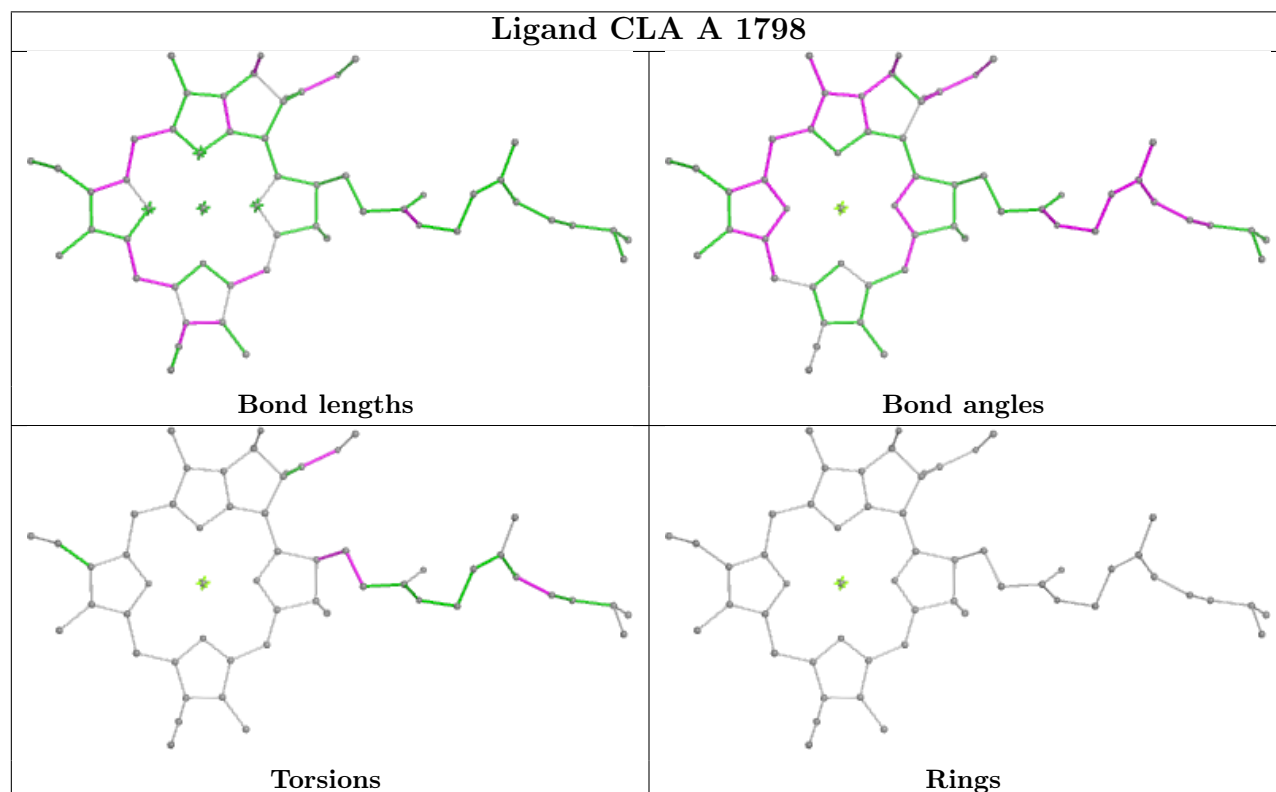


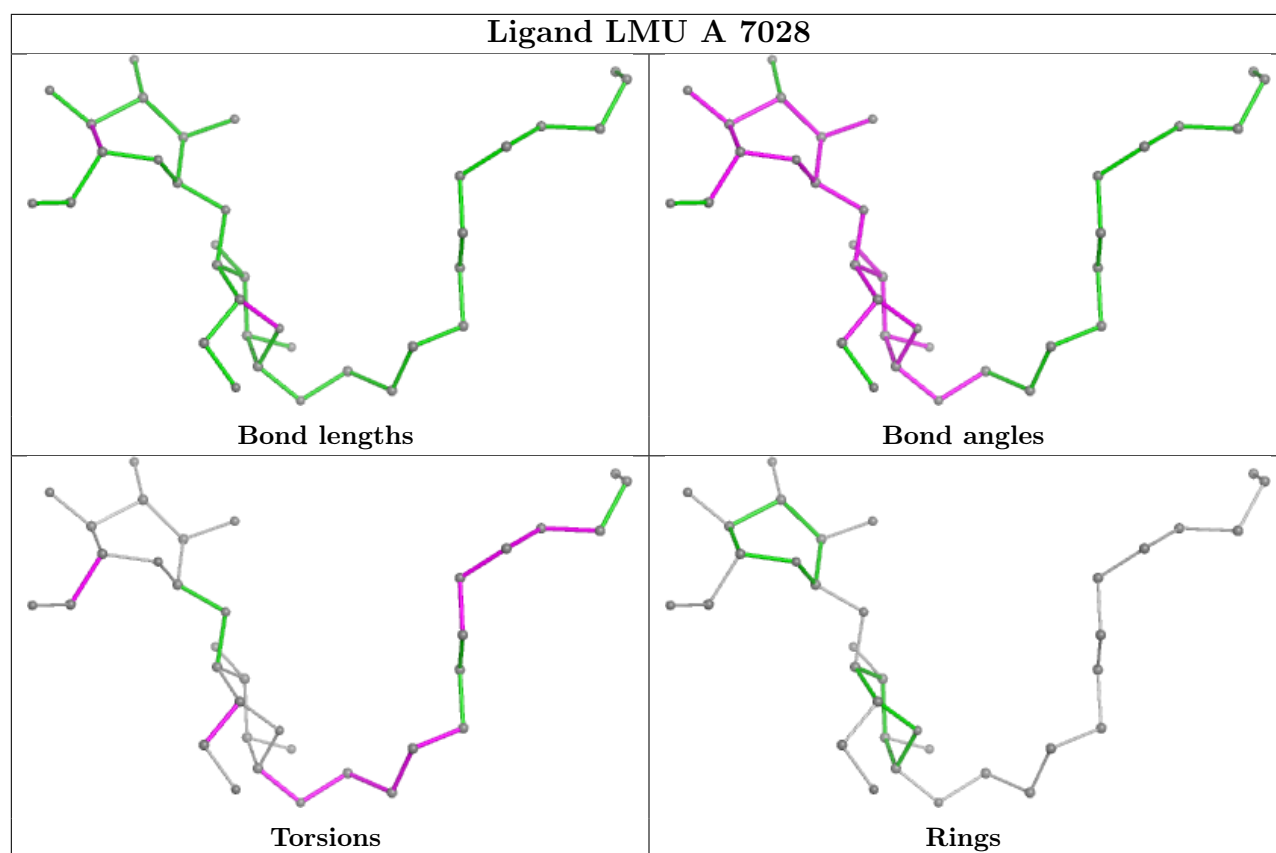


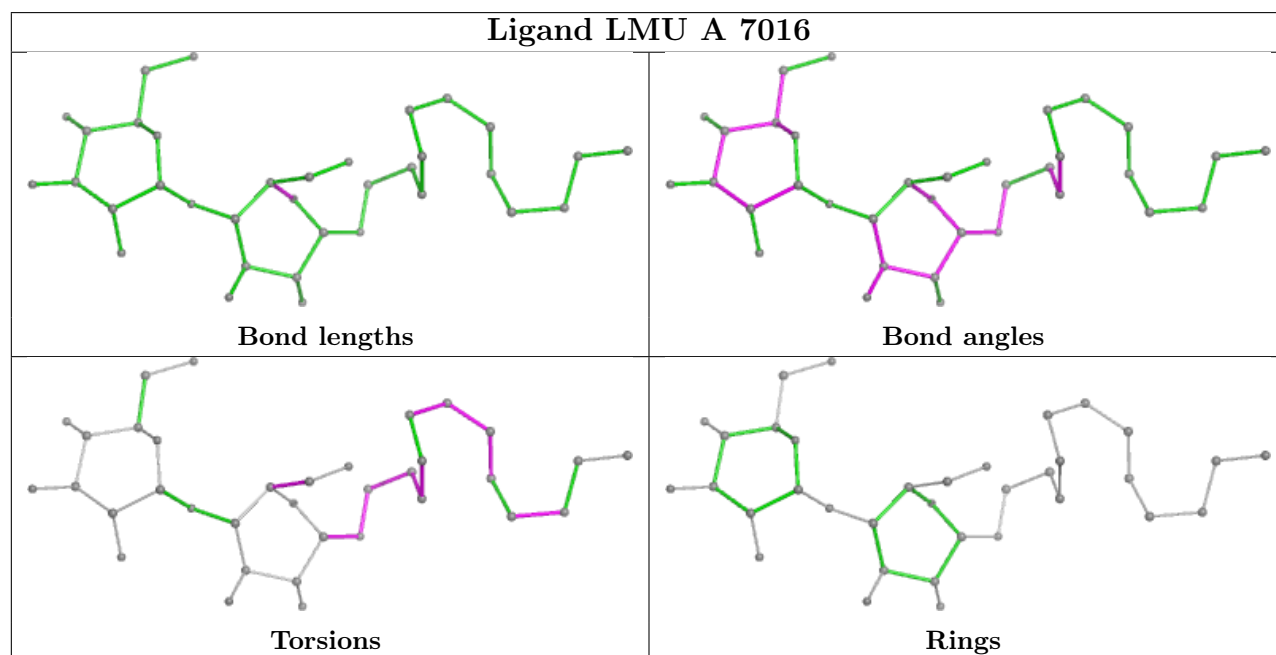
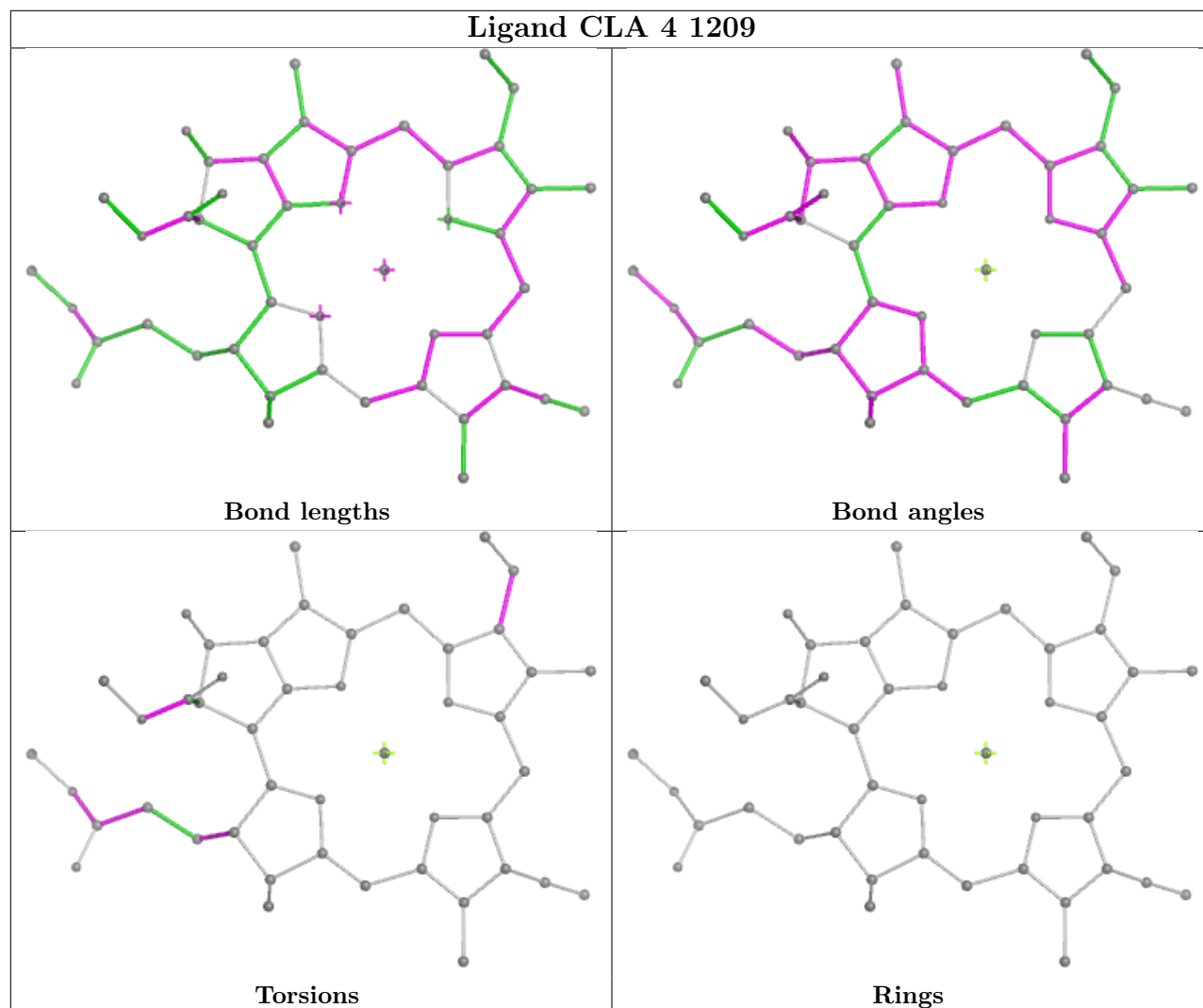
## Ligand LMU 2 7003

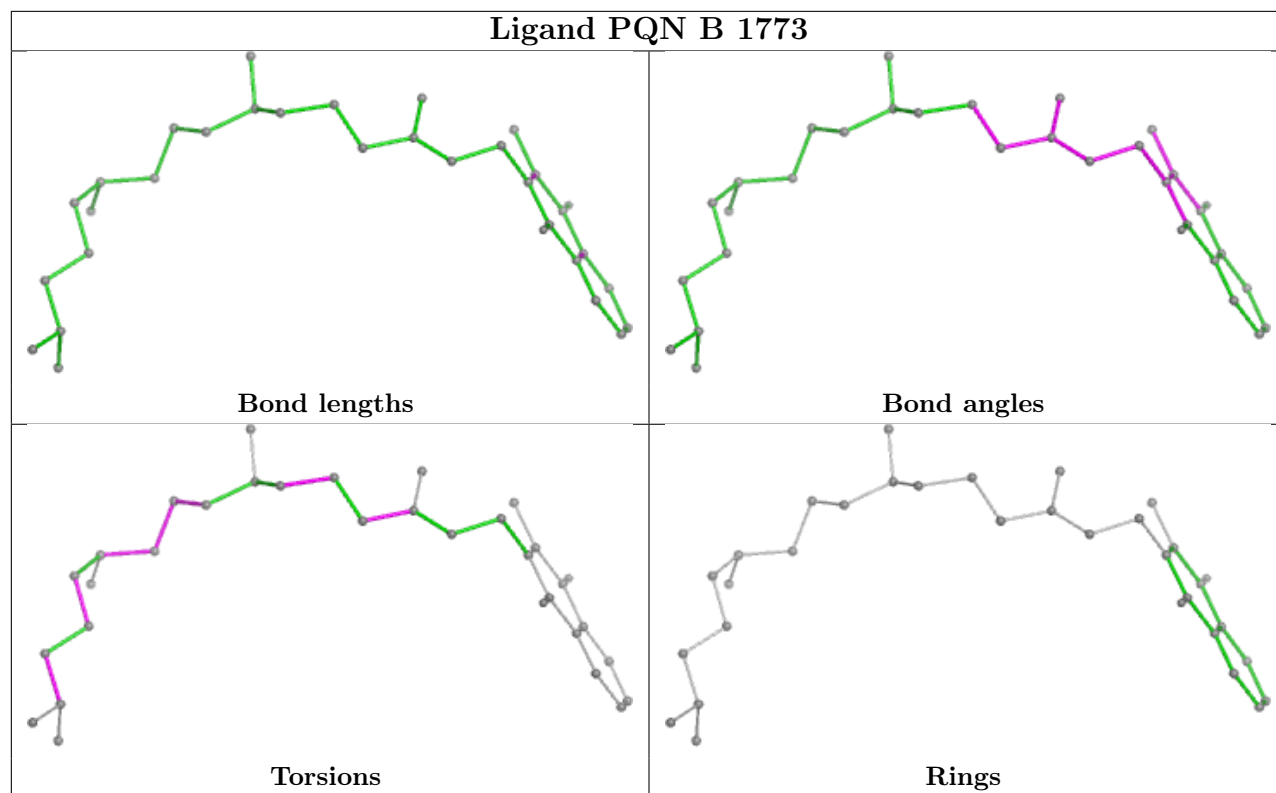


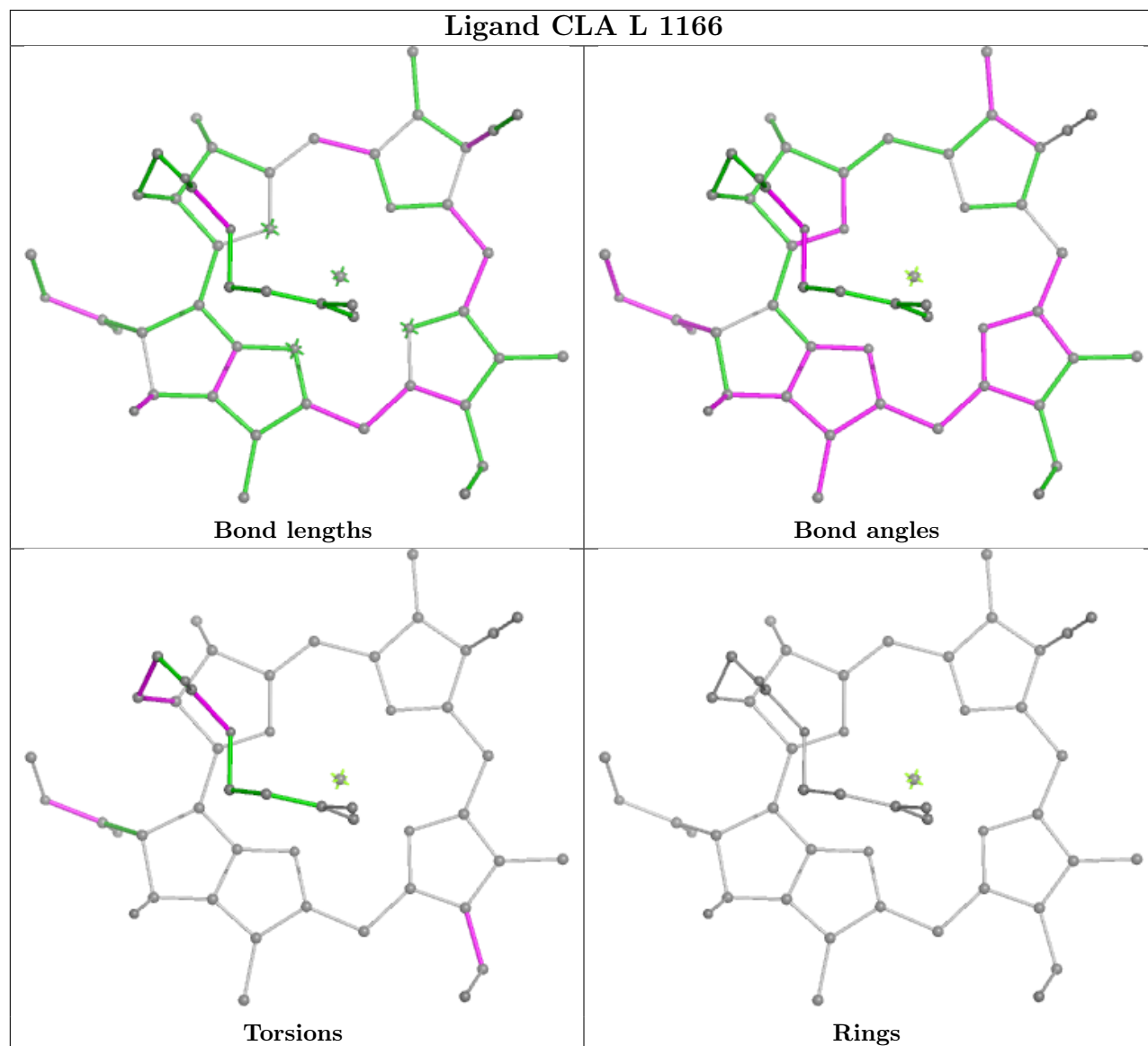
## Ligand CLA A 1798

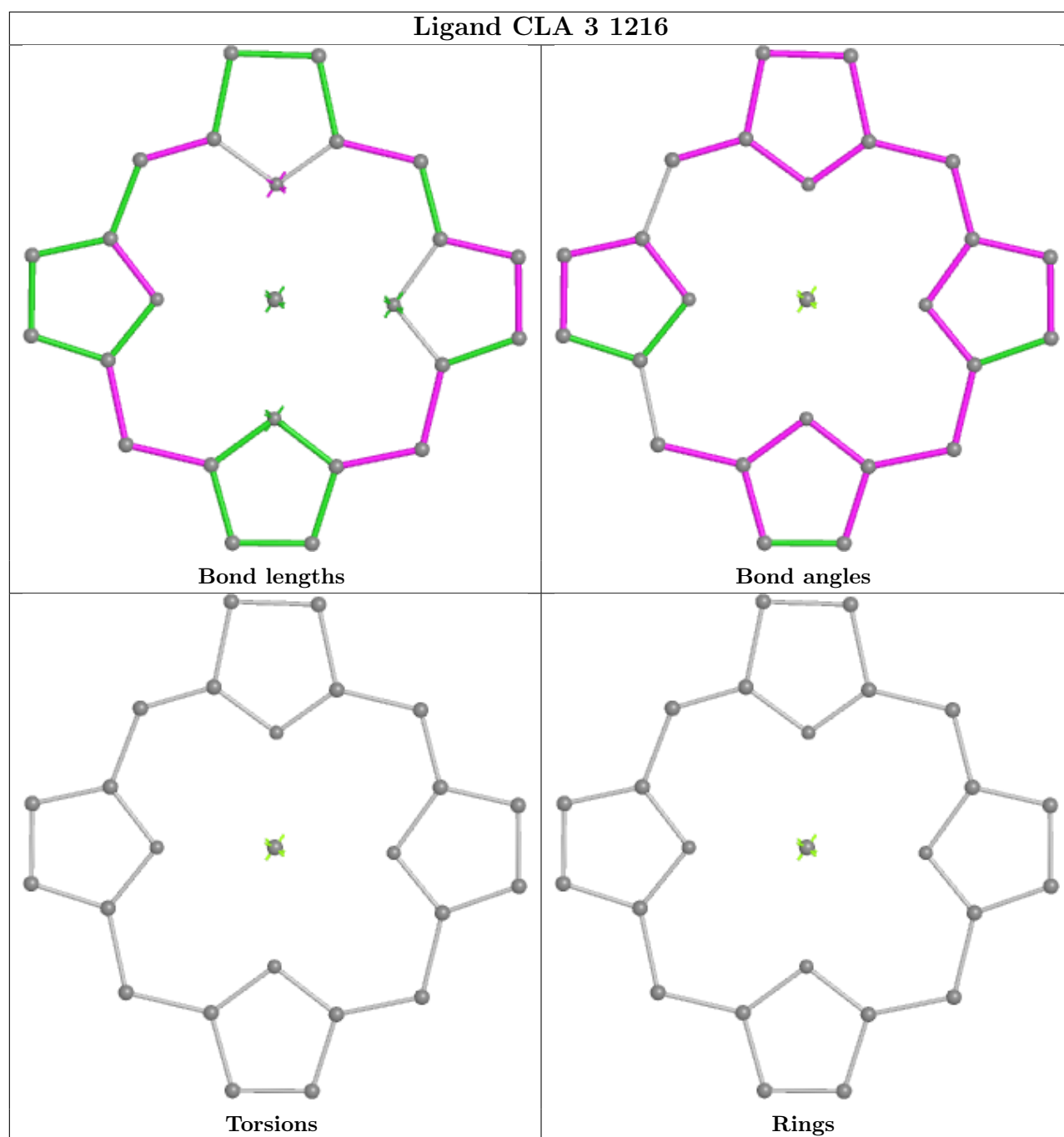


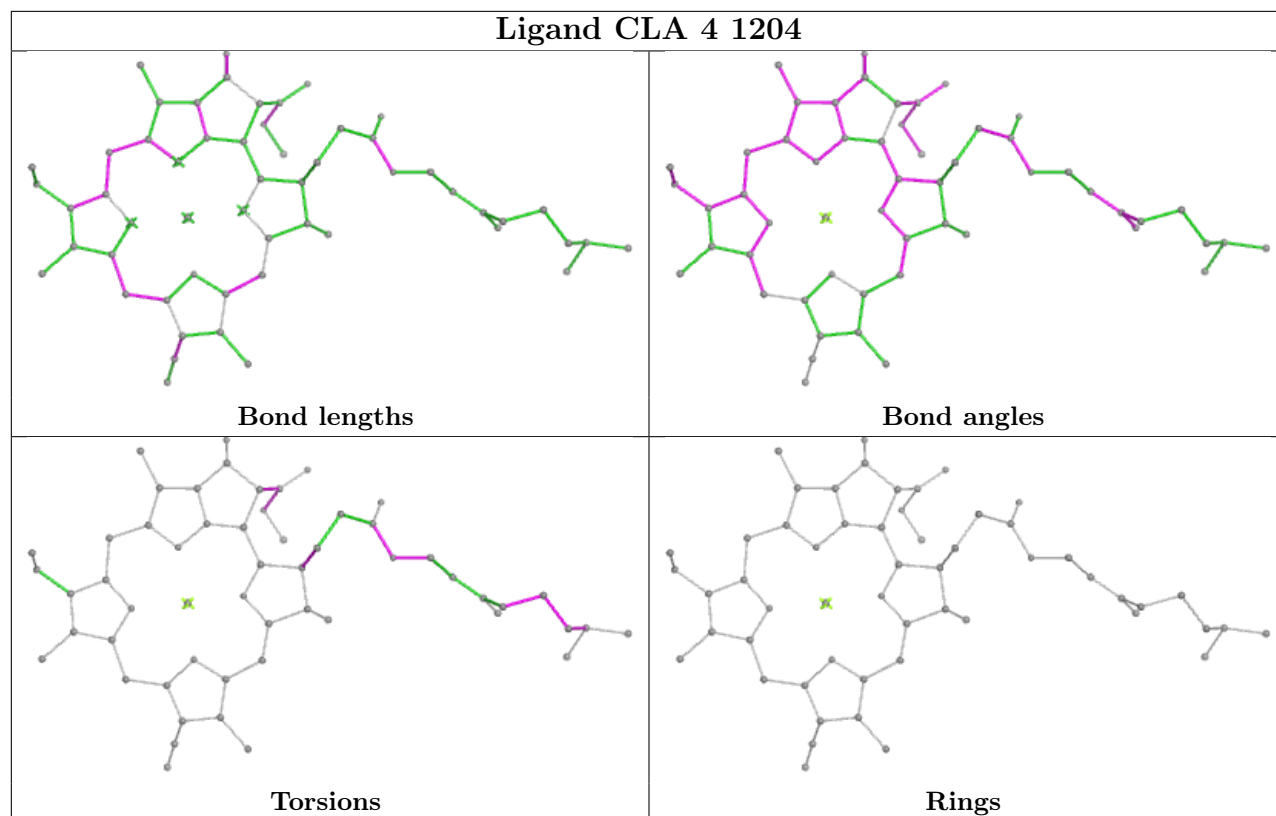






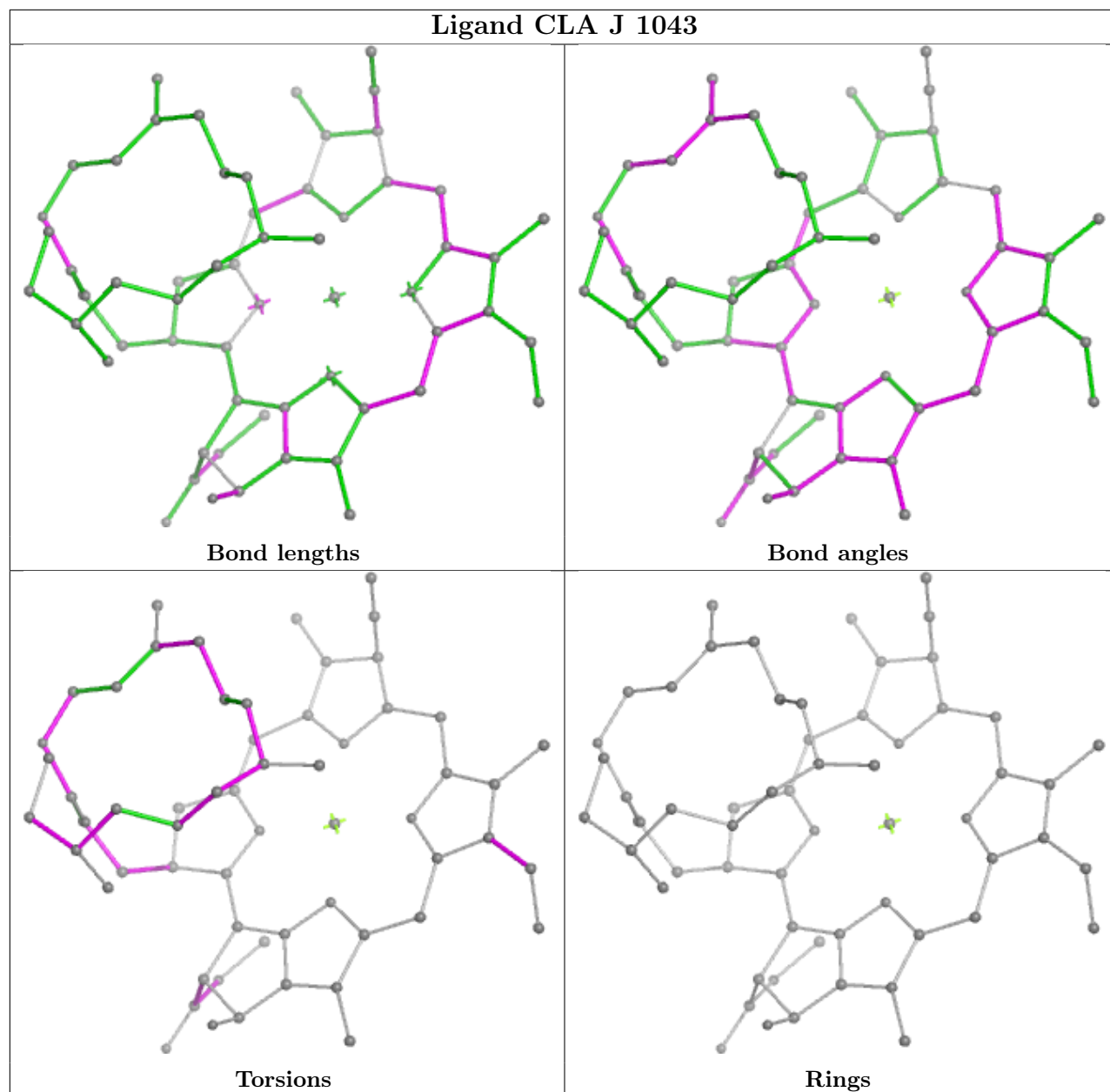




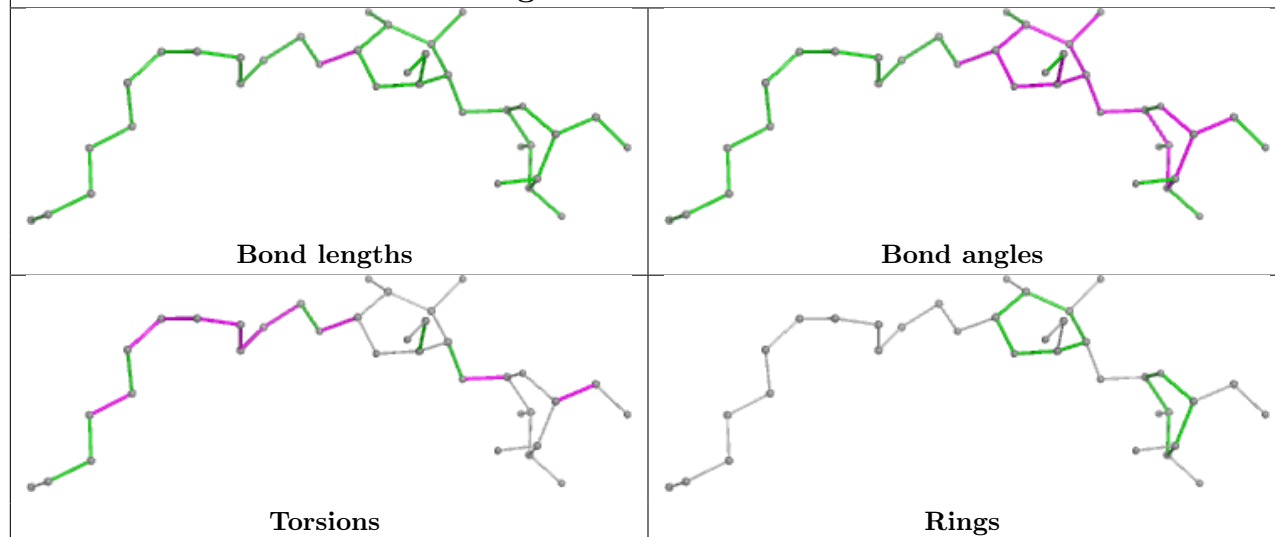




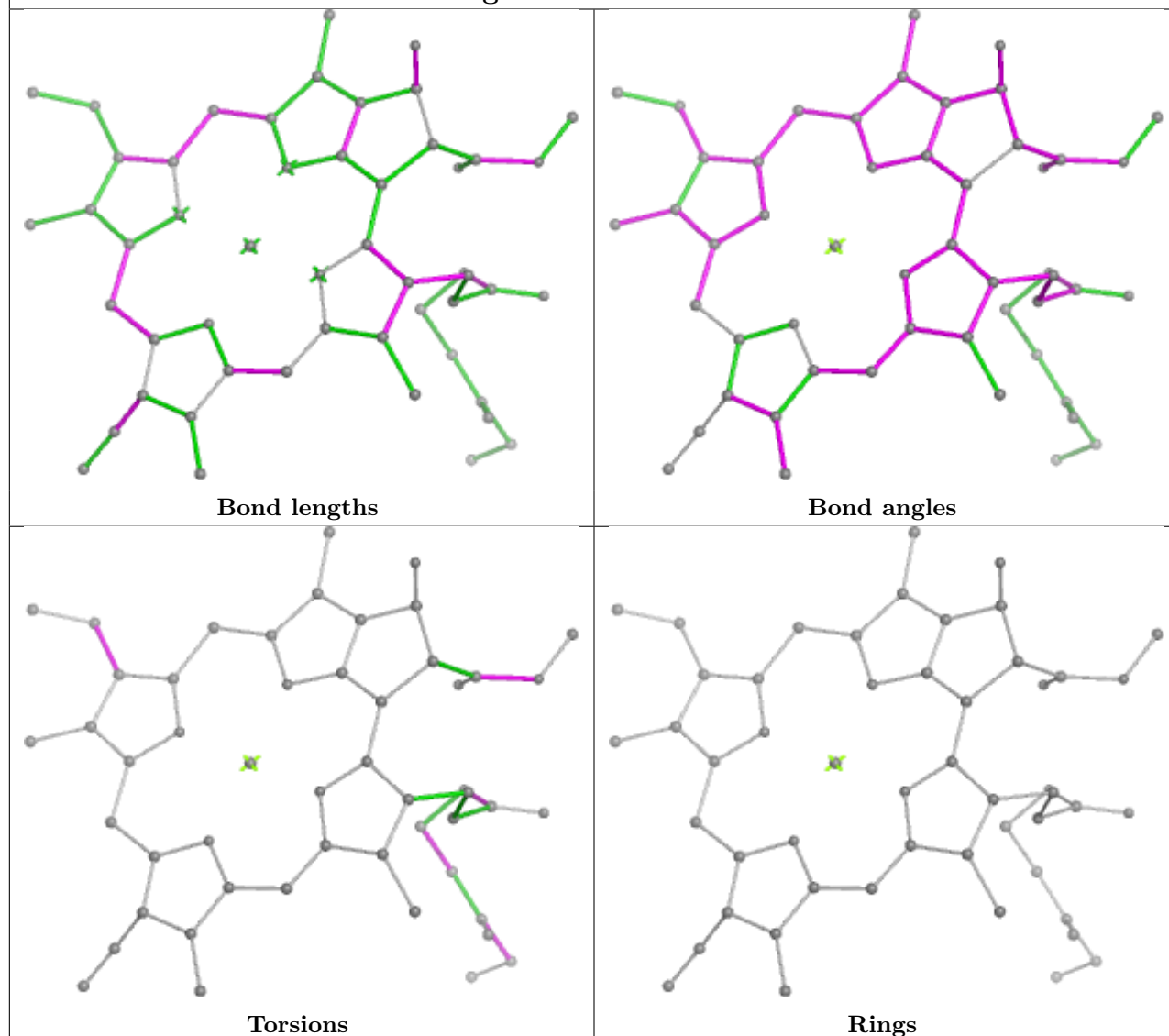
## Ligand CLA J 1043

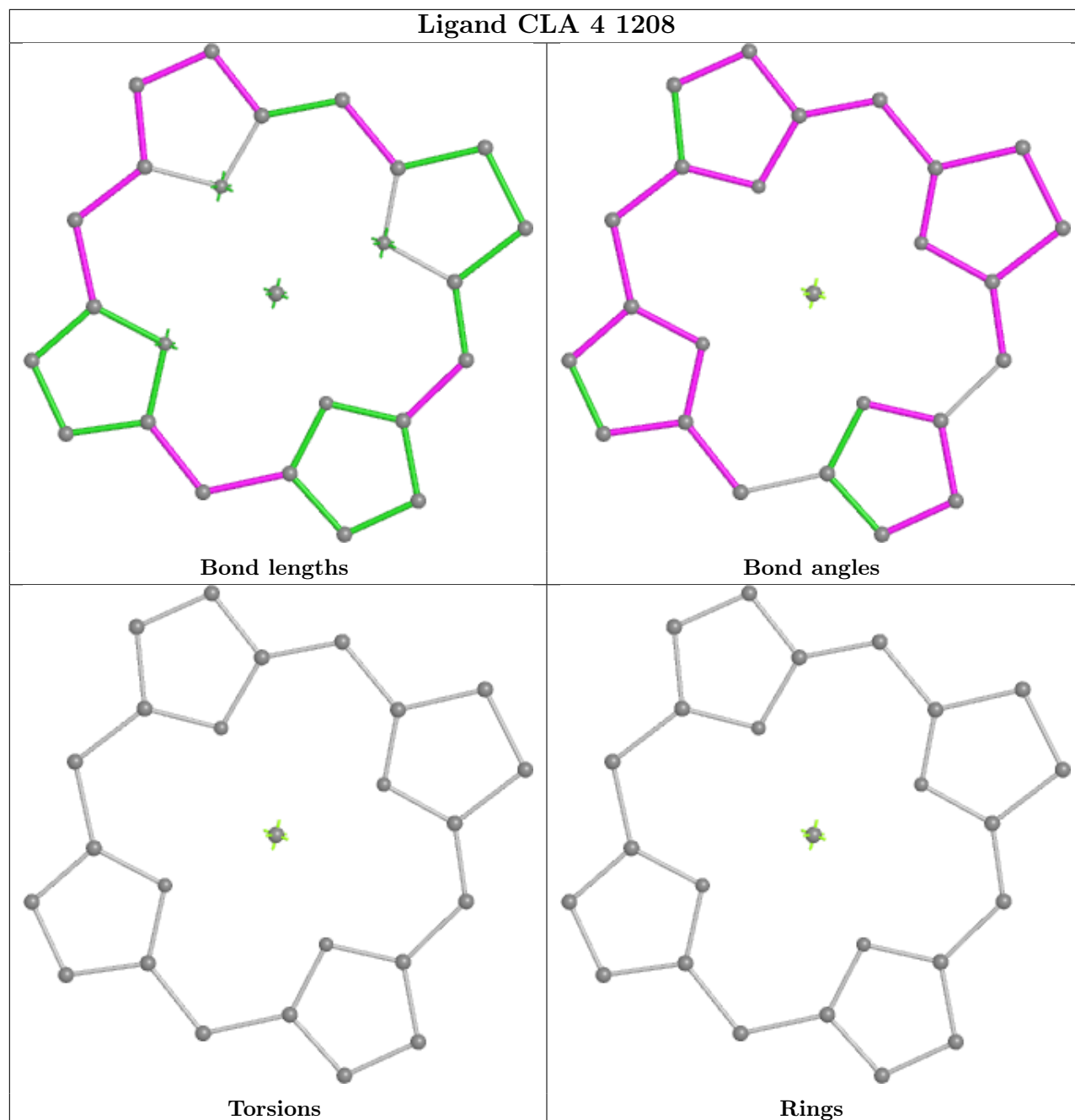


## Ligand LMU A 7027

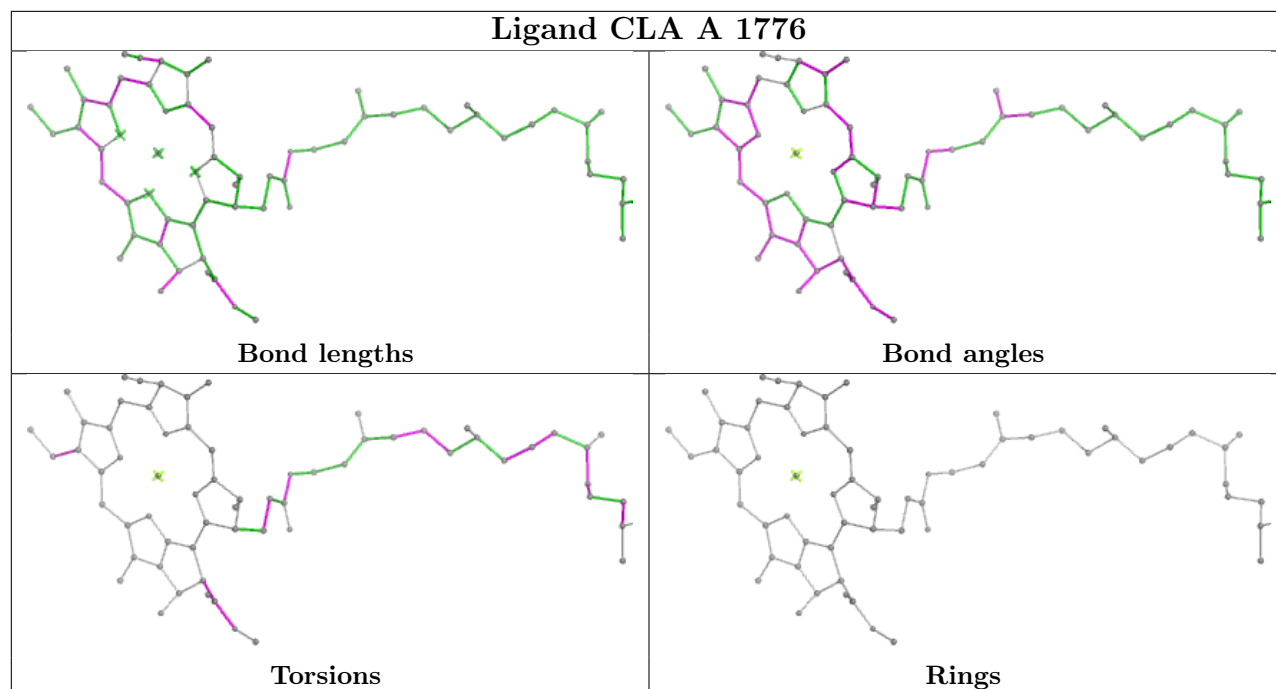


## Ligand CLA 1 1193

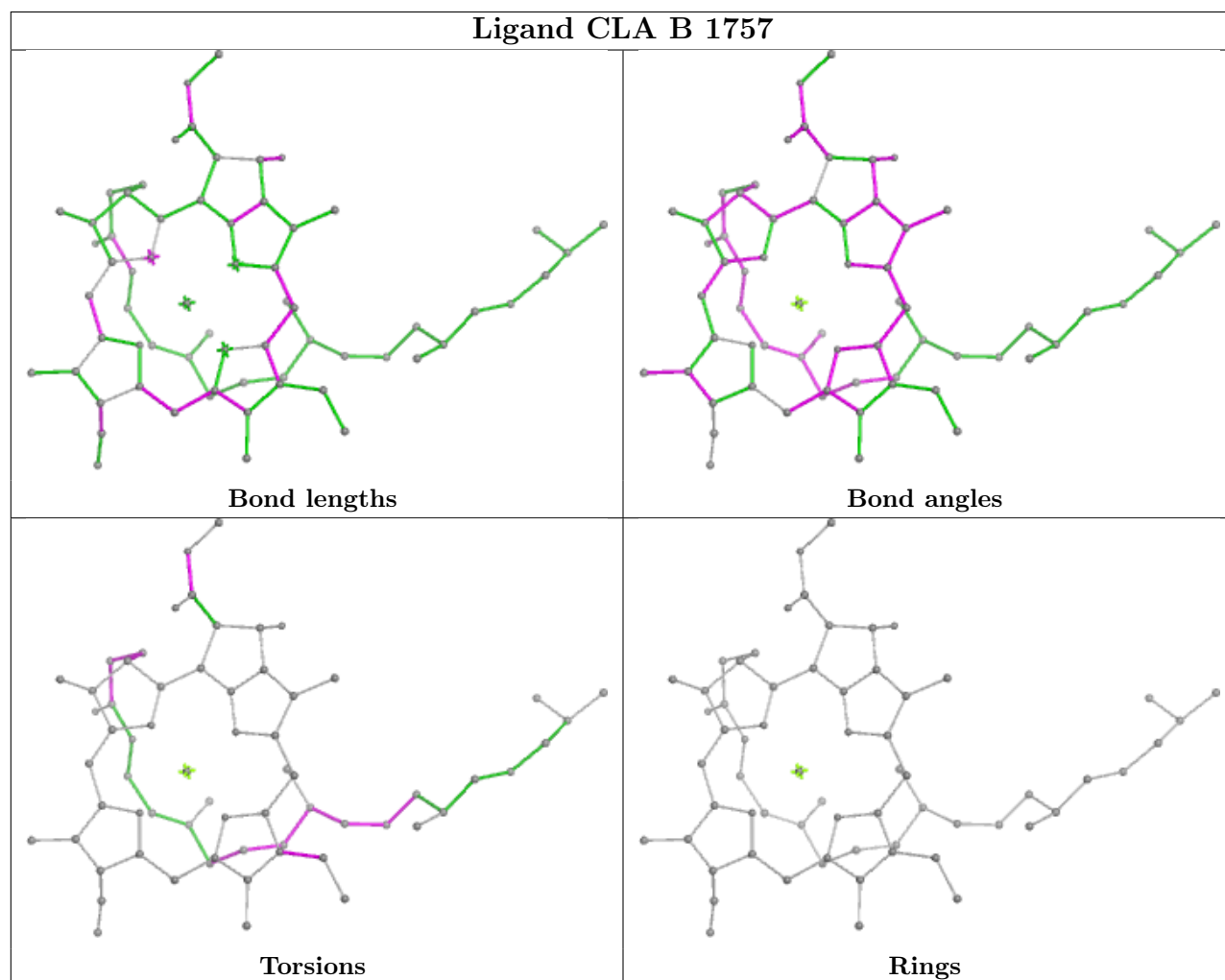


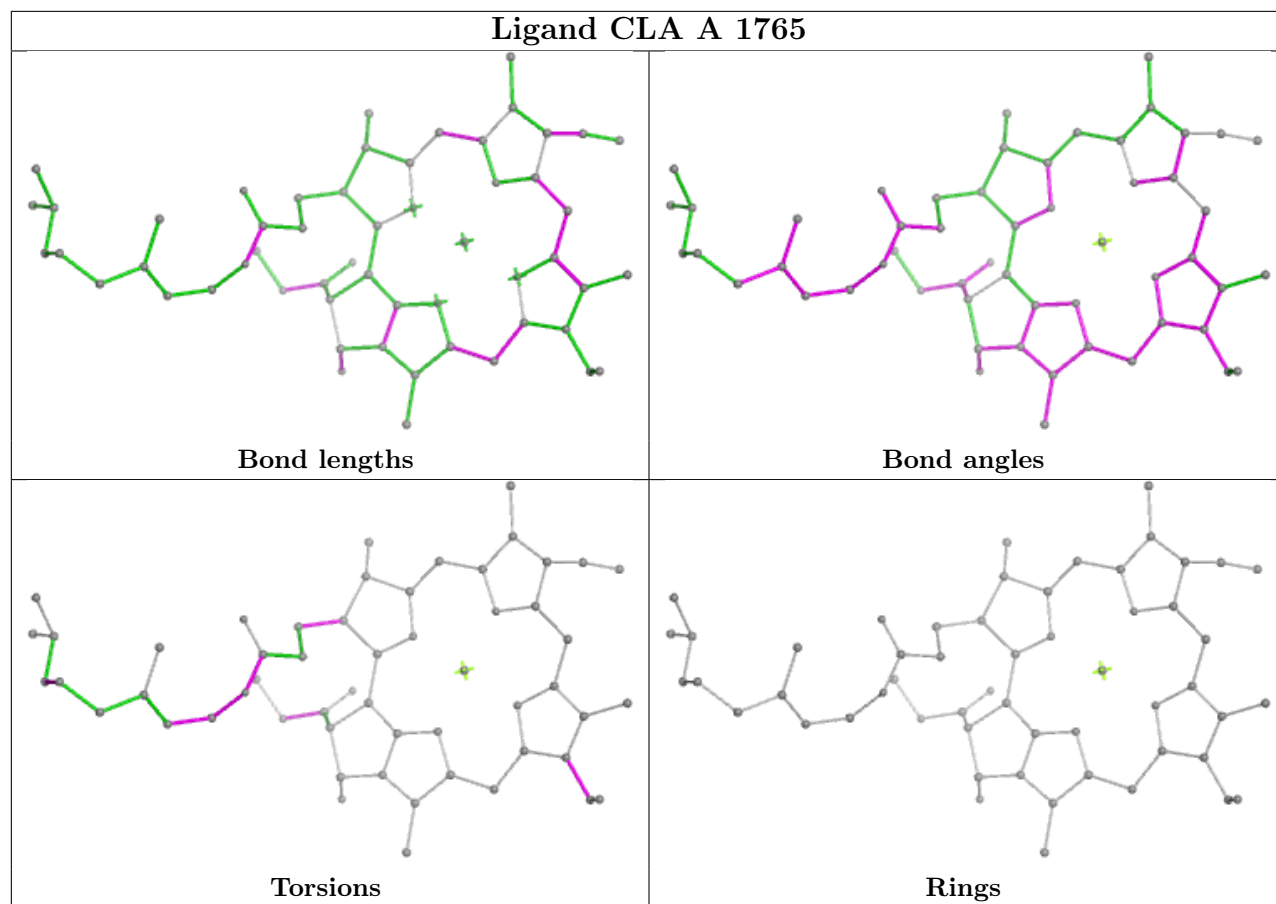


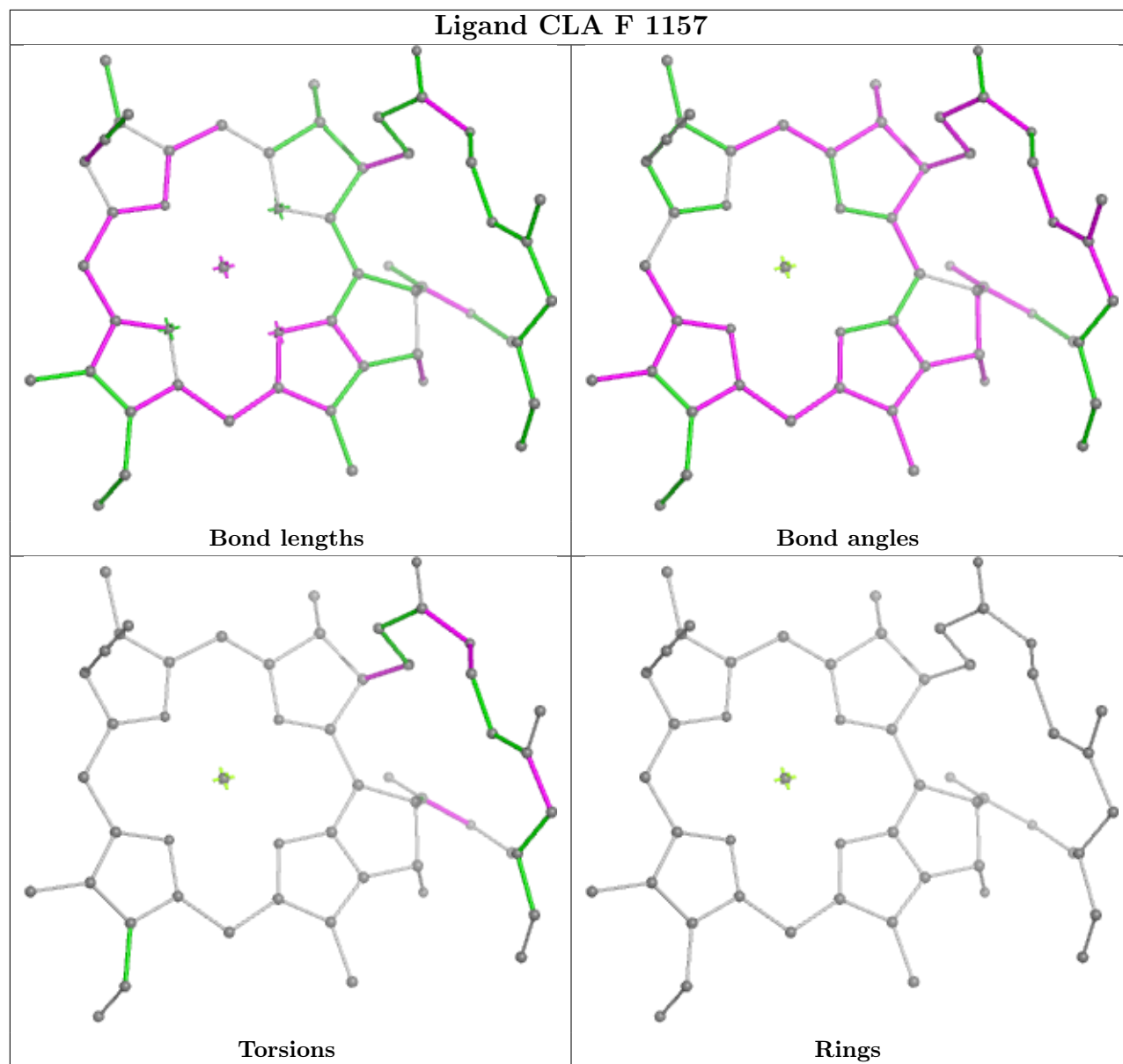
## Ligand CLA A 1776

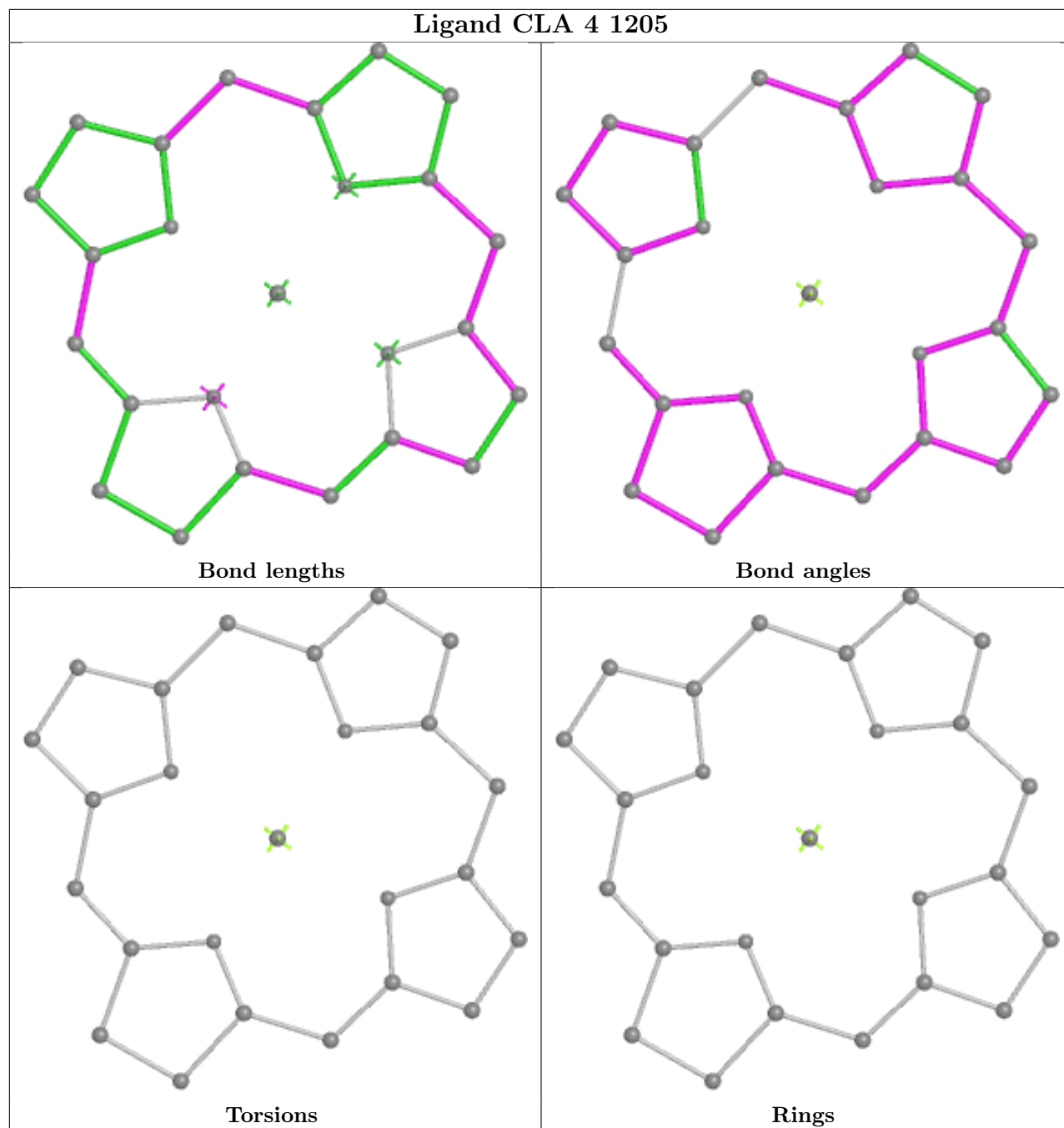


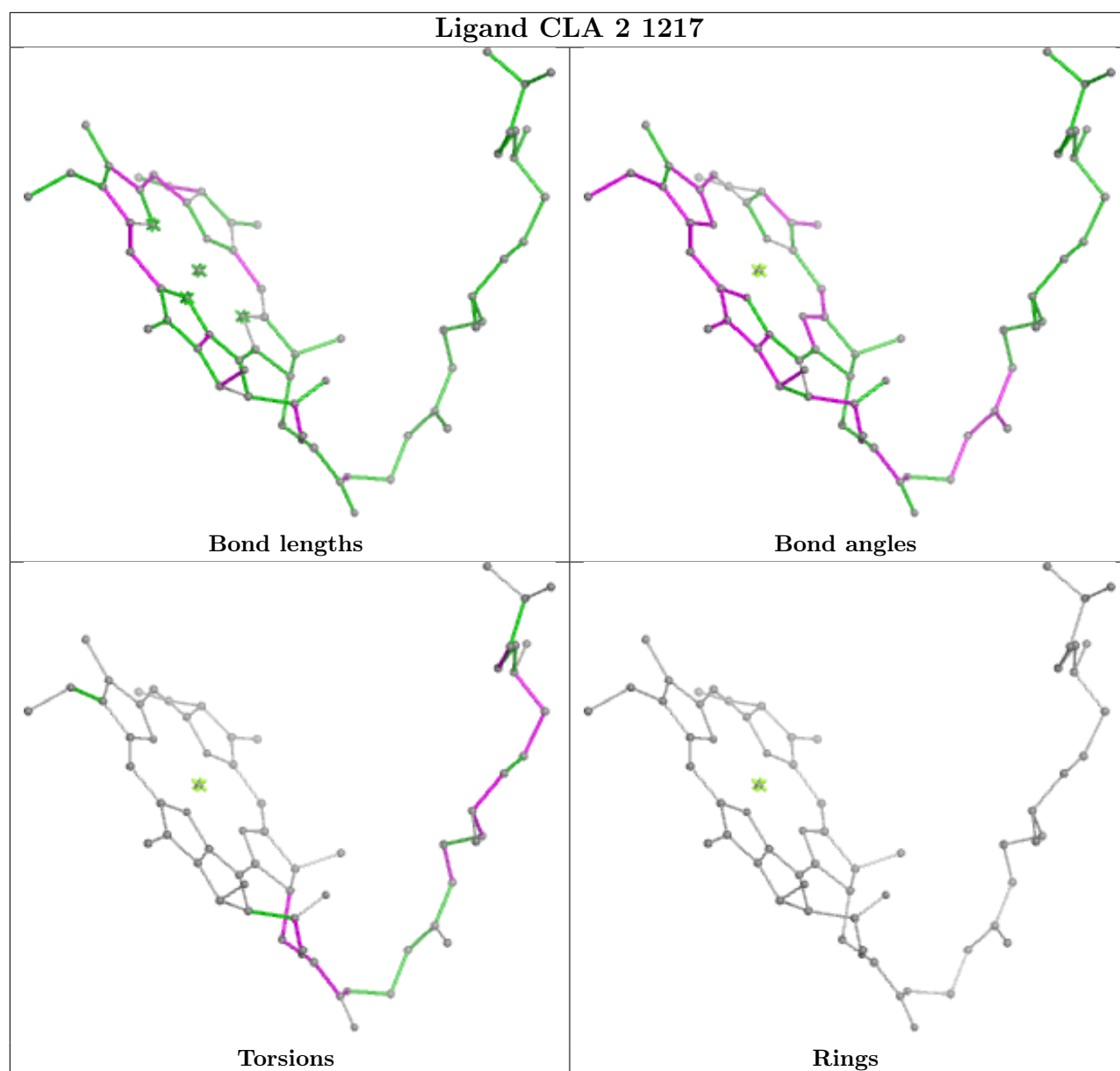
## Ligand CLA B 1757





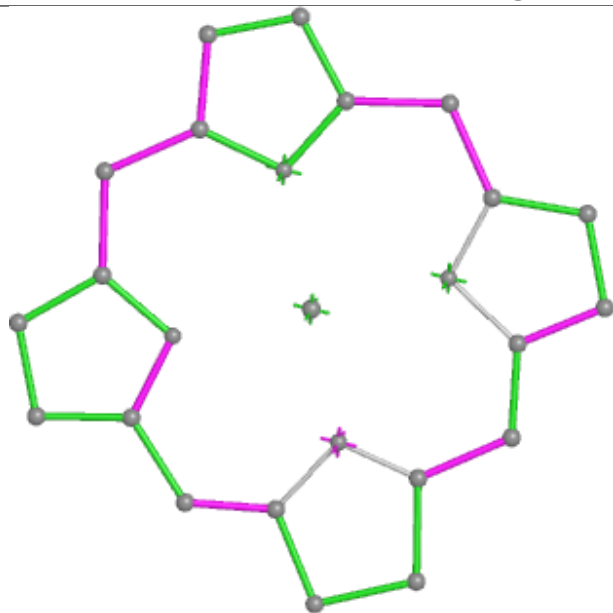




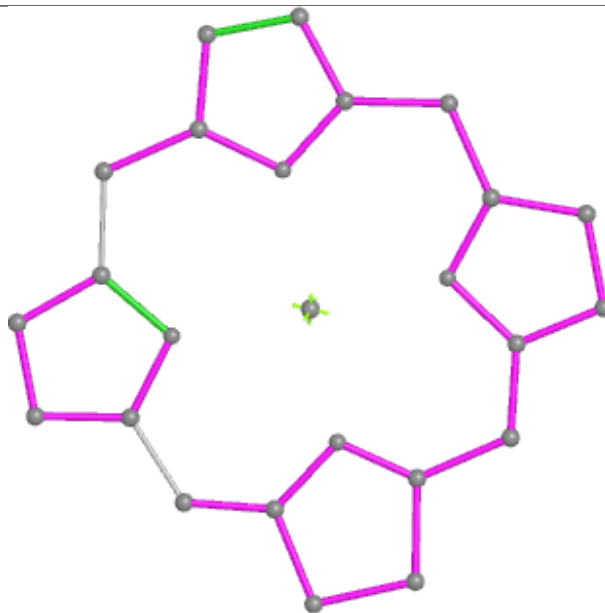




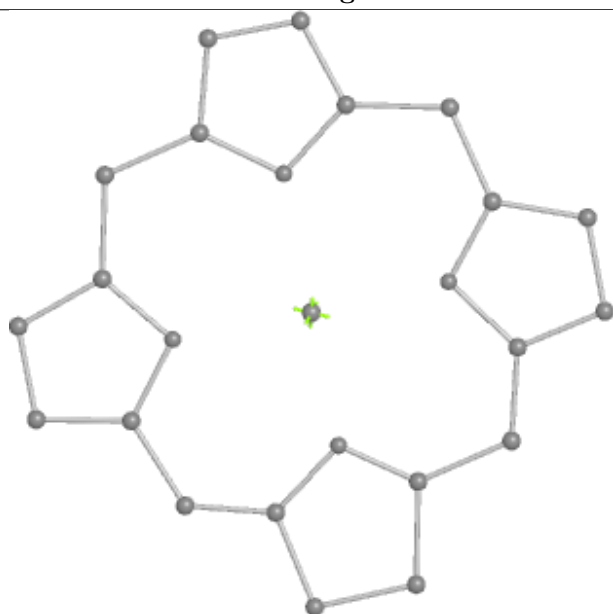
## Ligand CLA 3 3014



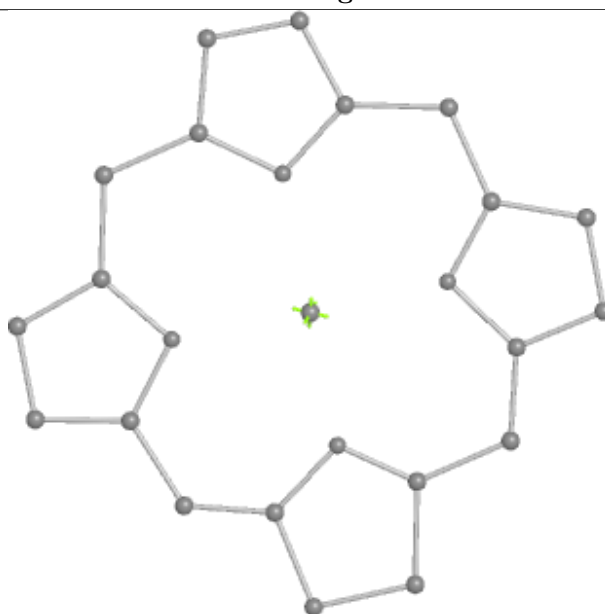
Bond lengths



Bond angles

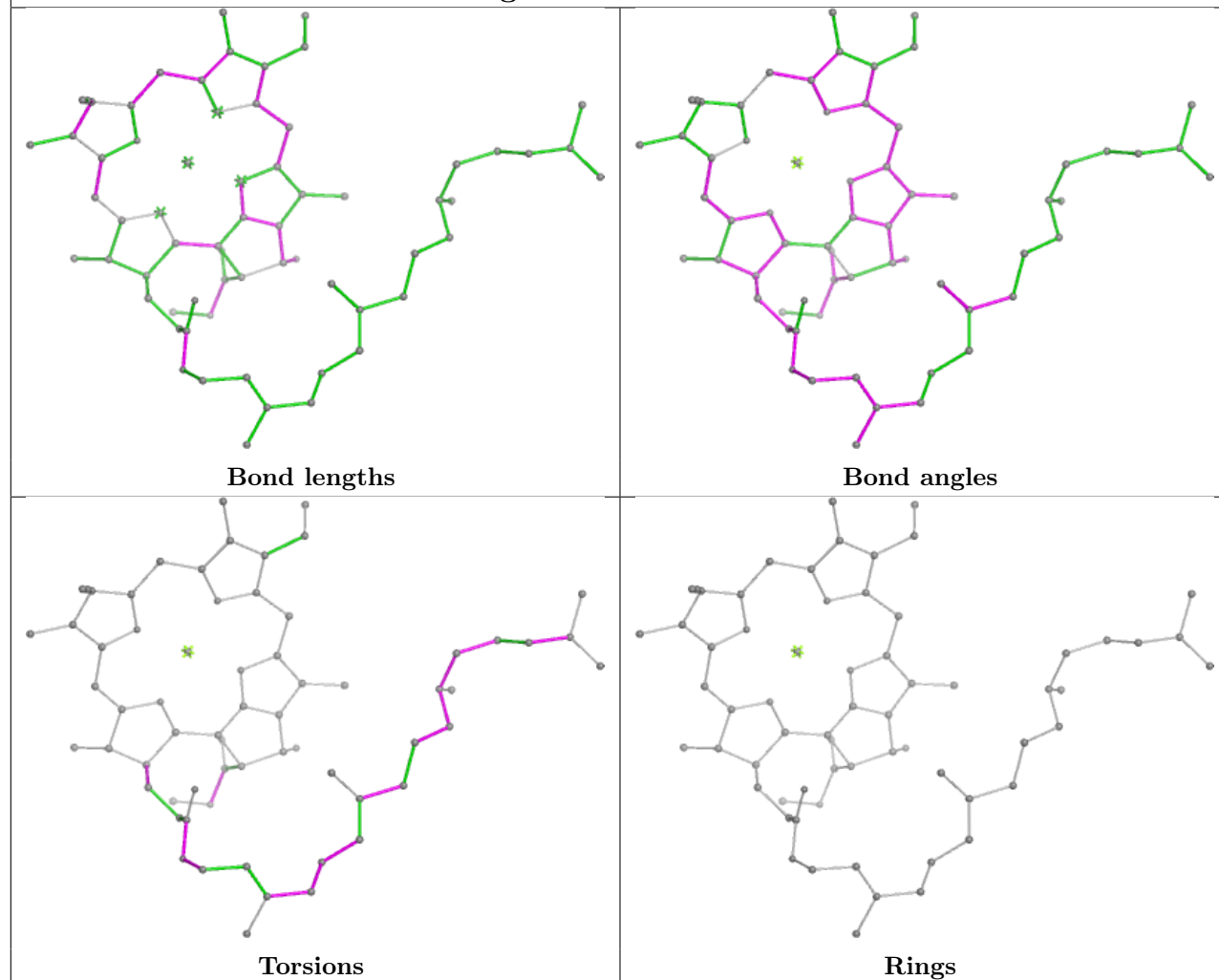


Torsions

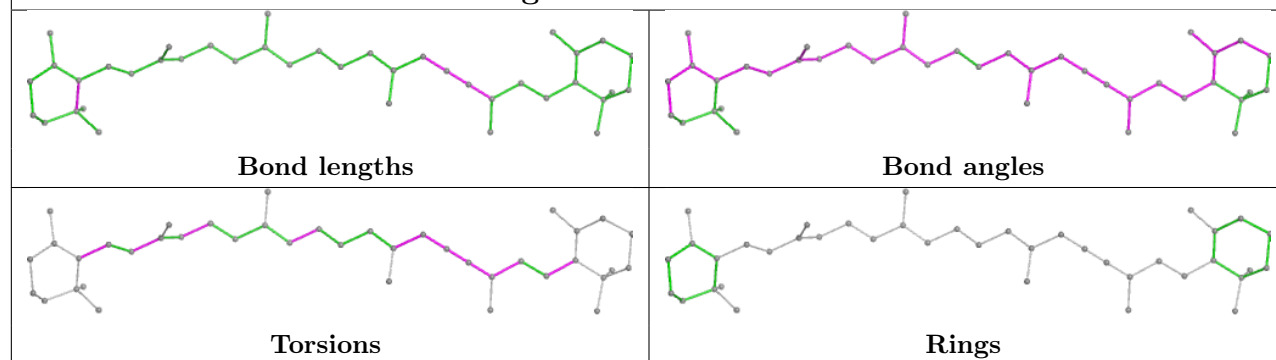


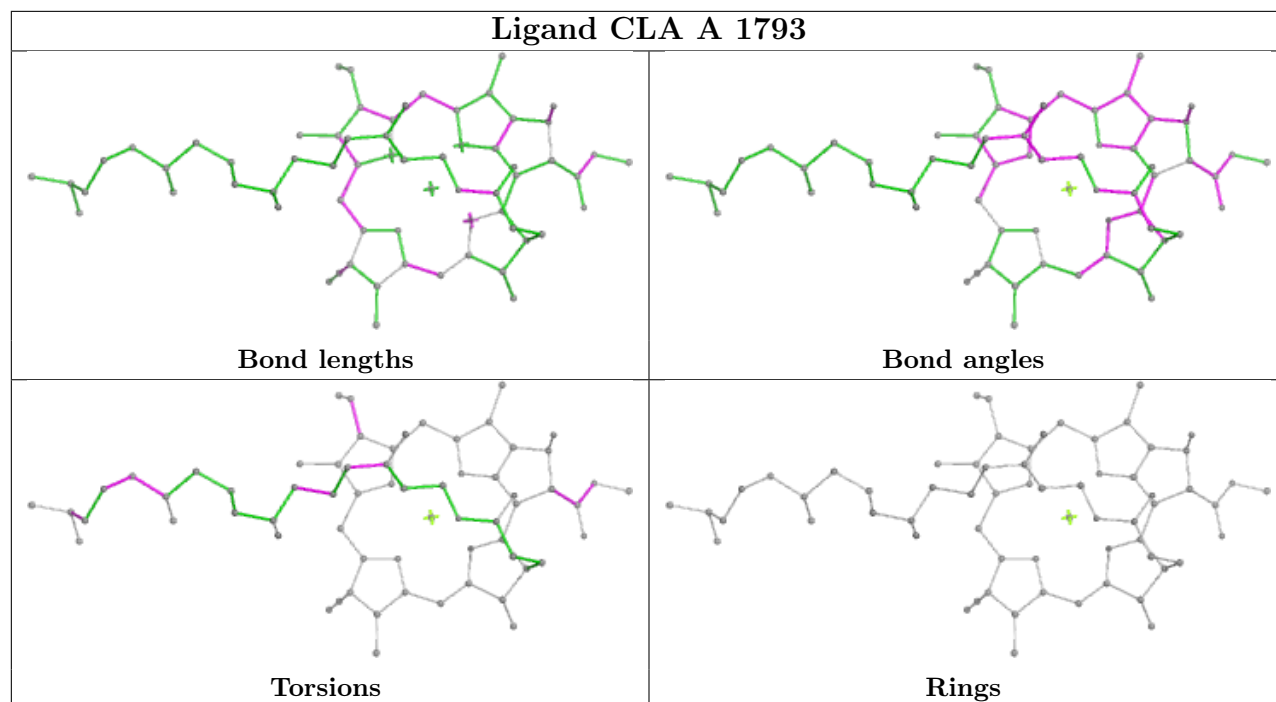
Rings

## Ligand CLA B 1762

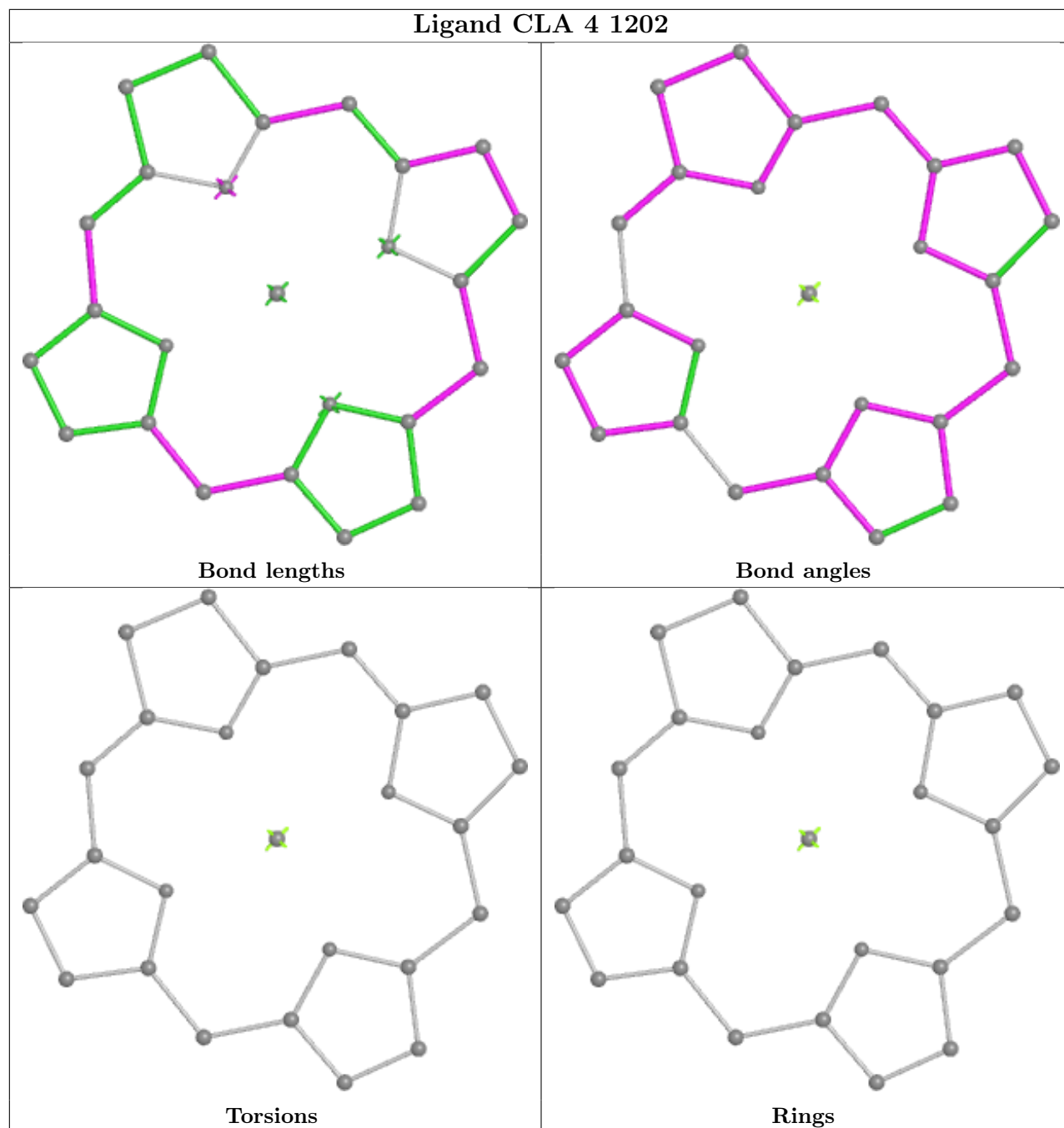


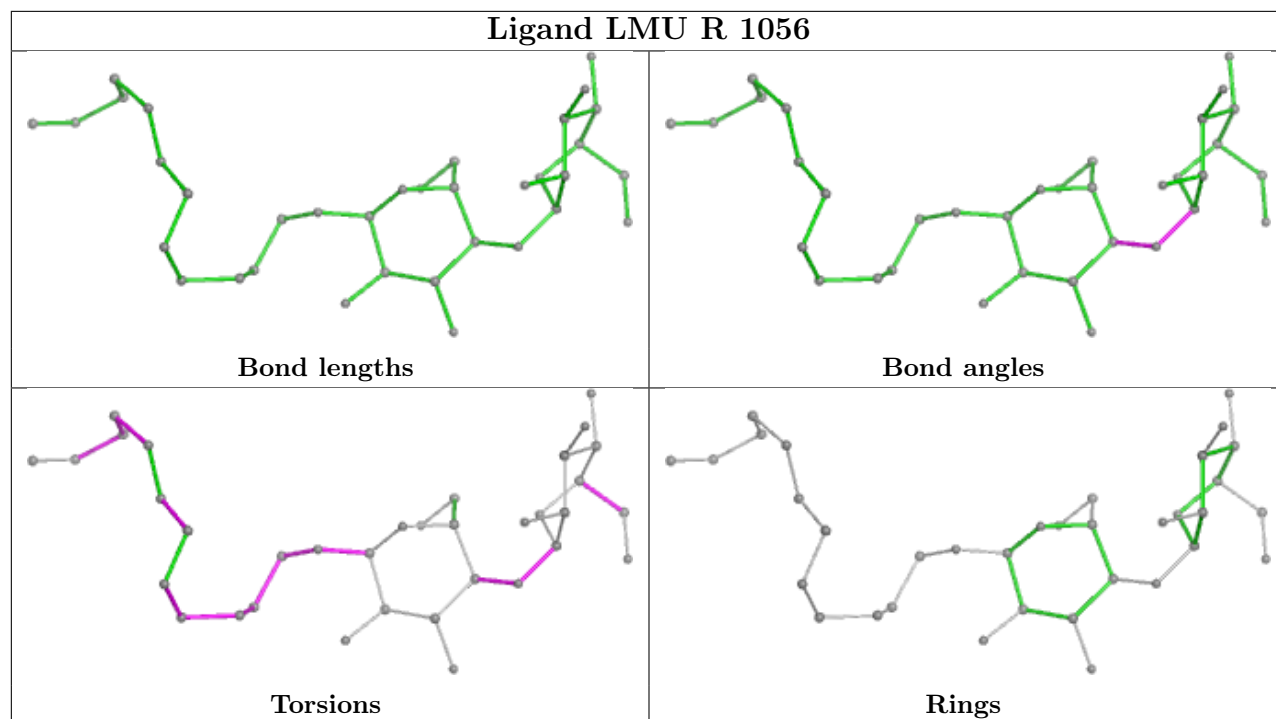
## Ligand BCR B 1777

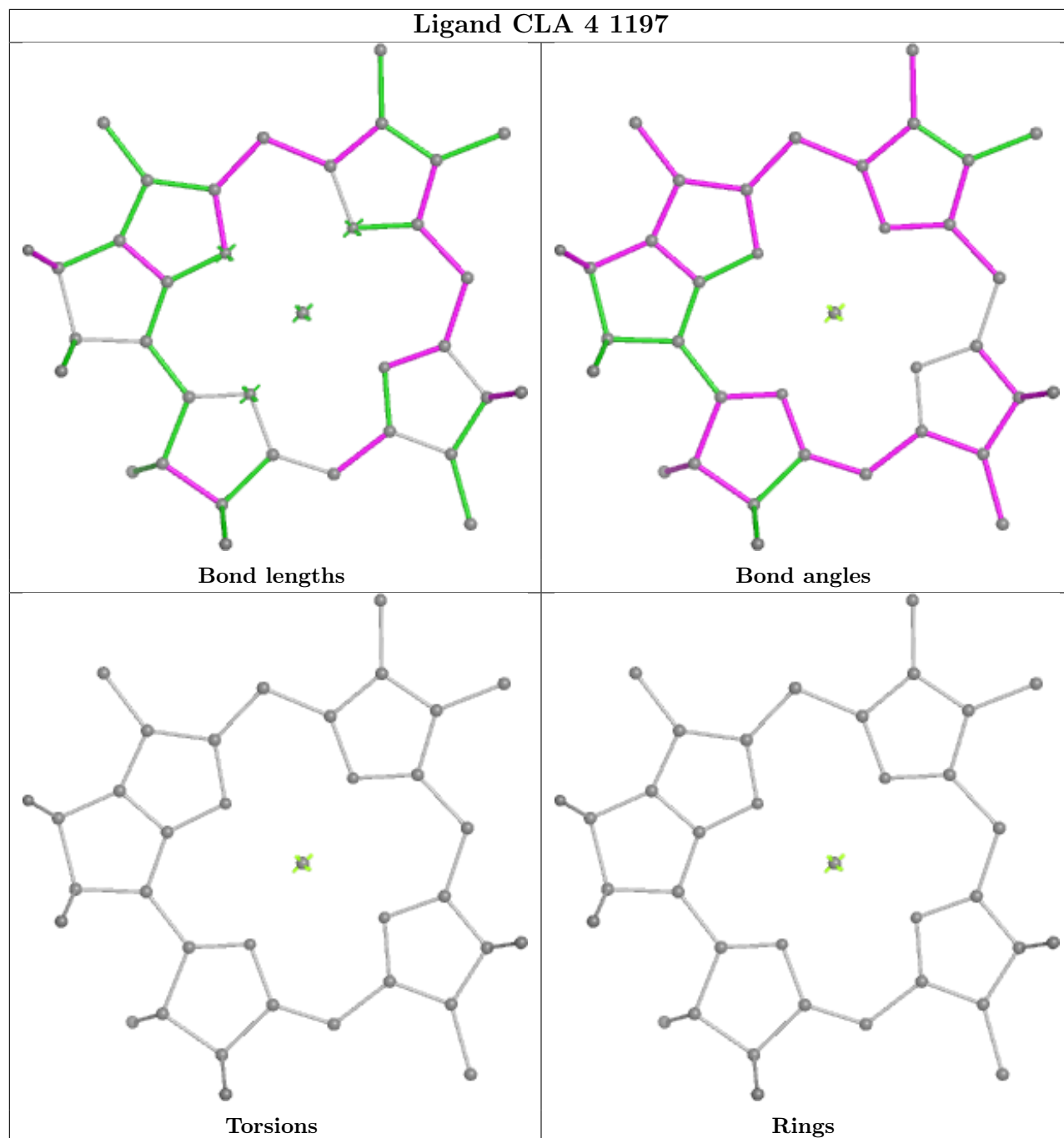


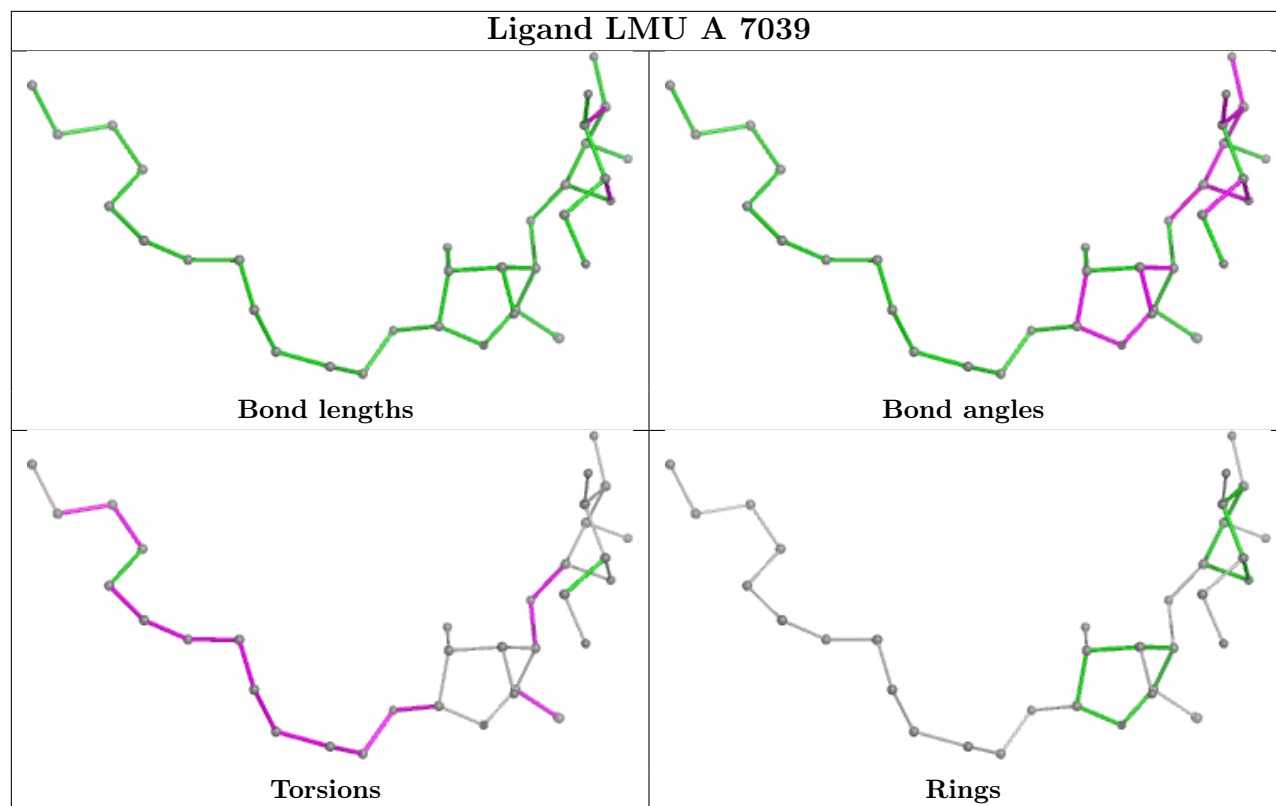


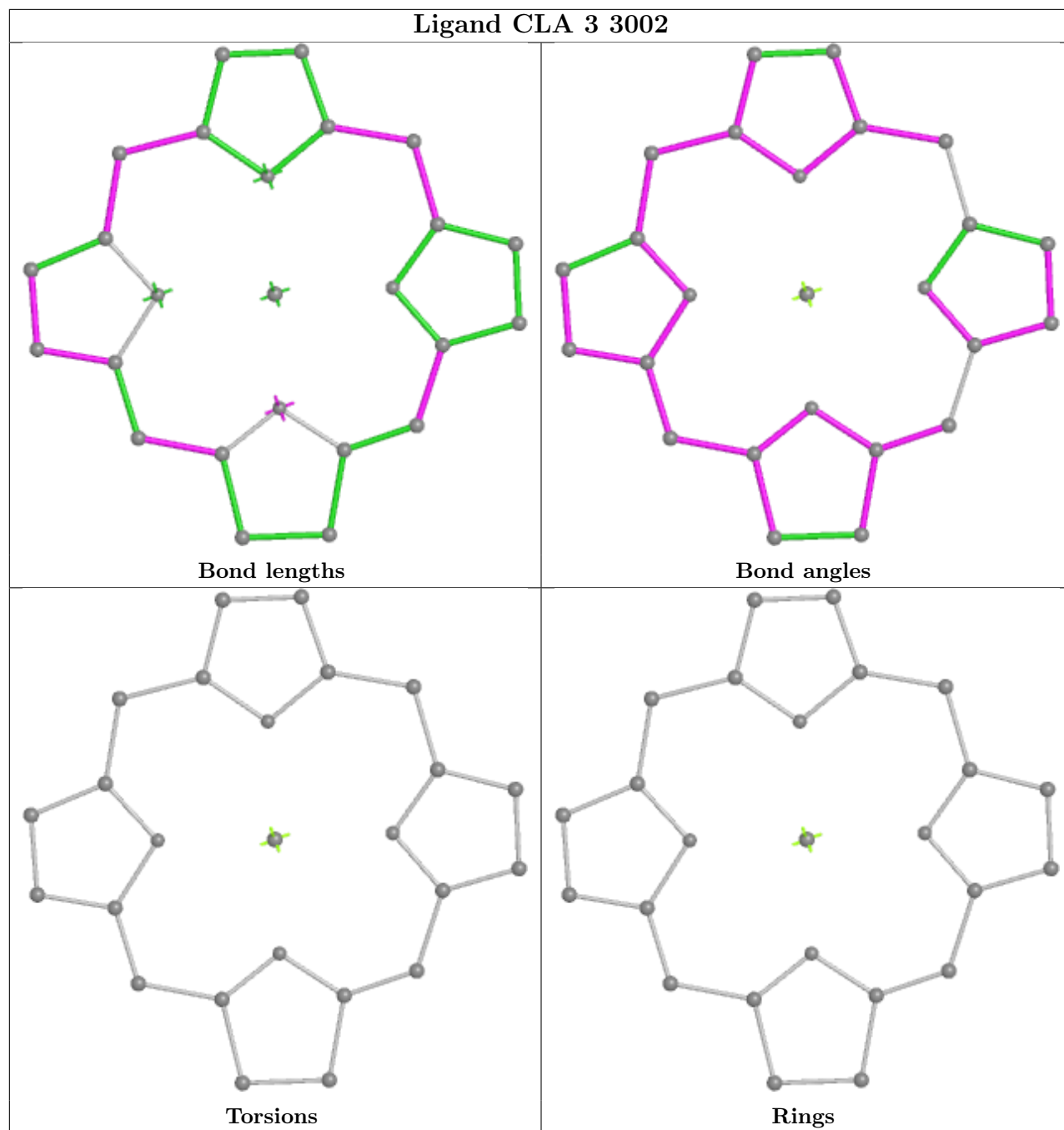
## Ligand CLA 4 1202



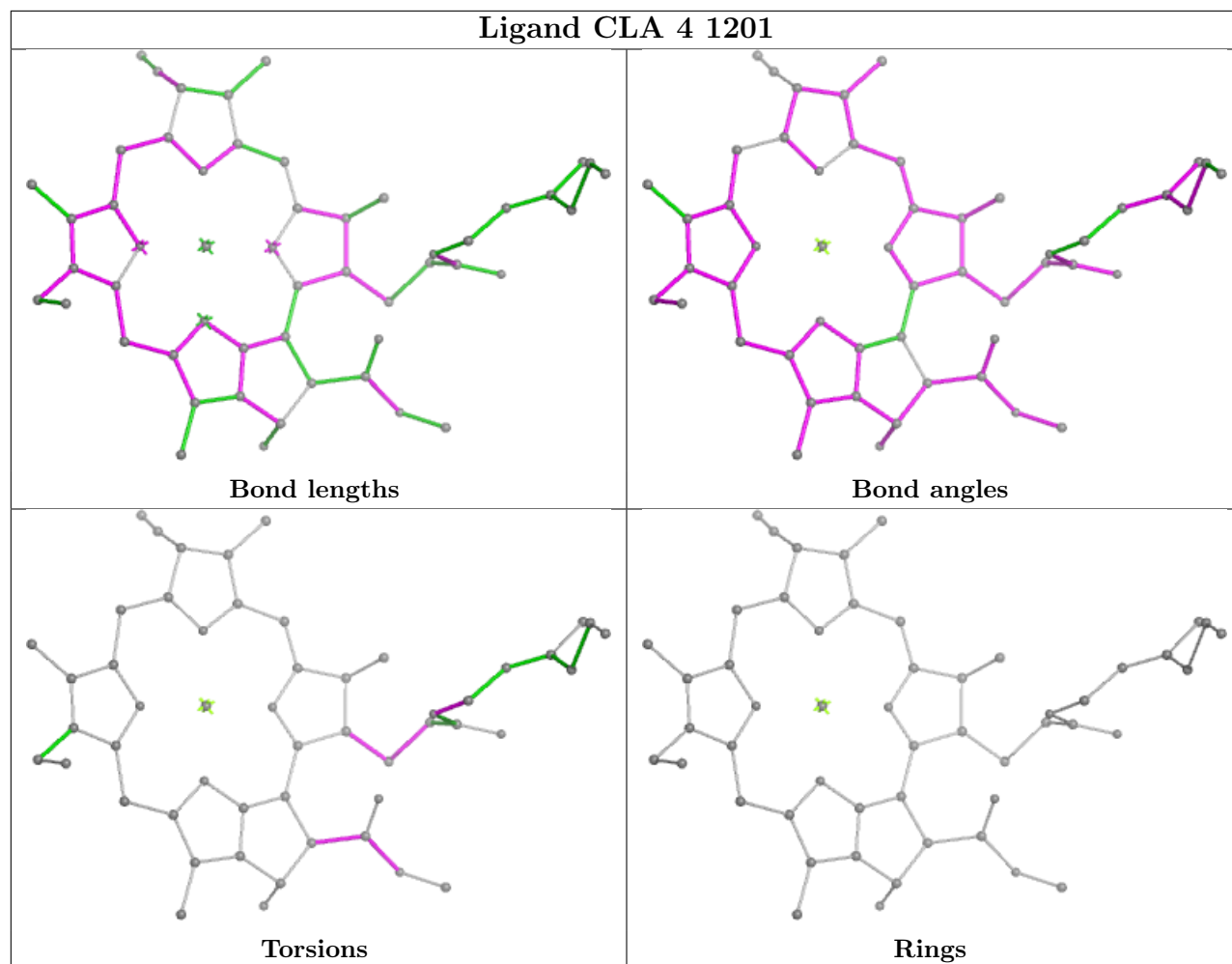




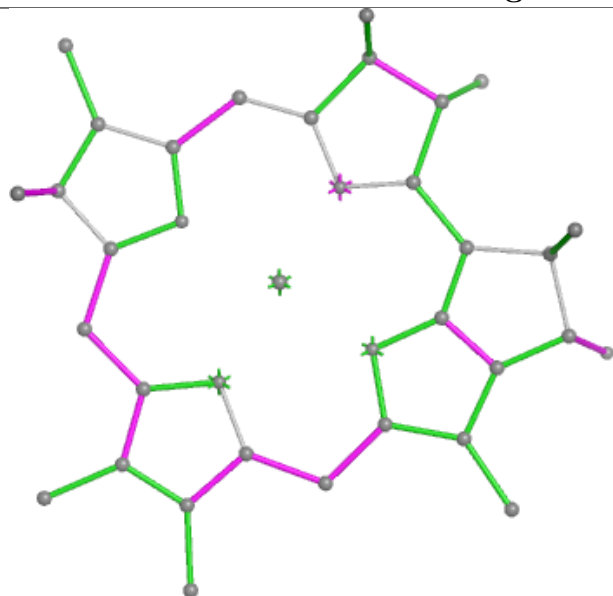




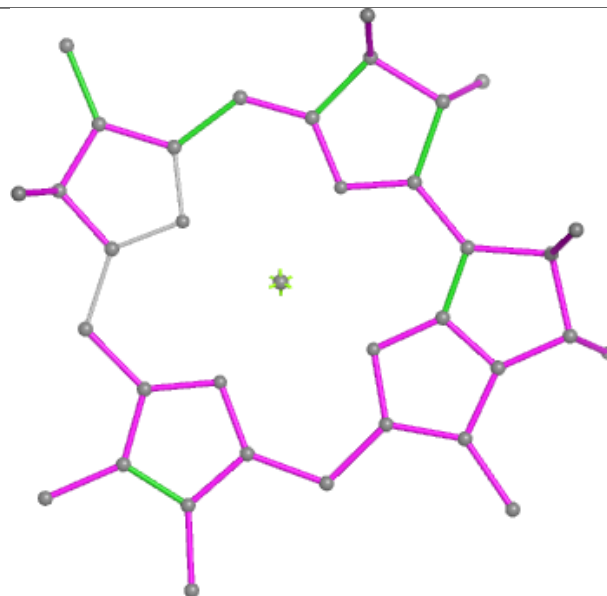




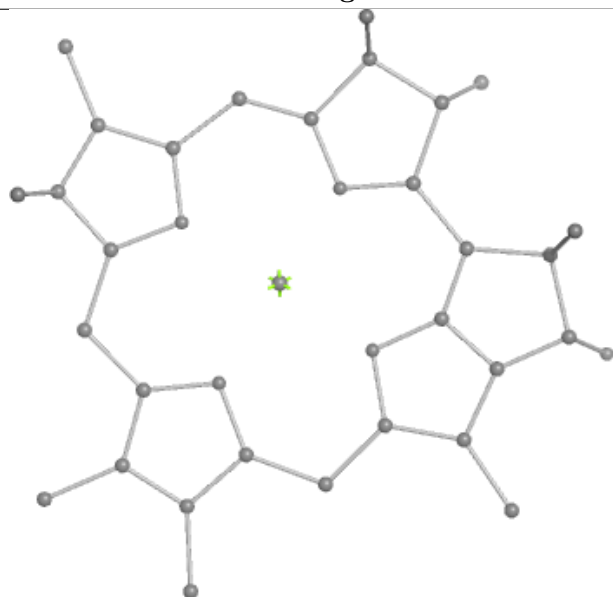
## Ligand CLA B 1772



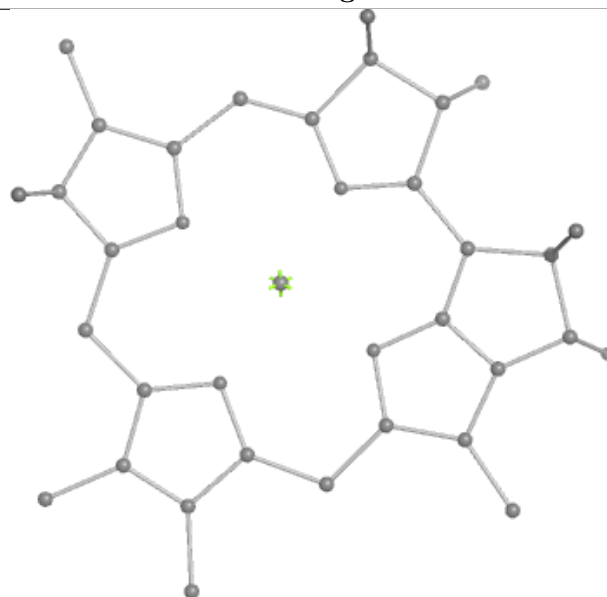
Bond lengths



Bond angles

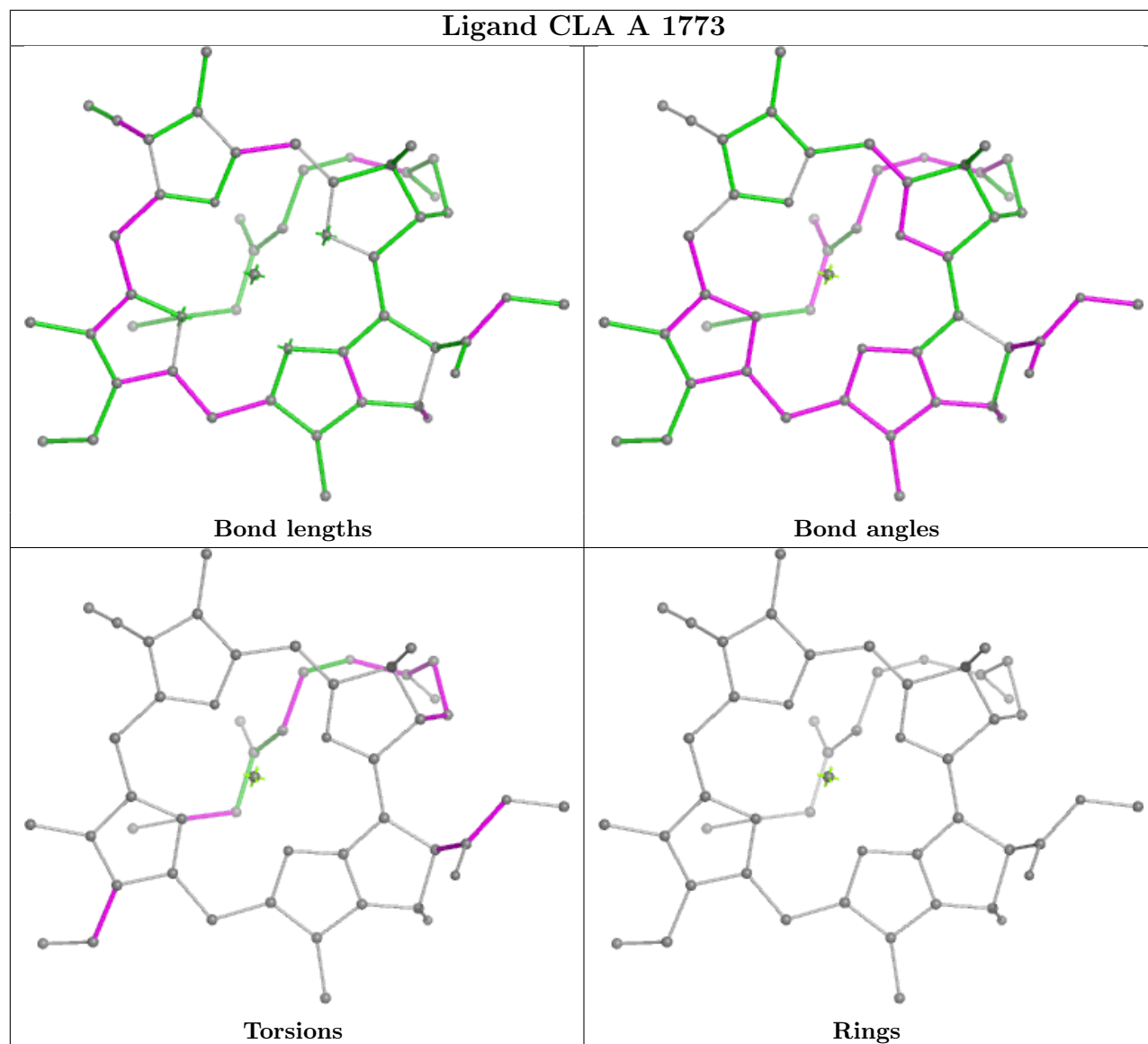


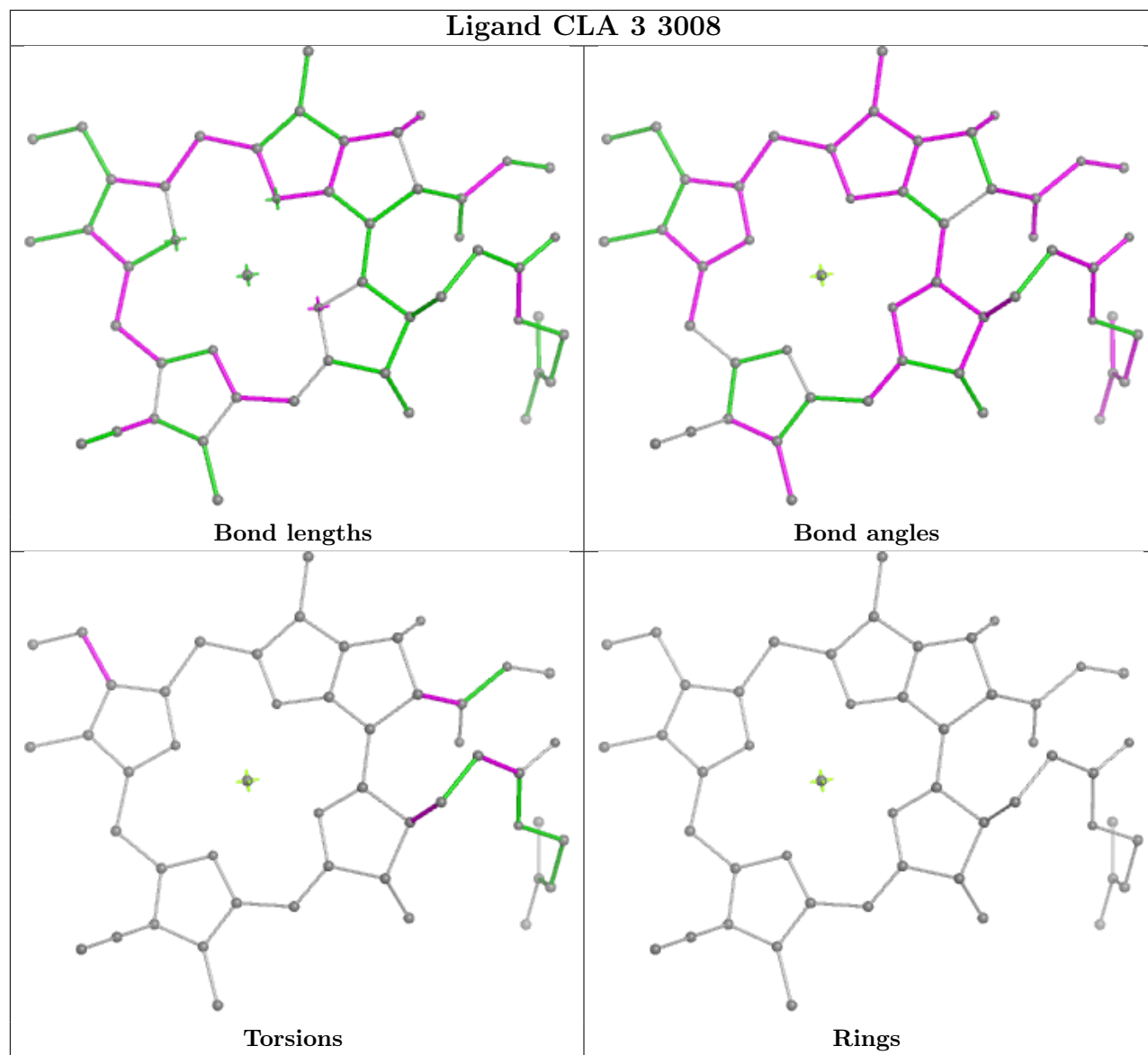
Torsions



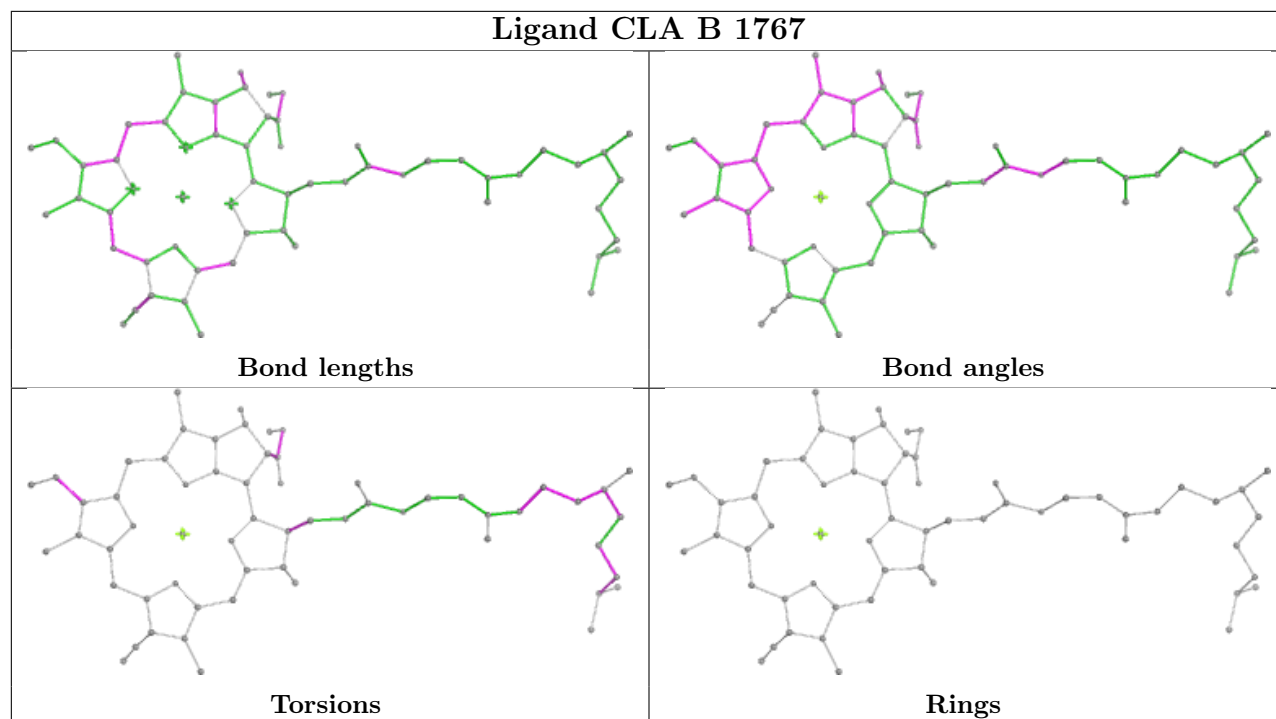
Rings

## Ligand CLA A 1773

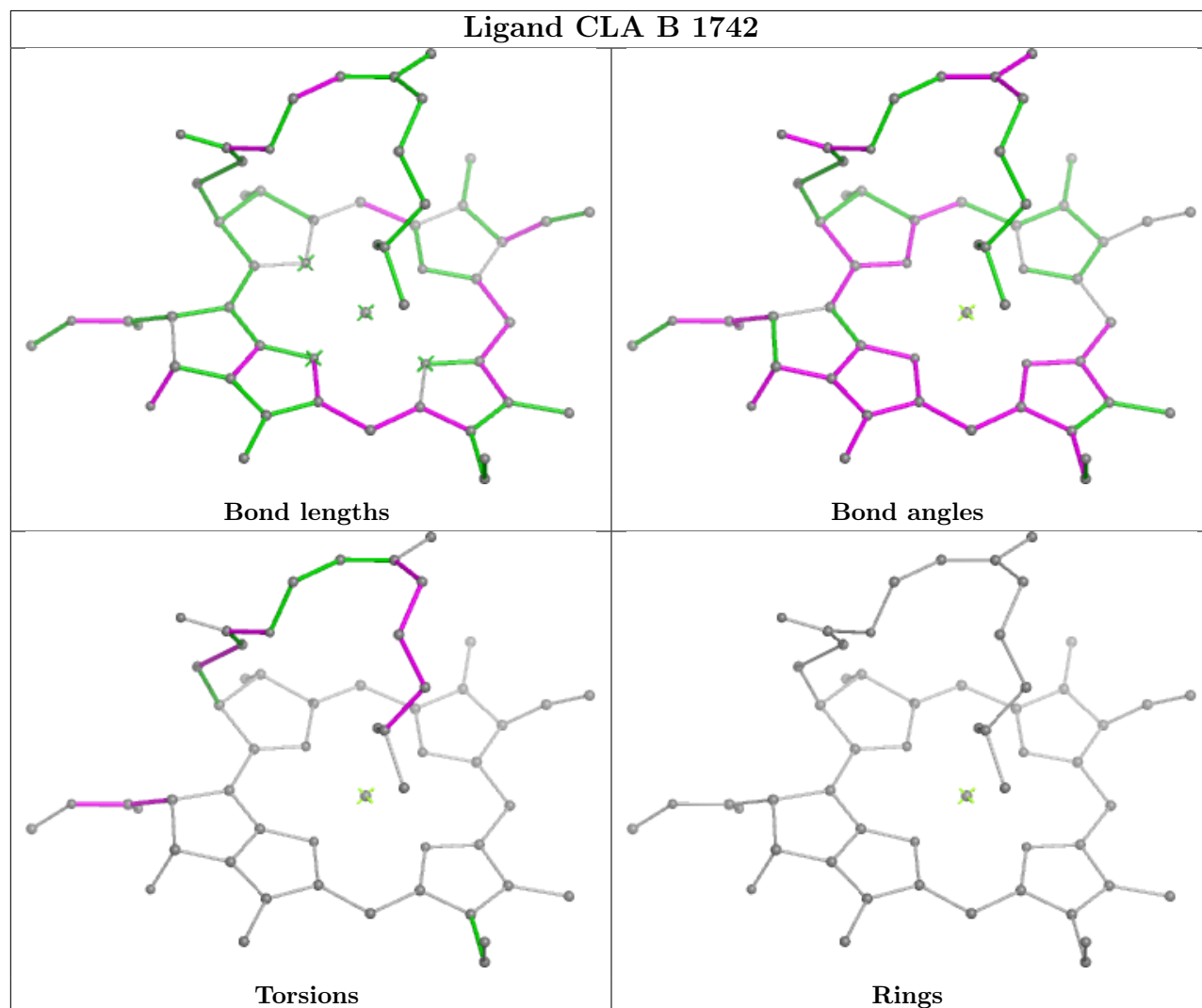




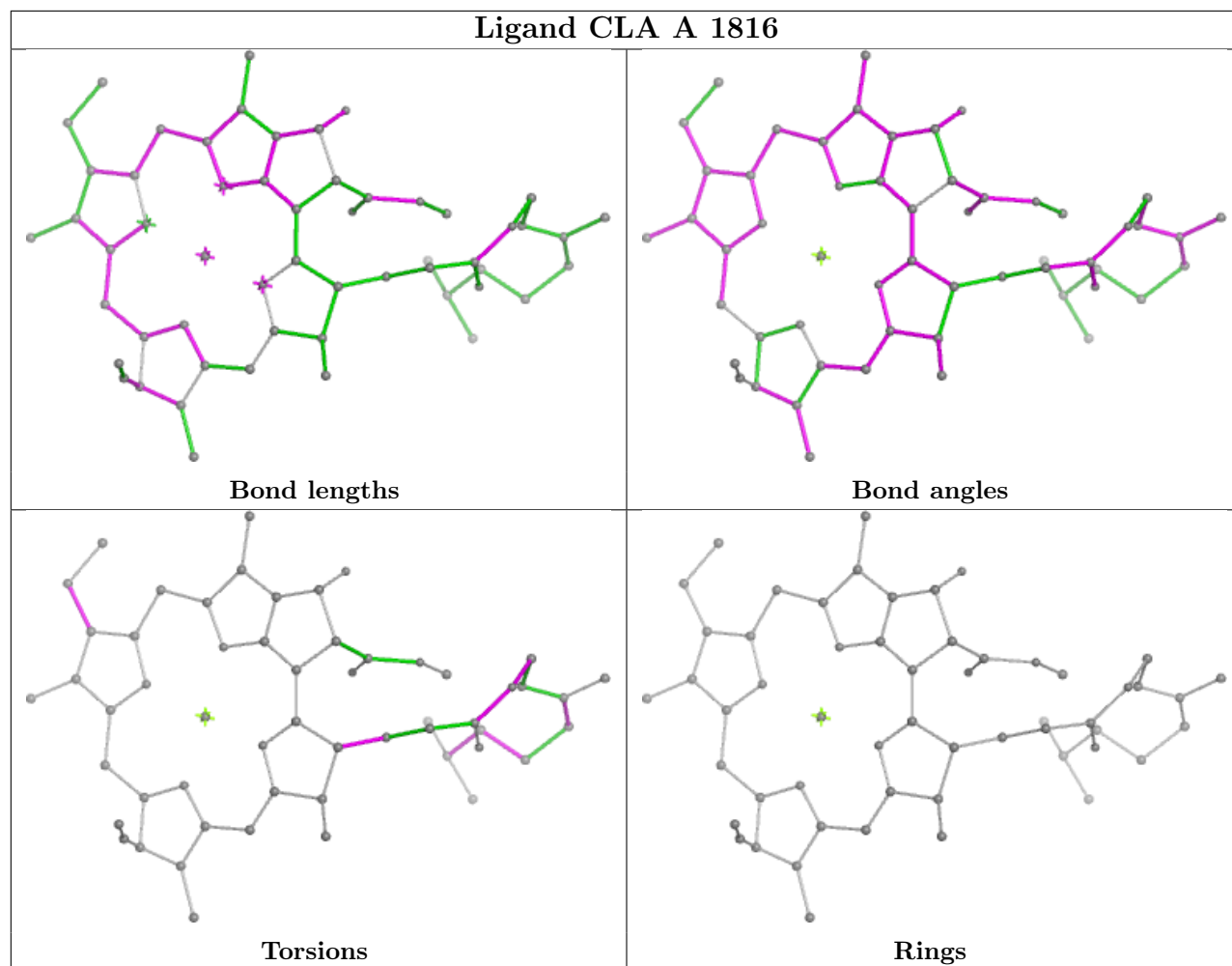
## Ligand CLA B 1767

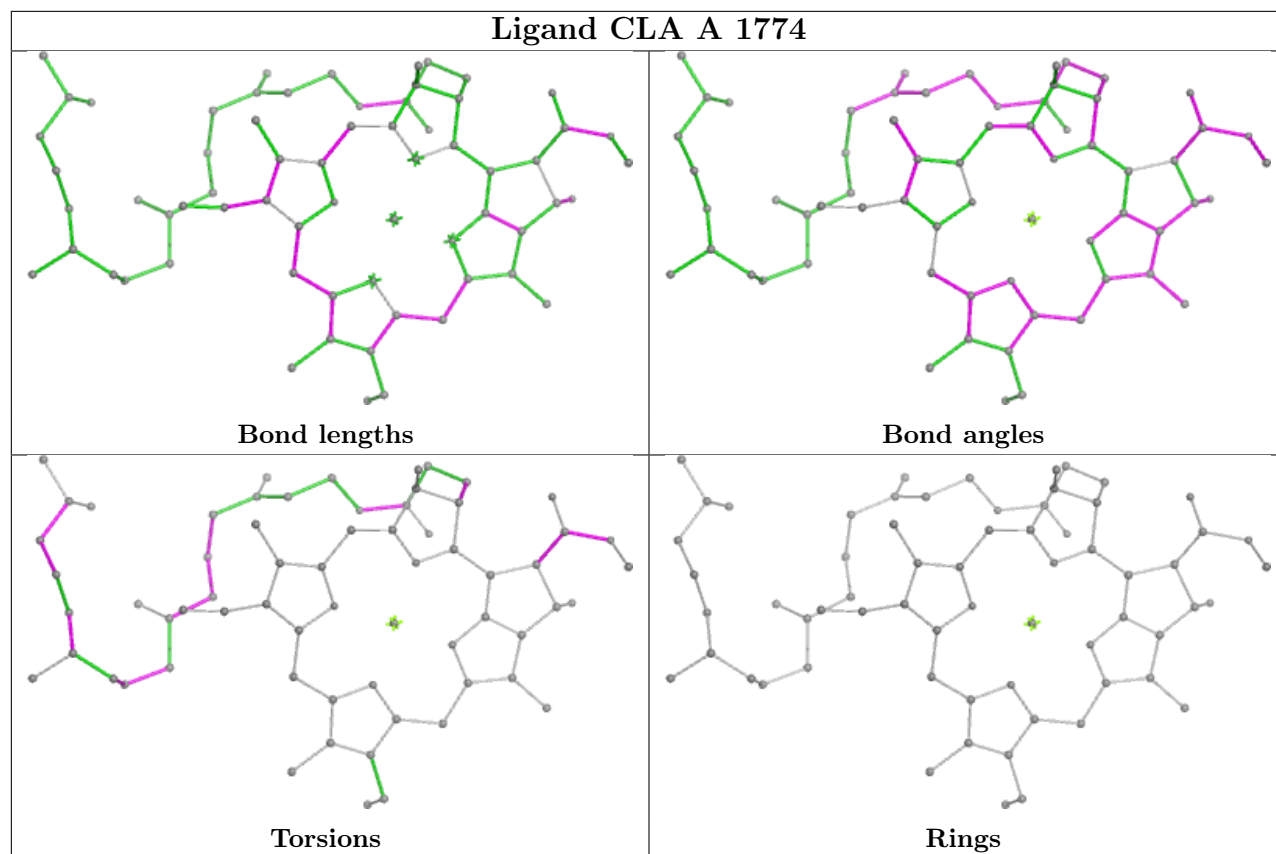


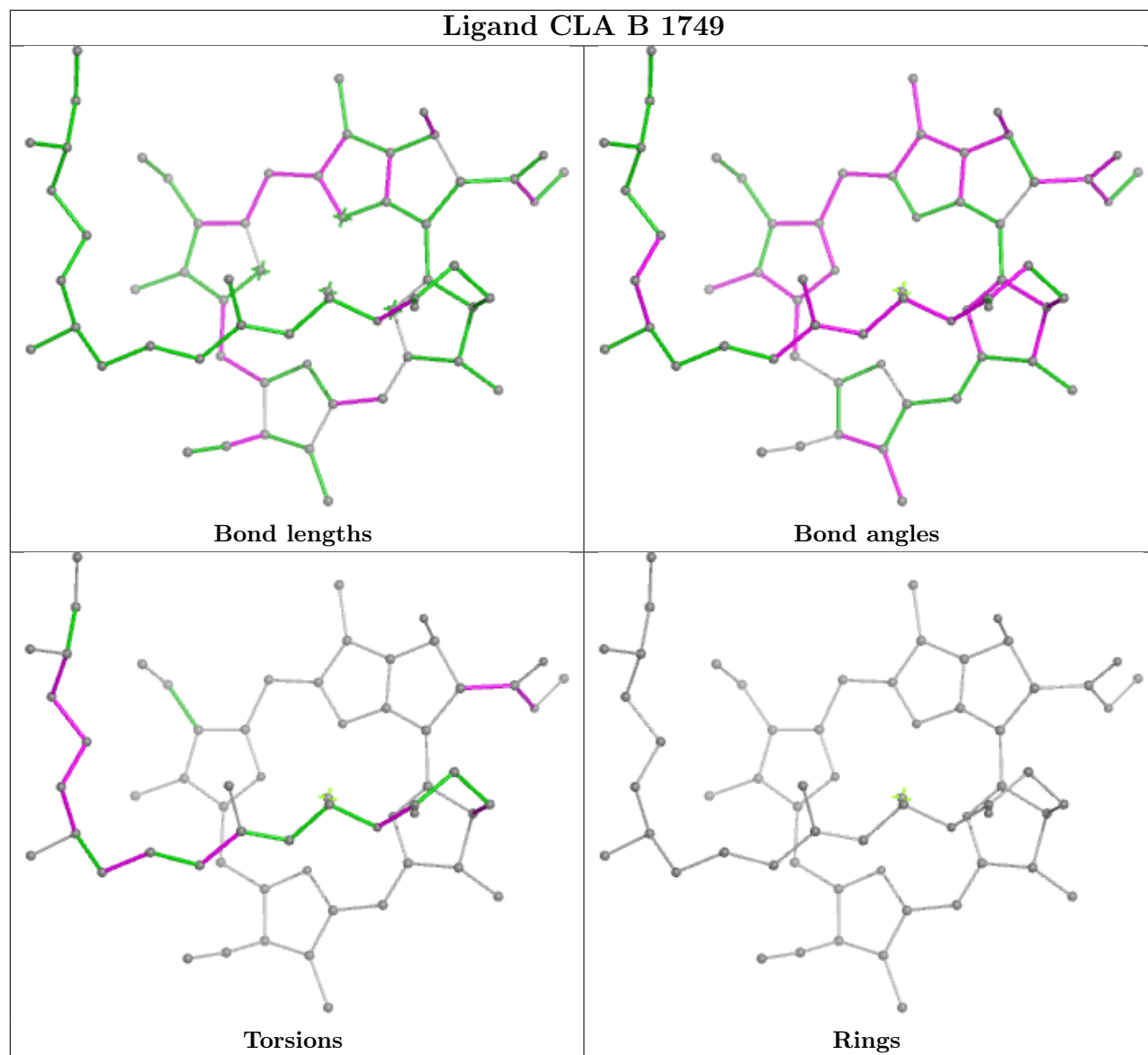
## Ligand CLA B 1742



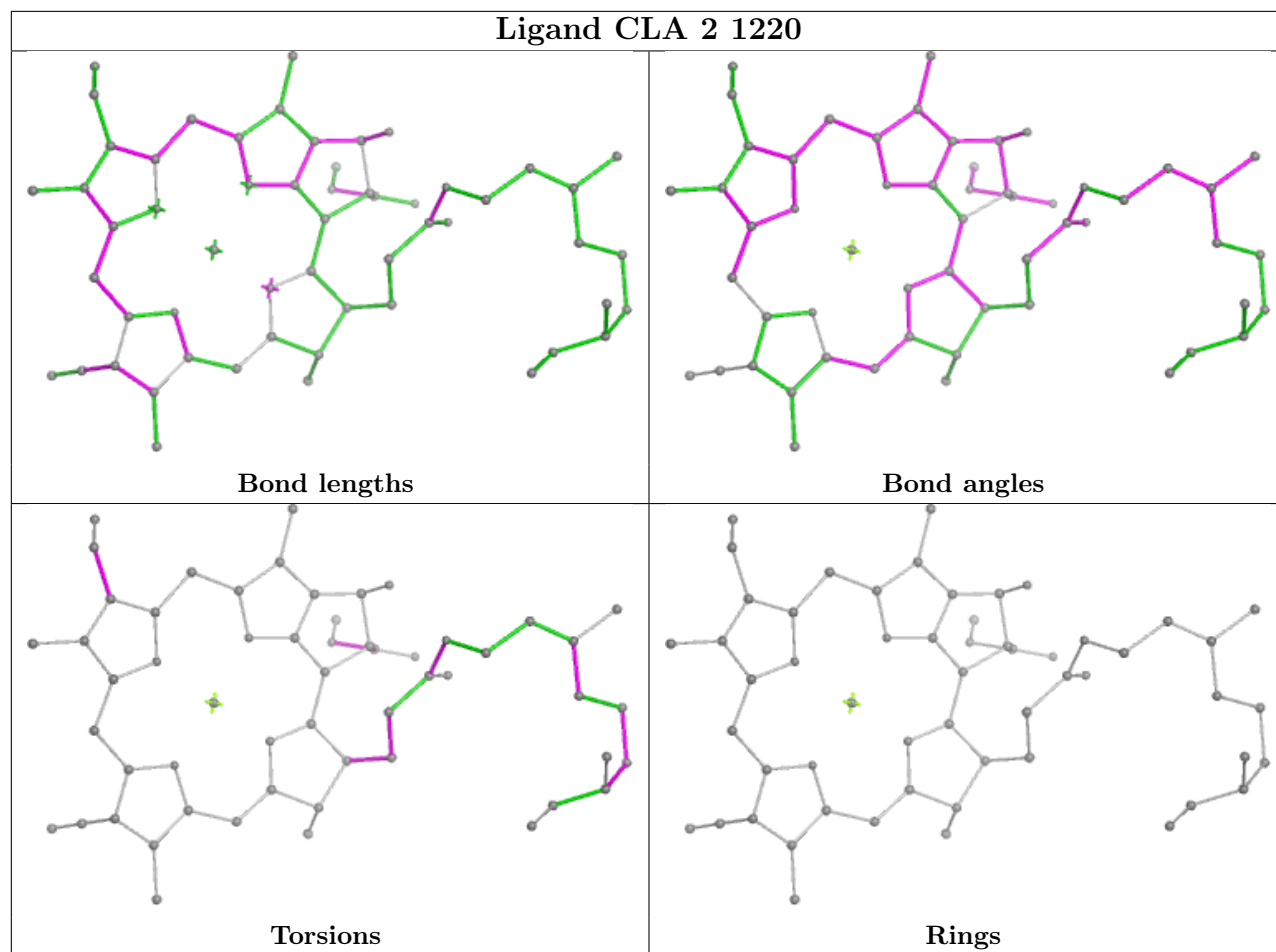
## Ligand CLA A 1816



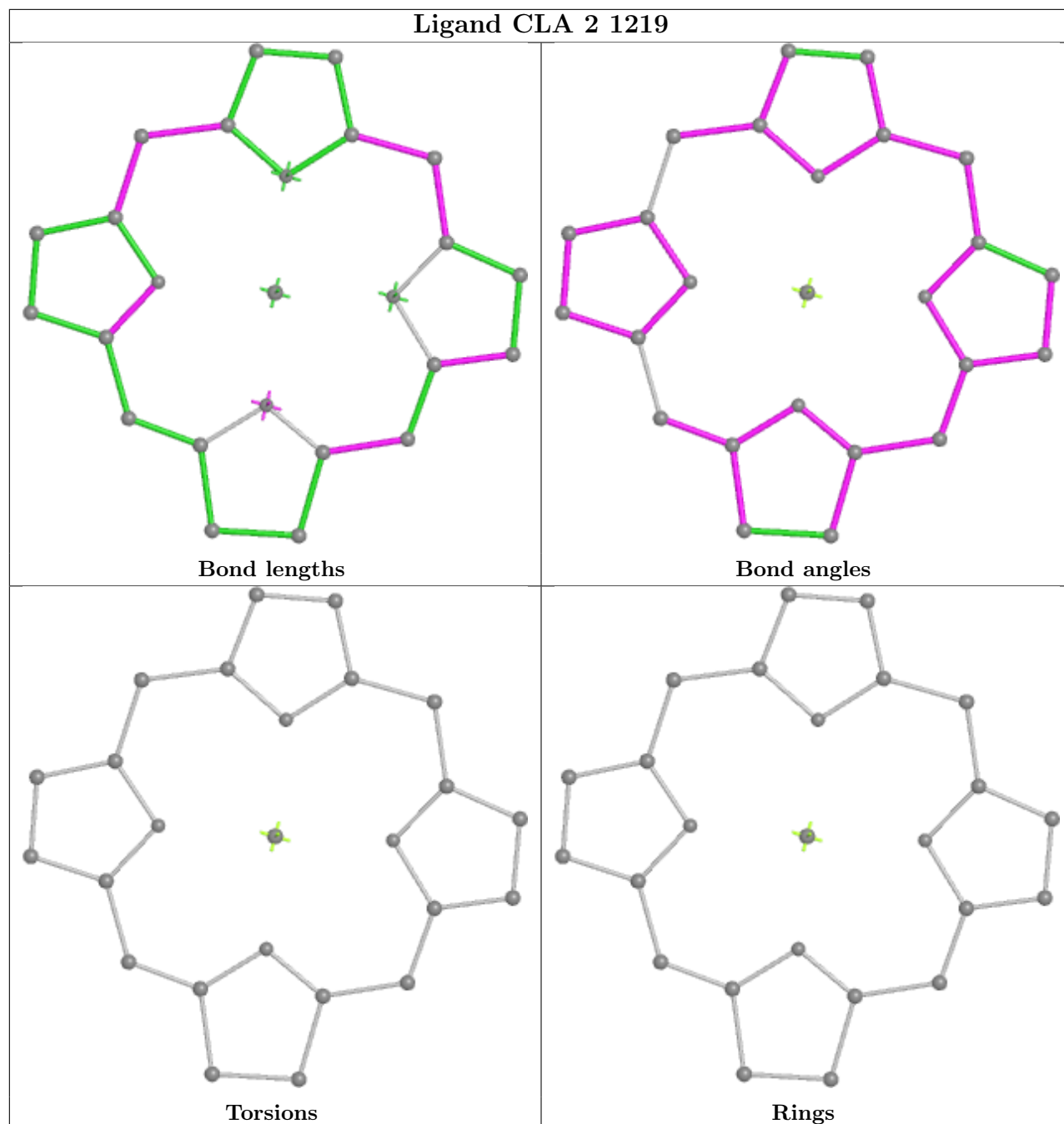


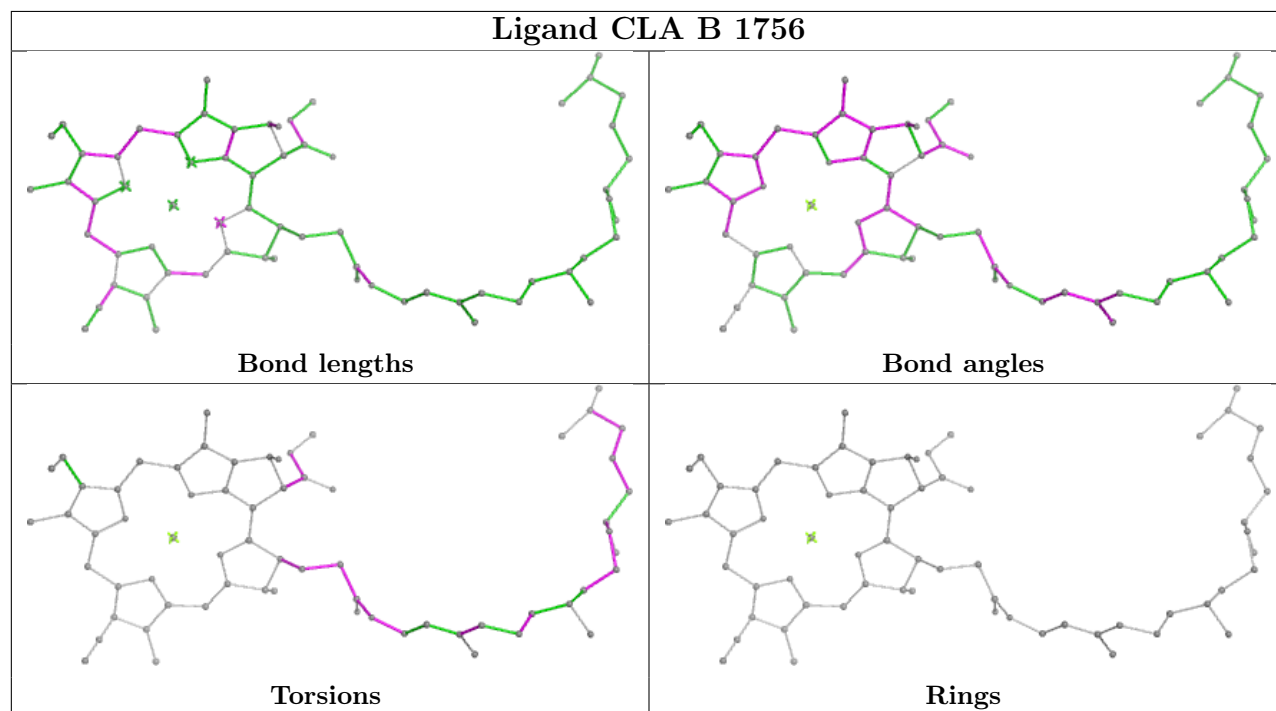
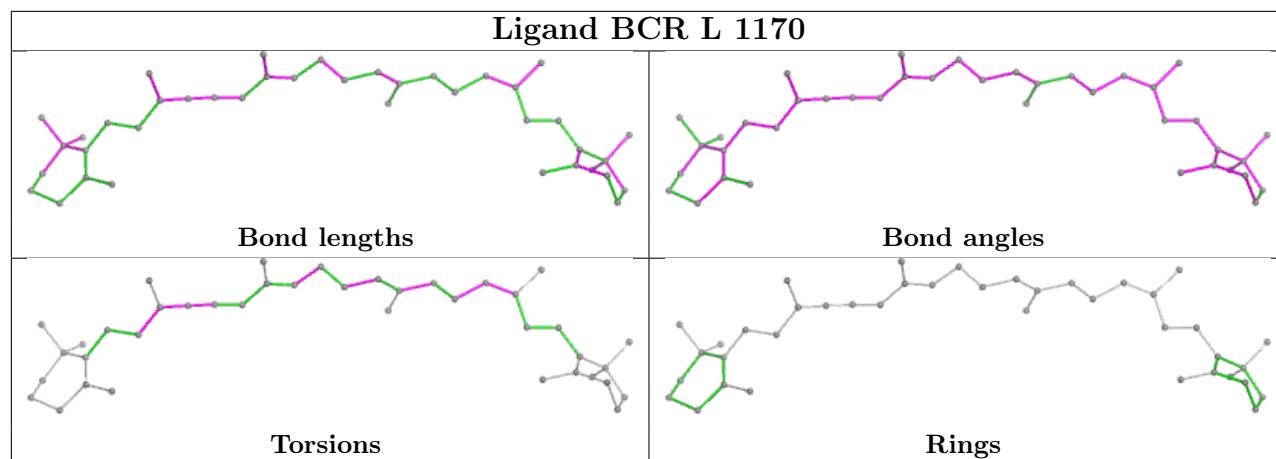


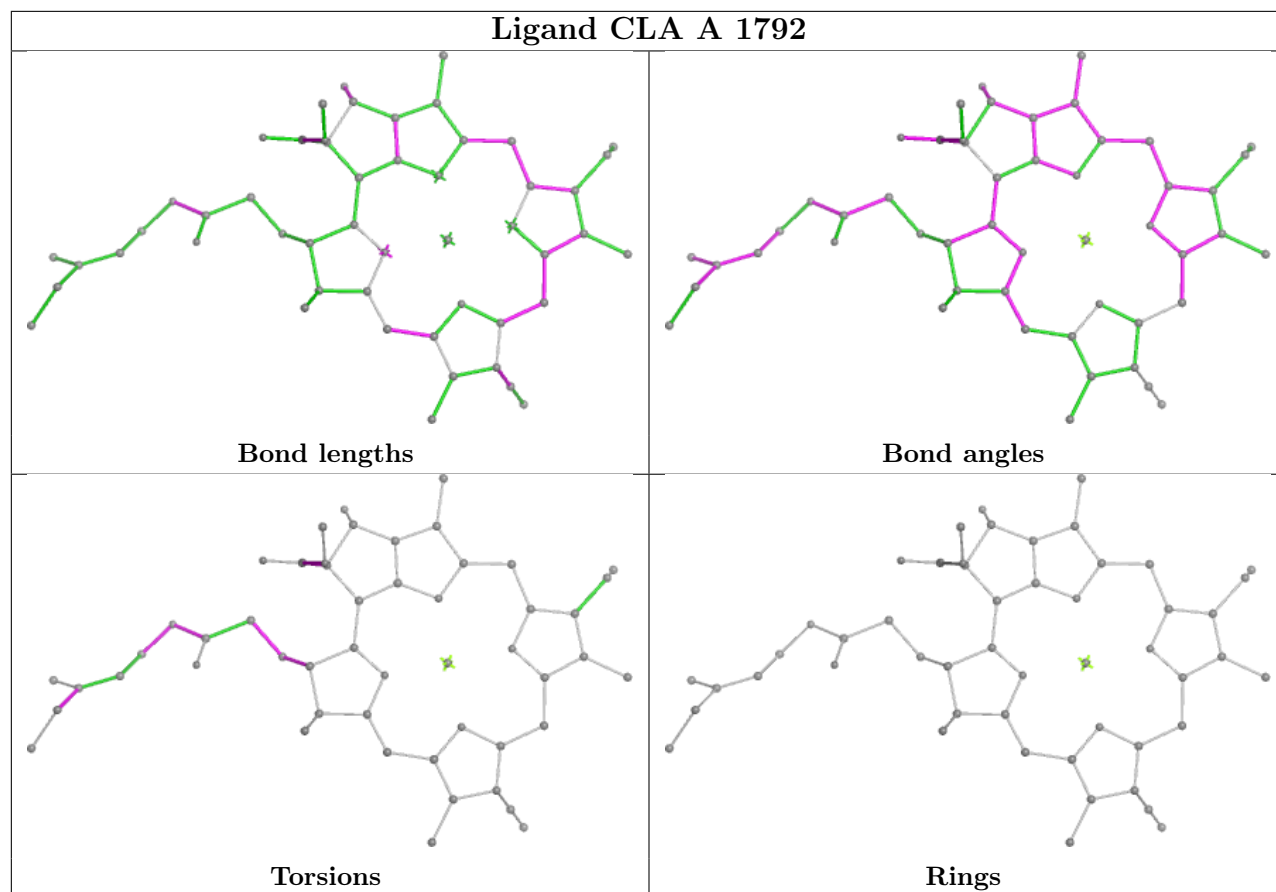




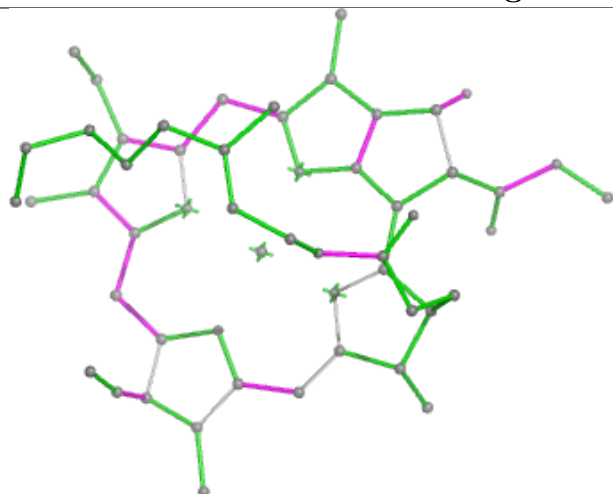
## Ligand CLA 2 1219



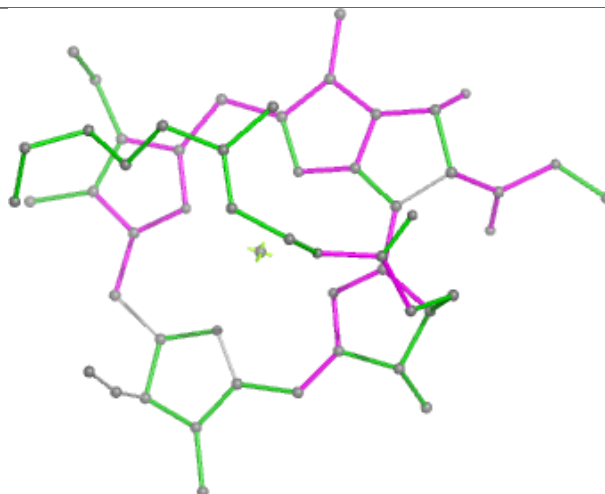




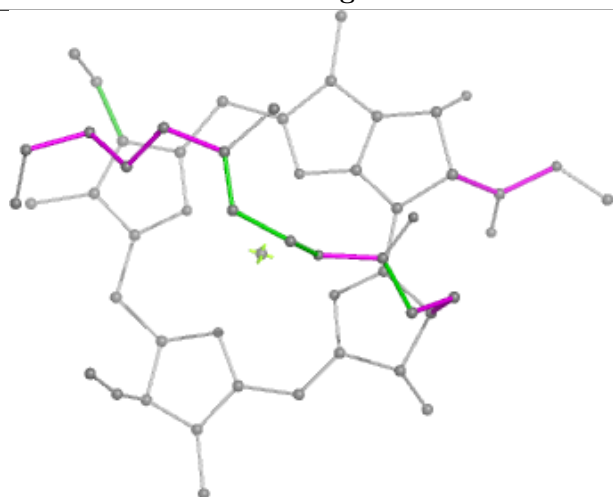
## Ligand CLA A 1768



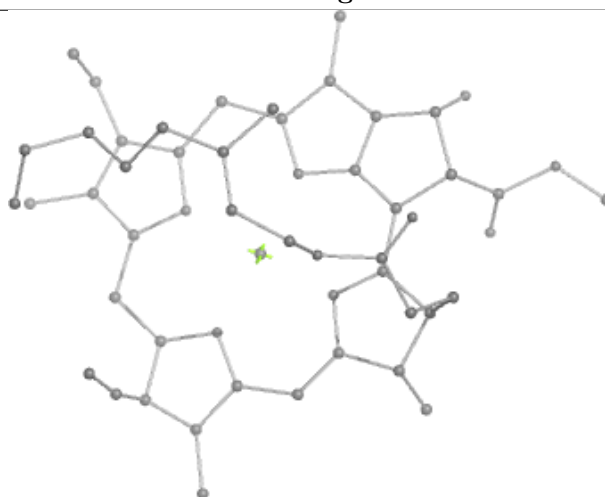
Bond lengths



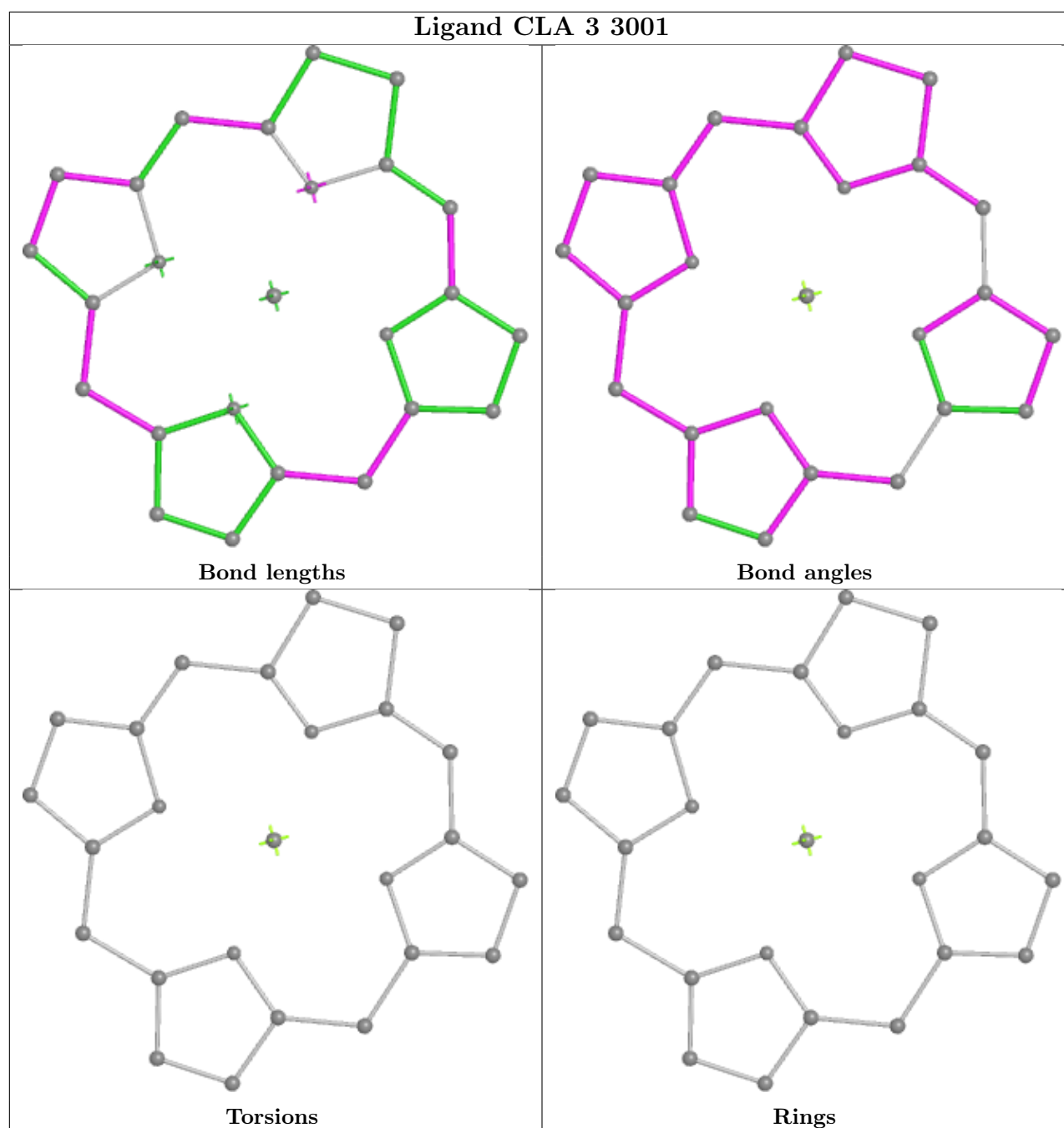
Bond angles

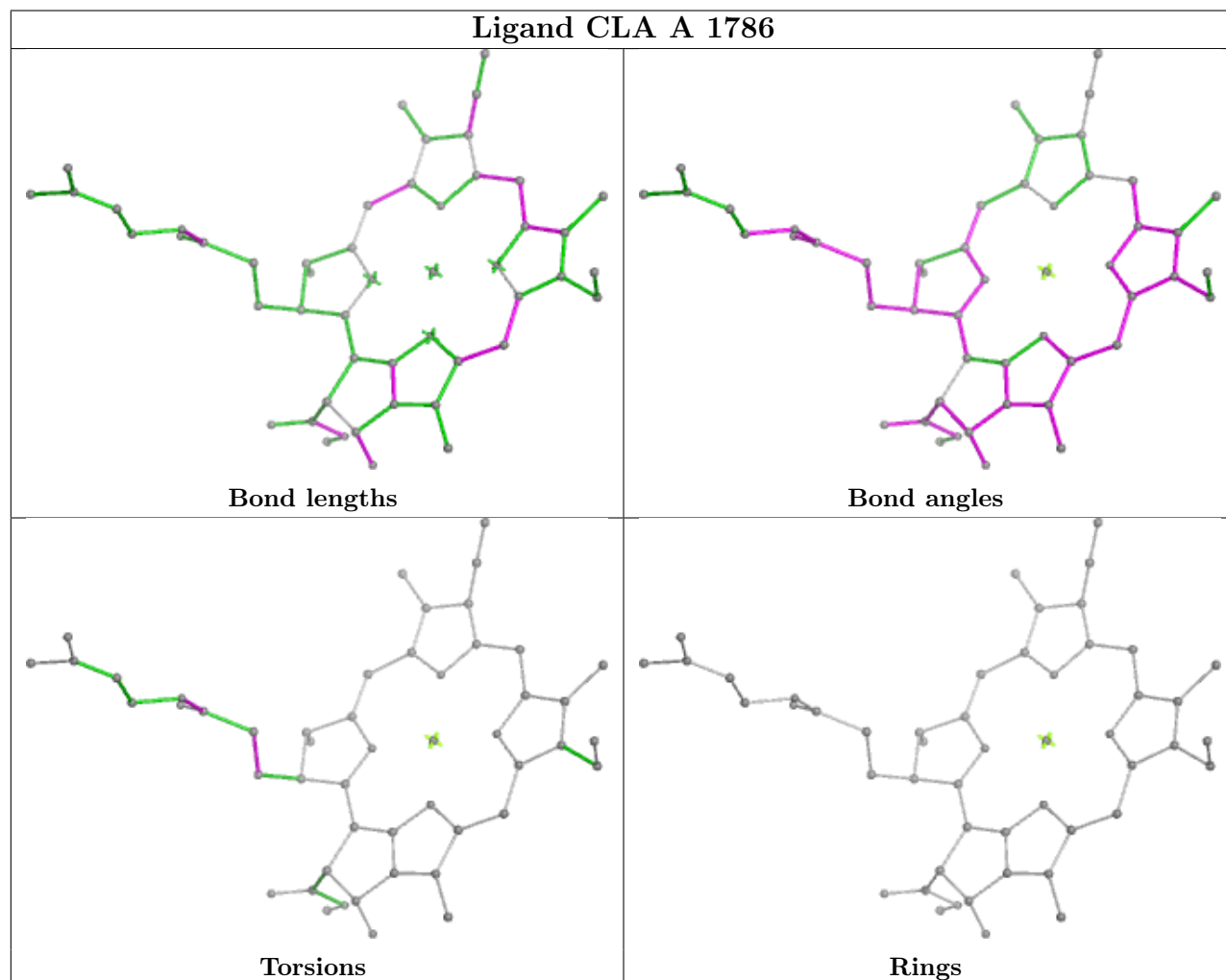
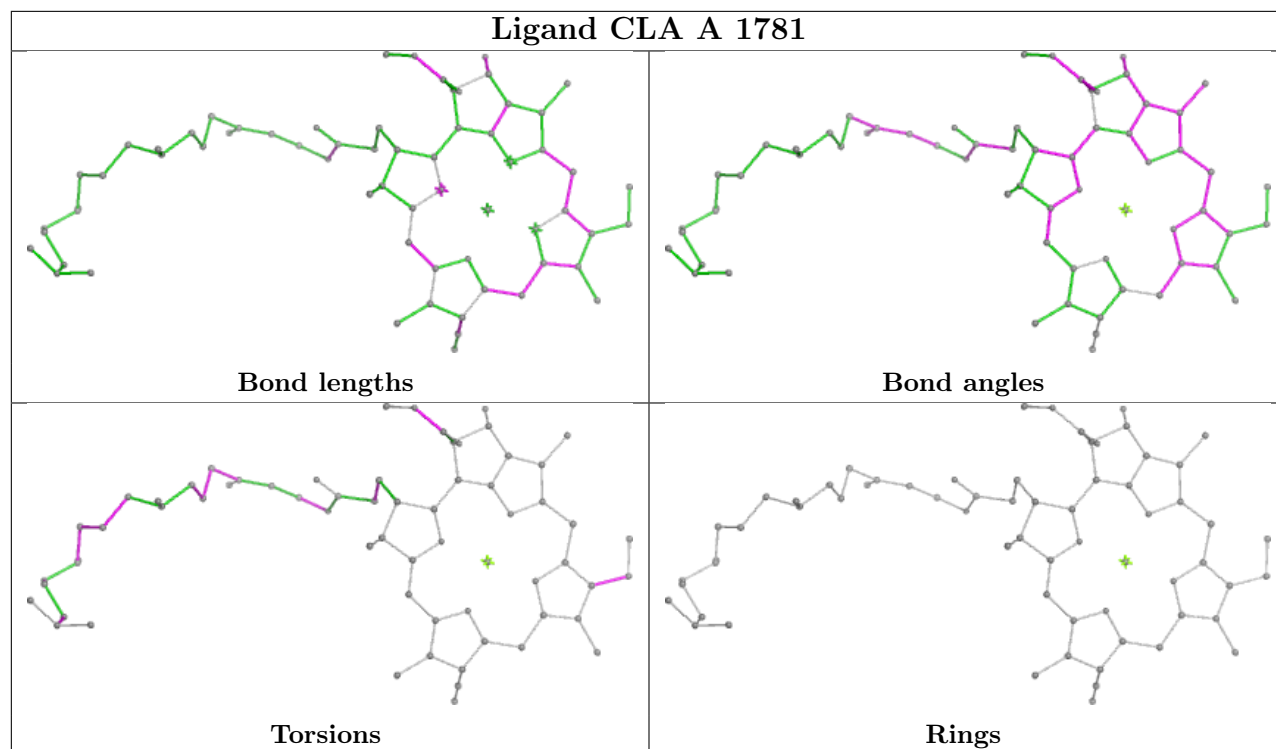


Torsions

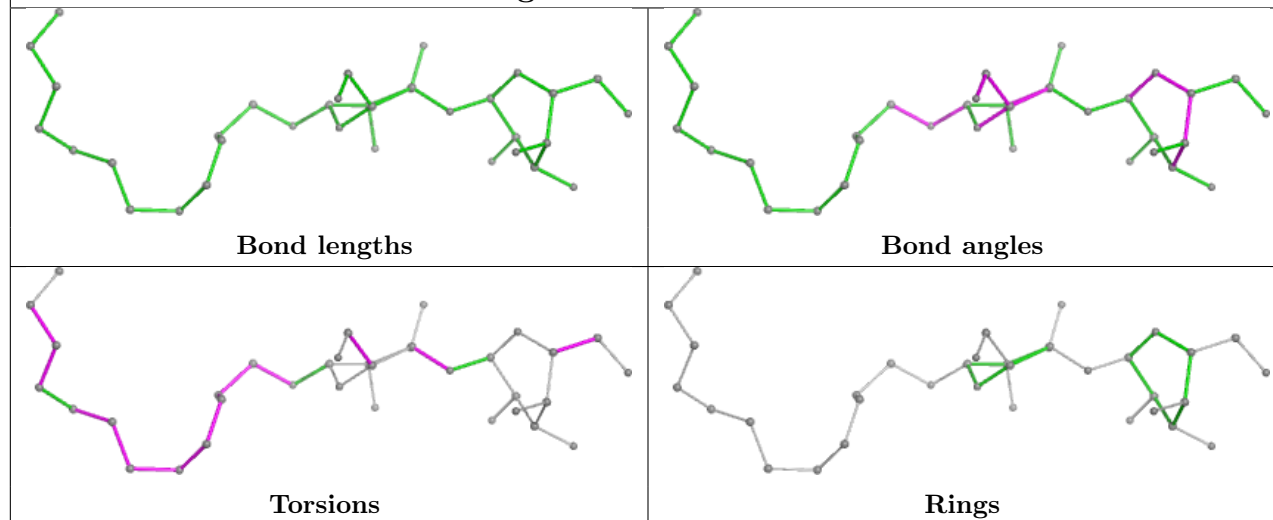


Rings

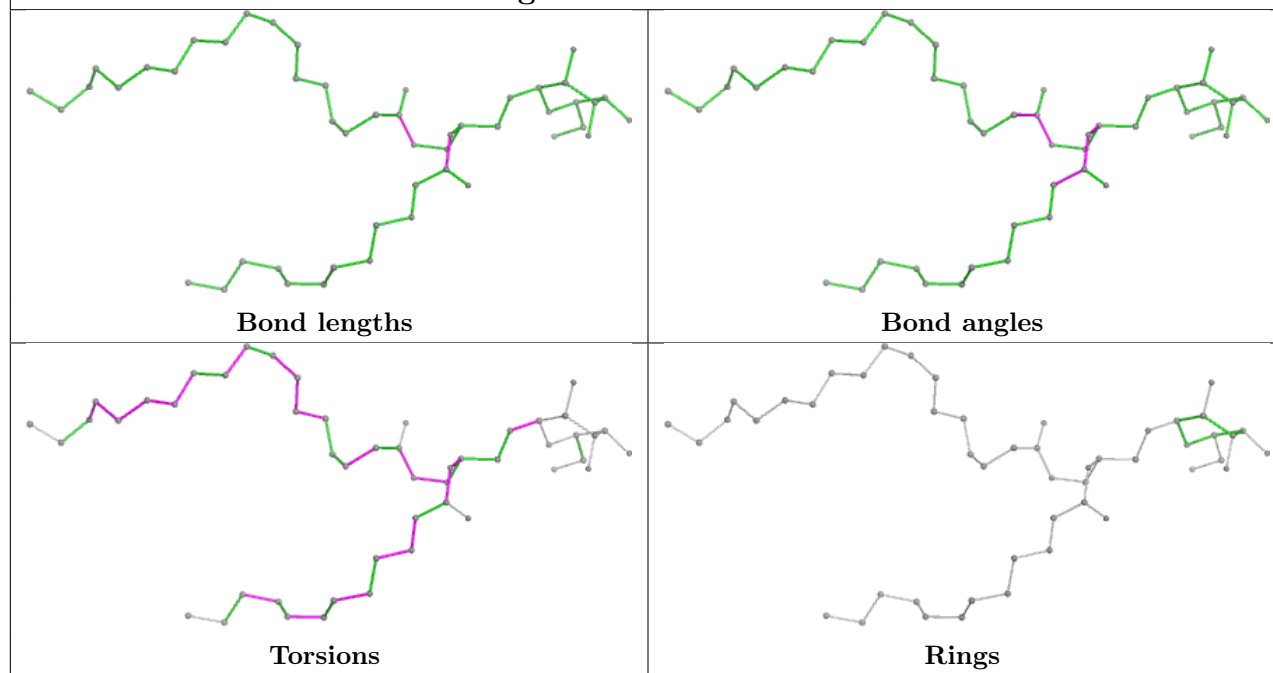




## Ligand LMU A 1809

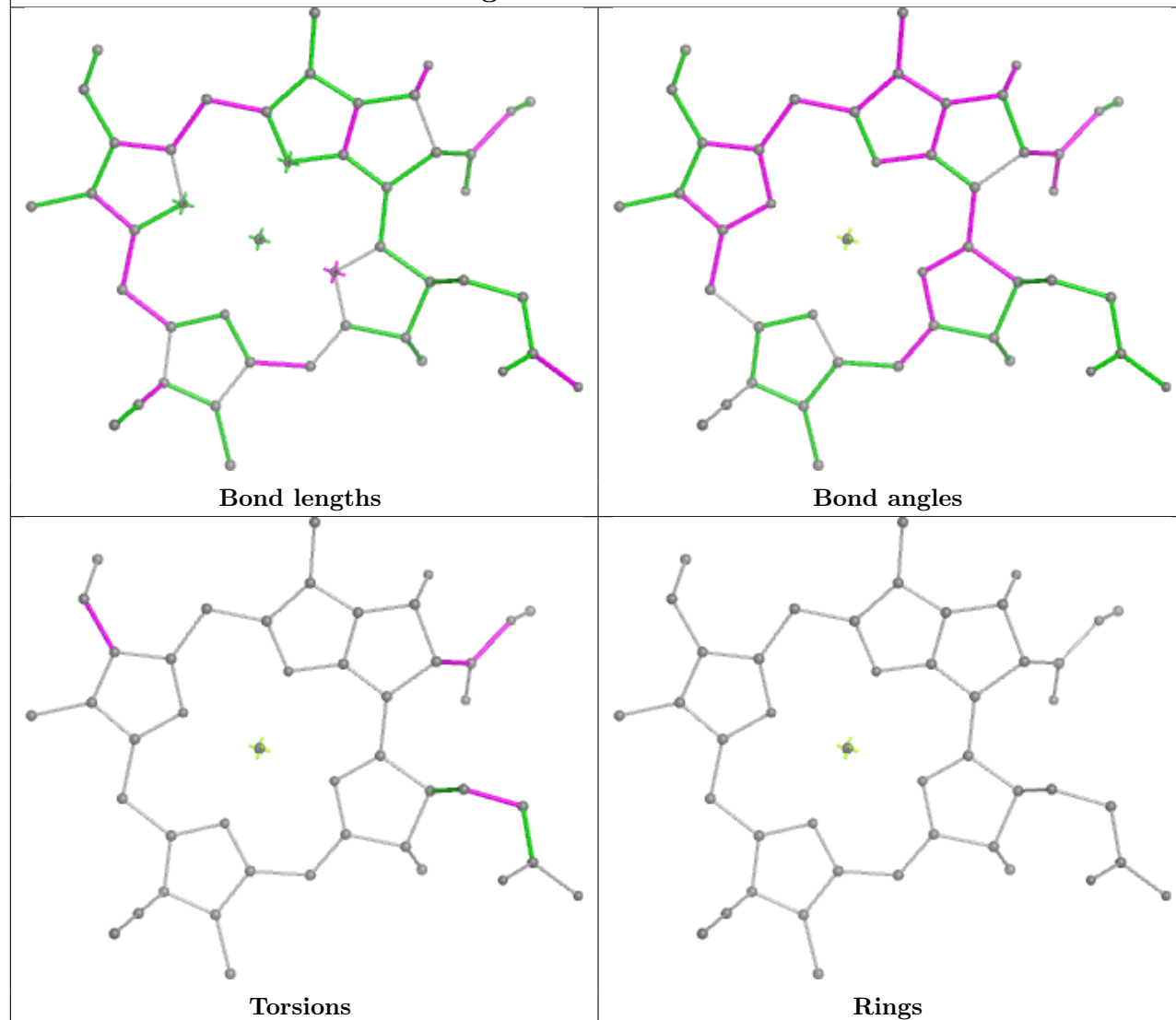


## Ligand LMG B 1783

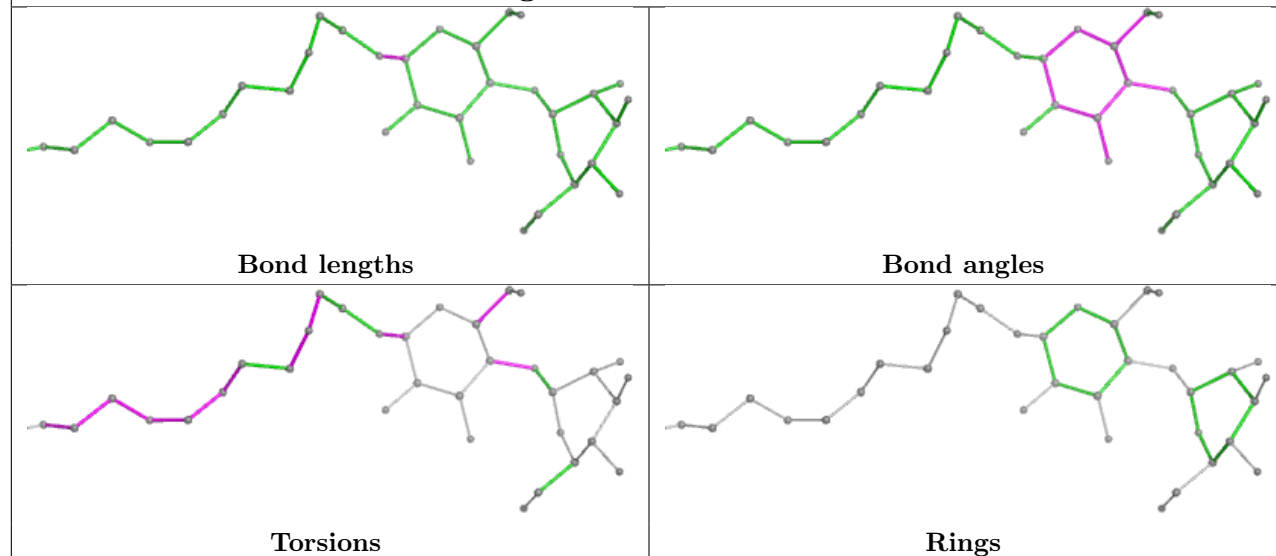


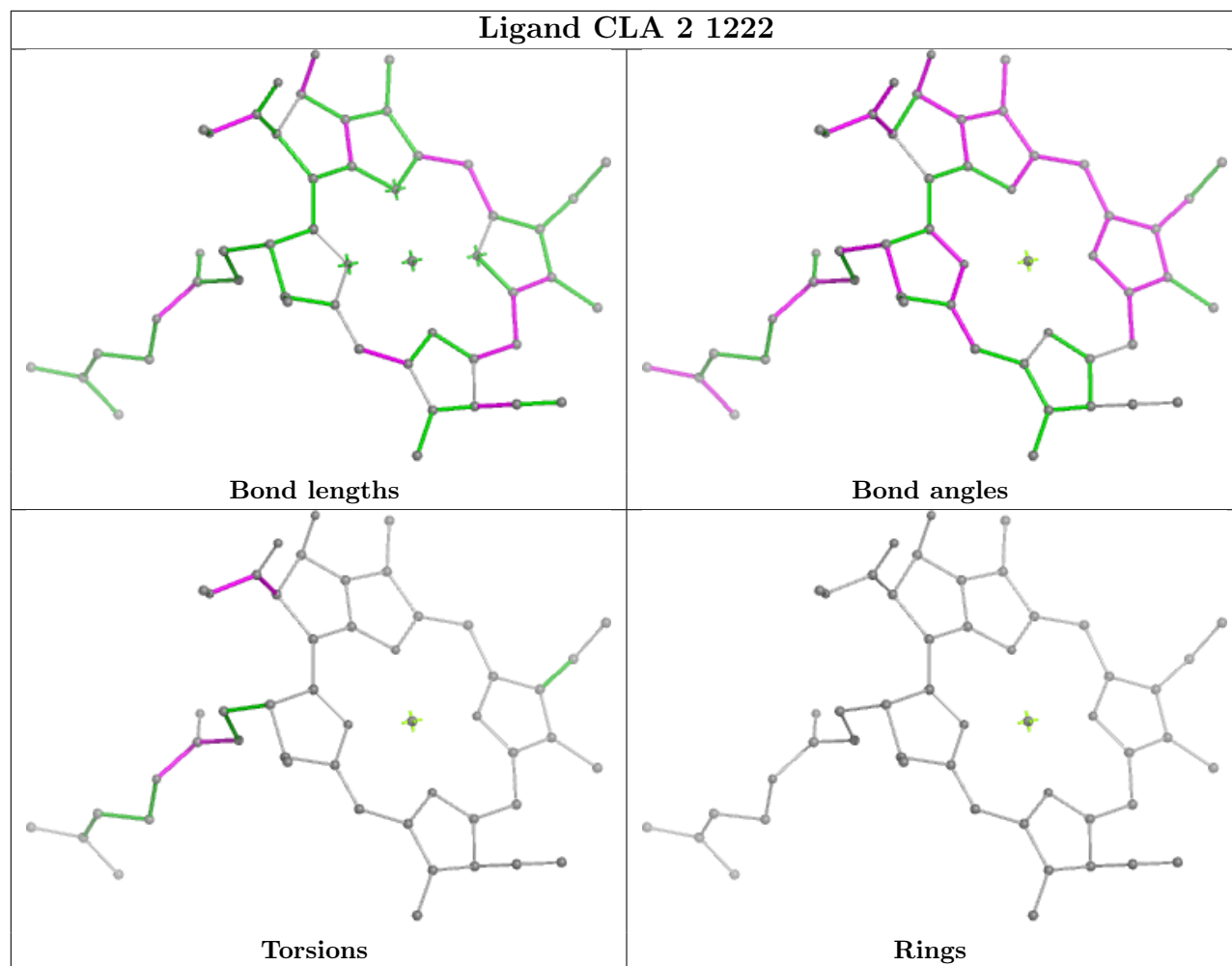


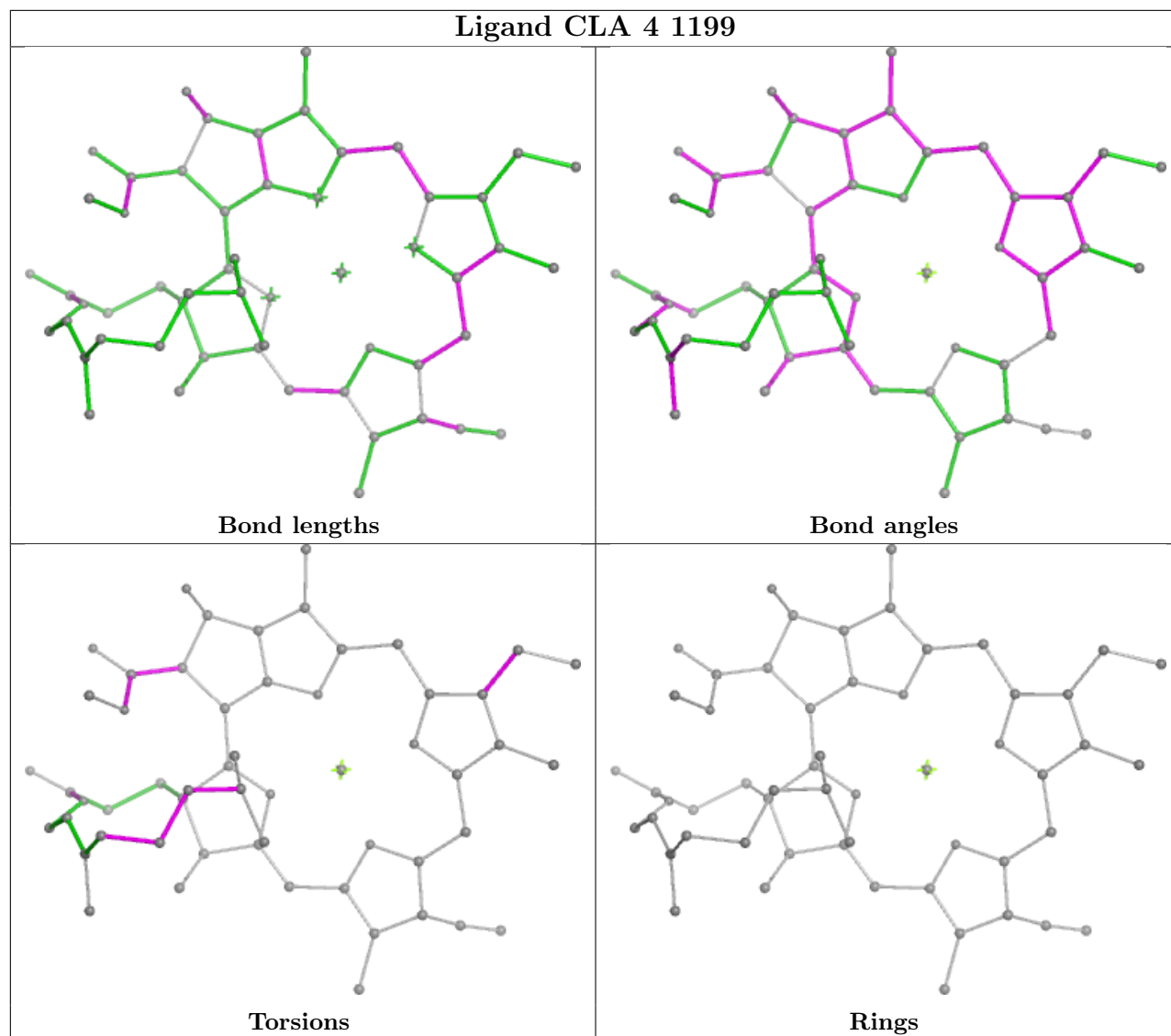
## Ligand CLA K 1142



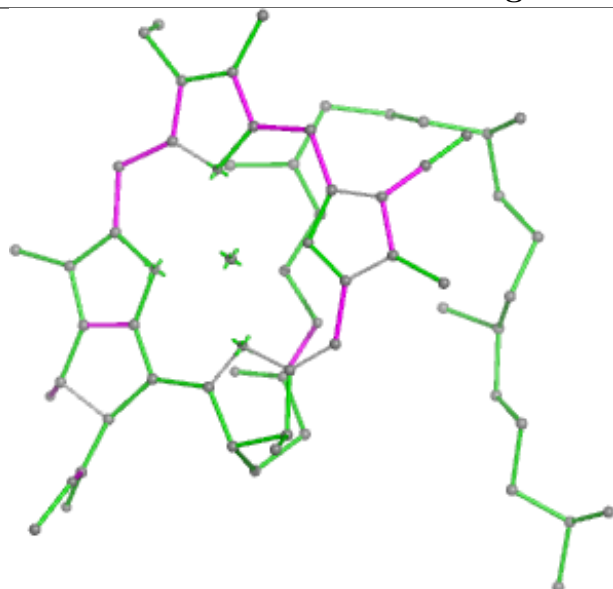
## Ligand LMU A 7035



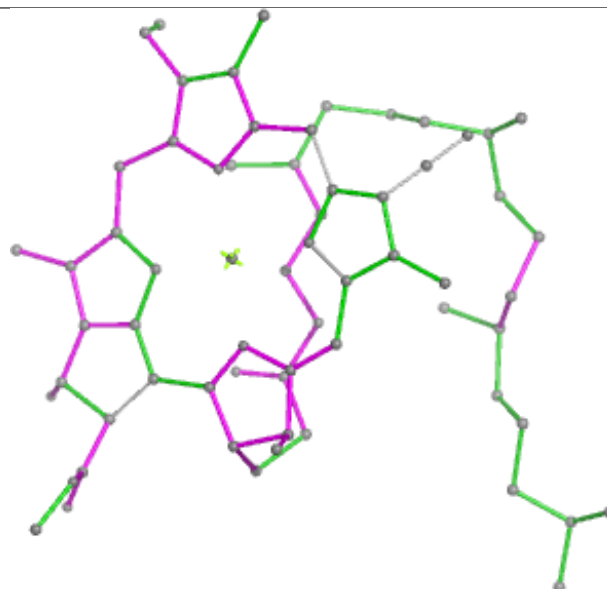




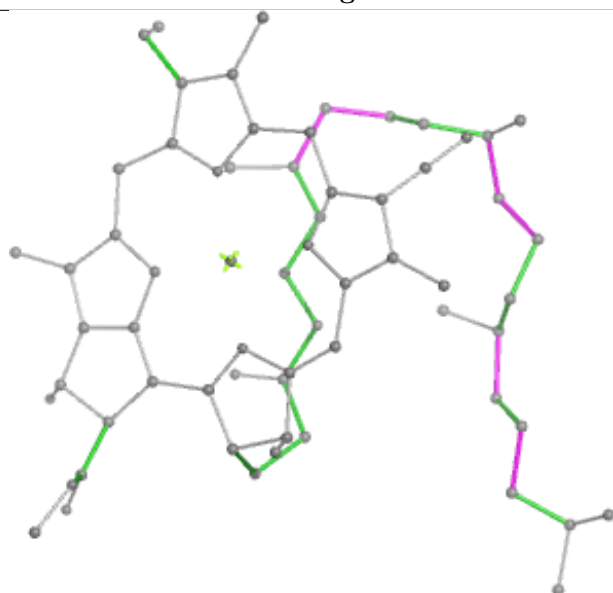
## Ligand CLA B 1739



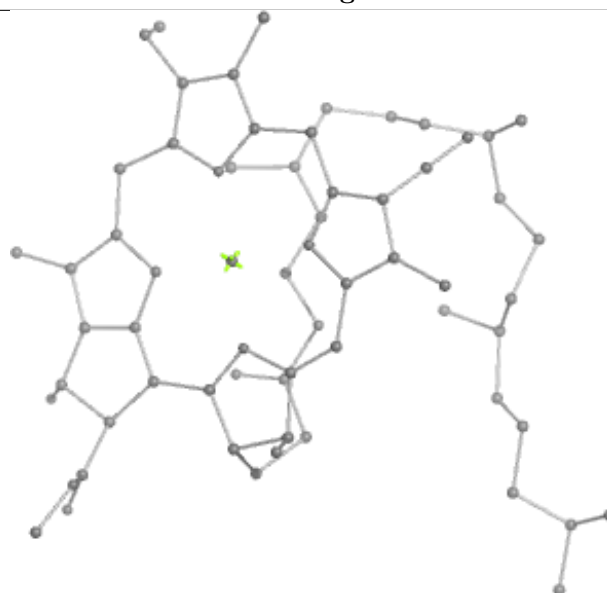
Bond lengths



Bond angles

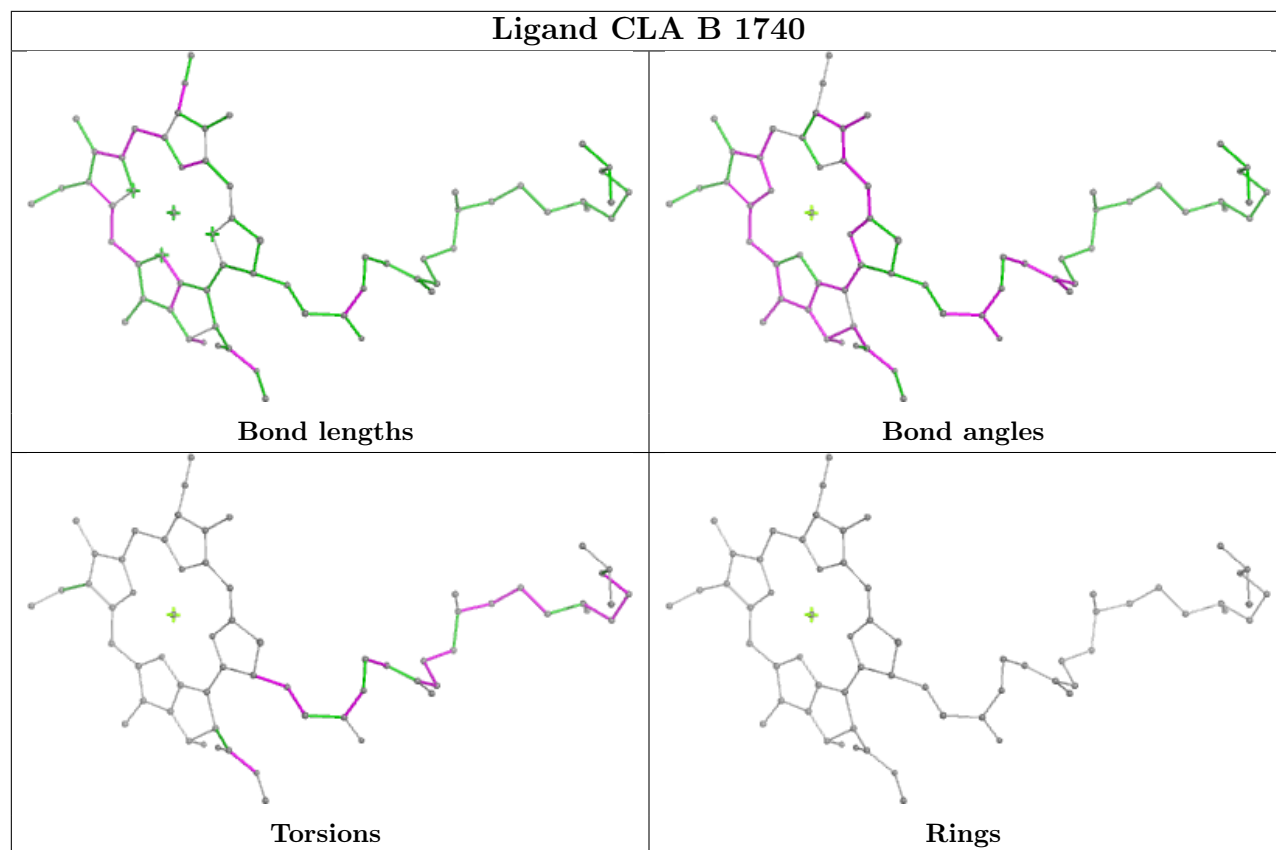


Torsions

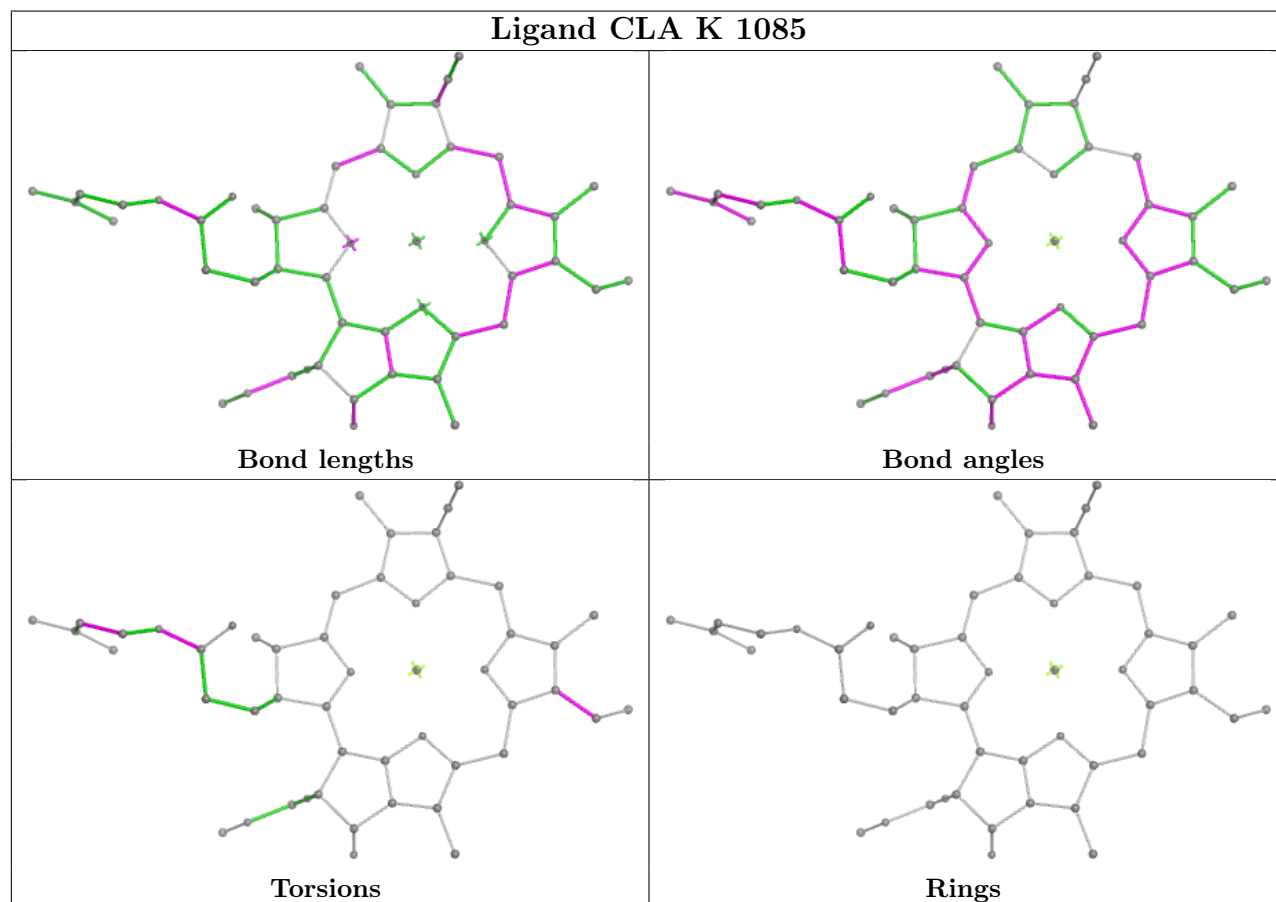


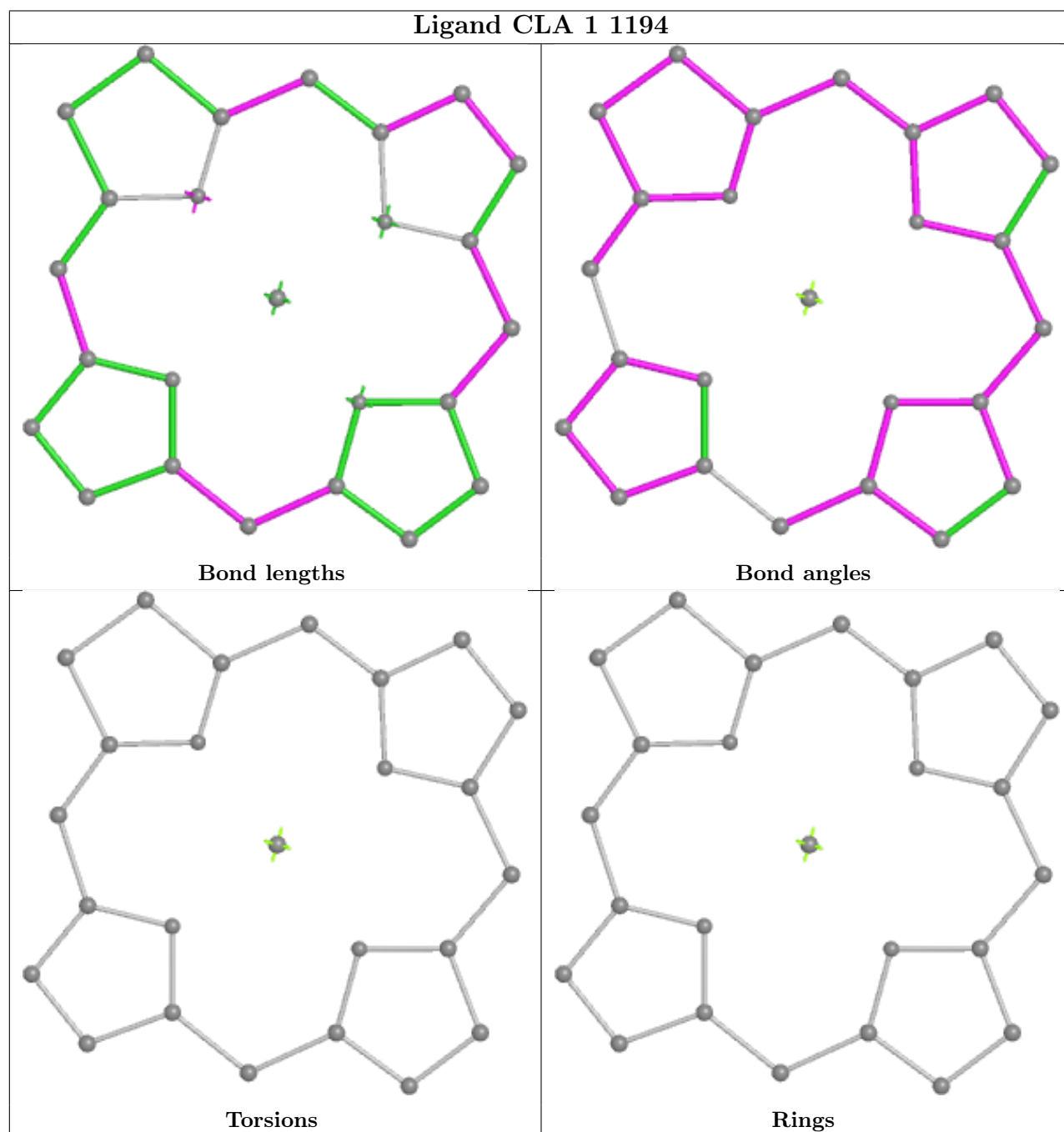
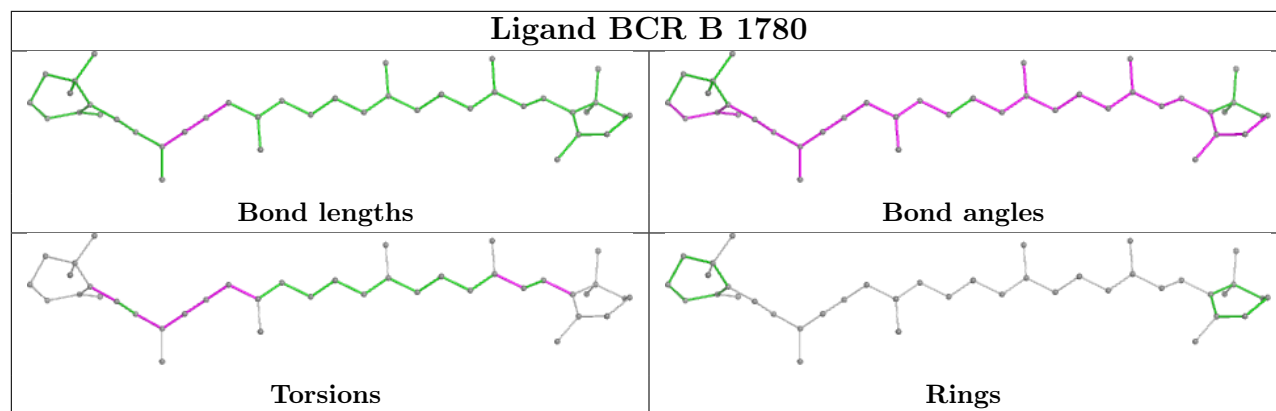
Rings

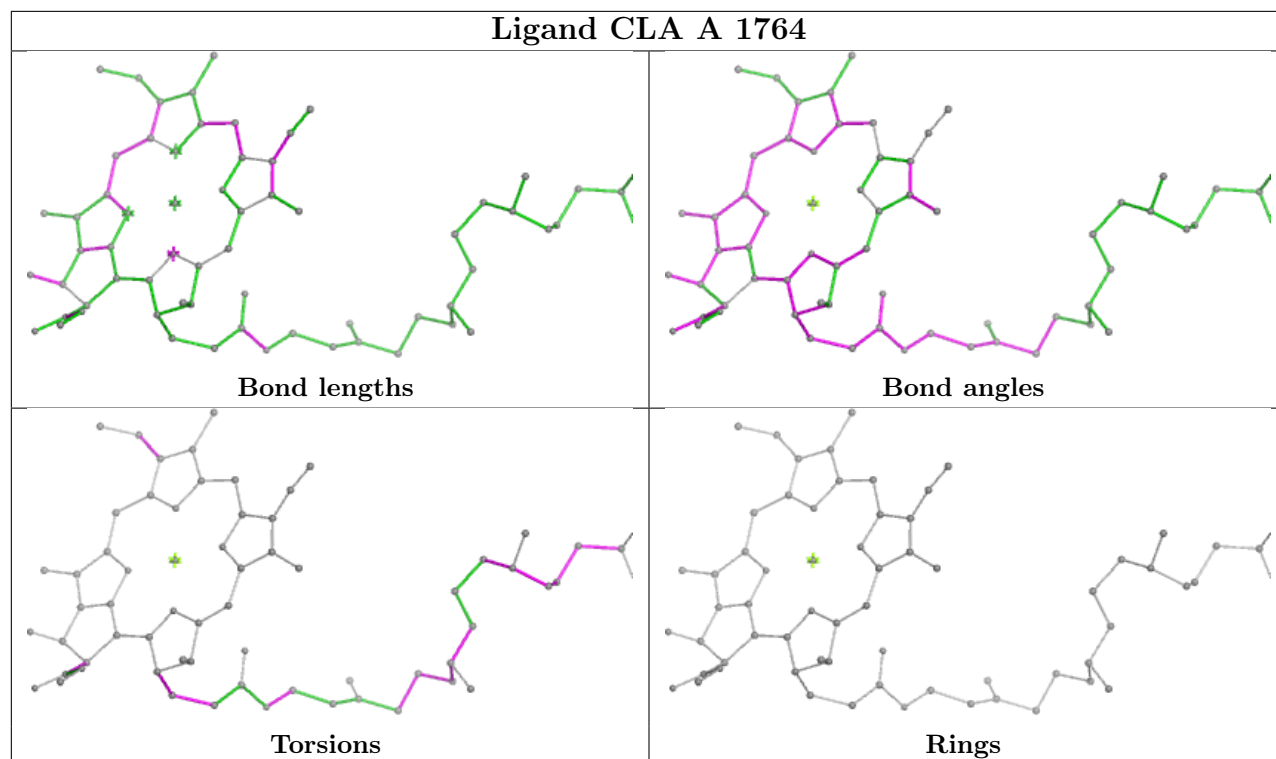
## Ligand CLA B 1740

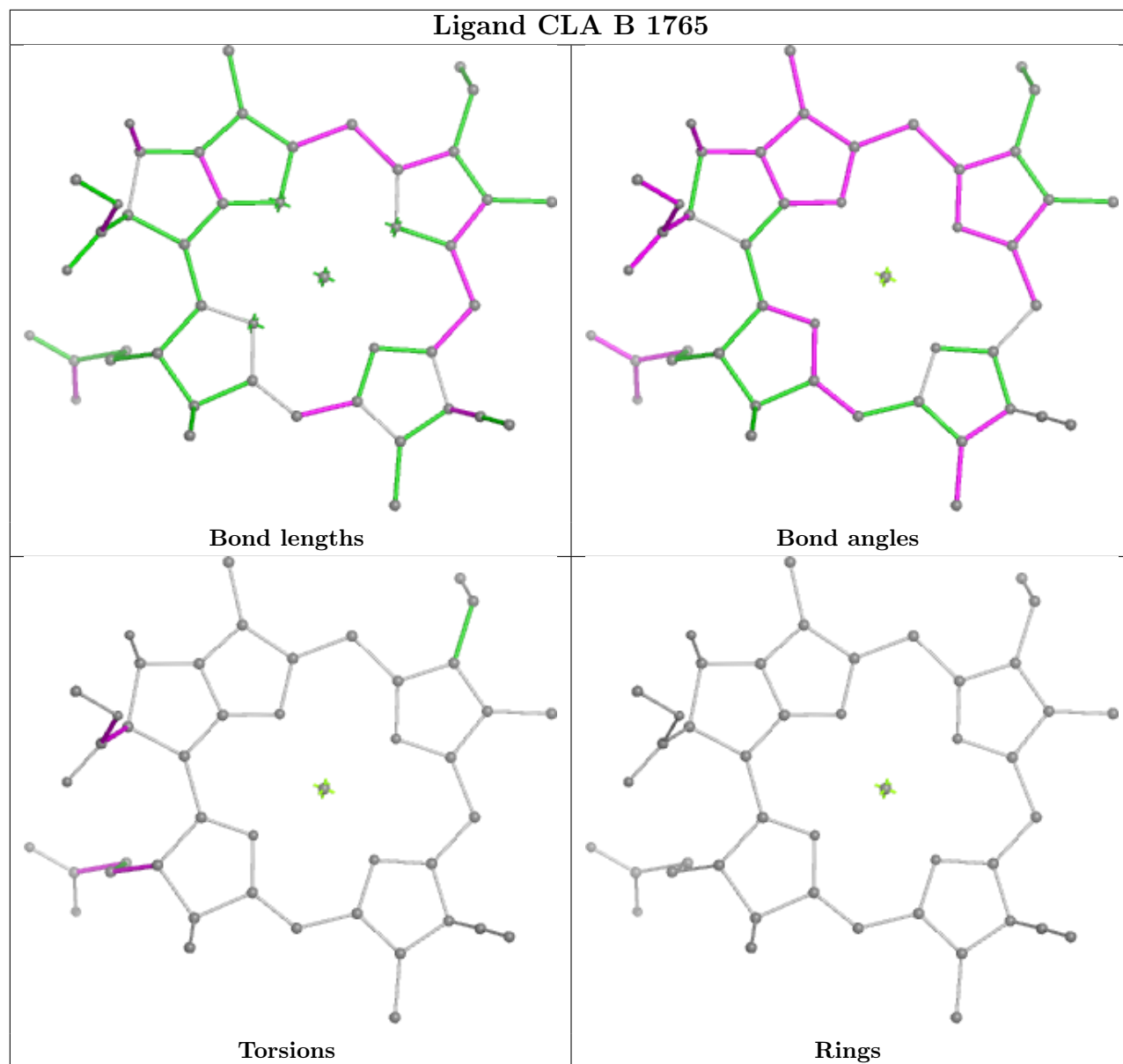


## Ligand CLA K 1085



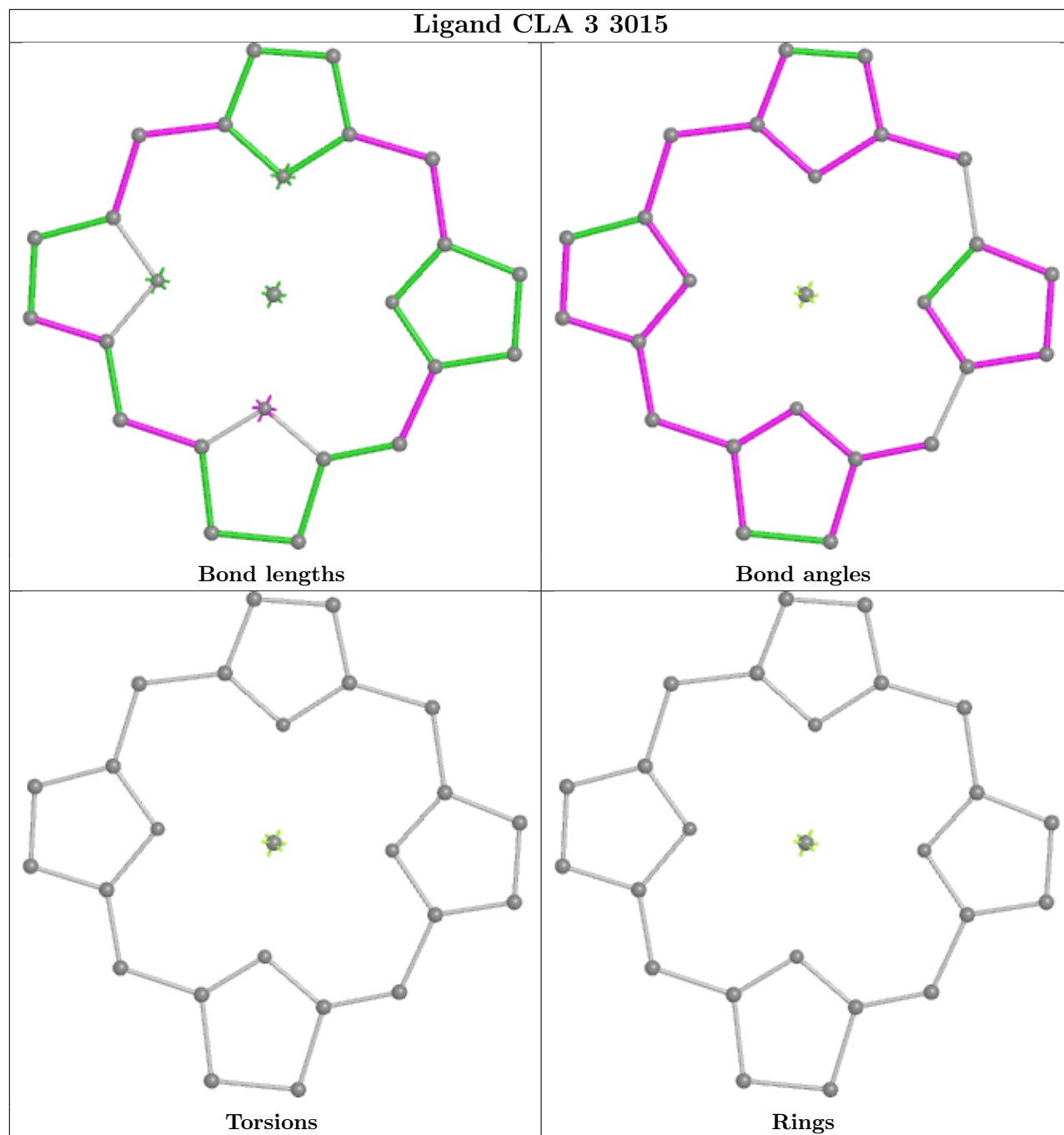


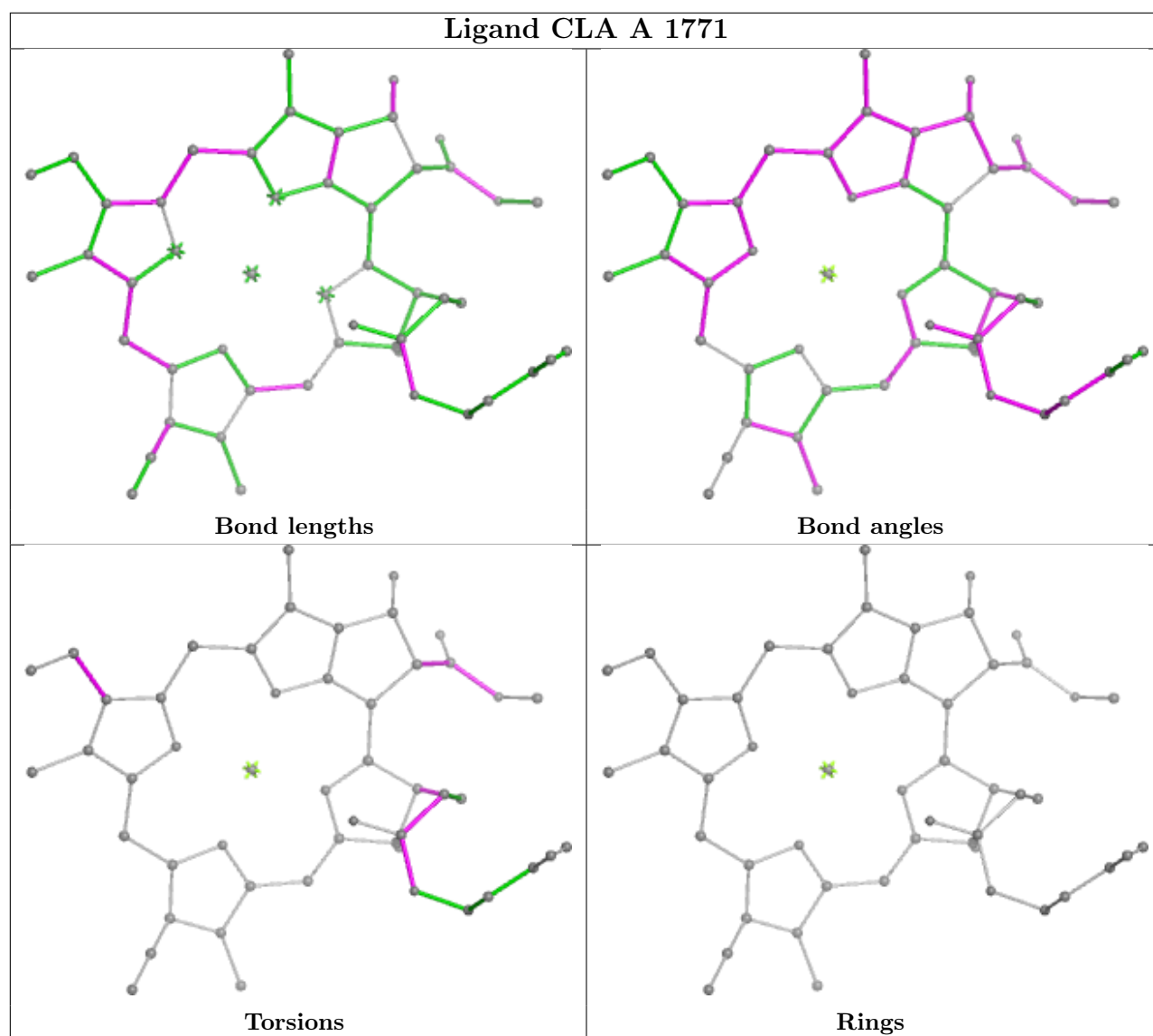




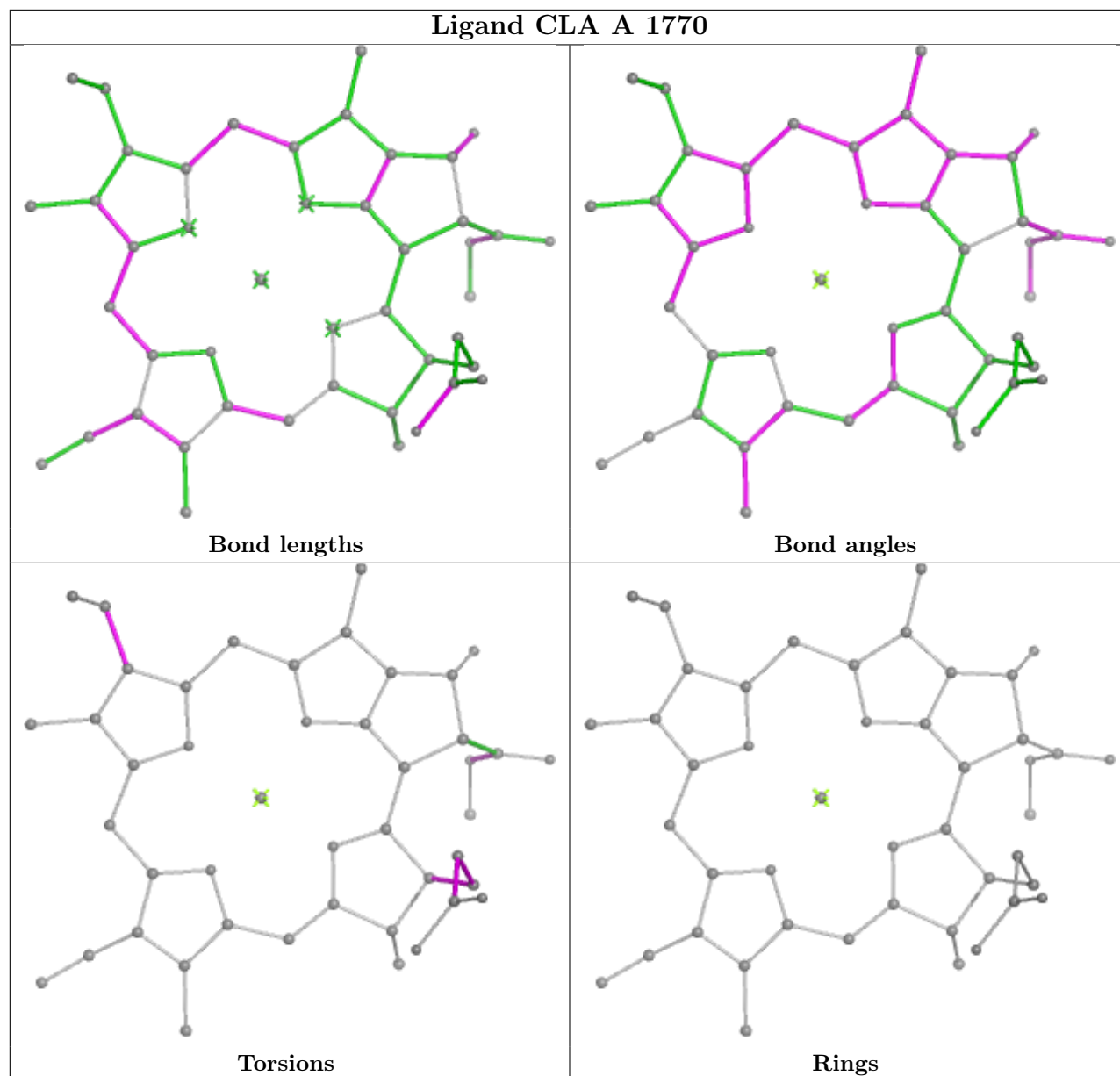


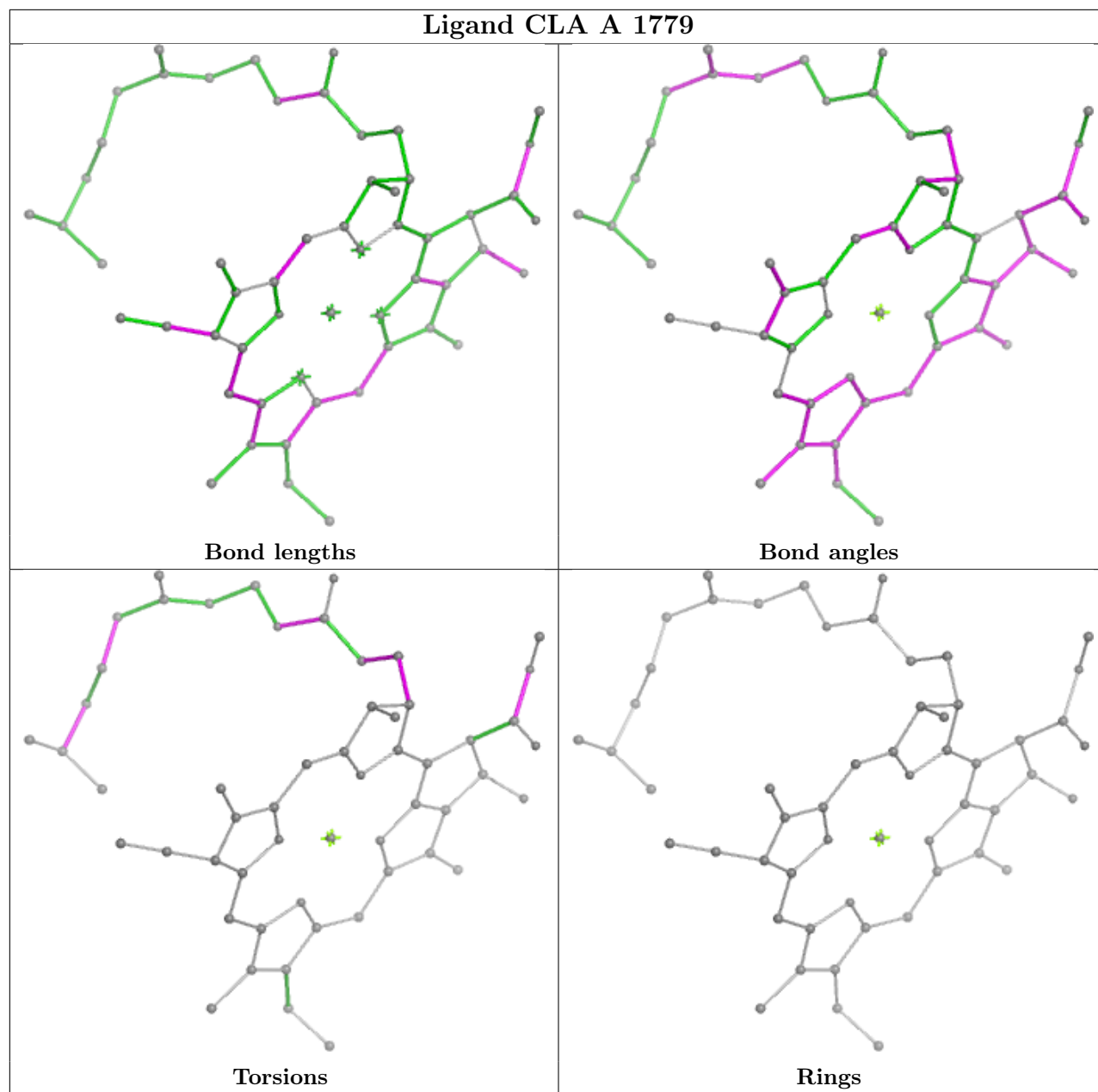
## Ligand CLA 3 3015

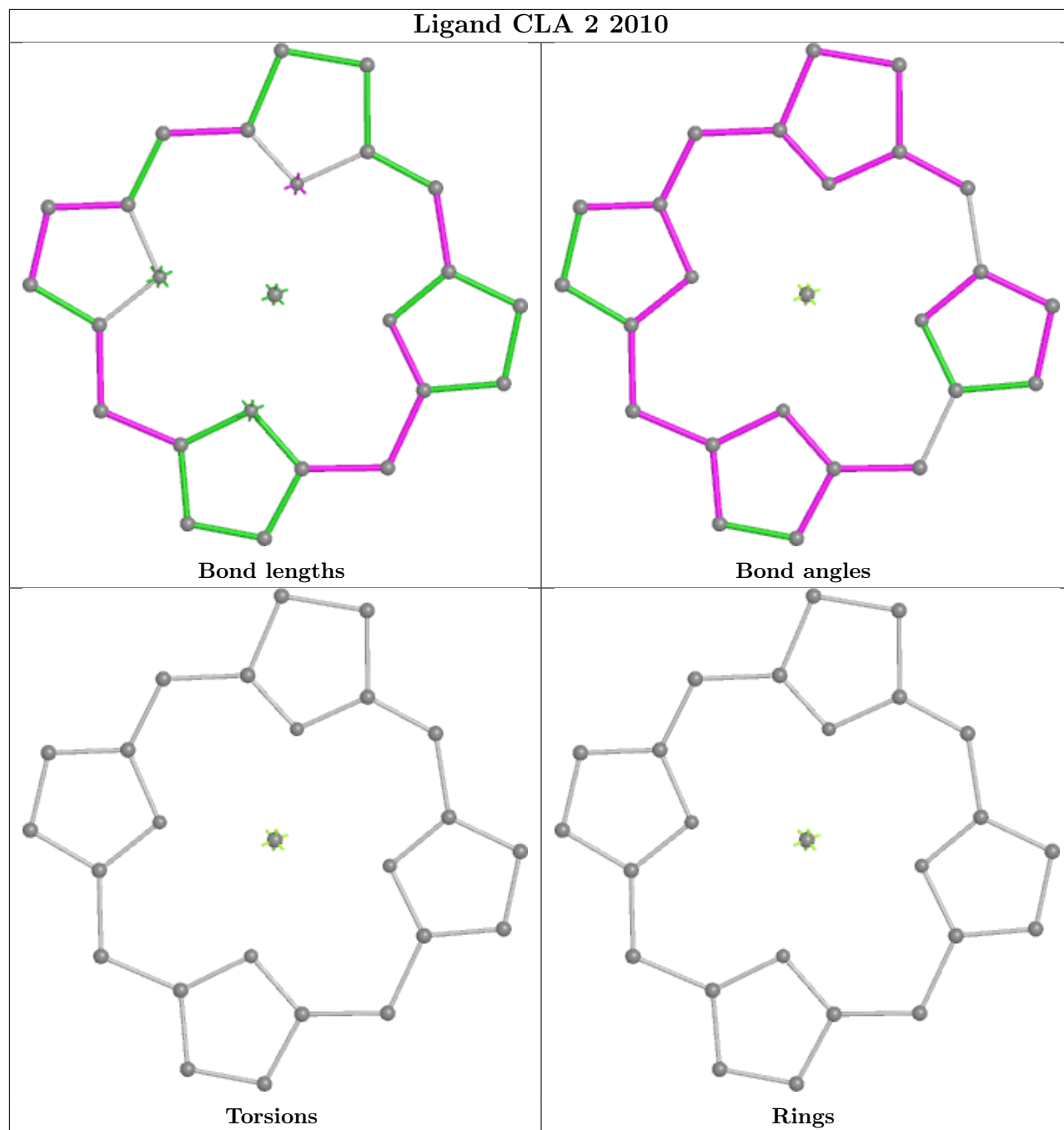




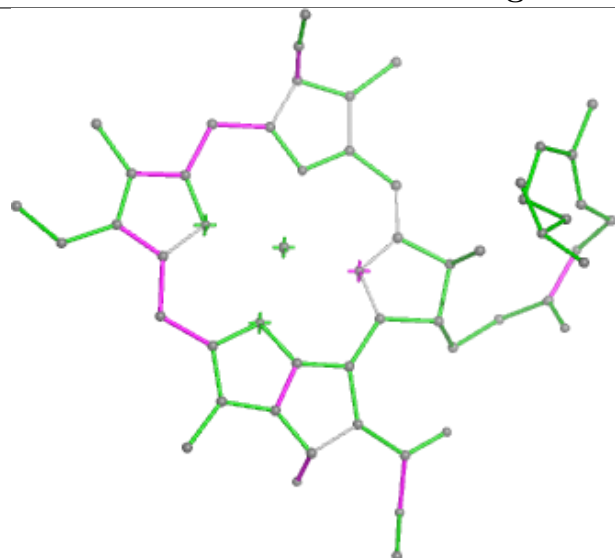
## Ligand CLA A 1770



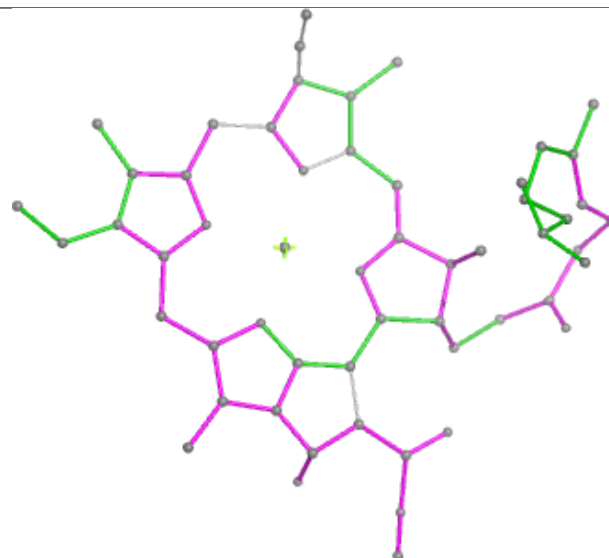




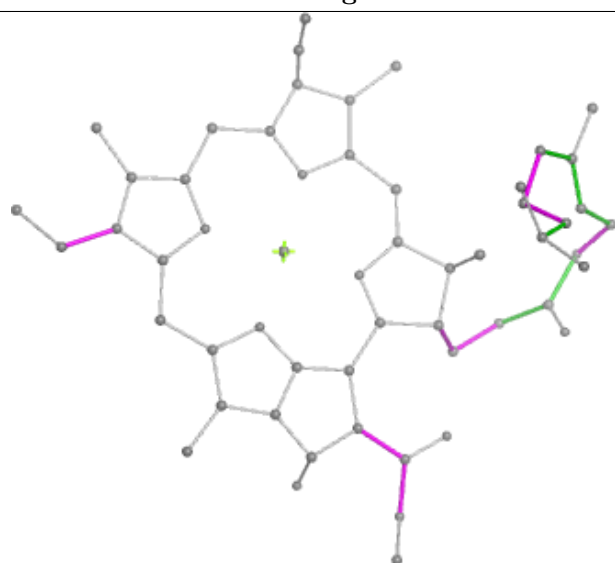
## Ligand CLA A 1815



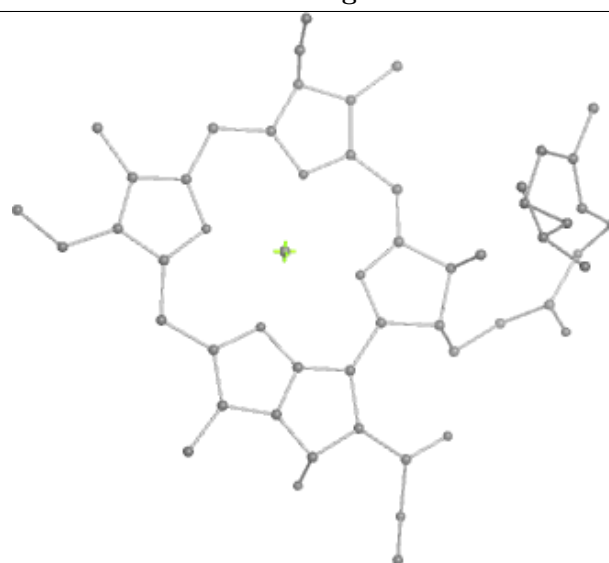
Bond lengths



Bond angles

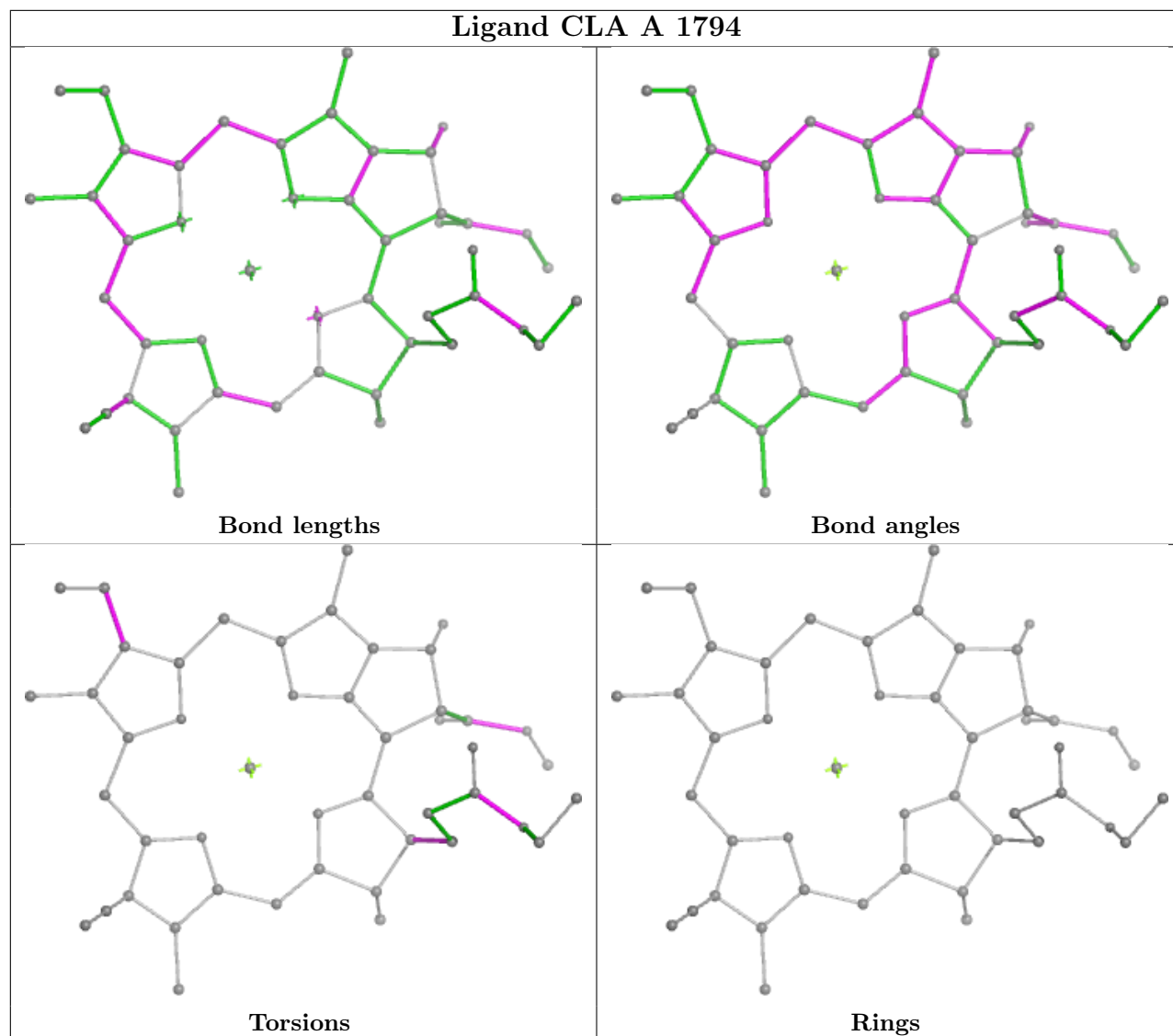


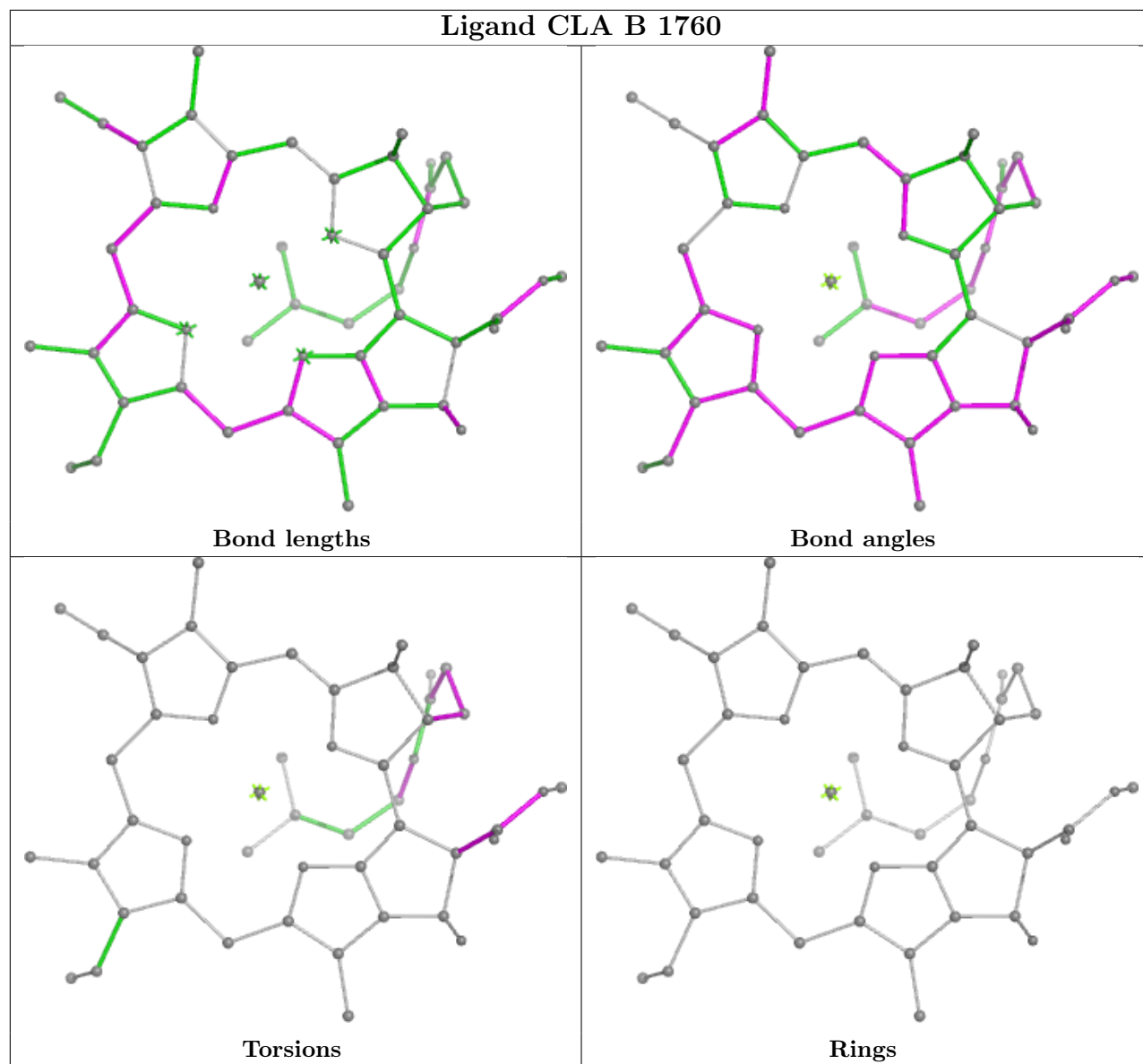
Torsions



Rings

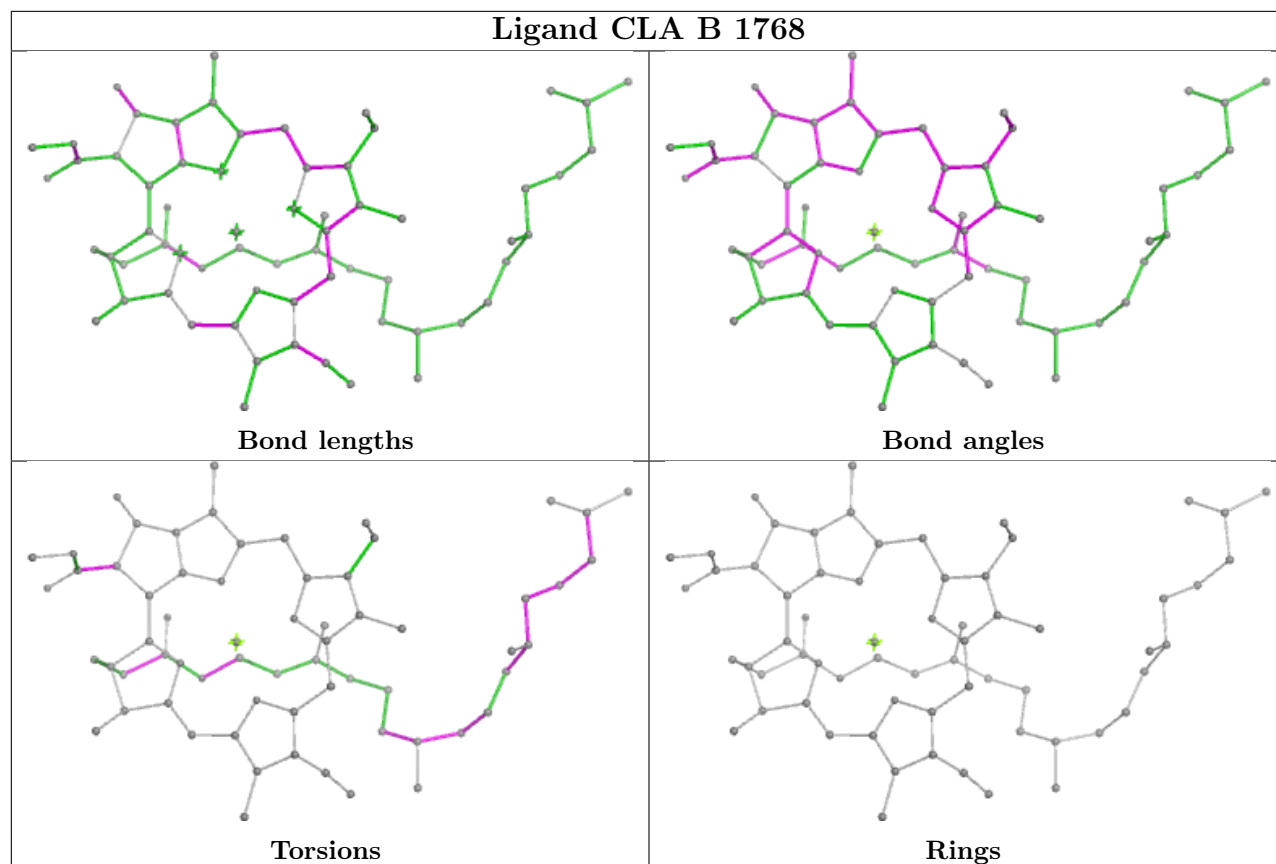
## Ligand CLA A 1794



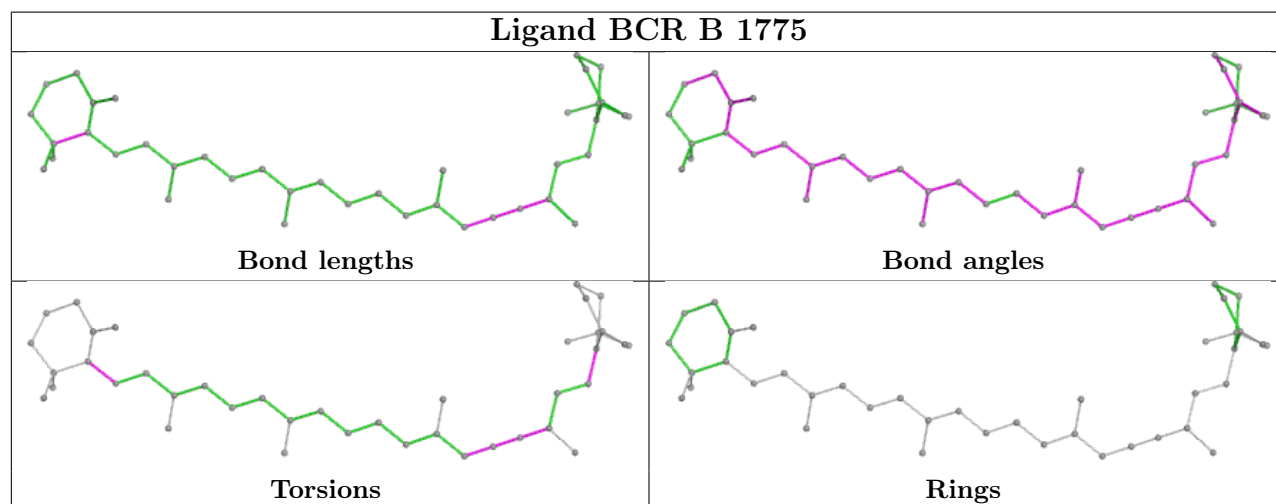




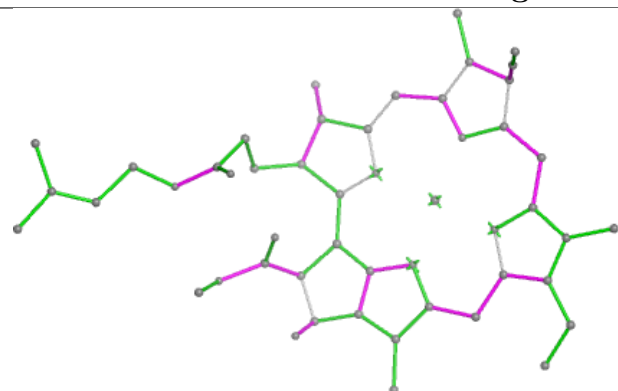
## Ligand CLA B 1768



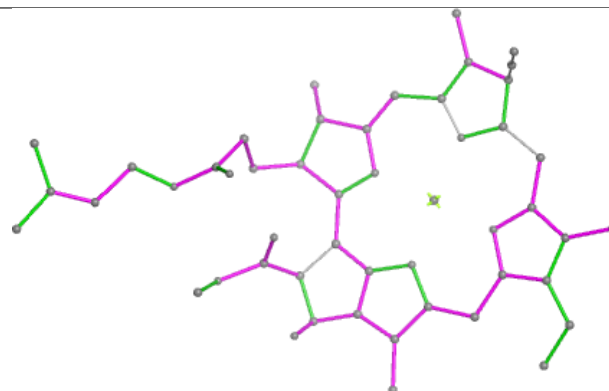
## Ligand BCR B 1775



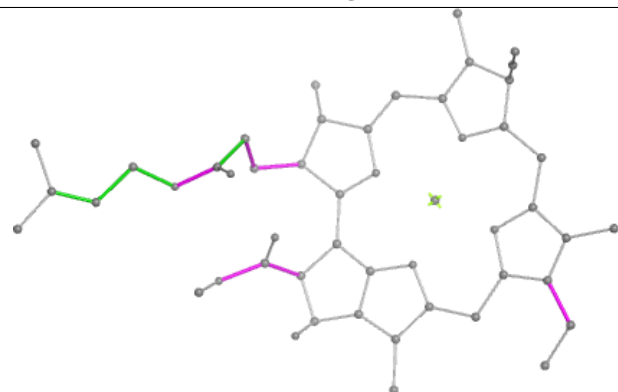
## Ligand CLA L 1168



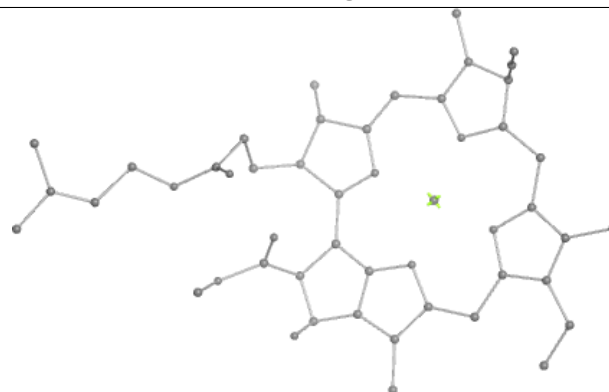
Bond lengths



Bond angles

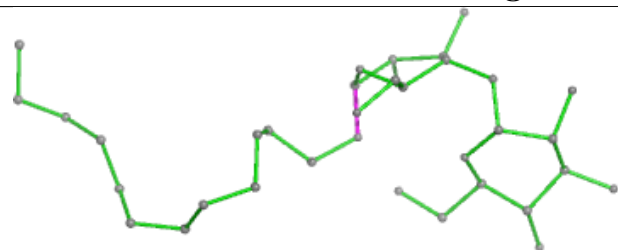


Torsions

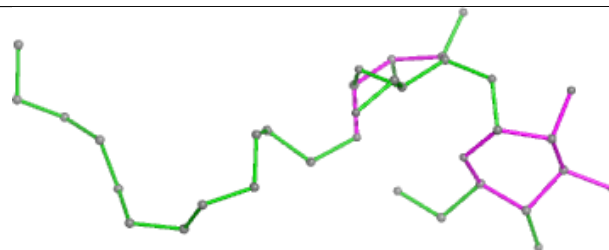


Rings

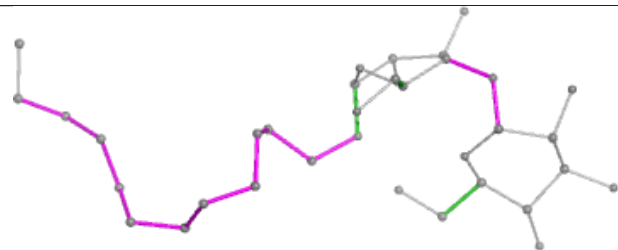
## Ligand LMU A 1810



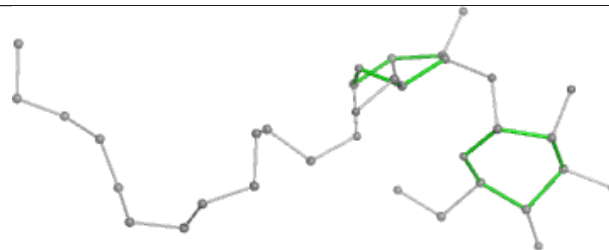
Bond lengths



Bond angles

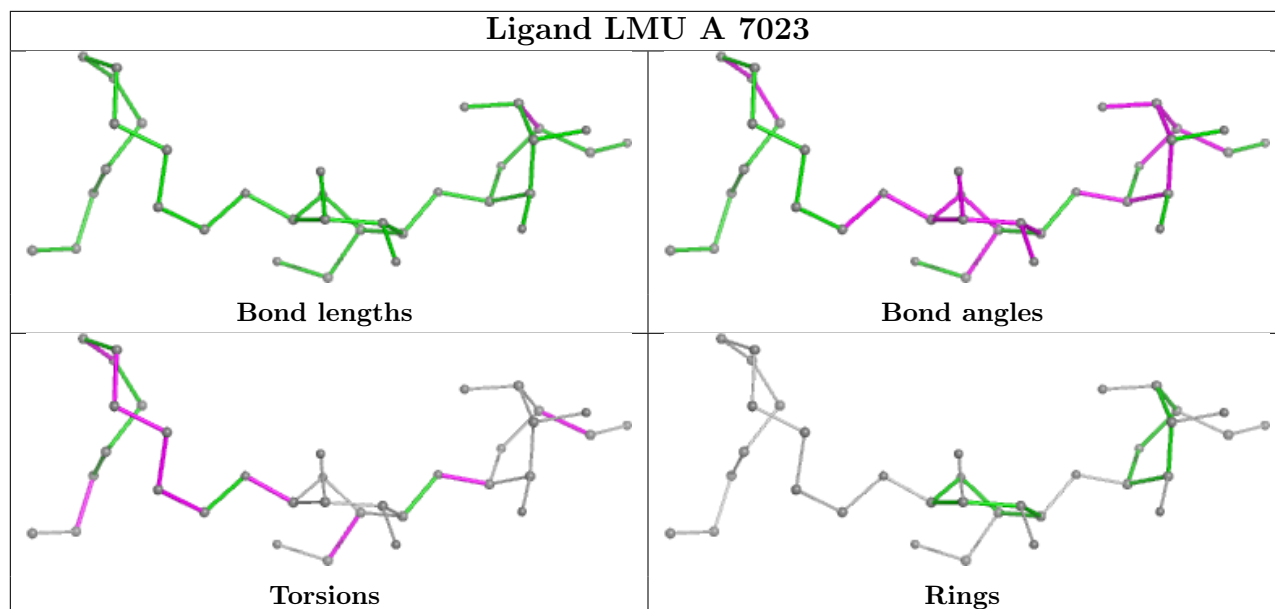


Torsions

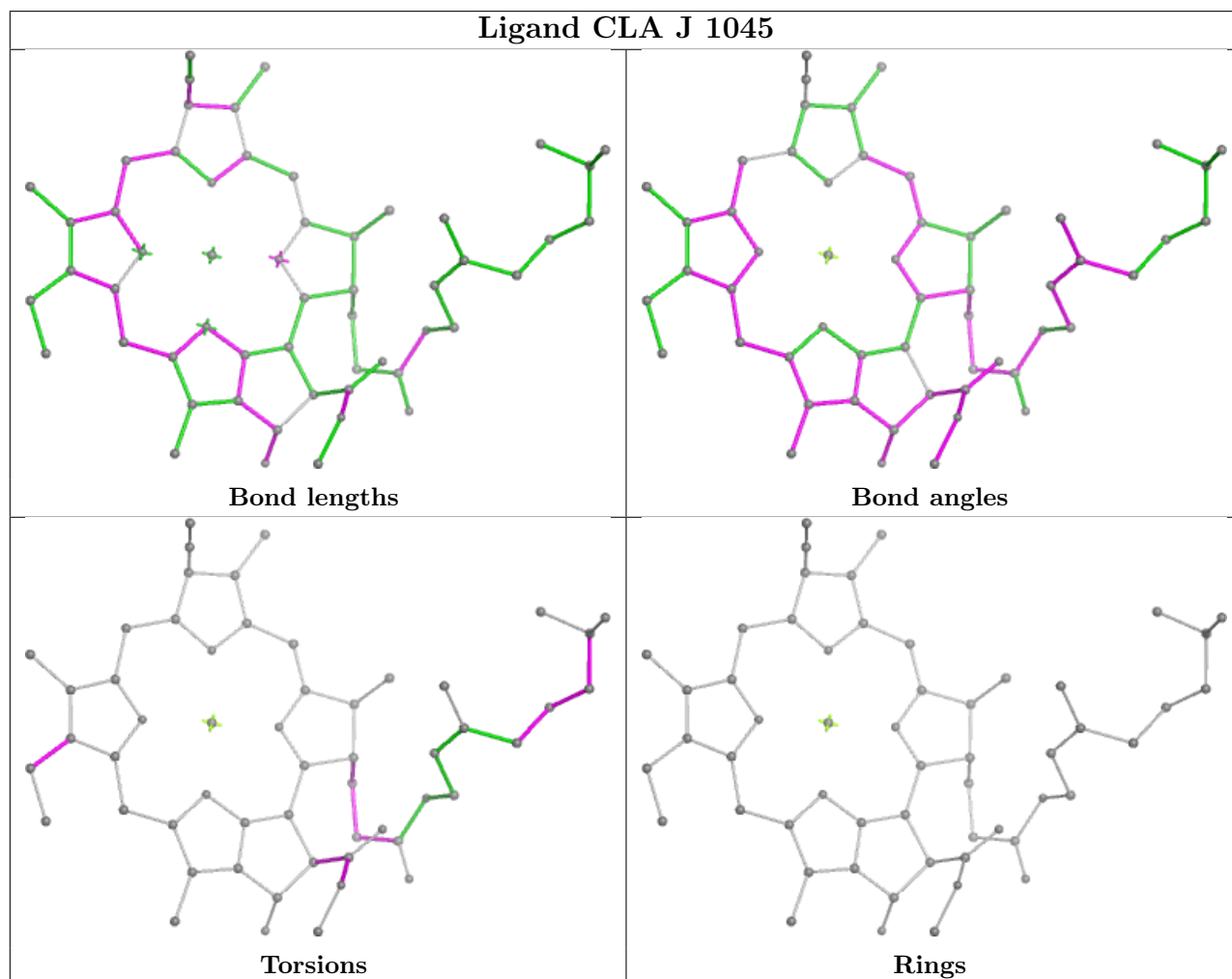


Rings

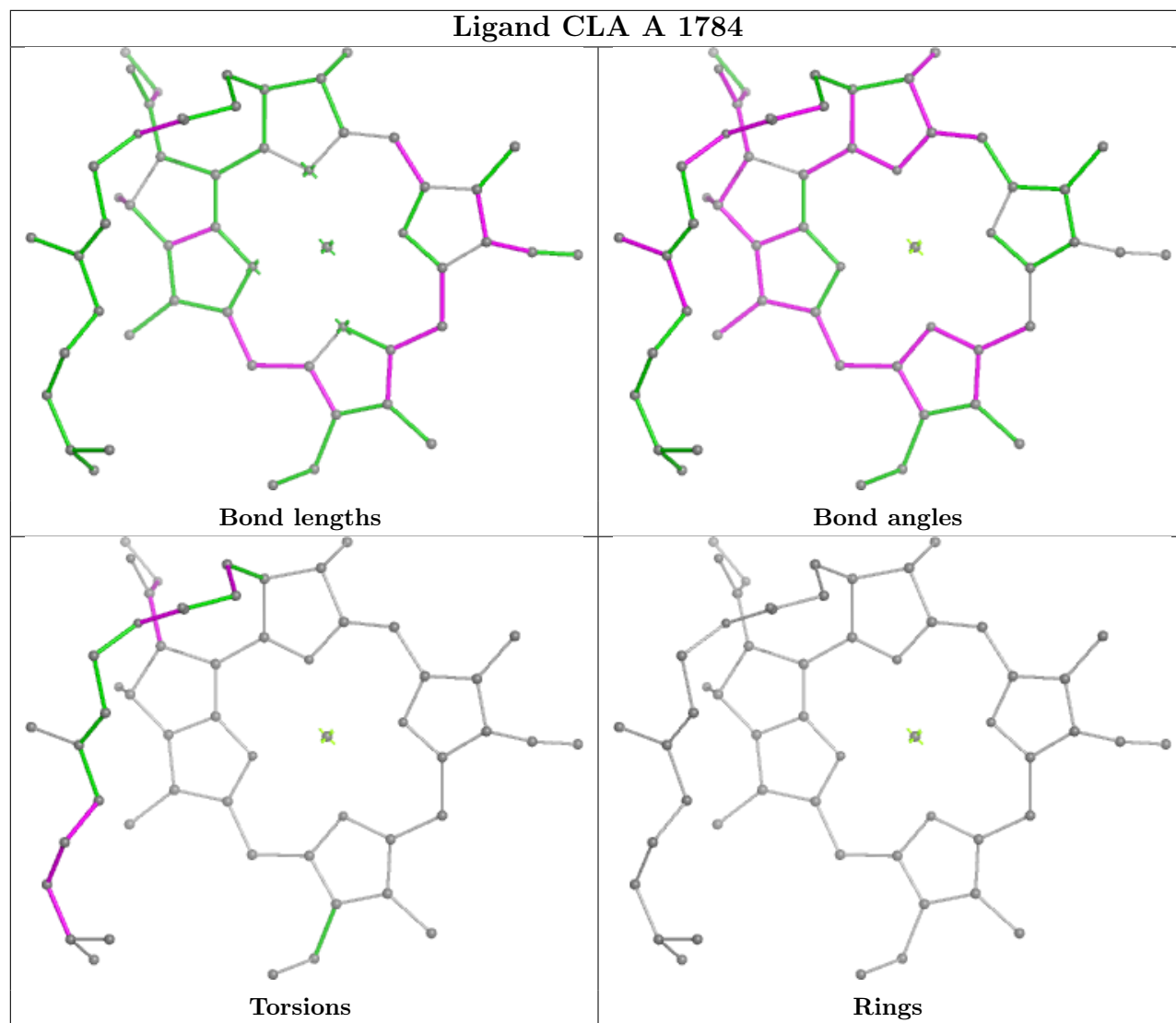
## Ligand LMU A 7023



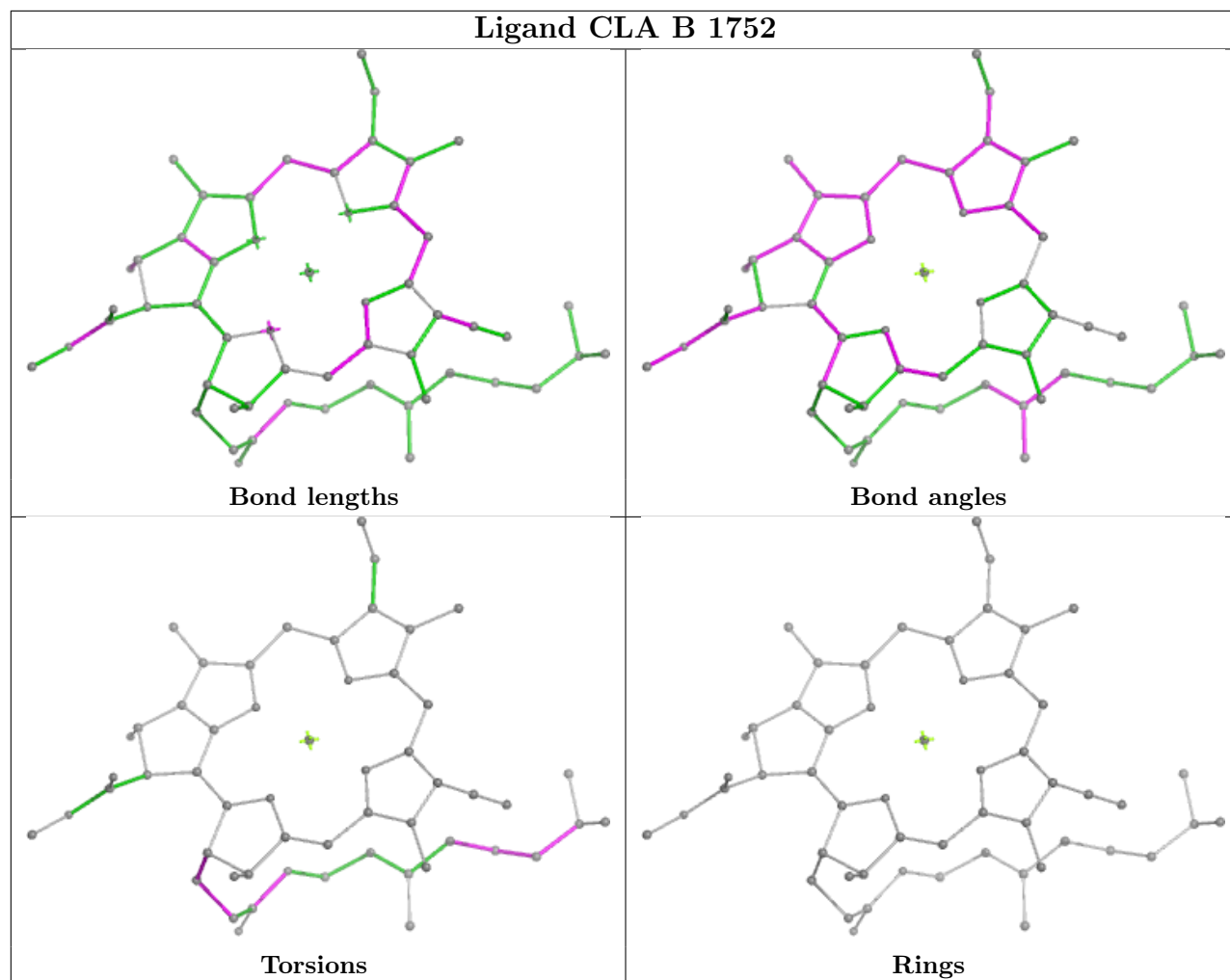
## Ligand CLA J 1045



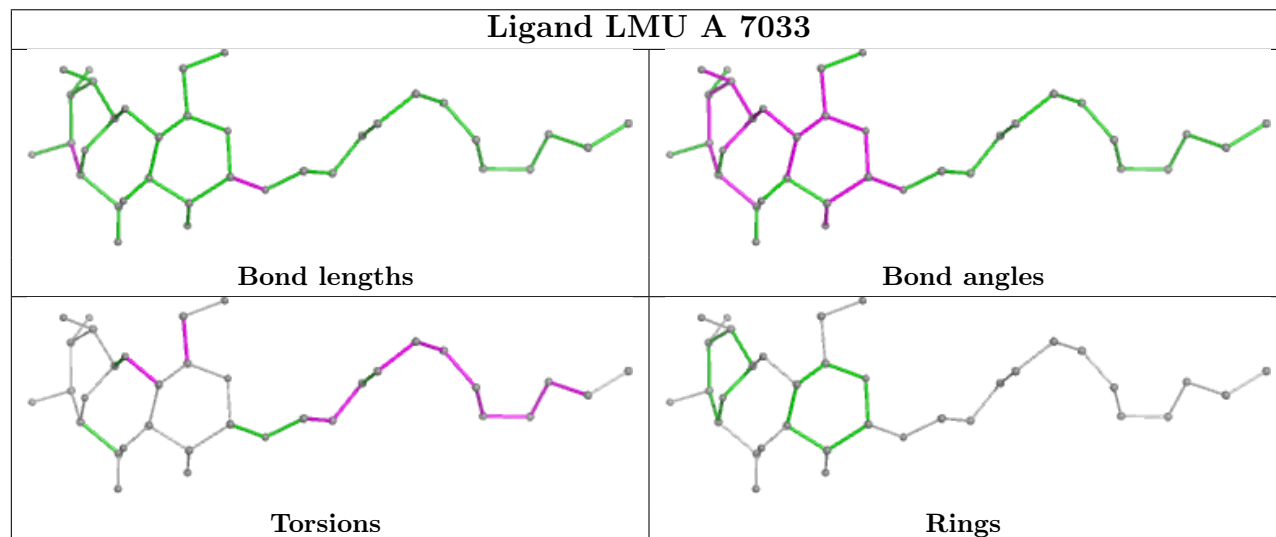
## Ligand CLA A 1784



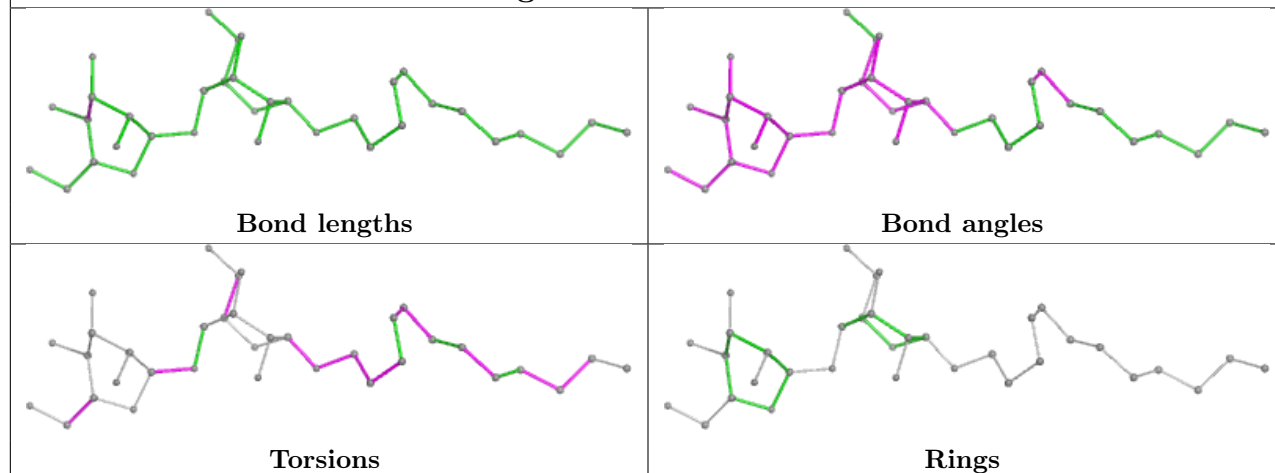
## Ligand CLA B 1752



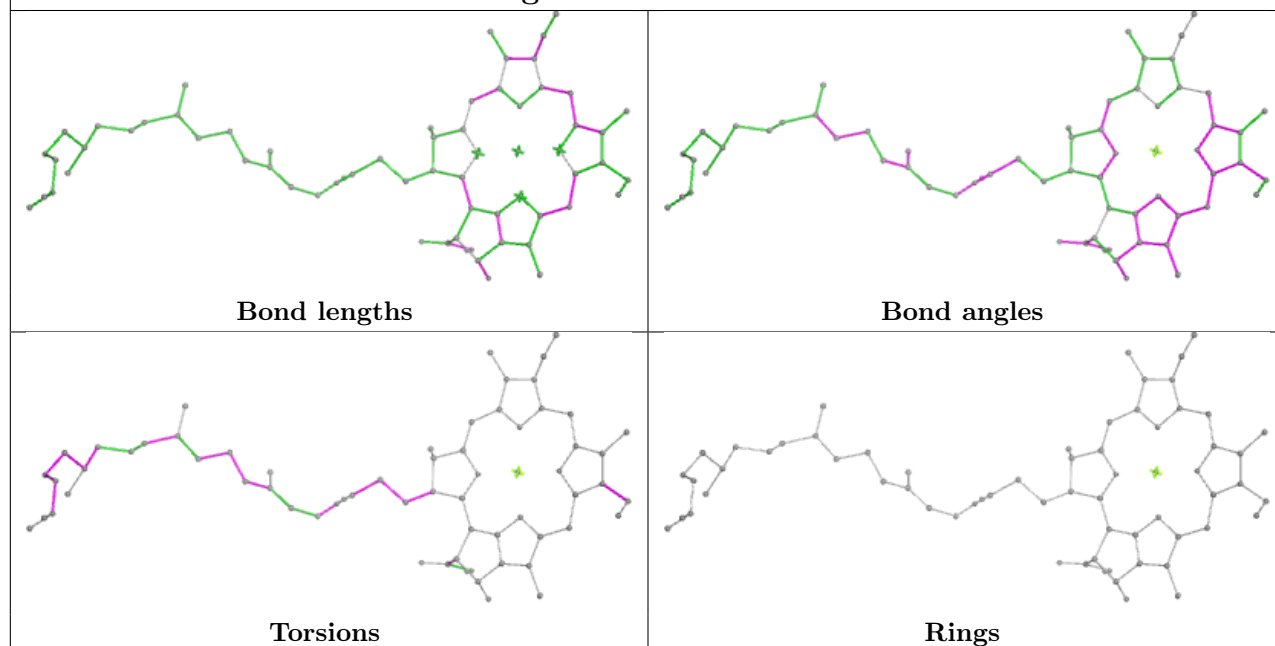
## Ligand LMU A 7033



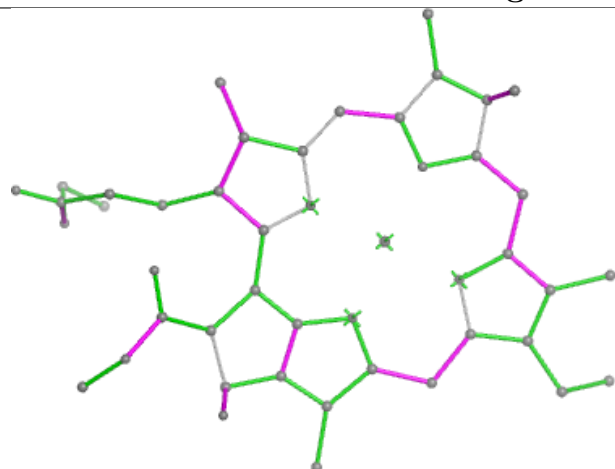
## Ligand LMU A 7037



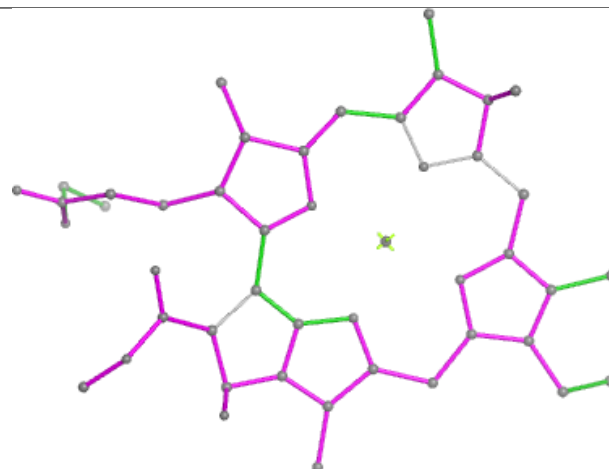
## Ligand CLA A 1761



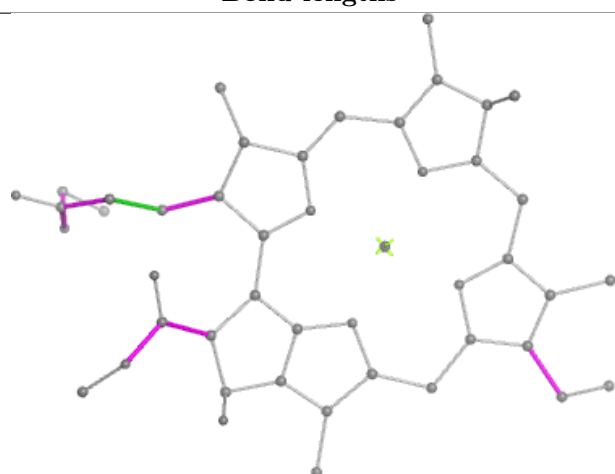
## Ligand CLA A 1817



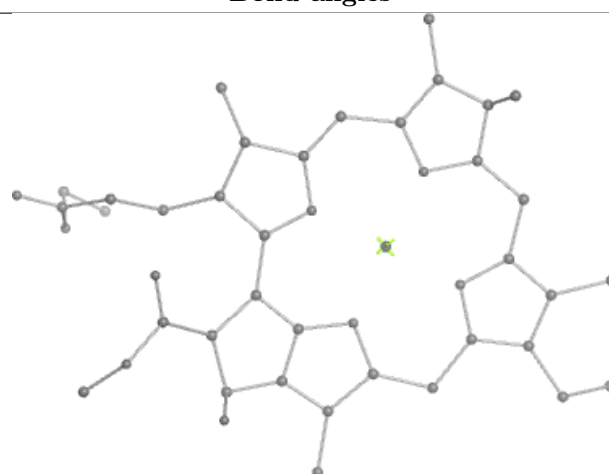
Bond lengths



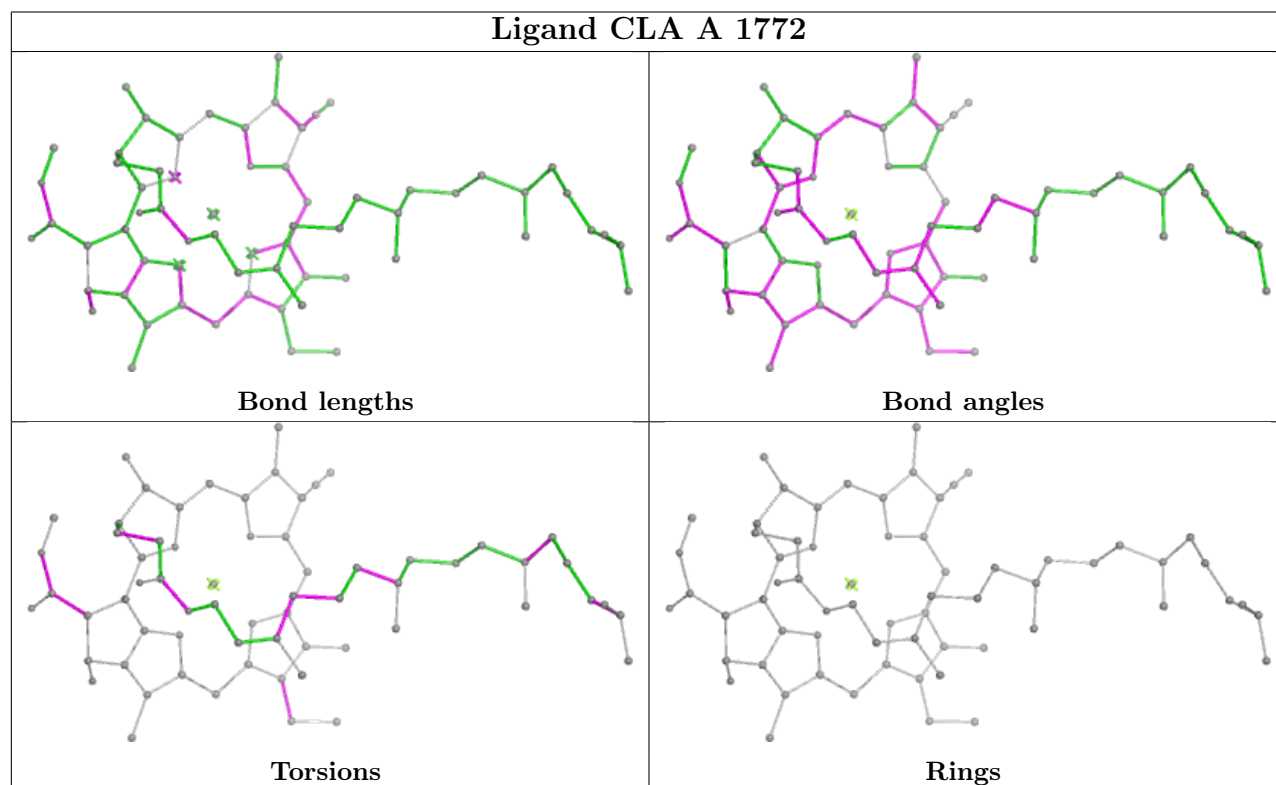
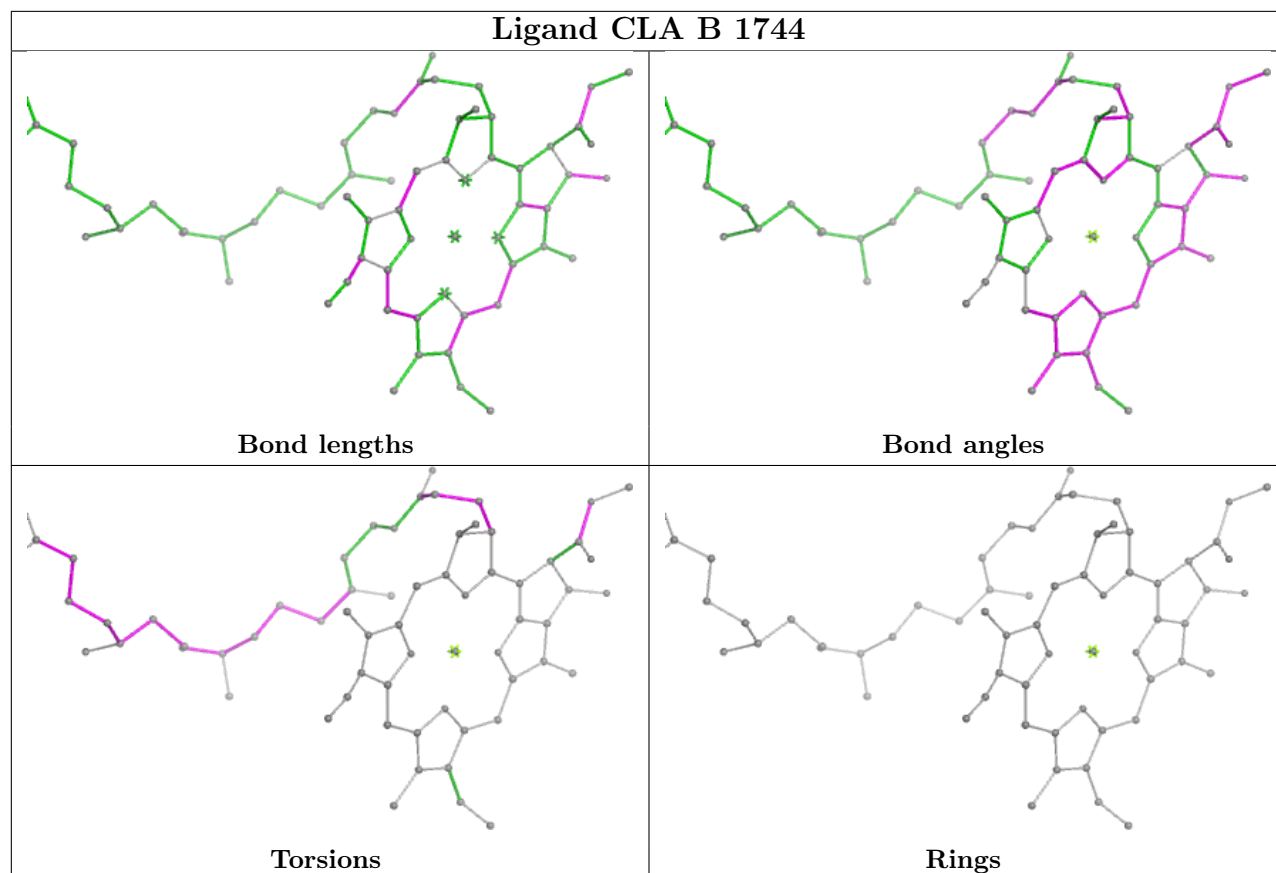
Bond angles



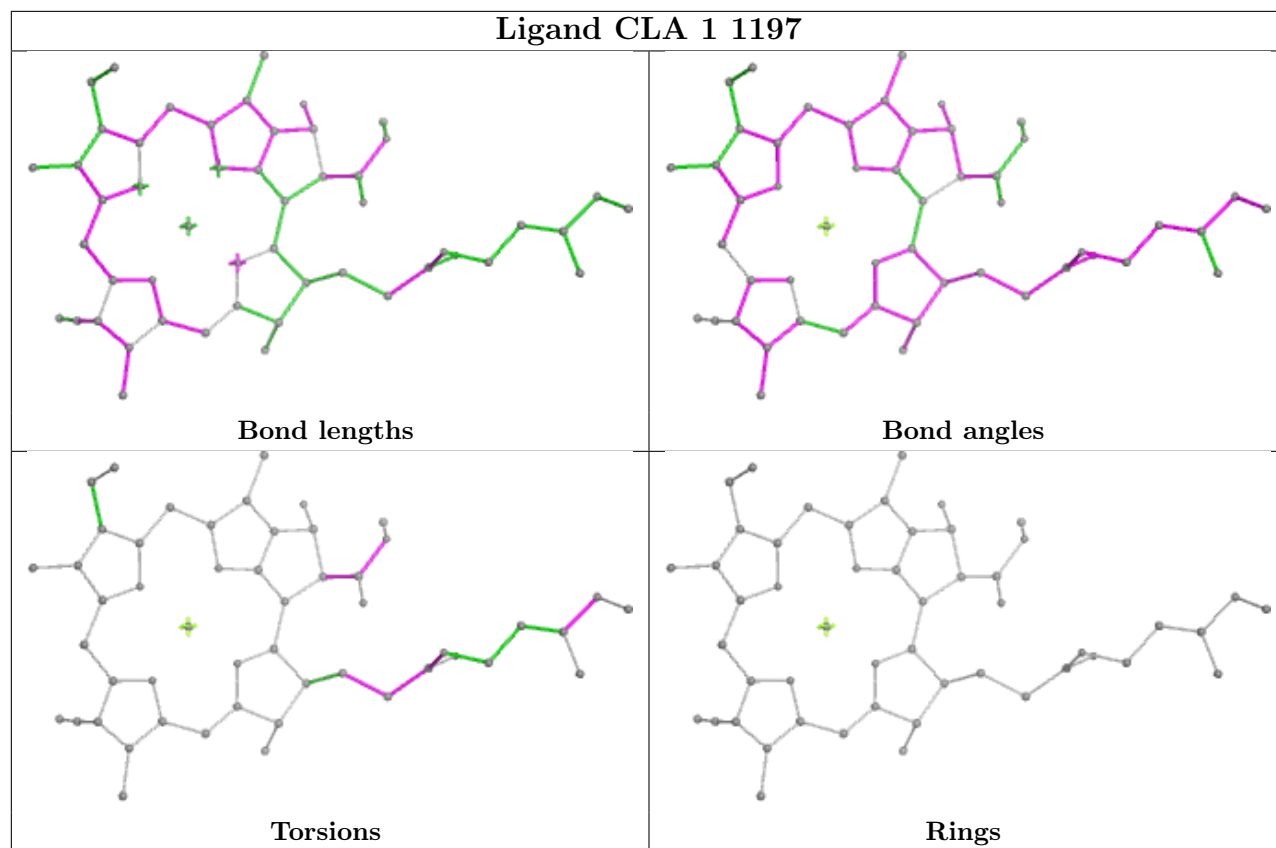
Torsions

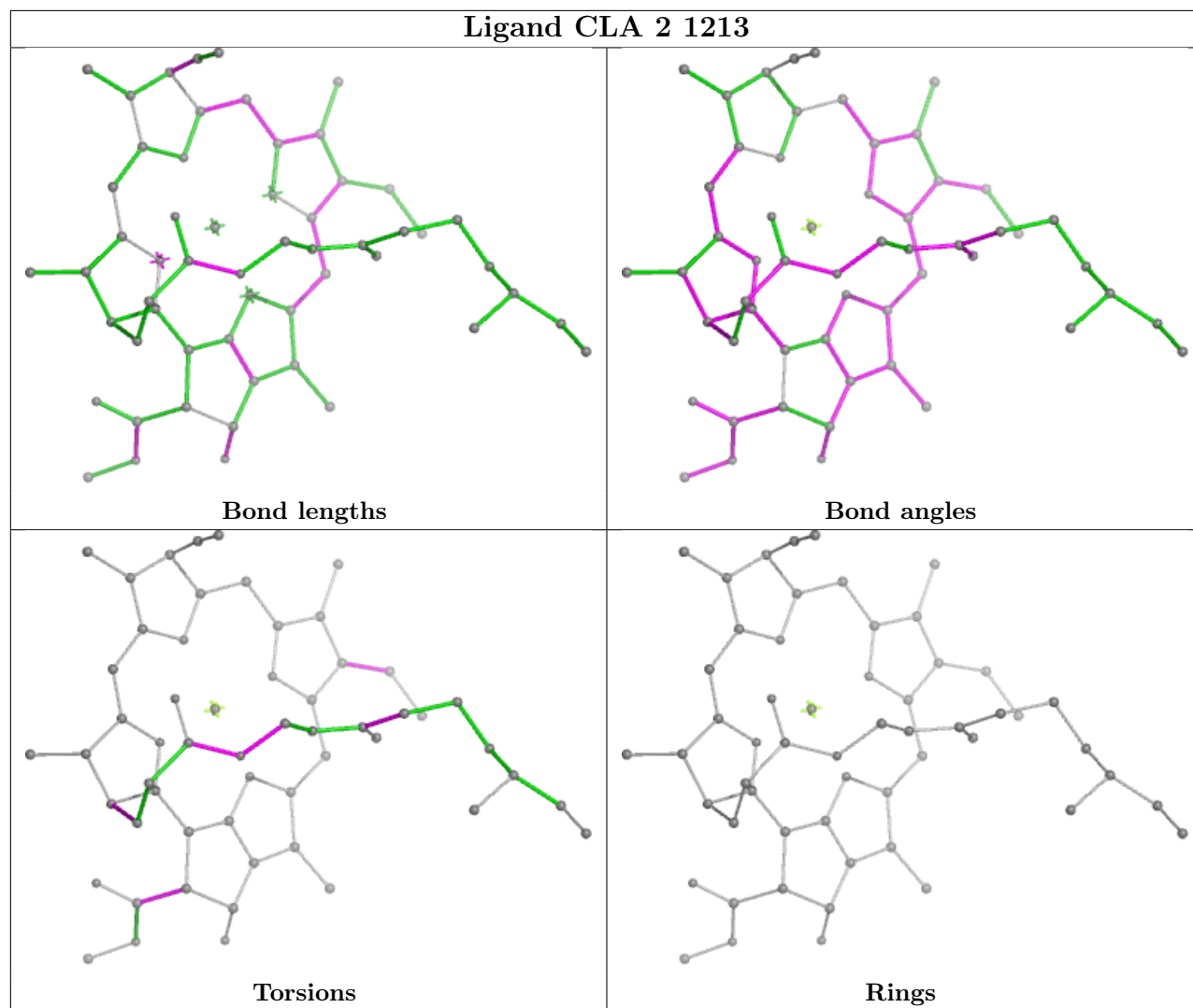


Rings

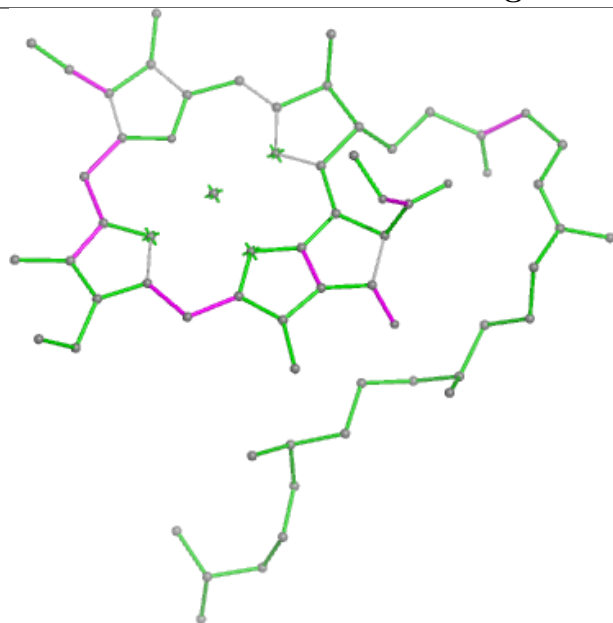




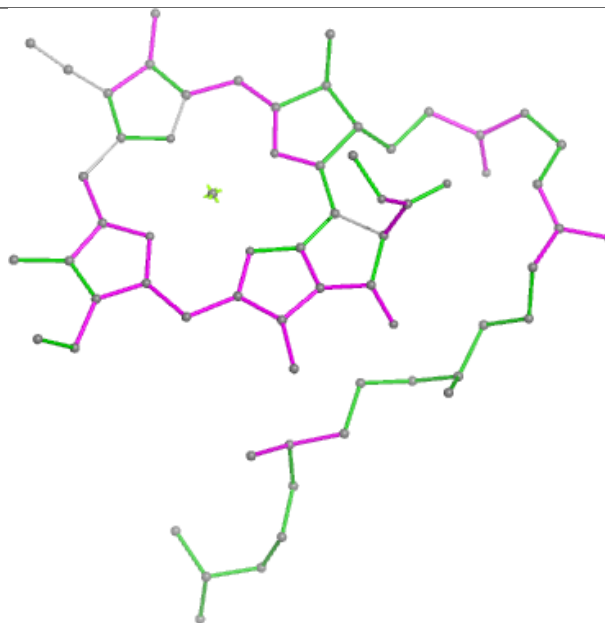




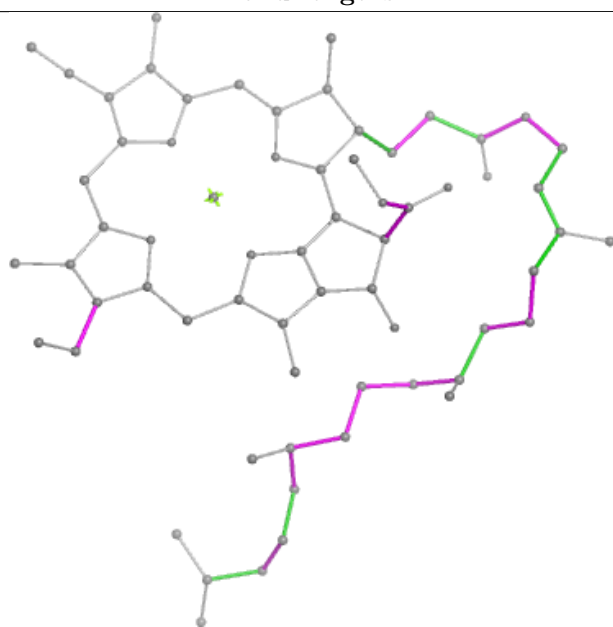
## Ligand CLA A 1780



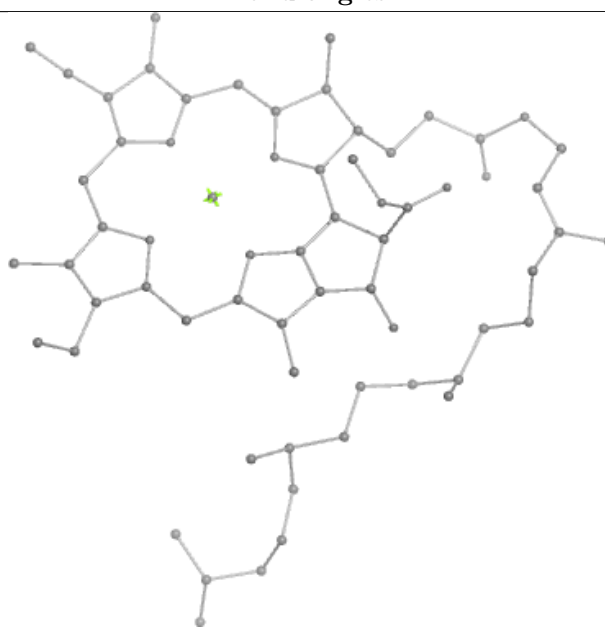
Bond lengths



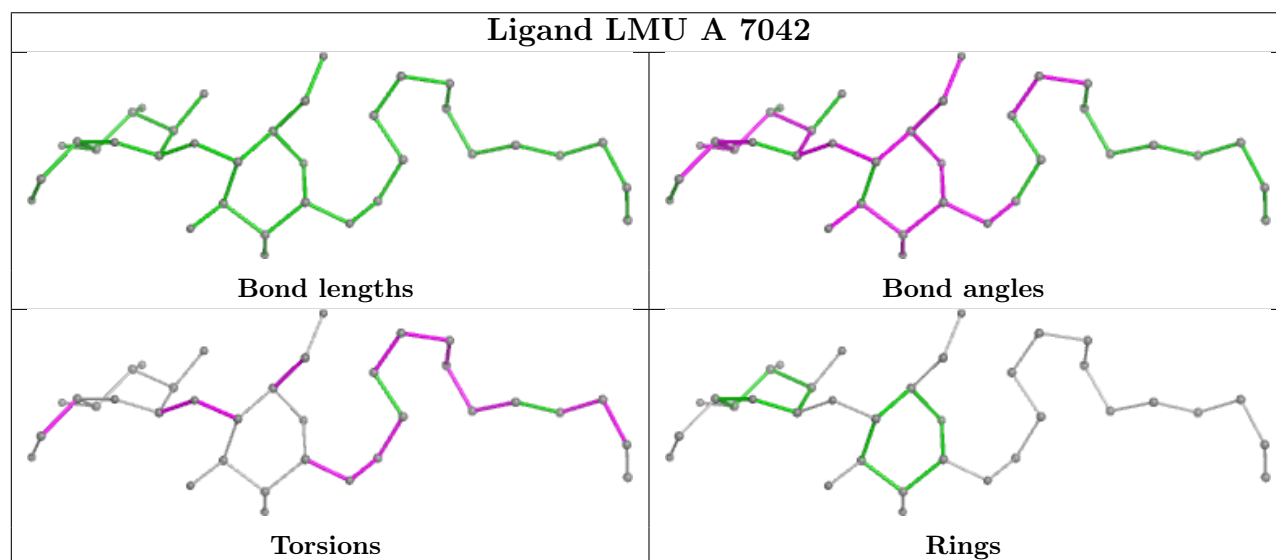
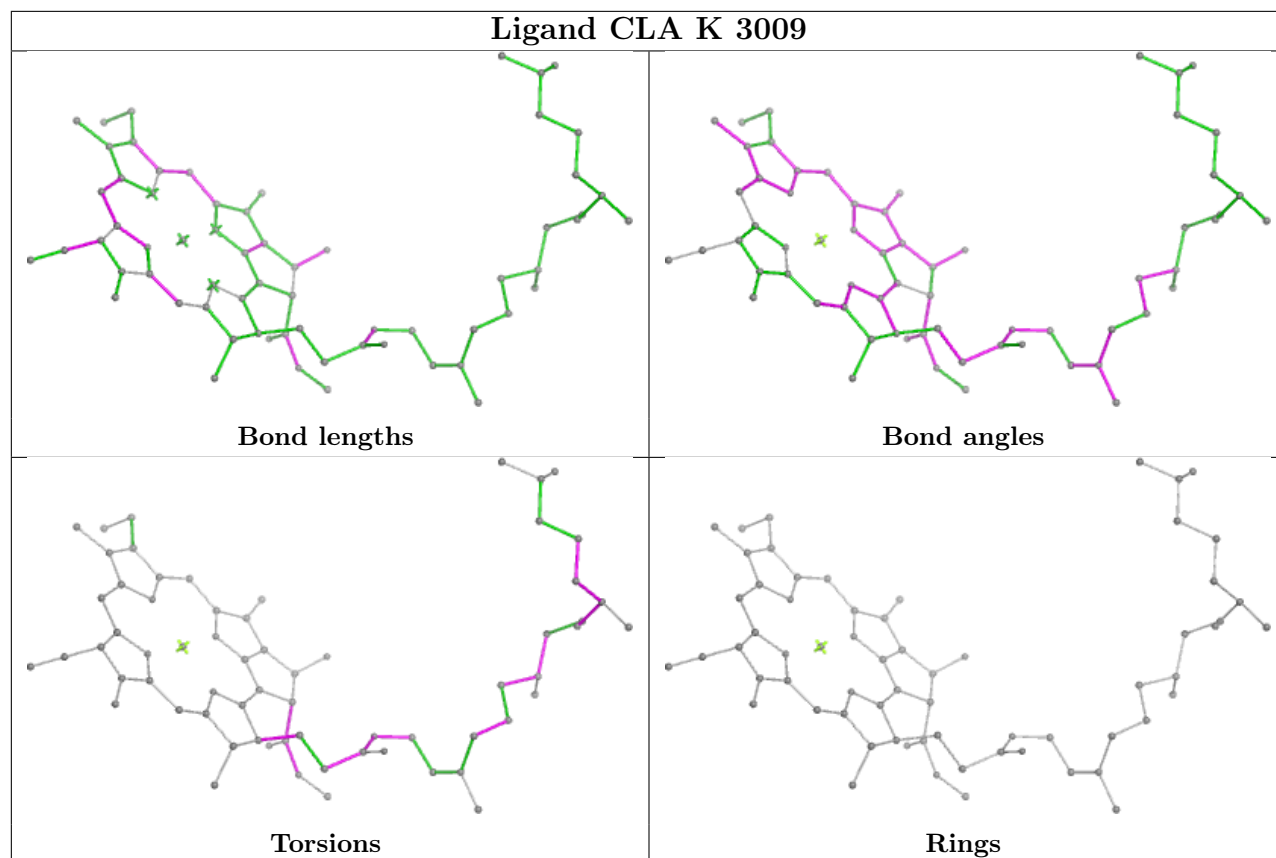
Bond angles

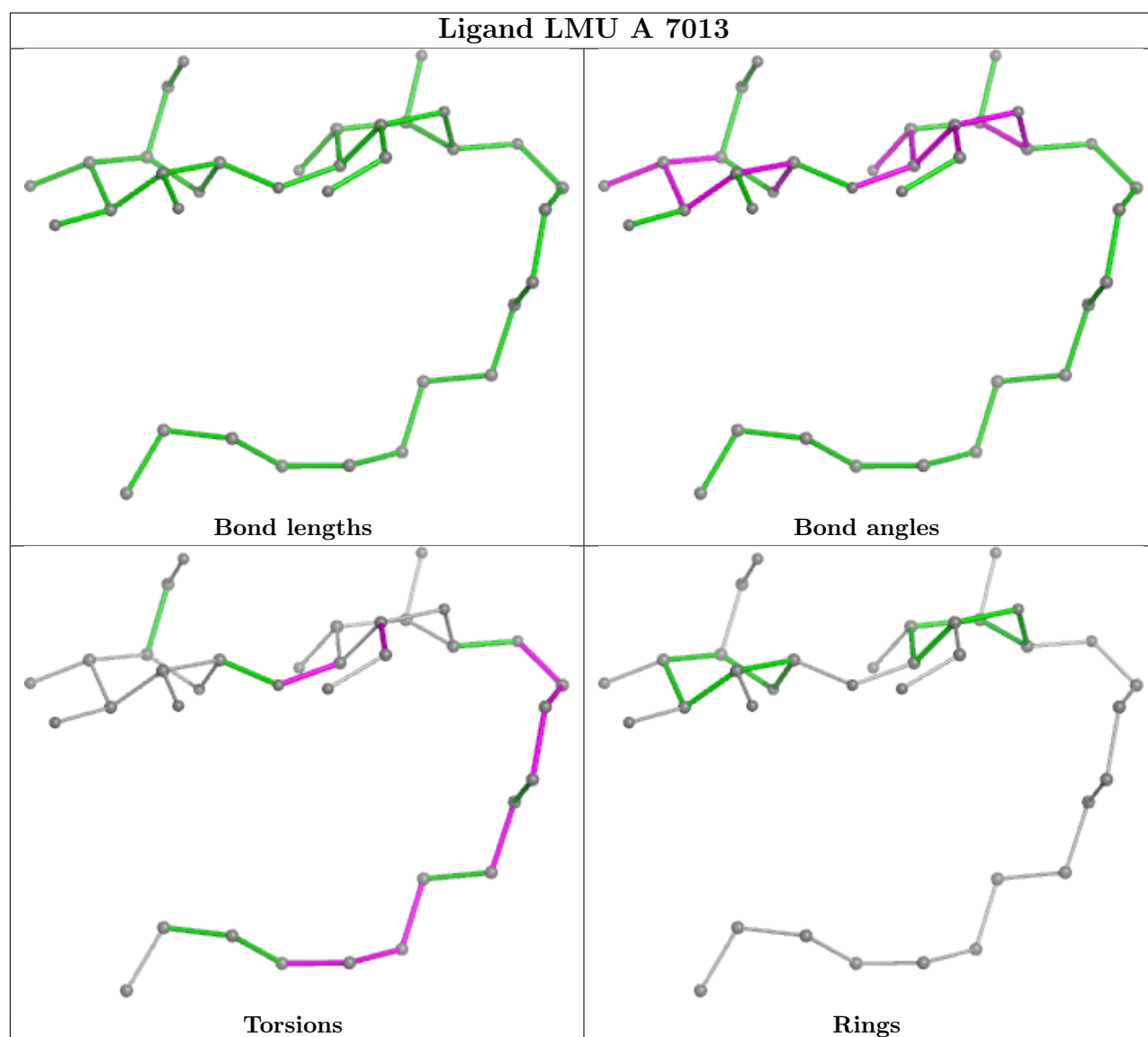


Torsions

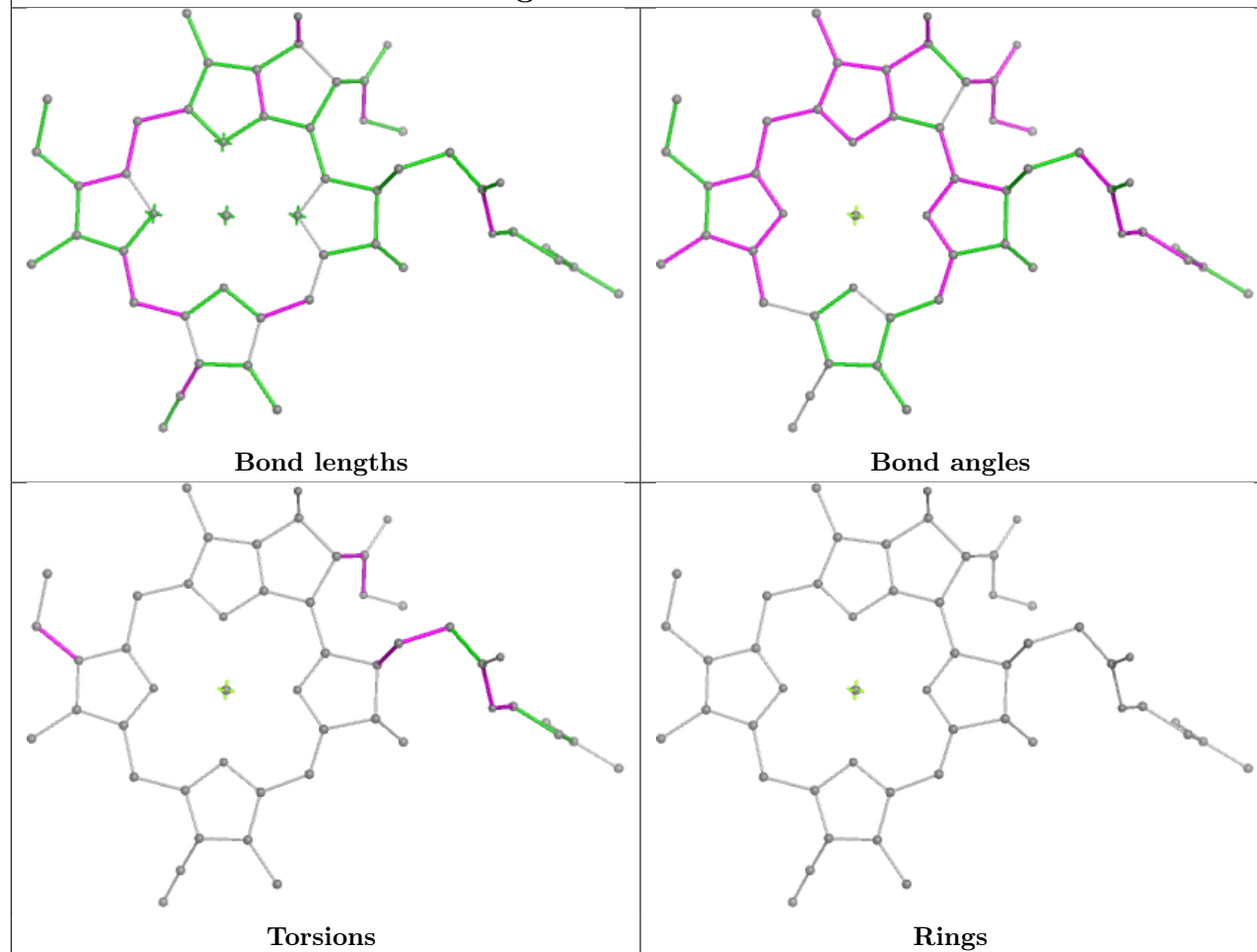


Rings

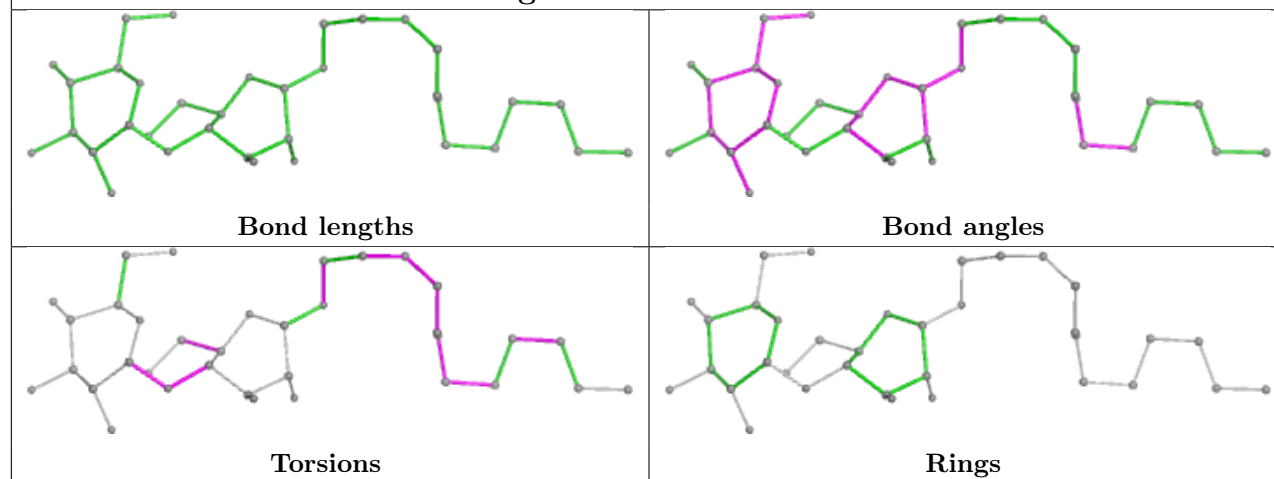


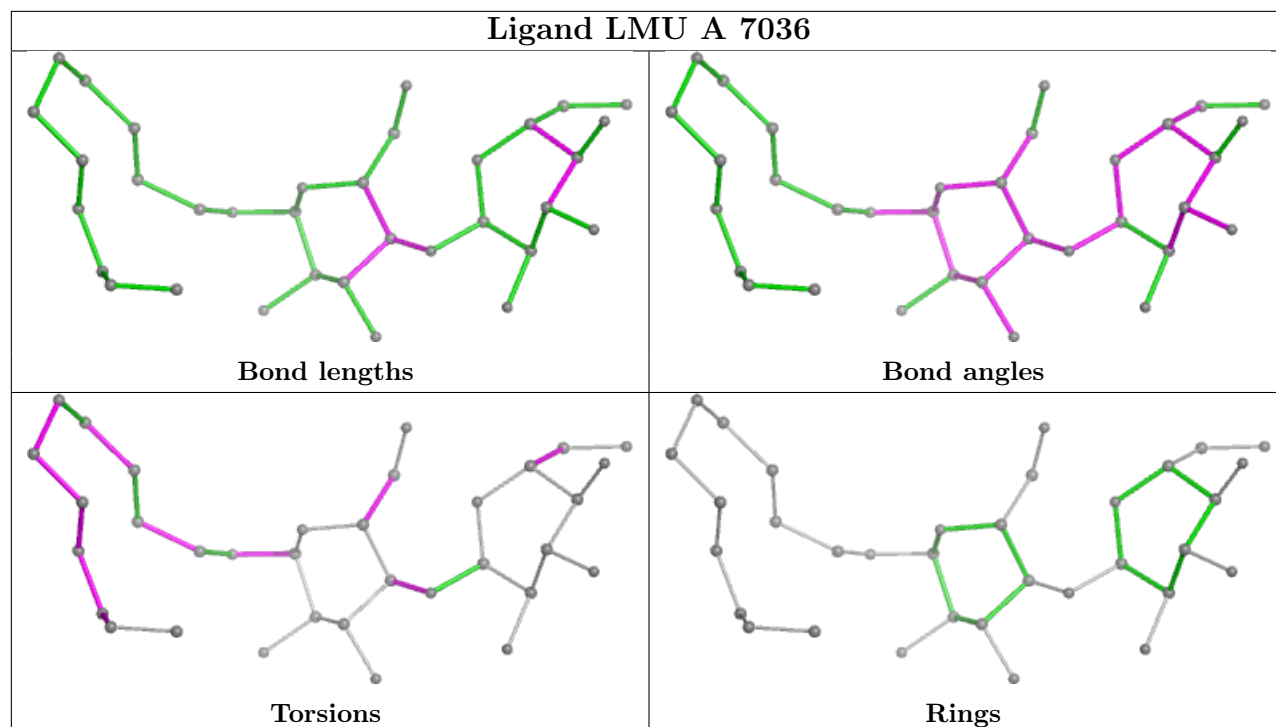


## Ligand CLA B 1761

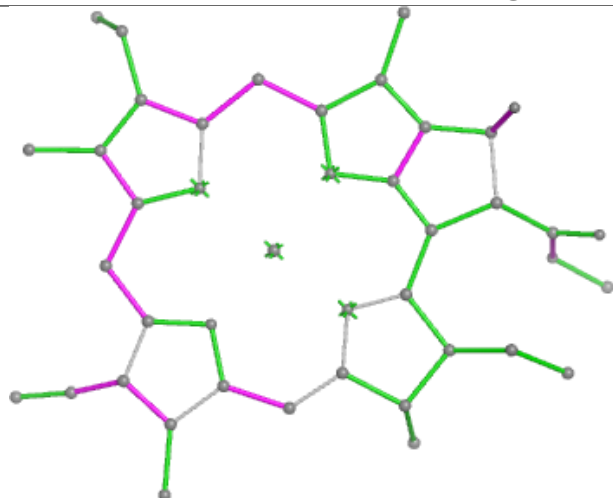


## Ligand LMU A 7020

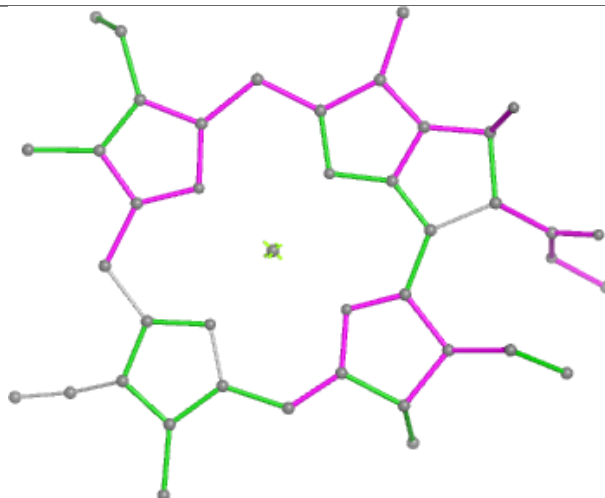




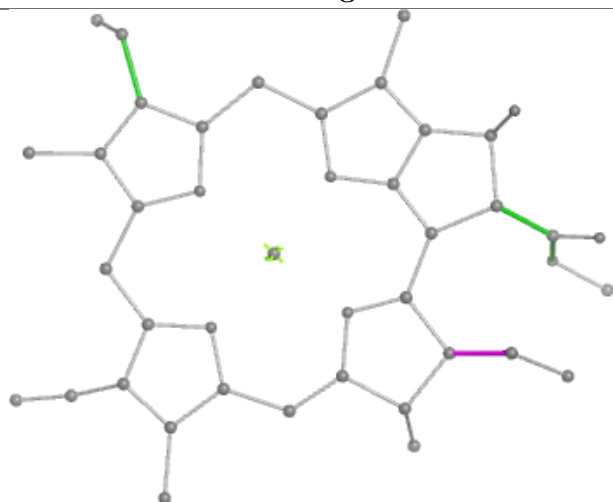
## Ligand CLA A 1778



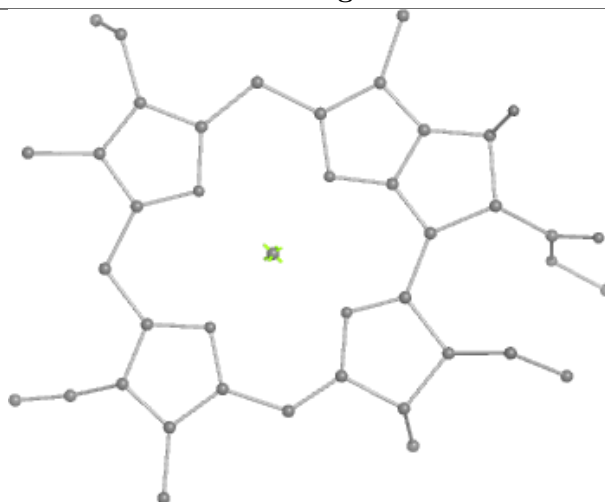
Bond lengths



Bond angles

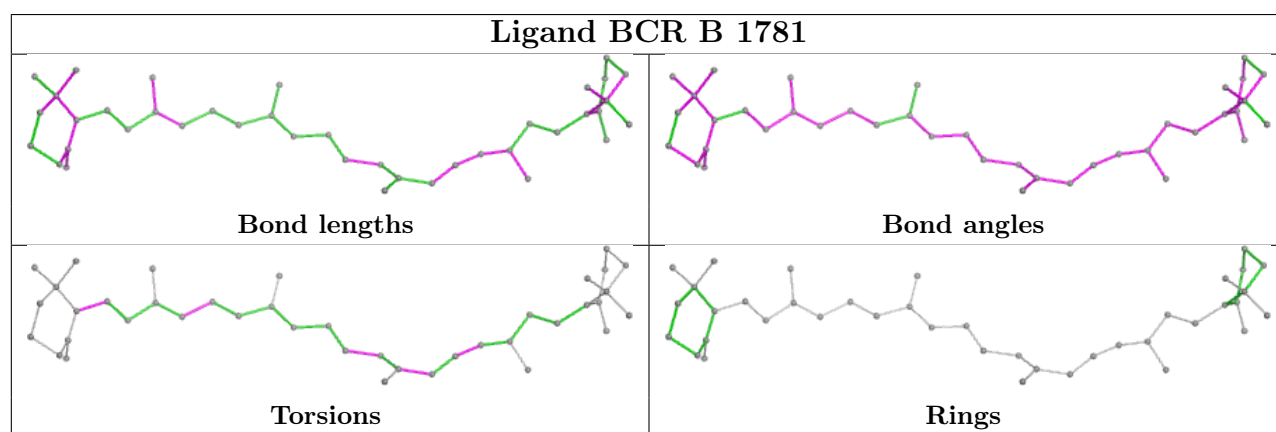
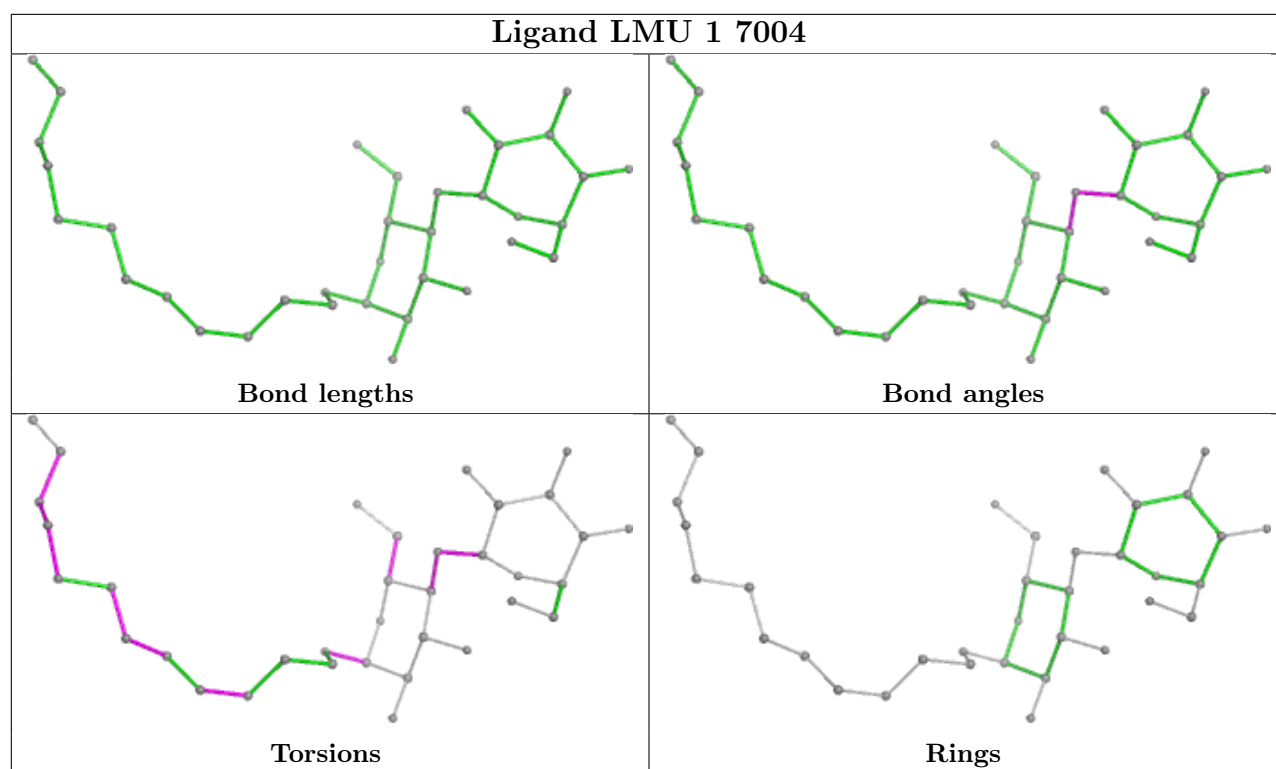


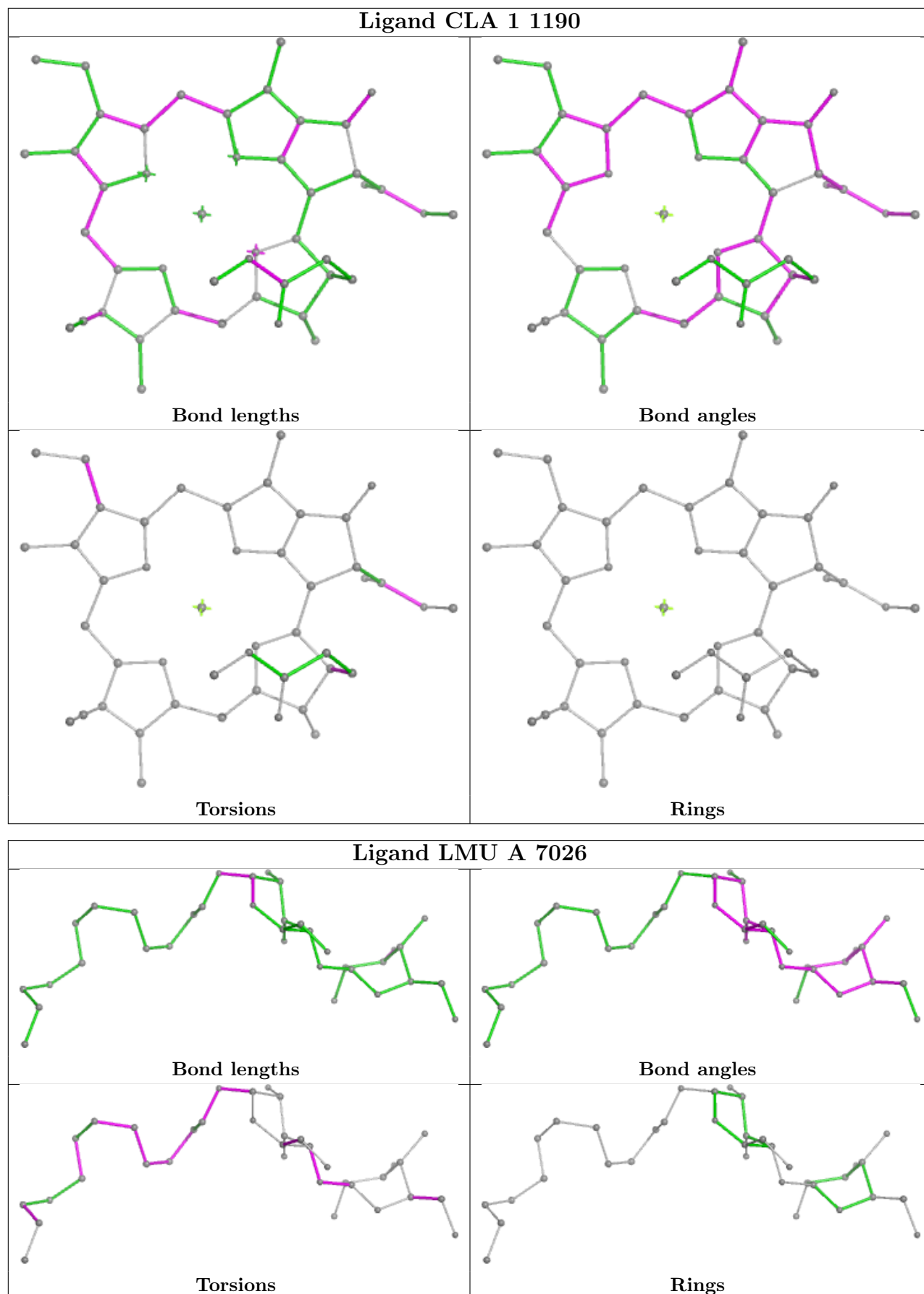
Torsions

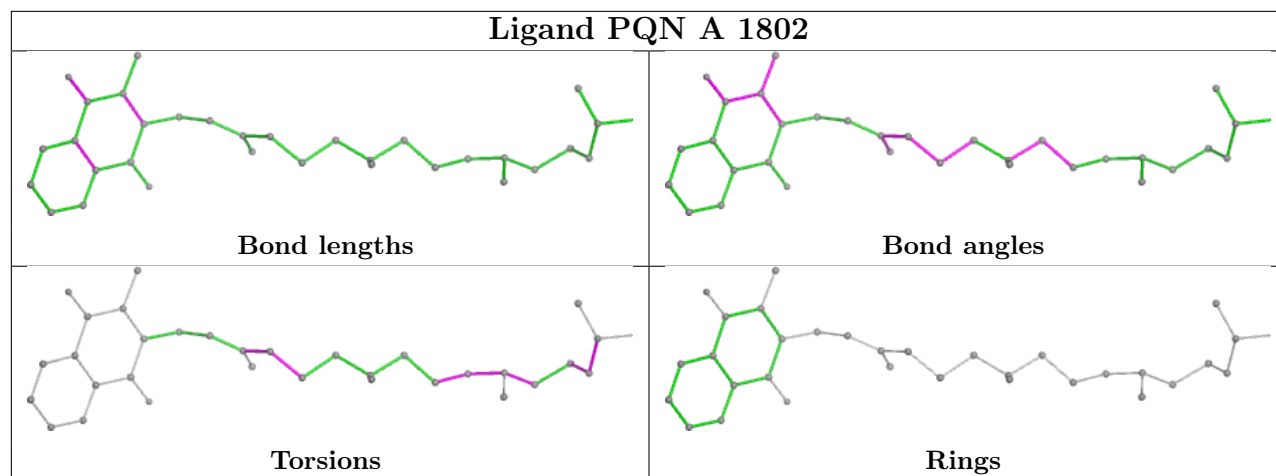


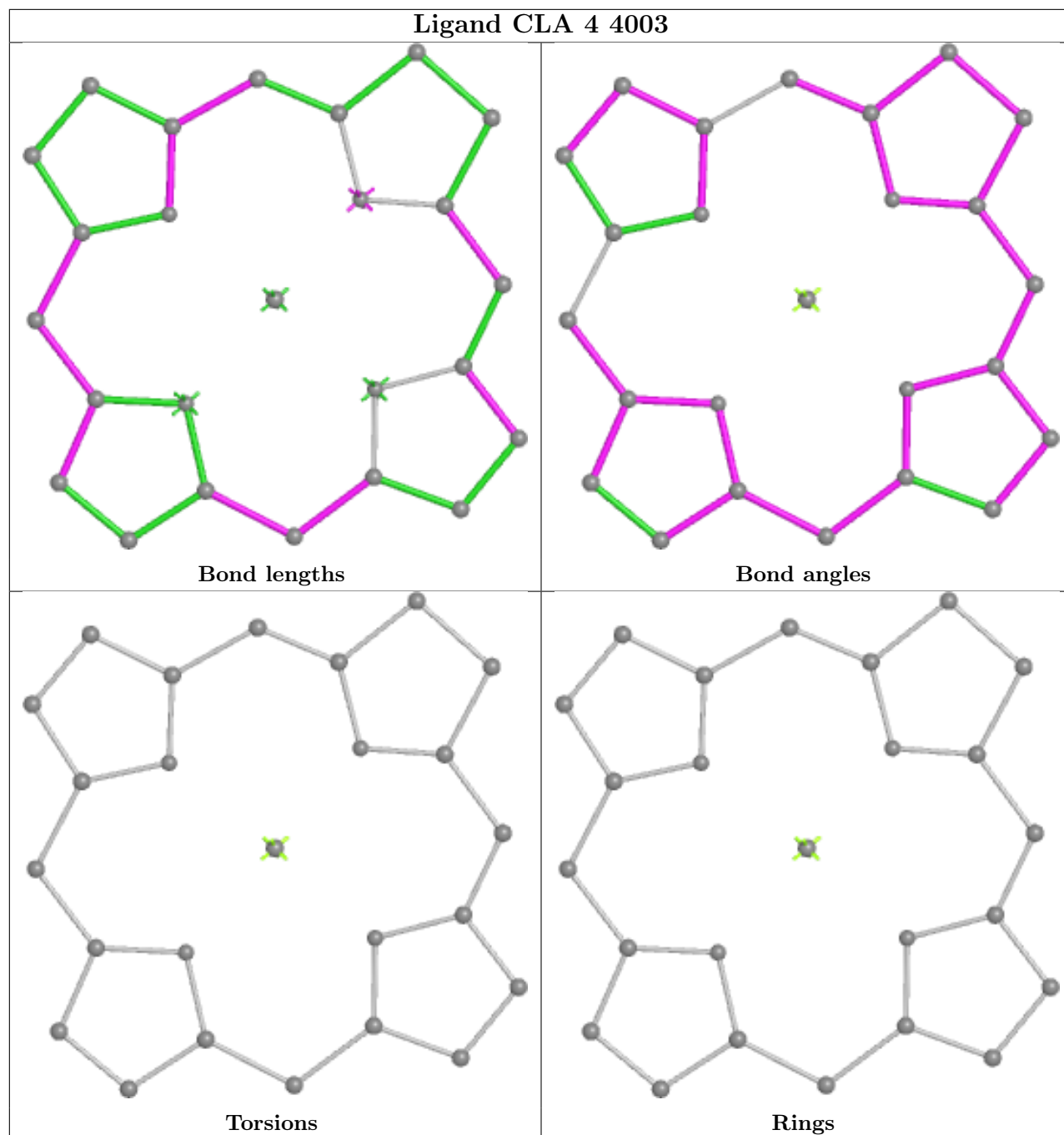
Rings

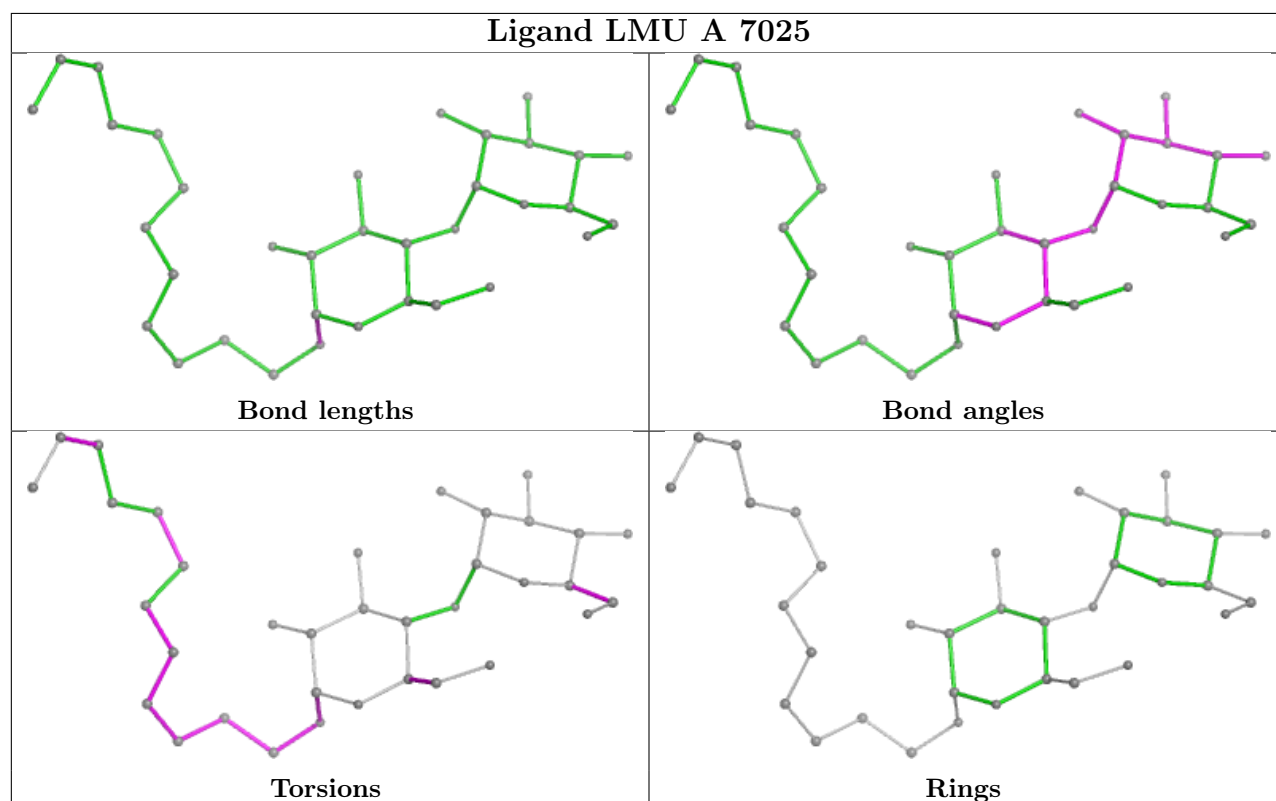
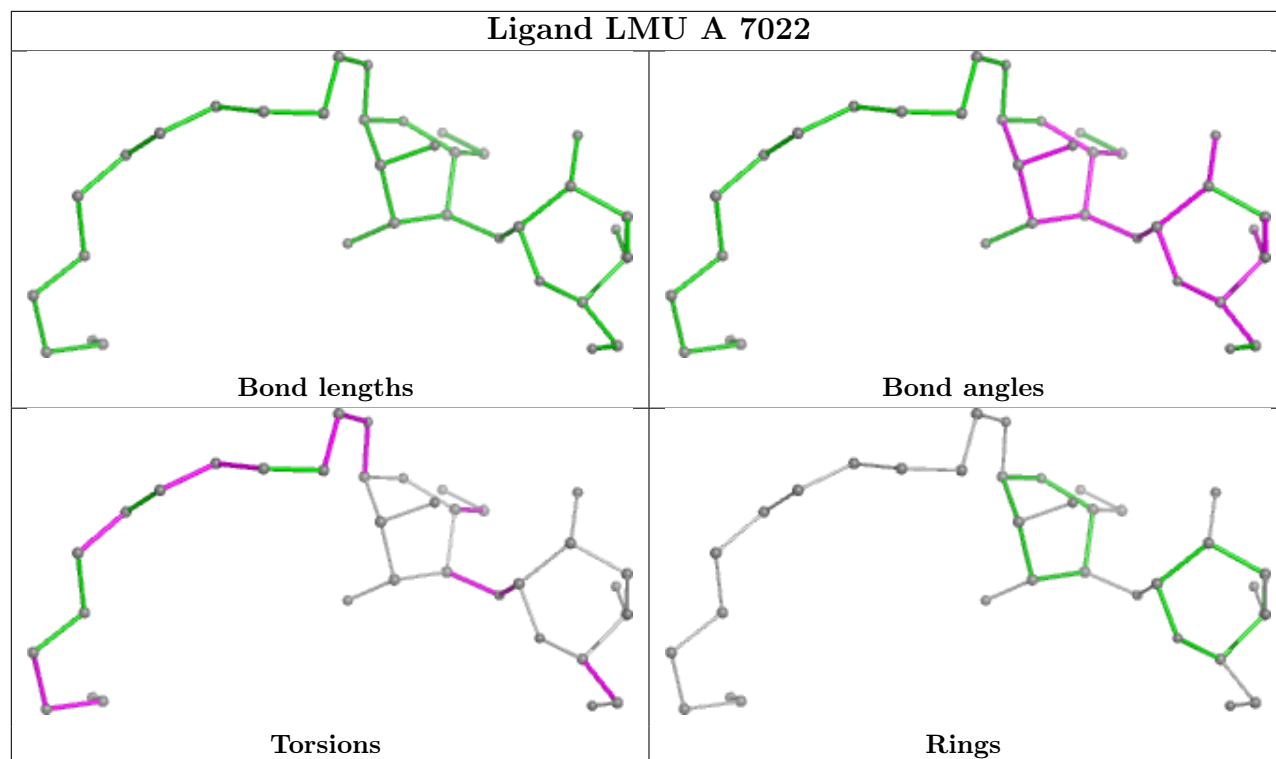


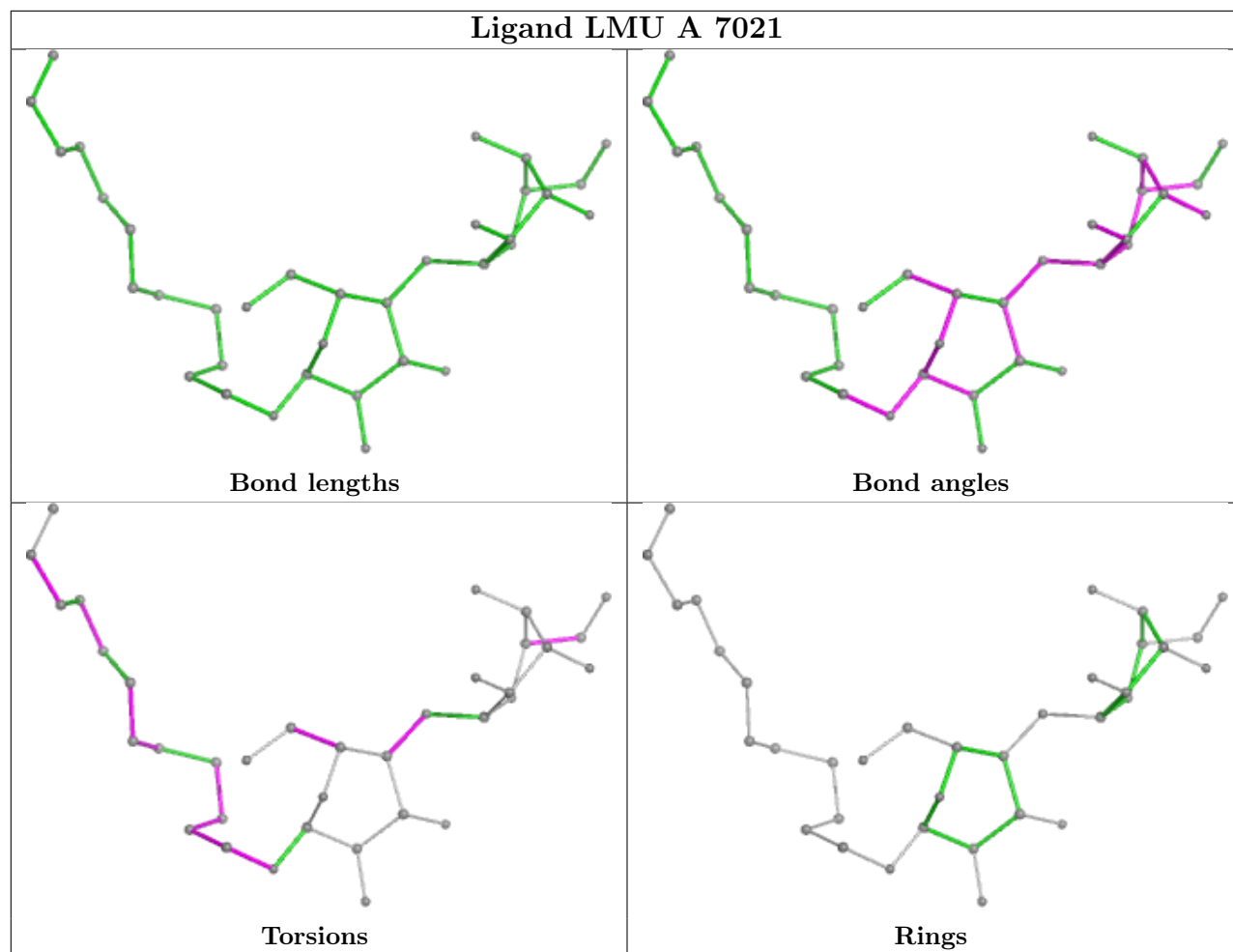




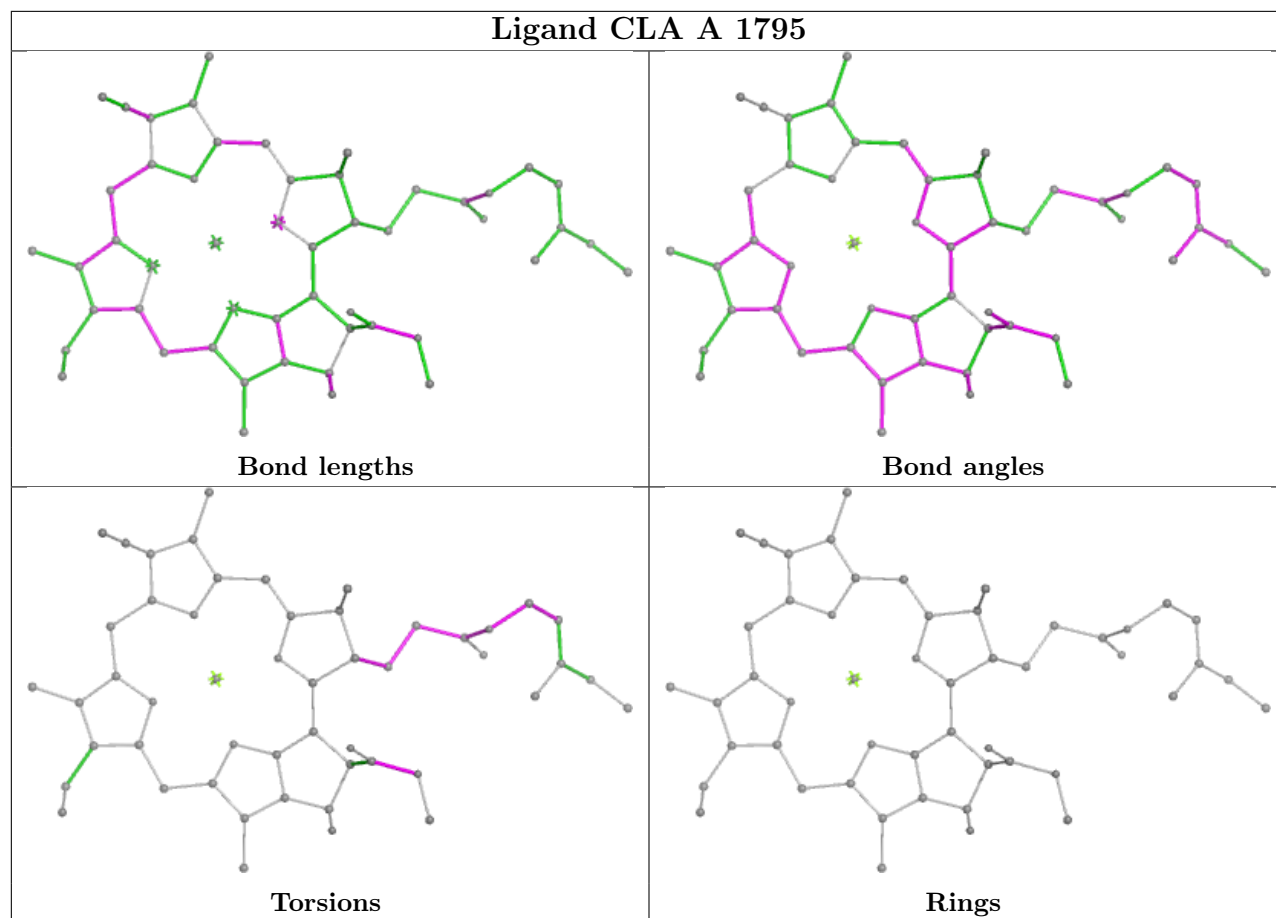


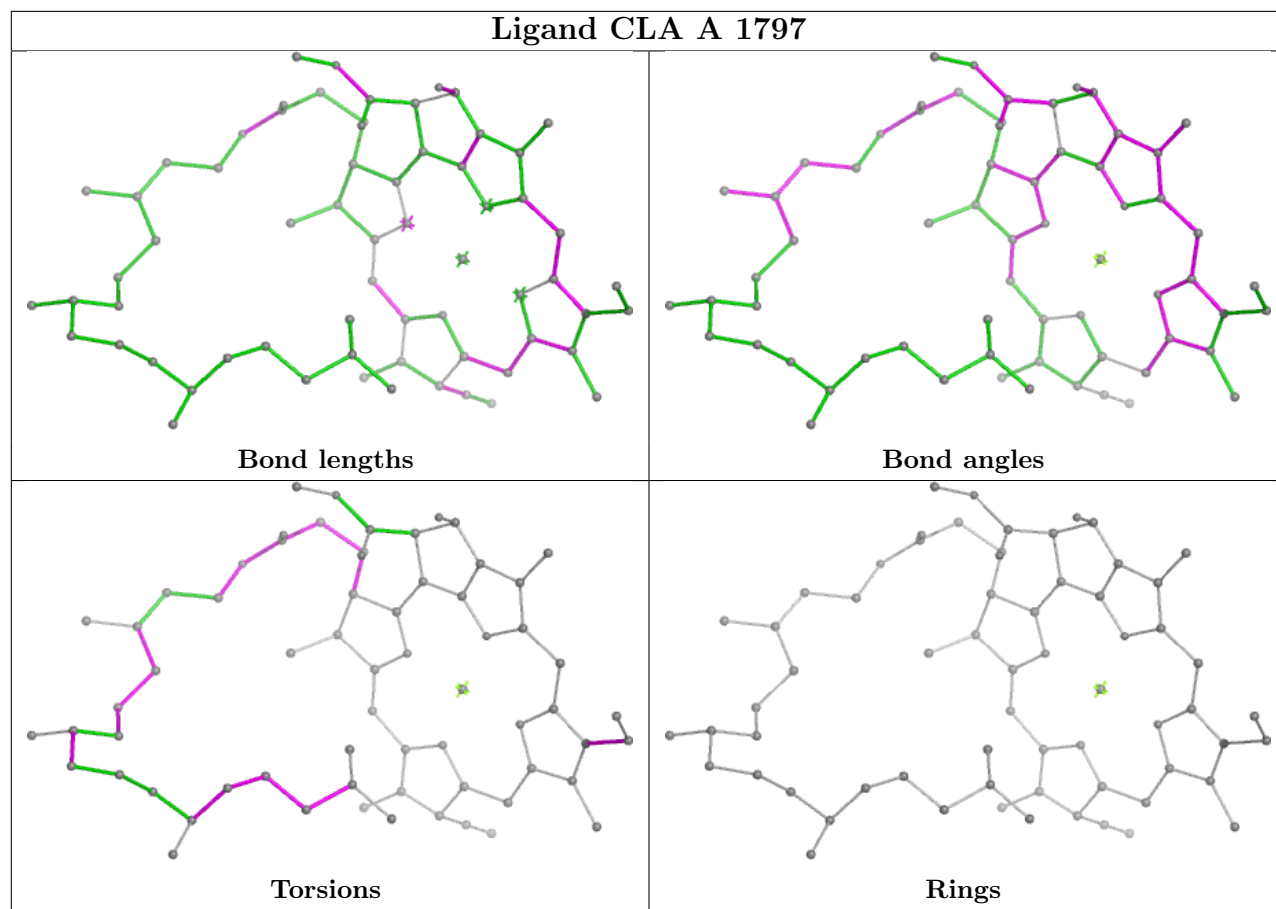




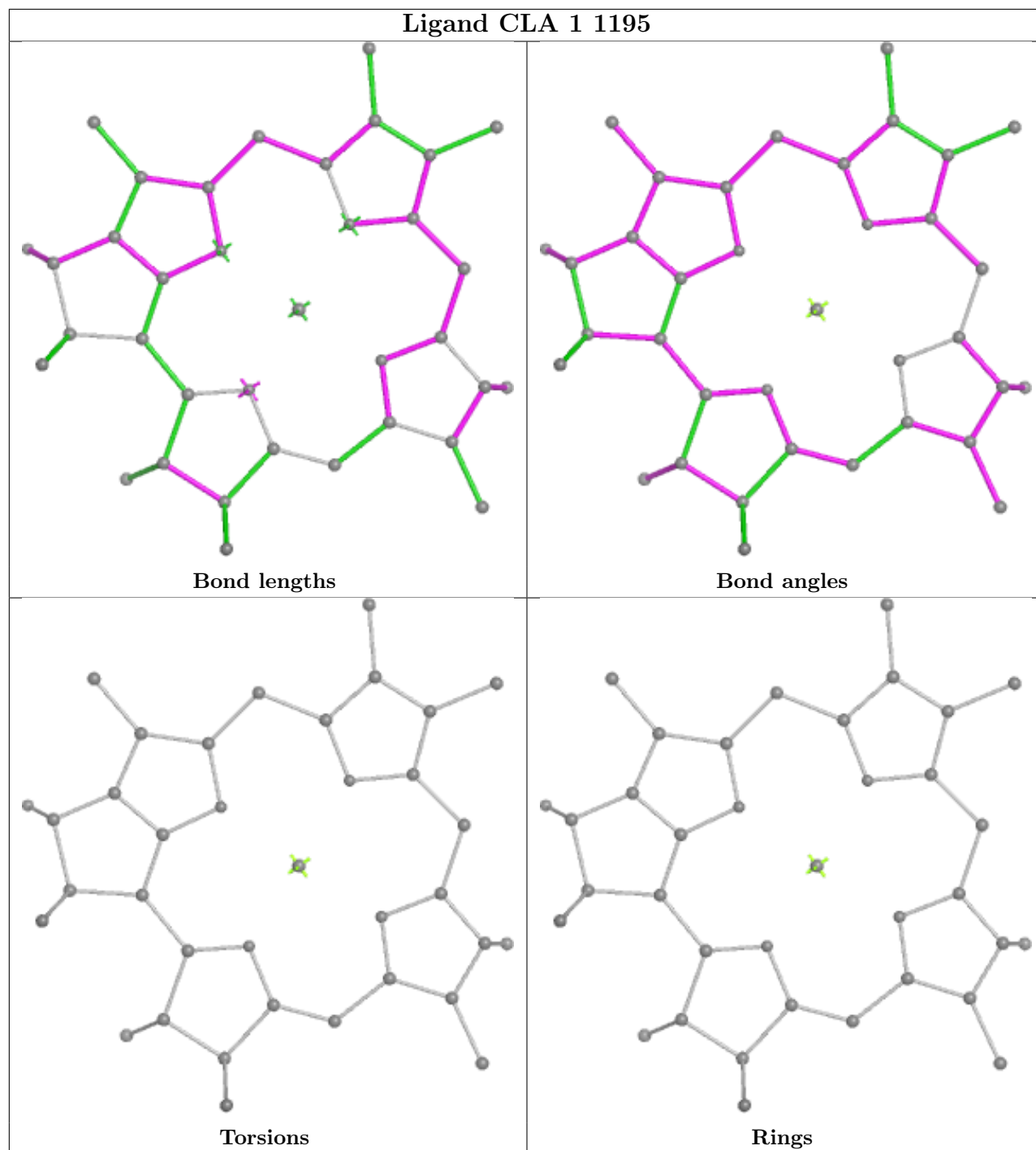


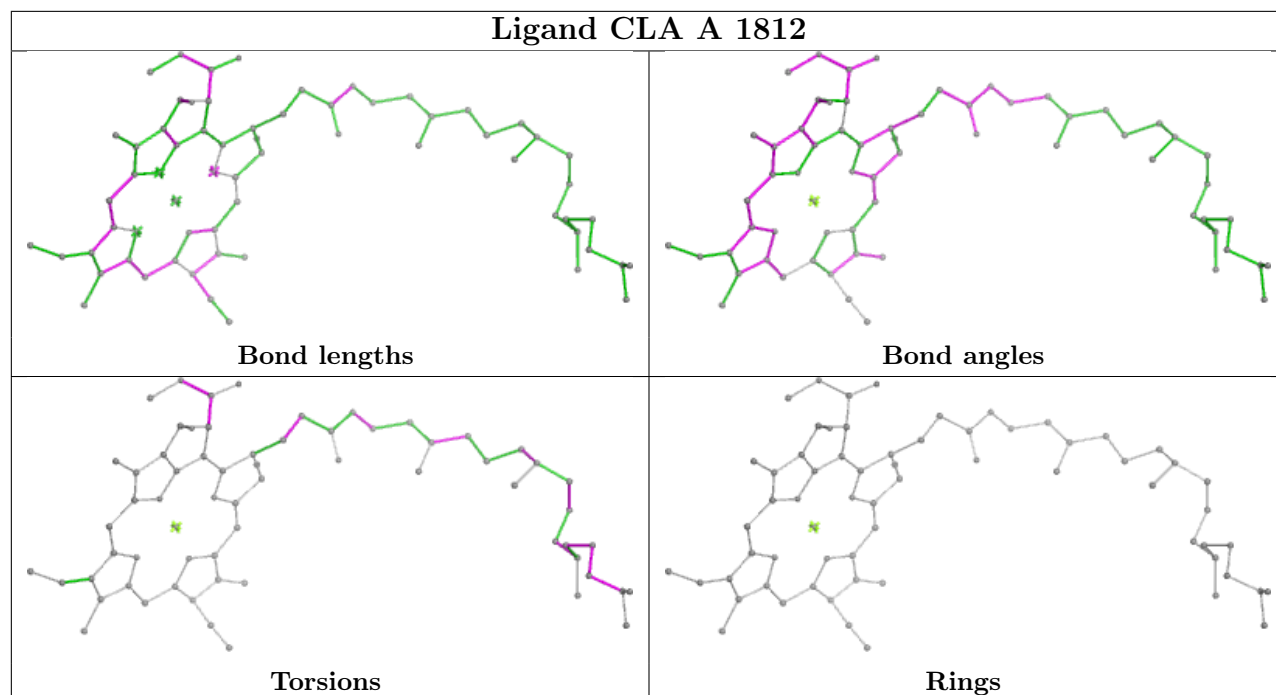
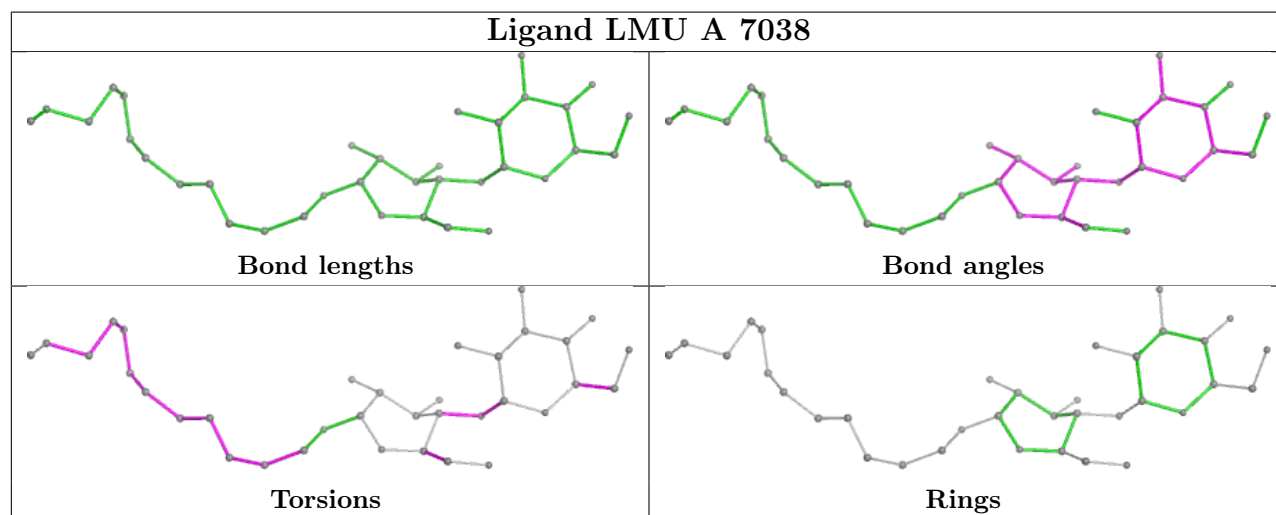
## Ligand CLA A 1795

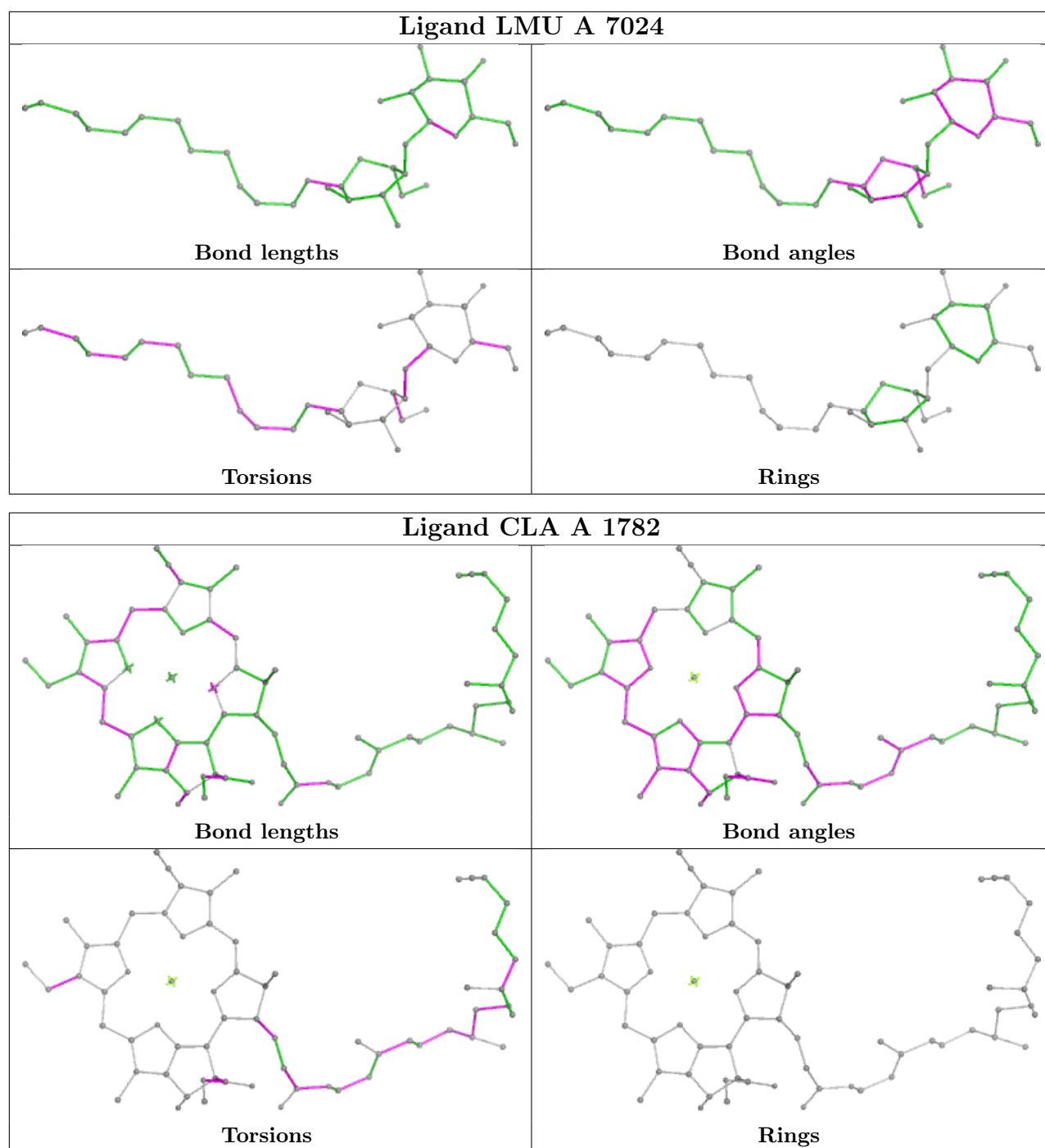








**Ligand CLA A 1812****Ligand LMU A 7038**



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	317:TYR	C	318:ARG	N	1.17

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	165/241 (68%)	2.32	86 (52%) 0 0	31, 61, 71, 72	0
2	2	176/269 (65%)	1.82	60 (34%) 1 1	33, 52, 64, 68	0
3	3	162/276 (58%)	2.26	82 (50%) 0 0	49, 79, 110, 112	0
4	4	166/251 (66%)	1.81	58 (34%) 1 1	21, 44, 57, 58	0
5	A	730/758 (96%)	1.29	141 (19%) 4 3	20, 20, 20, 20	0
6	B	733/734 (99%)	1.36	160 (21%) 3 2	20, 20, 20, 20	0
7	C	81/81 (100%)	1.71	27 (33%) 1 1	20, 20, 20, 20	0
8	D	138/212 (65%)	1.00	15 (10%) 12 12	20, 20, 20, 20	0
9	E	65/143 (45%)	0.98	8 (12%) 9 9	20, 20, 20, 20	0
10	F	154/231 (66%)	1.01	26 (16%) 5 4	20, 20, 20, 20	0
11	G	95/167 (56%)	0.76	7 (7%) 22 19	20, 20, 20, 20	0
12	H	69/144 (47%)	0.88	6 (8%) 17 16	20, 20, 20, 20	0
13	I	30/40 (75%)	0.42	0 100 100	20, 20, 20, 20	0
14	J	42/44 (95%)	0.79	1 (2%) 59 44	20, 20, 20, 20	0
15	K	84/131 (64%)	0.93	7 (8%) 19 17	20, 20, 20, 20	0
16	L	161/216 (74%)	1.01	27 (16%) 5 4	20, 20, 20, 20	0
17	N	85/170 (50%)	0.35	3 (3%) 47 35	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3136/4161 (75%)	1.36	714 (22%) 2 2	20, 20, 65, 112	0

All (714) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	B	491	ASN	11.1
2	2	123	PRO	10.7
1	1	92	GLY	9.6

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Mol	Chain	Res	Type	RSRZ
1	1	75	ALA	8.5
1	1	113	SER	8.5
5	A	266	ALA	8.4
5	A	220	ARG	8.3
1	1	42	SER	8.1
5	A	344	LYS	8.1
5	A	388	ASP	7.9
6	B	562	PRO	7.7
3	3	72	ALA	7.7
4	4	114	SER	7.6
5	A	505	PRO	7.6
5	A	617	SER	7.4
3	3	58	GLU	7.2
4	4	68	GLY	7.1
4	4	67	ILE	7.0
6	B	558	PRO	6.9
6	B	170	ASN	6.8
6	B	223	GLY	6.7
2	2	110	TRP	6.4
2	2	173	ALA	6.4
15	K	16	THR	6.2
5	A	126	ILE	6.2
5	A	610	SER	6.1
6	B	676	GLU	6.0
16	L	117	ALA	6.0
5	A	33	GLN	6.0
3	3	55	ALA	6.0
1	1	28	GLY	5.9
6	B	563	GLY	5.9
5	A	724	ALA	5.9
3	3	122	GLY	5.8
3	3	42	PRO	5.7
5	A	381	PRO	5.7
5	A	487	VAL	5.6
6	B	561	GLY	5.6
6	B	517	PHE	5.6
1	1	34	ALA	5.6
7	C	80	ALA	5.6
5	A	272	LEU	5.5
5	A	514	THR	5.4
1	1	32	VAL	5.4
3	3	40	SER	5.4

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Mol	Chain	Res	Type	RSRZ
1	1	33	PRO	5.3
6	B	584	LEU	5.3
5	A	659	ALA	5.3
5	A	752	ALA	5.3
4	4	73	PRO	5.3
5	A	191	PRO	5.3
5	A	470	LEU	5.3
6	B	258	LEU	5.2
1	1	41	GLU	5.2
5	A	518	GLY	5.2
6	B	527	LEU	5.2
4	4	125	SER	5.1
3	3	180	LYS	5.1
2	2	92	THR	5.1
6	B	484	PRO	5.1
1	1	46	HIS	5.0
3	3	75	PRO	5.0
16	L	80	ALA	5.0
6	B	292	ARG	5.0
1	1	19	PRO	4.9
3	3	91	PRO	4.9
3	3	54	LEU	4.9
3	3	83	LEU	4.9
2	2	53	ARG	4.9
3	3	80	LYS	4.8
2	2	119	VAL	4.8
3	3	67	LEU	4.8
7	C	9	ASP	4.7
2	2	169	LEU	4.7
5	A	185	HIS	4.7
2	2	43	TRP	4.7
5	A	484	LEU	4.7
5	A	485	GLN	4.7
6	B	470	THR	4.6
2	2	117	GLY	4.6
6	B	679	ALA	4.6
4	4	147	LEU	4.6
2	2	165	LYS	4.6
5	A	751	LEU	4.6
2	2	125	PHE	4.5
3	3	71	GLY	4.5
1	1	87	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
2	2	122	ASP	4.5
6	B	69	ALA	4.5
6	B	252	THR	4.5
6	B	271	THR	4.5
4	4	69	ILE	4.4
5	A	340	GLY	4.4
3	3	92	TRP	4.4
5	A	385	LEU	4.4
5	A	124	TRP	4.4
1	1	172	GLY	4.4
2	2	140	GLY	4.4
4	4	132	GLY	4.4
6	B	260	GLY	4.4
3	3	73	ILE	4.3
1	1	24	PHE	4.3
3	3	196	GLY	4.3
10	F	152	ASN	4.3
2	2	116	PRO	4.3
3	3	84	ILE	4.3
5	A	750	PHE	4.3
5	A	130	GLU	4.2
1	1	88	PRO	4.2
1	1	78	PRO	4.2
1	1	38	ARG	4.2
1	1	44	LEU	4.2
1	1	43	GLU	4.2
1	1	39	TYR	4.1
6	B	93	ASP	4.1
5	A	745	THR	4.1
6	B	171	ALA	4.1
2	2	141	LEU	4.1
3	3	78	LEU	4.1
5	A	329	ASP	4.1
5	A	391	THR	4.1
6	B	486	LEU	4.1
6	B	300	SER	4.1
1	1	117	ASP	4.0
5	A	433	ASP	4.0
6	B	212	PHE	4.0
6	B	272	ASP	4.0
1	1	152	ARG	4.0
3	3	187	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	1	37	GLU	4.0
6	B	205	GLU	4.0
7	C	41	SER	3.9
1	1	164	GLN	3.9
2	2	58	GLY	3.9
3	3	65	ALA	3.9
1	1	95	PRO	3.9
6	B	233	TYR	3.9
3	3	79	GLY	3.9
3	3	190	ALA	3.9
5	A	32	GLU	3.8
4	4	86	SER	3.8
8	D	141	VAL	3.8
1	1	129	ASP	3.8
4	4	135	GLY	3.8
4	4	63	VAL	3.8
3	3	68	GLY	3.8
1	1	94	LEU	3.8
4	4	93	ILE	3.8
6	B	667	TRP	3.8
6	B	702	ILE	3.8
6	B	682	HIS	3.8
3	3	82	GLY	3.7
6	B	147	PHE	3.7
3	3	181	LEU	3.7
6	B	367	THR	3.7
2	2	78	SER	3.7
5	A	160	SER	3.7
3	3	77	ILE	3.7
1	1	26	PRO	3.7
4	4	97	LEU	3.6
6	B	458	ILE	3.6
5	A	359	SER	3.6
5	A	247	GLU	3.6
5	A	376	MET	3.6
4	4	115	VAL	3.6
3	3	114	PHE	3.6
3	3	64	TYR	3.6
1	1	148	ILE	3.6
4	4	34	PRO	3.6
4	4	145	PRO	3.6
5	A	500	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
8	D	99	GLN	3.5
4	4	118	ASP	3.5
3	3	66	MET	3.5
5	A	265	GLY	3.5
3	3	199	VAL	3.5
6	B	502	ASN	3.5
3	3	107	TRP	3.5
3	3	184	VAL	3.5
8	D	108	GLU	3.5
1	1	169	PRO	3.5
2	2	170	ALA	3.5
6	B	255	LEU	3.5
6	B	40	GLY	3.5
3	3	60	ILE	3.5
1	1	173	PRO	3.5
8	D	71	GLY	3.5
7	C	6	LYS	3.5
6	B	346	SER	3.5
7	C	4	SER	3.5
2	2	55	ALA	3.5
5	A	471	GLY	3.5
5	A	707	ILE	3.5
6	B	560	ASP	3.5
1	1	79	GLY	3.4
16	L	159	TYR	3.4
4	4	89	THR	3.4
5	A	203	LEU	3.4
6	B	574	ASP	3.4
12	H	47	PHE	3.4
1	1	93	THR	3.4
6	B	350	GLN	3.4
5	A	657	LEU	3.4
1	1	55	PRO	3.4
5	A	527	VAL	3.4
10	F	111	GLU	3.4
4	4	104	ARG	3.4
10	F	64	GLY	3.4
4	4	117	GLN	3.3
6	B	610	ASN	3.3
5	A	181	ALA	3.3
5	A	584	PRO	3.3
6	B	645	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	2	163	GLU	3.3
16	L	81	GLY	3.3
10	F	76	ASP	3.3
5	A	662	SER	3.3
3	3	81	ALA	3.3
6	B	513	GLY	3.3
6	B	566	GLY	3.3
6	B	132	ASN	3.3
1	1	27	LEU	3.3
5	A	568	LEU	3.3
6	B	556	SER	3.3
15	K	53	ALA	3.3
7	C	54	CYS	3.3
5	A	299	ILE	3.3
6	B	492	ILE	3.3
5	A	635	THR	3.3
10	F	110	ASP	3.3
5	A	510	SER	3.3
5	A	494	ASN	3.3
8	D	137	ILE	3.3
4	4	126	LEU	3.3
10	F	107	ALA	3.2
4	4	109	ILE	3.2
6	B	457	PRO	3.2
9	E	84	LEU	3.2
1	1	74	TRP	3.2
6	B	183	PHE	3.2
2	2	157	LYS	3.2
7	C	78	GLY	3.2
6	B	319	HIS	3.2
1	1	47	CYS	3.2
3	3	191	MET	3.2
16	L	69	VAL	3.2
4	4	39	TRP	3.2
6	B	453	ILE	3.2
6	B	690	LEU	3.2
5	A	440	ASP	3.2
1	1	51	MET	3.2
2	2	166	ASN	3.2
2	2	138	PRO	3.1
2	2	139	GLY	3.1
1	1	134	SER	3.1

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Mol	Chain	Res	Type	RSRZ
6	B	113	VAL	3.1
1	1	175	GLU	3.1
6	B	262	HIS	3.1
1	1	84	TYR	3.1
1	1	105	ILE	3.1
5	A	249	ILE	3.1
6	B	263	PRO	3.1
5	A	157	GLY	3.1
5	A	517	GLY	3.1
1	1	21	ASP	3.1
1	1	35	ASN	3.1
3	3	53	TRP	3.1
5	A	34	TRP	3.1
16	L	65	VAL	3.1
6	B	274	ALA	3.1
6	B	570	ILE	3.1
5	A	128	GLY	3.1
5	A	345	GLY	3.1
3	3	113	LEU	3.1
8	D	86	LEU	3.1
1	1	82	ALA	3.1
1	1	130	PRO	3.0
1	1	111	GLN	3.0
1	1	76	ALA	3.0
7	C	8	TYR	3.0
3	3	76	GLU	3.0
5	A	293	GLY	3.0
14	J	4	PHE	3.0
8	D	151	LYS	3.0
4	4	157	GLY	3.0
5	A	182	GLY	3.0
1	1	150	ASN	3.0
2	2	191	ASN	3.0
5	A	71	LEU	3.0
2	2	182	ILE	3.0
6	B	208	ARG	3.0
16	L	96	SER	3.0
5	A	643	ALA	3.0
4	4	83	TYR	3.0
4	4	133	TYR	3.0
8	D	116	ASP	3.0
3	3	89	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
16	L	115	ALA	3.0
6	B	321	GLY	2.9
12	H	76	VAL	2.9
11	G	27	GLN	2.9
6	B	734	GLY	2.9
7	C	67	VAL	2.9
7	C	56	SER	2.9
3	3	90	LEU	2.9
10	F	124	PRO	2.9
1	1	40	LYS	2.9
3	3	173	GLU	2.9
4	4	66	SER	2.9
1	1	36	LEU	2.9
16	L	116	PRO	2.9
5	A	497	ALA	2.9
7	C	11	CYS	2.9
3	3	115	VAL	2.9
4	4	142	ASN	2.9
6	B	217	PRO	2.9
2	2	113	ILE	2.9
2	2	179	PHE	2.9
1	1	96	THR	2.8
1	1	145	VAL	2.8
4	4	101	VAL	2.8
4	4	131	VAL	2.8
2	2	210	PRO	2.8
1	1	112	ARG	2.8
3	3	95	THR	2.8
5	A	551	VAL	2.8
7	C	5	VAL	2.8
5	A	100	GLY	2.8
2	2	152	SER	2.8
4	4	50	TRP	2.8
5	A	586	ARG	2.8
15	K	44	GLU	2.8
5	A	693	LEU	2.8
5	A	341	GLN	2.8
6	B	181	GLY	2.8
5	A	486	PRO	2.8
5	A	532	ILE	2.8
6	B	337	ALA	2.8
5	A	264	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
5	A	362	LEU	2.8
6	B	135	LEU	2.8
16	L	86	LEU	2.8
6	B	131	THR	2.8
7	C	10	THR	2.8
2	2	181	HIS	2.8
10	F	63	CYS	2.8
17	N	77	CYS	2.8
3	3	116	PHE	2.8
5	A	360	ILE	2.8
6	B	493	TRP	2.8
1	1	140	LEU	2.8
2	2	114	LEU	2.8
3	3	125	GLU	2.8
5	A	304	LEU	2.8
6	B	620	LEU	2.8
6	B	366	THR	2.8
5	A	588	GLY	2.8
2	2	205	PHE	2.8
5	A	106	TYR	2.7
9	E	56	ASP	2.7
16	L	134	ASP	2.7
7	C	60	THR	2.7
10	F	98	GLY	2.7
2	2	207	ALA	2.7
5	A	386	ALA	2.7
7	C	17	CYS	2.7
6	B	555	TYR	2.7
10	F	135	SER	2.7
12	H	30	SER	2.7
4	4	134	PRO	2.7
5	A	263	ALA	2.7
5	A	509	ALA	2.7
3	3	202	LEU	2.7
6	B	568	CYS	2.7
16	L	93	VAL	2.7
5	A	248	PHE	2.7
7	C	37	LYS	2.7
15	K	49	THR	2.7
5	A	744	ALA	2.7
3	3	104	TYR	2.7
6	B	197	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	3	117	GLU	2.7
5	A	407	ILE	2.7
1	1	146	LYS	2.7
6	B	732	LYS	2.7
3	3	69	ALA	2.7
3	3	74	ALA	2.7
6	B	427	LEU	2.7
6	B	582	TRP	2.7
9	E	74	TYR	2.7
7	C	55	GLU	2.6
3	3	93	PHE	2.6
5	A	196	PHE	2.6
1	1	186	HIS	2.6
10	F	32	TYR	2.6
1	1	45	ILE	2.6
6	B	251	GLY	2.6
6	B	397	ASP	2.6
6	B	642	SER	2.6
12	H	26	SER	2.6
4	4	36	ASN	2.6
6	B	210	ASN	2.6
16	L	82	ALA	2.6
1	1	81	GLN	2.6
11	G	74	TRP	2.6
5	A	749	PHE	2.6
4	4	51	ALA	2.6
6	B	448	THR	2.6
1	1	159	VAL	2.6
7	C	52	LYS	2.6
4	4	161	LEU	2.6
10	F	143	GLU	2.6
2	2	206	ALA	2.6
5	A	607	ASN	2.6
5	A	685	VAL	2.6
6	B	67	HIS	2.6
9	E	66	VAL	2.6
4	4	110	LYS	2.6
1	1	18	ALA	2.6
1	1	115	GLU	2.6
3	3	43	GLU	2.6
3	3	126	HIS	2.6
4	4	192	THR	2.6

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Mol	Chain	Res	Type	RSRZ
6	B	114	ASN	2.6
2	2	164	ILE	2.5
6	B	632	ILE	2.5
6	B	358	TYR	2.5
1	1	64	GLY	2.5
8	D	63	GLY	2.5
16	L	84	GLY	2.5
2	2	175	MET	2.5
1	1	83	THR	2.5
2	2	133	THR	2.5
3	3	112	THR	2.5
6	B	511	THR	2.5
4	4	47	ASN	2.5
6	B	487	ASN	2.5
5	A	153	TRP	2.5
6	B	498	LEU	2.5
6	B	291	TYR	2.5
6	B	221	GLY	2.5
3	3	166	PRO	2.5
5	A	77	LYS	2.5
7	C	25	VAL	2.5
2	2	62	ILE	2.5
7	C	12	ILE	2.5
6	B	569	ASP	2.5
6	B	724	PHE	2.5
16	L	88	ALA	2.5
17	N	2	VAL	2.5
4	4	70	ILE	2.5
6	B	12	ILE	2.5
3	3	120	LEU	2.5
5	A	270	PHE	2.5
6	B	340	SER	2.5
5	A	354	TRP	2.5
4	4	174	GLY	2.5
6	B	259	GLY	2.5
5	A	45	ALA	2.5
5	A	245	PRO	2.5
6	B	454	LEU	2.5
10	F	62	LEU	2.5
6	B	98	GLN	2.5
6	B	118	SER	2.5
6	B	479	SER	2.5

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Mol	Chain	Res	Type	RSRZ
6	B	619	TRP	2.5
8	D	50	TRP	2.5
5	A	49	ASP	2.5
1	1	50	ALA	2.5
3	3	108	ALA	2.5
4	4	124	TYR	2.5
4	4	144	ALA	2.5
5	A	384	TYR	2.5
6	B	303	TYR	2.5
3	3	70	VAL	2.5
4	4	172	VAL	2.5
1	1	181	LEU	2.4
3	3	123	PHE	2.4
2	2	121	THR	2.4
4	4	122	LYS	2.4
6	B	27	THR	2.4
17	N	56	LYS	2.4
1	1	72	GLN	2.4
1	1	80	GLY	2.4
2	2	87	TYR	2.4
5	A	198	ASP	2.4
5	A	122	VAL	2.4
6	B	438	VAL	2.4
9	E	65	VAL	2.4
2	2	66	GLU	2.4
3	3	194	ILE	2.4
6	B	268	LEU	2.4
5	A	506	GLY	2.4
6	B	209	TRP	2.4
6	B	195	VAL	2.4
6	B	670	TYR	2.4
16	L	102	TYR	2.4
3	3	41	ASP	2.4
5	A	368	LEU	2.4
3	3	198	PHE	2.4
6	B	595	HIS	2.4
3	3	47	GLY	2.4
4	4	173	THR	2.4
8	D	34	GLY	2.4
1	1	106	ALA	2.4
5	A	127	VAL	2.4
1	1	177	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	3	189	LEU	2.4
4	4	181	LEU	2.4
5	A	743	ILE	2.4
5	A	98	PHE	2.4
6	B	31	PHE	2.4
6	B	29	HIS	2.4
5	A	696	GLY	2.4
1	1	178	ALA	2.4
2	2	59	ALA	2.4
2	2	50	VAL	2.4
6	B	343	VAL	2.4
5	A	660	GLN	2.4
6	B	608	GLN	2.4
9	E	82	TYR	2.4
6	B	613	SER	2.4
2	2	63	PHE	2.4
5	A	161	GLU	2.4
10	F	4	GLY	2.4
6	B	123	TRP	2.4
16	L	140	THR	2.4
6	B	347	LEU	2.3
1	1	31	GLU	2.3
6	B	559	CYS	2.3
16	L	78	GLU	2.3
6	B	204	GLY	2.3
5	A	195	TRP	2.3
5	A	548	THR	2.3
6	B	533	ILE	2.3
16	L	9	GLN	2.3
6	B	697	PRO	2.3
4	4	87	SER	2.3
4	4	62	GLU	2.3
5	A	682	ALA	2.3
10	F	101	GLY	2.3
16	L	34	ALA	2.3
5	A	567	ARG	2.3
1	1	58	LEU	2.3
2	2	54	TRP	2.3
6	B	341	LEU	2.3
6	B	469	LYS	2.3
6	B	478	LEU	2.3
7	C	69	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
10	F	6	THR	2.3
3	3	111	TYR	2.3
5	A	512	SER	2.3
2	2	176	GLY	2.3
3	3	151	GLY	2.3
5	A	123	VAL	2.3
10	F	73	VAL	2.3
3	3	98	ILE	2.3
1	1	165	GLN	2.3
3	3	201	ALA	2.3
6	B	423	SER	2.3
12	H	25	GLY	2.3
1	1	25	ASP	2.3
1	1	49	TRP	2.3
4	4	106	TRP	2.3
2	2	126	PRO	2.3
2	2	161	THR	2.3
6	B	8	PHE	2.3
1	1	53	ALA	2.3
6	B	473	GLY	2.3
15	K	65	ALA	2.3
5	A	705	GLU	2.3
6	B	354	SER	2.3
6	B	227	THR	2.2
6	B	261	PHE	2.2
9	E	79	THR	2.2
15	K	63	CYS	2.2
5	A	699	TYR	2.2
1	1	54	VAL	2.2
7	C	49	VAL	2.2
3	3	62	GLY	2.2
3	3	119	ALA	2.2
10	F	71	LEU	2.2
1	1	109	GLU	2.2
6	B	124	TRP	2.2
4	4	112	PRO	2.2
5	A	616	PHE	2.2
3	3	88	THR	2.2
5	A	461	TYR	2.2
5	A	516	GLY	2.2
6	B	713	PHE	2.2
4	4	105	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
6	B	694	ARG	2.2
5	A	589	THR	2.2
5	A	186	TYR	2.2
1	1	85	LEU	2.2
5	A	296	LEU	2.2
6	B	175	LEU	2.2
6	B	334	LEU	2.2
2	2	60	ALA	2.2
11	G	51	ALA	2.2
2	2	103	GLY	2.2
5	A	117	GLY	2.2
6	B	646	TRP	2.2
16	L	49	PRO	2.2
6	B	214	ASP	2.2
5	A	493	GLN	2.2
6	B	117	TYR	2.2
6	B	437	TYR	2.2
11	G	22	VAL	2.2
5	A	415	ALA	2.2
1	1	20	GLY	2.2
3	3	188	ARG	2.2
5	A	82	HIS	2.2
10	F	38	PRO	2.2
10	F	137	PRO	2.2
5	A	80	SER	2.2
6	B	420	SER	2.2
11	G	9	SER	2.2
2	2	159	LEU	2.2
4	4	59	LEU	2.2
5	A	733	VAL	2.2
8	D	33	THR	2.2
10	F	66	ASP	2.2
3	3	57	GLY	2.1
5	A	236	GLY	2.1
5	A	613	ILE	2.1
6	B	309	ILE	2.1
5	A	76	ARG	2.1
8	D	115	LYS	2.1
16	L	145	PHE	2.1
5	A	686	TRP	2.1
5	A	608	SER	2.1
6	B	571	SER	2.1

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Mol	Chain	Res	Type	RSRZ
6	B	701	SER	2.1
7	C	2	SER	2.1
16	L	106	SER	2.1
5	A	105	ASN	2.1
1	1	99	ALA	2.1
2	2	183	TYR	2.1
7	C	40	ALA	2.1
7	C	66	ARG	2.1
4	4	40	PHE	2.1
6	B	446	PHE	2.1
1	1	141	GLU	2.1
1	1	147	GLU	2.1
2	2	77	PRO	2.1
8	D	90	LEU	2.1
3	3	110	SER	2.1
6	B	567	THR	2.1
3	3	105	ASN	2.1
2	2	180	GLN	2.1
16	L	141	GLY	2.1
3	3	140	LYS	2.1
4	4	38	ARG	2.1
5	A	753	ARG	2.1
4	4	121	PHE	2.1
1	1	174	LEU	2.1
4	4	37	LEU	2.1
16	L	118	LEU	2.1
1	1	89	VAL	2.1
5	A	219	ALA	2.1
6	B	250	ALA	2.1
6	B	658	ALA	2.1
5	A	143	ILE	2.1
5	A	353	SER	2.1
8	D	32	SER	2.1
10	F	11	SER	2.1
16	L	33	ILE	2.1
5	A	742	GLY	2.1
6	B	618	GLY	2.1
6	B	441	ASP	2.1
3	3	167	LEU	2.1
6	B	237	PRO	2.1
6	B	616	LEU	2.1
9	E	36	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
5	A	594	ALA	2.1
3	3	94	ARG	2.1
3	3	182	LYS	2.1
4	4	146	THR	2.1
11	G	5	SER	2.1
5	A	197	GLN	2.1
4	4	180	ASN	2.1
3	3	169	PHE	2.1
2	2	171	MET	2.1
6	B	655	LEU	2.1
16	L	101	MET	2.1
6	B	712	HIS	2.1
10	F	138	VAL	2.1
2	2	198	ALA	2.0
6	B	362	ALA	2.0
7	C	42	ALA	2.0
6	B	372	TYR	2.0
5	A	94	SER	2.0
5	A	217	SER	2.0
10	F	116	GLN	2.0
10	F	128	SER	2.0
6	B	332	PHE	2.0
10	F	35	ASP	2.0
5	A	371	VAL	2.0
2	2	109	ARG	2.0
6	B	573	TRP	2.0
6	B	621	ARG	2.0
6	B	657	TRP	2.0
6	B	116	ALA	2.0
6	B	455	ILE	2.0
6	B	723	ALA	2.0
15	K	27	ALA	2.0
2	2	89	THR	2.0
2	2	137	TYR	2.0
3	3	106	TYR	2.0
7	C	68	TYR	2.0
11	G	11	SER	2.0
12	H	22	ASP	2.0
6	B	625	TRP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	J	1046	25/65	0.43	0.17	5,42,60,60	0
22	BCR	A	1803	40/40	0.50	0.24	20,20,20,20	0
21	LMU	A	7013	35/35	0.57	0.16	20,20,20,20	0
20	CLA	L	1505	55/65	0.58	0.17	20,20,20,20	0
20	CLA	3	1217	25/65	0.58	0.19	20,20,20,20	0
20	CLA	1	1199	25/65	0.58	0.22	20,20,20,20	0
20	CLA	2	1218	65/65	0.59	0.18	20,20,20,20	0
22	BCR	A	1808	40/40	0.59	0.22	20,20,20,20	0
21	LMU	A	7037	35/35	0.60	0.18	20,20,20,20	0
20	CLA	2	1212	51/65	0.61	0.20	20,20,20,20	0
22	BCR	3	1220	40/40	0.61	0.19	20,20,20,20	0
20	CLA	4	4003	25/65	0.61	0.17	20,20,20,20	0
20	CLA	I	1033	55/65	0.61	0.16	20,20,20,20	0
21	LMU	2	1225	35/35	0.62	0.16	20,20,20,20	0
20	CLA	A	1797	65/65	0.62	0.17	20,20,20,20	0
20	CLA	B	1746	46/65	0.63	0.21	20,20,20,20	0
20	CLA	B	1766	51/65	0.63	0.17	20,20,20,20	0
20	CLA	3	1214	25/65	0.63	0.19	20,20,20,20	0
21	LMU	A	7041	35/35	0.63	0.16	20,20,20,20	0
20	CLA	3	1219	65/65	0.63	0.17	20,20,20,20	0
20	CLA	K	1142	45/65	0.63	0.16	20,20,20,20	0
20	CLA	A	1801	55/65	0.63	0.19	20,20,20,20	0
20	CLA	B	1745	60/65	0.64	0.18	20,20,20,20	0
21	LMU	1	7004	35/35	0.65	0.15	20,20,20,20	0
20	CLA	2	1216	25/65	0.65	0.17	20,20,20,20	0
20	CLA	4	4007	52/65	0.65	0.16	20,20,20,20	0
20	CLA	1	1191	36/65	0.65	0.15	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	J	1044	61/65	0.65	0.17	20,20,20,20	0
20	CLA	A	1799	50/65	0.65	0.15	20,20,20,20	0
20	CLA	2	1220	56/65	0.65	0.16	2,36,60,60	0
20	CLA	4	1200	50/65	0.65	0.19	20,20,20,20	0
20	CLA	3	3007	42/65	0.66	0.16	20,20,20,20	0
20	CLA	K	3009	65/65	0.67	0.17	20,20,20,20	0
21	LMU	A	7010	35/35	0.67	0.15	20,20,20,20	0
20	CLA	3	1218	65/65	0.67	0.17	20,20,20,20	0
20	CLA	4	4014	47/65	0.67	0.17	20,20,20,20	0
21	LMU	A	7017	35/35	0.68	0.13	20,20,20,20	0
20	CLA	B	1755	58/65	0.68	0.23	20,20,20,20	0
20	CLA	A	1816	55/65	0.68	0.14	20,20,20,20	0
21	LMU	A	7009	34/35	0.68	0.15	20,20,20,20	0
20	CLA	4	1196	55/65	0.68	0.17	20,20,20,20	0
22	BCR	A	1805	40/40	0.68	0.21	20,20,20,20	0
20	CLA	1	1198	61/65	0.68	0.15	2,35,60,60	0
20	CLA	R	1054	57/65	0.69	0.16	20,20,20,20	0
20	CLA	A	1815	55/65	0.69	0.14	20,20,20,20	0
21	LMU	A	7015	35/35	0.69	0.14	20,20,20,20	0
20	CLA	1	1197	51/65	0.69	0.15	20,20,20,20	0
20	CLA	F	1156	41/65	0.69	0.17	20,20,20,20	0
20	CLA	B	1765	45/65	0.70	0.15	20,20,20,20	0
20	CLA	J	1043	61/65	0.70	0.15	20,20,20,20	0
21	LMU	A	7043	35/35	0.70	0.13	20,20,20,20	0
20	CLA	4	1198	65/65	0.70	0.17	20,20,20,20	0
20	CLA	4	1199	55/65	0.70	0.16	20,20,20,20	0
20	CLA	G	1099	51/65	0.70	0.14	20,20,20,20	0
21	LMU	A	7034	35/35	0.70	0.15	20,20,20,20	0
21	LMU	A	1809	35/35	0.71	0.14	20,20,20,20	0
21	LMU	A	1810	35/35	0.71	0.14	20,20,20,20	0
21	LMU	A	7038	35/35	0.71	0.13	20,20,20,20	0
20	CLA	A	1766	45/65	0.71	0.16	20,20,20,20	0
20	CLA	A	1770	45/65	0.71	0.19	20,20,20,20	0
20	CLA	A	1791	45/65	0.71	0.16	20,20,20,20	0
20	CLA	1	1193	51/65	0.71	0.14	20,20,20,20	0
20	CLA	1	1200	51/65	0.71	0.15	20,20,20,20	0
21	LMU	A	7030	35/35	0.71	0.12	20,20,20,20	0
20	CLA	3	1213	25/65	0.72	0.15	20,20,20,20	0
20	CLA	K	1146	50/65	0.72	0.14	20,20,20,20	0
21	LMU	A	7025	35/35	0.72	0.15	20,20,20,20	0
21	LMU	A	7027	35/35	0.72	0.13	20,20,20,20	0
20	CLA	A	1798	55/65	0.72	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	LMU	A	7031	35/35	0.72	0.13	20,20,20,20	0
20	CLA	2	1215	50/65	0.72	0.17	20,20,20,20	0
20	CLA	A	1763	46/65	0.72	0.17	20,20,20,20	0
20	CLA	F	1157	53/65	0.72	0.14	20,20,20,20	0
20	CLA	3	3001	25/65	0.72	0.15	20,20,20,20	0
20	CLA	2	1223	50/65	0.72	0.20	20,20,20,20	0
20	CLA	A	1775	36/65	0.72	0.15	20,20,20,20	0
20	CLA	3	3014	25/65	0.72	0.15	20,20,20,20	0
20	CLA	B	1751	46/65	0.72	0.19	20,20,20,20	0
20	CLA	K	1085	50/65	0.72	0.15	20,20,20,20	0
22	BCR	I	1032	40/40	0.72	0.15	20,20,20,20	0
20	CLA	2	1213	56/65	0.73	0.16	20,20,20,20	0
21	LMU	3	7005	35/35	0.73	0.14	20,20,20,20	0
21	LMU	A	7020	35/35	0.73	0.13	20,20,20,20	0
20	CLA	1	1187	46/65	0.73	0.14	20,20,20,20	0
21	LMU	A	7047	35/35	0.73	0.13	20,20,20,20	0
20	CLA	A	1780	65/65	0.73	0.24	20,20,20,20	0
21	LMU	A	7028	35/35	0.73	0.13	20,20,20,20	0
20	CLA	3	1215	25/65	0.73	0.15	20,20,20,20	0
20	CLA	3	3002	25/65	0.73	0.14	20,20,20,20	0
22	BCR	B	1776	40/40	0.73	0.18	20,20,20,20	0
22	BCR	B	1780	40/40	0.73	0.27	20,20,20,20	0
20	CLA	2	1227	25/65	0.73	0.13	20,20,20,20	0
20	CLA	2	1217	65/65	0.74	0.15	20,20,20,20	0
21	LMU	K	1086	35/35	0.74	0.12	20,20,20,20	0
20	CLA	4	1204	55/65	0.74	0.17	20,20,20,20	0
20	CLA	A	1778	42/65	0.74	0.14	20,20,20,20	0
20	CLA	4	1208	25/65	0.74	0.14	20,20,20,20	0
20	CLA	1	1194	25/65	0.74	0.15	20,20,20,20	0
20	CLA	R	1055	65/65	0.74	0.14	20,20,20,20	0
21	LMU	A	7042	35/35	0.74	0.14	20,20,20,20	0
21	LMU	1	1202	35/35	0.74	0.12	20,20,20,20	0
20	CLA	H	1079	65/65	0.75	0.20	20,20,20,20	0
20	CLA	L	1168	50/65	0.75	0.18	20,20,20,20	0
21	LMU	2	7003	35/35	0.75	0.13	20,20,20,20	0
22	BCR	A	1806	40/40	0.75	0.20	20,20,20,20	0
21	LMU	2	7006	35/35	0.75	0.13	20,20,20,20	0
21	LMU	A	7036	34/35	0.75	0.13	20,20,20,20	0
20	CLA	1	1192	61/65	0.75	0.14	20,20,20,20	0
21	LMU	R	1057	35/35	0.75	0.12	20,20,20,20	0
21	LMU	A	7019	35/35	0.76	0.12	20,20,20,20	0
20	CLA	1	1188	47/65	0.76	0.15	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	A	1817	46/65	0.76	0.13	20,20,20,20	0
21	LMU	B	1782	25/35	0.76	0.12	20,20,20,20	0
21	LMU	4	1210	35/35	0.76	0.12	20,20,20,20	0
20	CLA	3	1212	36/65	0.76	0.13	20,20,20,20	0
20	CLA	1	1189	47/65	0.76	0.14	20,20,20,20	0
24	LMG	B	1783	49/55	0.76	0.22	20,20,20,20	0
20	CLA	4	1203	25/65	0.77	0.15	20,20,20,20	0
20	CLA	3	3008	50/65	0.77	0.13	20,20,20,20	0
20	CLA	2	1224	65/65	0.77	0.15	20,20,20,20	0
20	CLA	L	1166	50/65	0.77	0.16	20,20,20,20	0
22	BCR	A	1804	40/40	0.77	0.18	20,20,20,20	0
20	CLA	B	1764	45/65	0.77	0.17	20,20,20,20	0
20	CLA	4	1209	46/65	0.77	0.13	20,20,20,20	0
22	BCR	A	1807	40/40	0.77	0.22	20,20,20,20	0
21	LMU	A	7021	35/35	0.77	0.12	20,20,20,20	0
22	BCR	B	1774	40/40	0.77	0.20	20,20,20,20	0
22	BCR	B	1775	40/40	0.77	0.20	20,20,20,20	0
21	LMU	A	7023	35/35	0.77	0.12	20,20,20,20	0
20	CLA	A	1767	65/65	0.77	0.18	20,20,20,20	0
20	CLA	B	1772	36/65	0.77	0.13	20,20,20,20	0
20	CLA	4	1202	25/65	0.77	0.15	20,20,20,20	0
20	CLA	A	1776	65/65	0.78	0.18	20,20,20,20	0
20	CLA	J	1045	55/65	0.78	0.13	2,33,60,60	0
20	CLA	B	1762	65/65	0.78	0.20	20,20,20,20	0
20	CLA	A	1771	50/65	0.78	0.15	20,20,20,20	0
20	CLA	A	1772	65/65	0.78	0.17	2,35,60,60	0
22	BCR	B	1779	40/40	0.78	0.18	20,20,20,20	0
20	CLA	A	1787	65/65	0.78	0.18	20,20,20,20	0
20	CLA	1	1195	36/65	0.78	0.14	20,20,20,20	0
22	BCR	L	1169	40/40	0.78	0.18	20,20,20,20	0
21	LMU	A	7033	35/35	0.78	0.12	20,20,20,20	0
20	CLA	1	1196	36/65	0.79	0.16	20,20,20,20	0
20	CLA	1	1201	25/65	0.79	0.13	20,20,20,20	0
20	CLA	2	1219	25/65	0.79	0.14	20,20,20,20	0
21	LMU	A	7022	35/35	0.79	0.13	20,20,20,20	0
21	LMU	A	7040	35/35	0.79	0.12	20,20,20,20	0
20	CLA	3	1216	25/65	0.79	0.12	20,20,20,20	0
20	CLA	2	2010	25/65	0.79	0.15	20,20,20,20	0
21	LMU	A	7026	35/35	0.79	0.12	20,20,20,20	0
20	CLA	3	3011	65/65	0.79	0.13	20,20,20,20	0
20	CLA	1	1190	46/65	0.79	0.14	20,20,20,20	0
20	CLA	B	1741	54/65	0.79	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	LMU	R	1056	35/35	0.79	0.12	20,20,20,20	0
20	CLA	B	1742	55/65	0.79	0.18	20,20,20,20	0
20	CLA	3	3015	25/65	0.79	0.13	20,20,20,20	0
20	CLA	A	1782	65/65	0.80	0.16	20,20,20,20	0
20	CLA	2	1221	25/65	0.80	0.15	20,20,20,20	0
20	CLA	B	1756	65/65	0.80	0.18	20,20,20,20	0
20	CLA	4	1197	36/65	0.80	0.17	20,20,20,20	0
20	CLA	B	1735	65/65	0.80	0.22	20,20,20,20	0
20	CLA	A	1769	54/65	0.80	0.17	20,20,20,20	0
20	CLA	A	1761	65/65	0.80	0.21	20,20,20,20	0
20	CLA	B	1744	65/65	0.80	0.17	20,20,20,20	0
20	CLA	4	1205	25/65	0.80	0.18	20,20,20,20	0
20	CLA	A	1781	65/65	0.80	0.17	20,20,20,20	0
20	CLA	A	1760	55/65	0.81	0.17	20,20,20,20	0
20	CLA	A	1768	54/65	0.81	0.13	20,20,20,20	0
20	CLA	B	1736	45/65	0.81	0.17	20,20,20,20	0
20	CLA	B	1740	65/65	0.81	0.19	20,20,20,20	0
20	CLA	B	1761	50/65	0.81	0.16	20,20,20,20	0
20	CLA	A	1777	51/65	0.81	0.14	20,20,20,20	0
21	LMU	L	1171	35/35	0.81	0.11	20,20,20,20	0
22	BCR	B	1777	40/40	0.81	0.22	20,20,20,20	0
22	BCR	B	1778	40/40	0.81	0.22	20,20,20,20	0
21	LMU	A	7035	35/35	0.81	0.13	20,20,20,20	0
20	CLA	B	1763	50/65	0.81	0.20	20,20,20,20	0
20	CLA	A	1813	65/65	0.81	0.19	20,20,20,20	0
20	CLA	4	1207	36/65	0.81	0.17	20,20,20,20	0
20	CLA	A	1774	65/65	0.81	0.21	20,20,20,20	0
20	CLA	2	1214	25/65	0.82	0.12	20,20,20,20	0
20	CLA	B	1753	65/65	0.82	0.16	20,20,20,20	0
20	CLA	A	1786	50/65	0.82	0.15	20,20,20,20	0
20	CLA	2	1222	50/65	0.82	0.15	20,20,20,20	0
20	CLA	4	1201	52/65	0.82	0.12	20,20,20,20	0
20	CLA	I	1031	60/65	0.82	0.17	20,20,20,20	0
20	CLA	A	1792	51/65	0.83	0.17	20,20,20,20	0
20	CLA	A	1812	65/65	0.83	0.20	20,20,20,20	0
20	CLA	A	1773	52/65	0.83	0.17	20,20,20,20	0
20	CLA	A	1789	65/65	0.83	0.18	20,20,20,20	0
20	CLA	F	1155	36/65	0.83	0.15	20,20,20,20	0
20	CLA	B	1747	59/65	0.83	0.16	20,20,20,20	0
20	CLA	L	1167	47/65	0.83	0.16	20,20,20,20	0
20	CLA	A	1765	55/65	0.83	0.18	20,20,20,20	0
23	PQN	A	1802	33/33	0.83	0.23	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
21	LMU	A	7016	35/35	0.83	0.10	20,20,20,20	0
20	CLA	A	1784	55/65	0.84	0.18	20,20,20,20	0
20	CLA	B	1759	65/65	0.84	0.19	20,20,20,20	0
20	CLA	A	1793	65/65	0.84	0.18	20,20,20,20	0
20	CLA	A	1795	51/65	0.84	0.20	20,20,20,20	0
20	CLA	A	1796	65/65	0.84	0.16	20,20,20,20	0
20	CLA	A	1785	65/65	0.84	0.18	20,20,20,20	0
20	CLA	4	1206	25/65	0.84	0.15	20,20,20,20	0
20	CLA	B	1743	65/65	0.84	0.17	20,20,20,20	0
20	CLA	B	1767	60/65	0.84	0.19	20,20,20,20	0
21	LMU	A	7024	35/35	0.84	0.10	20,20,20,20	0
21	LMU	A	7039	35/35	0.84	0.10	20,20,20,20	0
20	CLA	B	1769	47/65	0.84	0.20	20,20,20,20	0
20	CLA	B	1770	65/65	0.84	0.18	20,20,20,20	0
20	CLA	B	1749	61/65	0.85	0.17	20,20,20,20	0
20	CLA	B	1750	50/65	0.85	0.16	20,20,20,20	0
20	CLA	A	1790	50/65	0.85	0.15	20,20,20,20	0
20	CLA	B	1752	55/65	0.85	0.14	20,20,20,20	0
20	CLA	A	1759	50/65	0.85	0.14	20,20,20,20	0
20	CLA	A	1764	65/65	0.85	0.22	20,20,20,20	0
20	CLA	A	1788	65/65	0.85	0.15	20,20,20,20	0
22	BCR	B	1781	40/40	0.85	0.16	20,20,20,20	0
20	CLA	A	1762	57/65	0.85	0.16	20,20,20,20	0
21	LMU	A	7032	35/35	0.85	0.10	20,20,20,20	0
20	CLA	B	1748	60/65	0.85	0.21	20,20,20,20	0
20	CLA	B	1787	65/65	0.85	0.20	20,20,20,20	0
22	BCR	L	1170	40/40	0.86	0.18	20,20,20,20	0
20	CLA	B	1758	65/65	0.86	0.21	20,20,20,20	0
20	CLA	A	1800	65/65	0.86	0.15	20,20,20,20	0
26	UNL	B	8057	23/-	0.86	0.09	20,20,20,20	0
20	CLA	B	1737	65/65	0.87	0.18	20,20,20,20	0
20	CLA	A	1779	55/65	0.87	0.16	20,20,20,20	0
20	CLA	B	1768	65/65	0.87	0.18	20,20,20,20	0
20	CLA	B	1757	65/65	0.87	0.18	20,20,20,20	0
20	CLA	A	1794	47/65	0.87	0.17	20,20,20,20	0
20	CLA	B	1771	65/65	0.87	0.17	20,20,20,20	0
20	CLA	B	1754	54/65	0.87	0.18	20,20,20,20	0
20	CLA	B	1785	65/65	0.87	0.20	20,20,20,20	0
23	PQN	B	1773	33/33	0.88	0.18	20,20,20,20	0
20	CLA	B	1738	65/65	0.88	0.17	20,20,20,20	0
20	CLA	B	1786	65/65	0.88	0.18	20,20,20,20	0
20	CLA	B	1760	50/65	0.89	0.14	20,20,20,20	0

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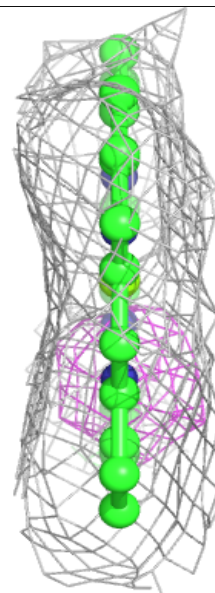
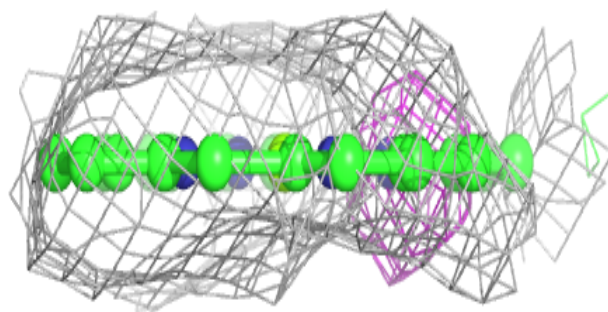
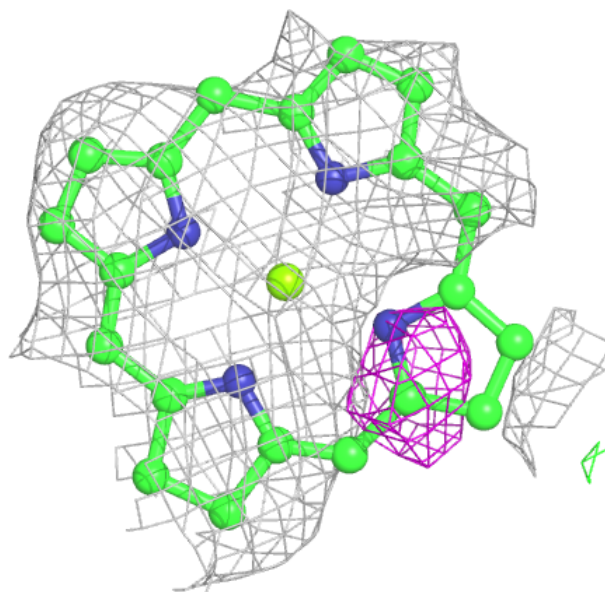
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	CLA	B	1739	65/65	0.89	0.20	20,20,20,20	0
20	CLA	A	1811	65/65	0.89	0.23	20,20,20,20	0
20	CLA	A	1783	65/65	0.89	0.18	20,20,20,20	0
25	SF4	C	1082	8/8	0.98	0.06	20,20,20,20	0
25	SF4	C	1083	8/8	0.99	0.05	20,20,20,20	0
25	SF4	B	1784	8/8	0.99	0.05	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

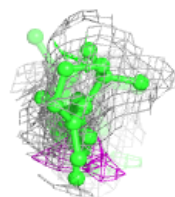
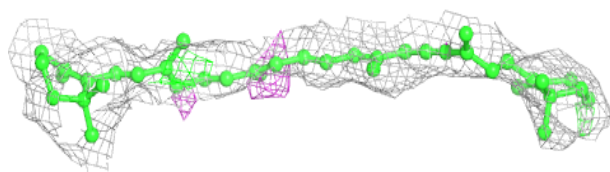
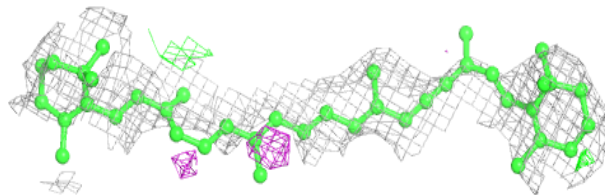
**Electron density around CLA J 1046:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BCR A 1803:**

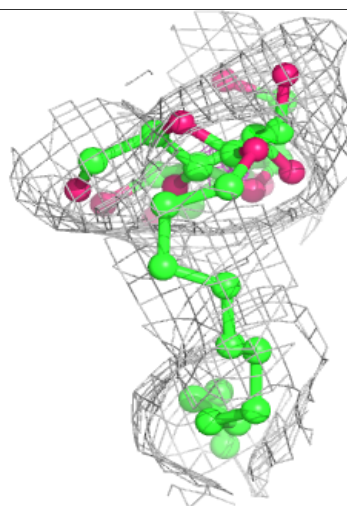
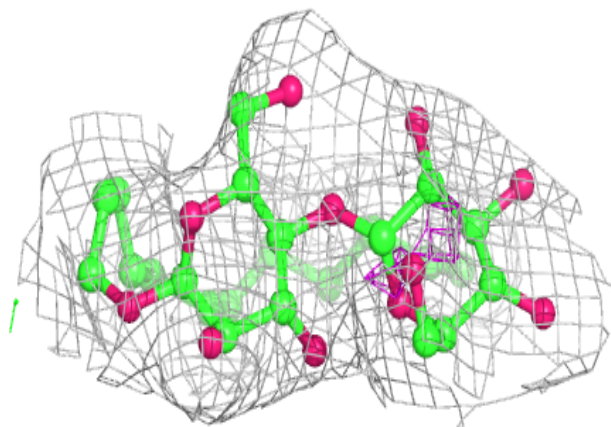
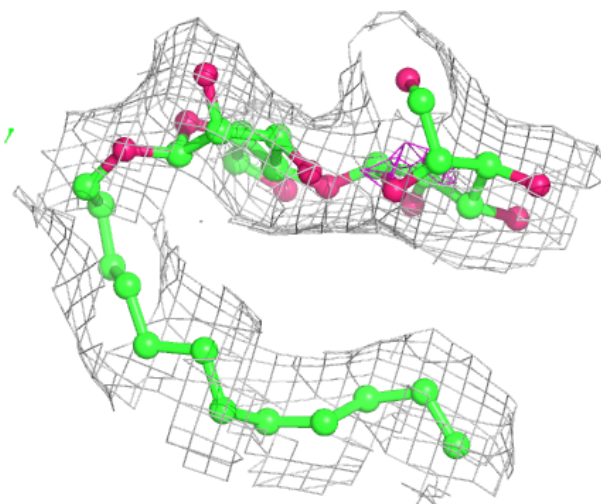
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





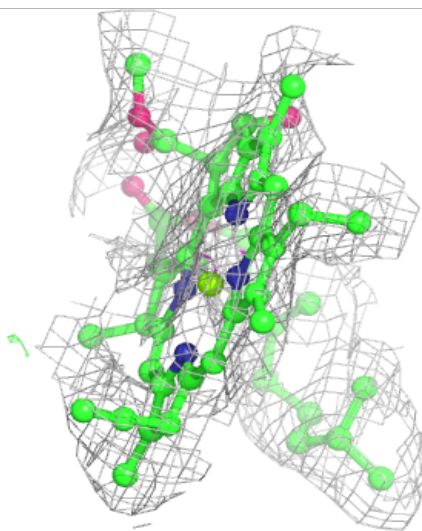
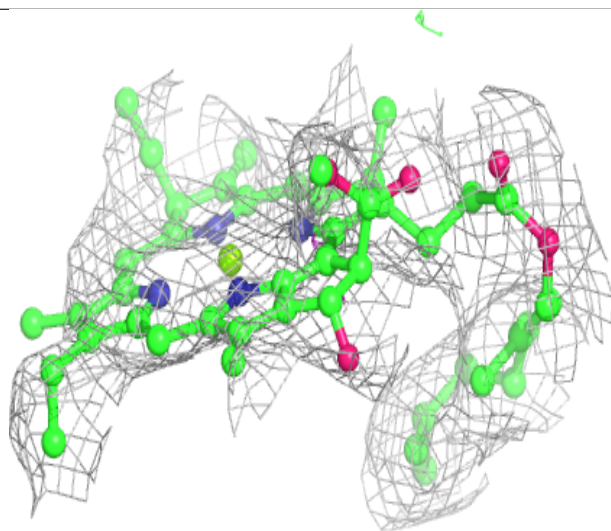
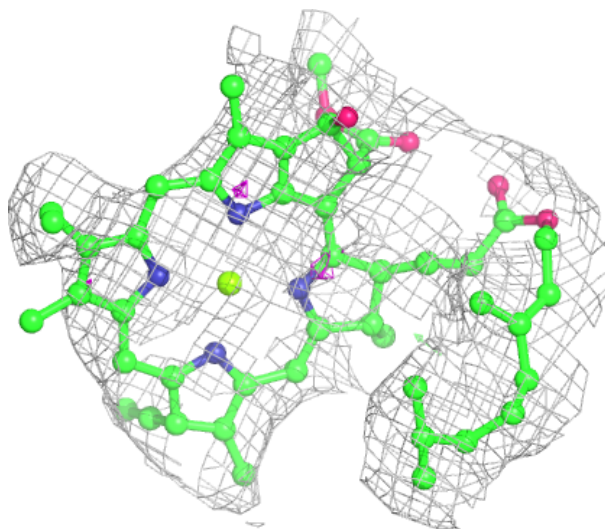
**Electron density around LMU A 7013:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA L 1505:**

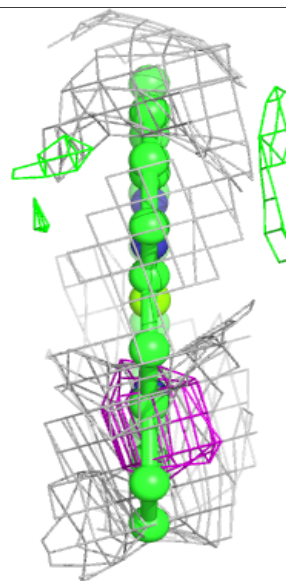
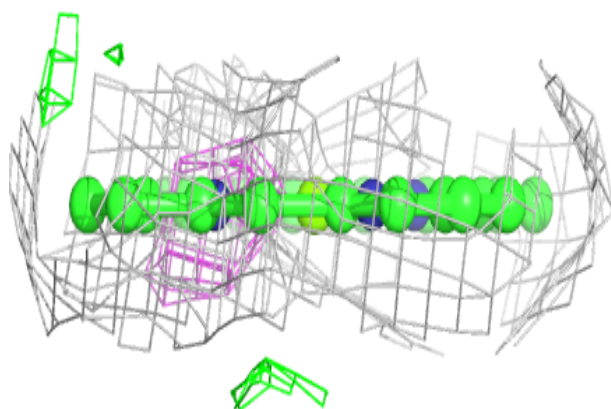
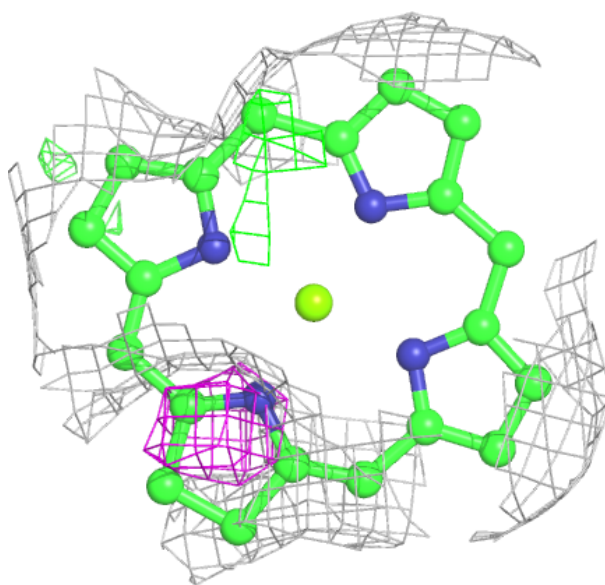
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





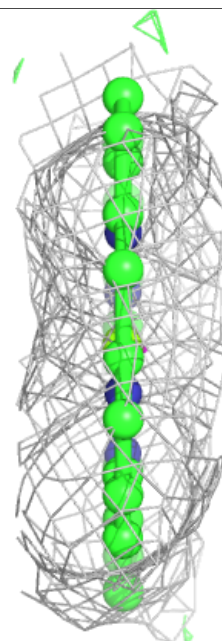
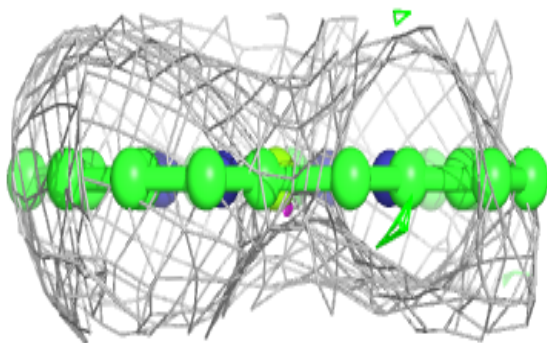
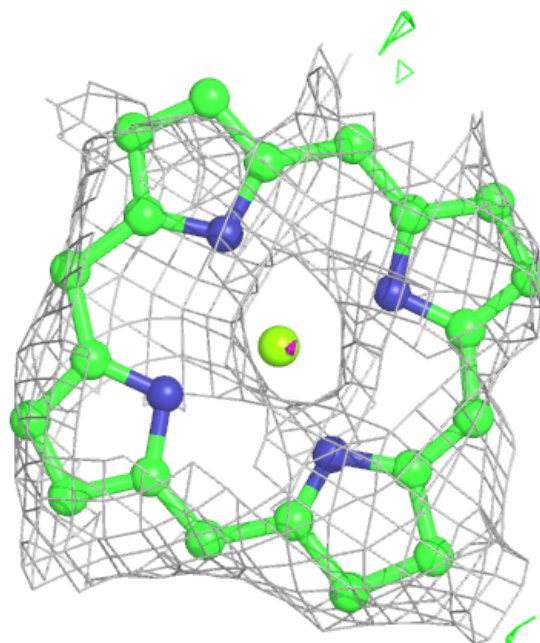
**Electron density around CLA 3 1217:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



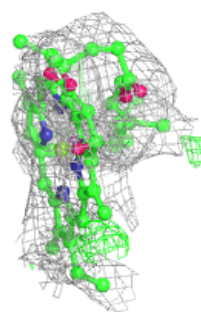
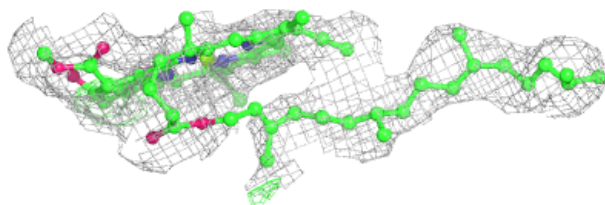
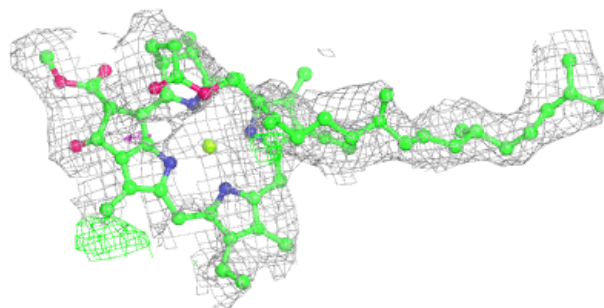
**Electron density around CLA 1 1199:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

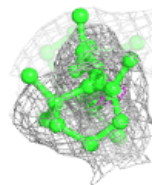
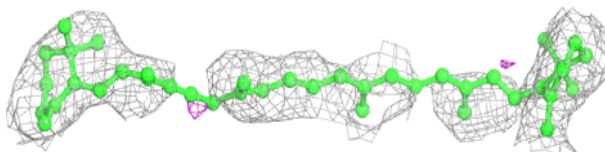
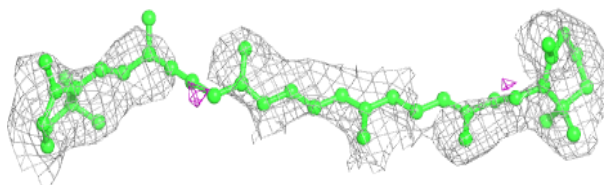


**Electron density around CLA 2 1218:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

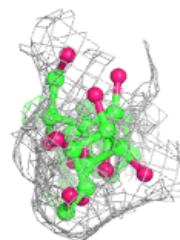
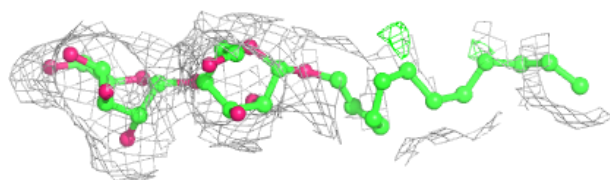
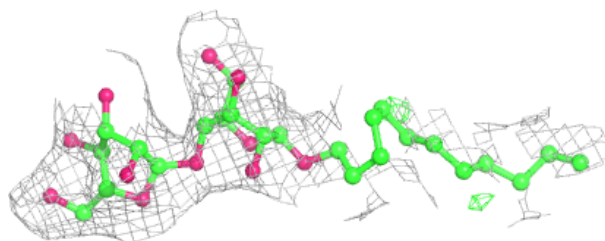
**Electron density around BCR A 1808:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



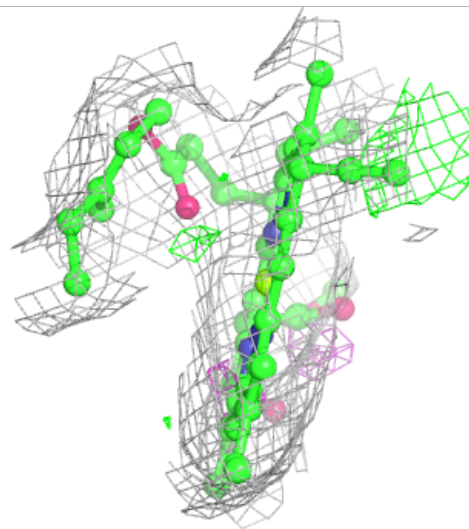
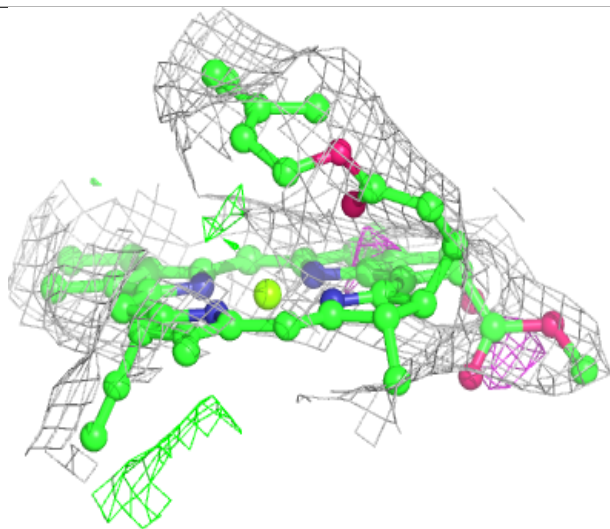
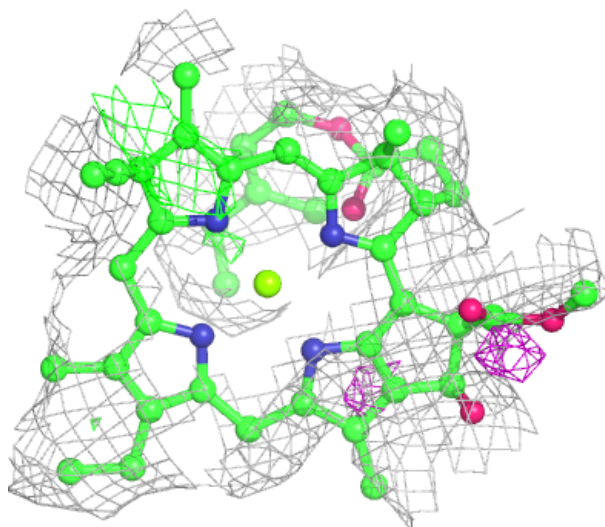
**Electron density around LMU A 7037:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



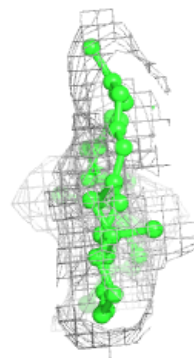
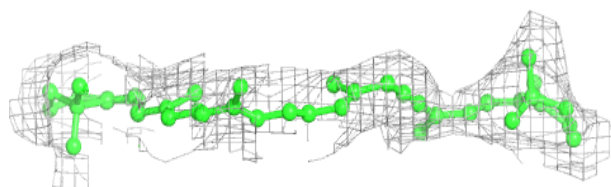
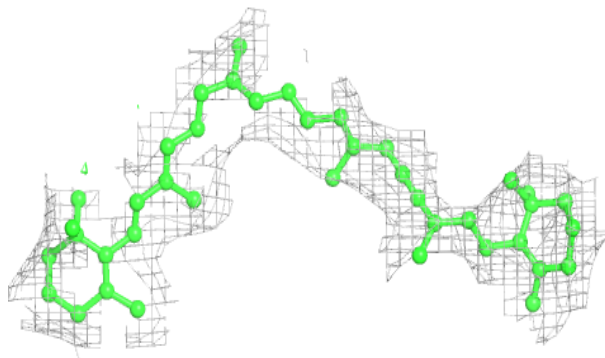
**Electron density around CLA 2 1212:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BCR 3 1220:**

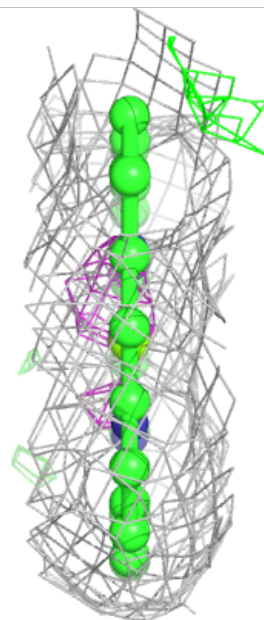
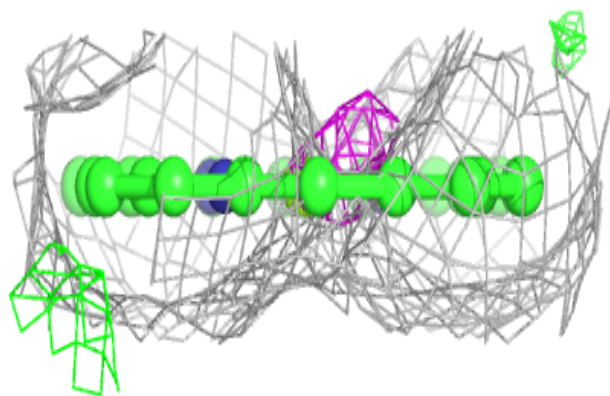
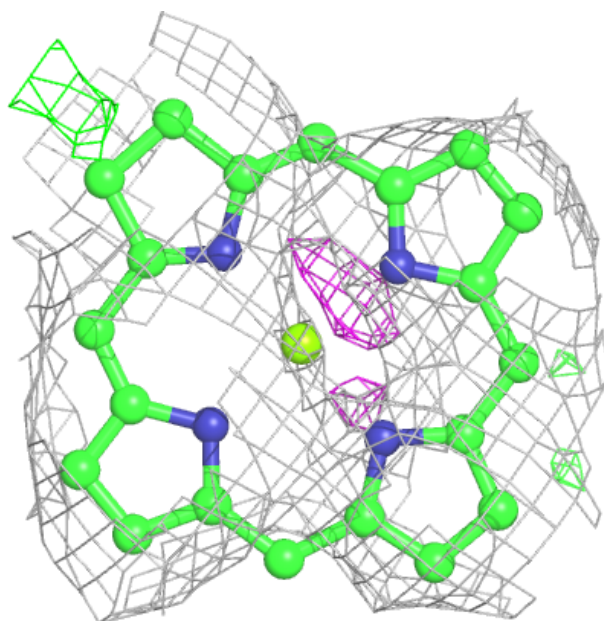
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





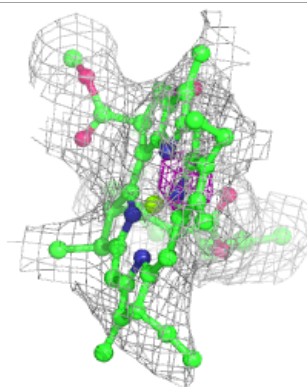
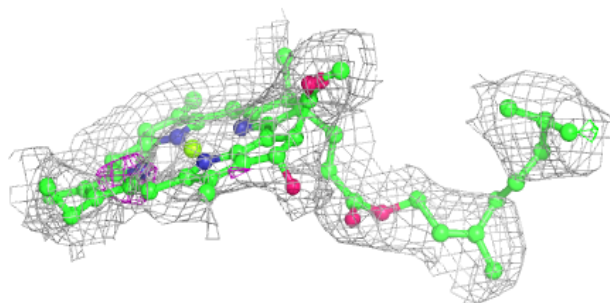
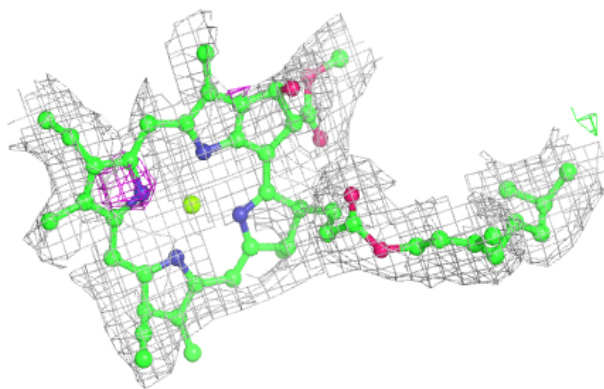
**Electron density around CLA 4 4003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

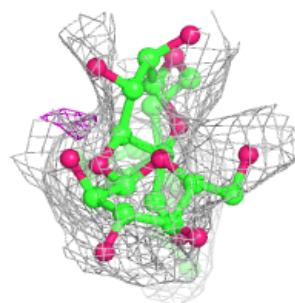
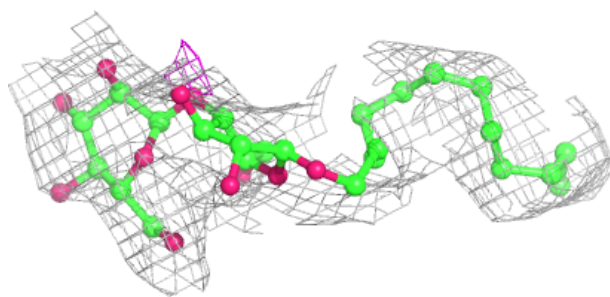
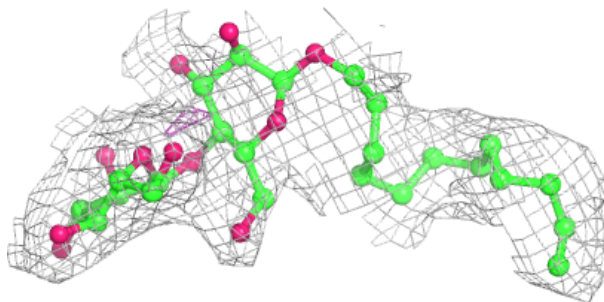


**Electron density around CLA I 1033:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMU 2 1225:**

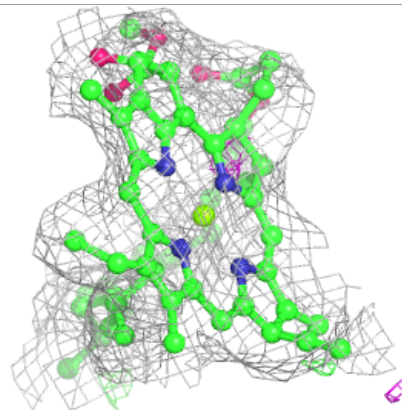
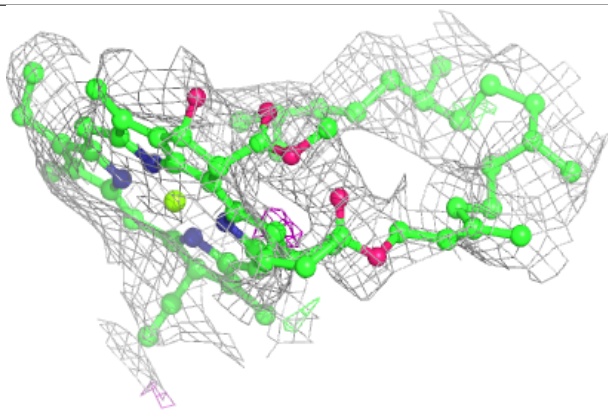
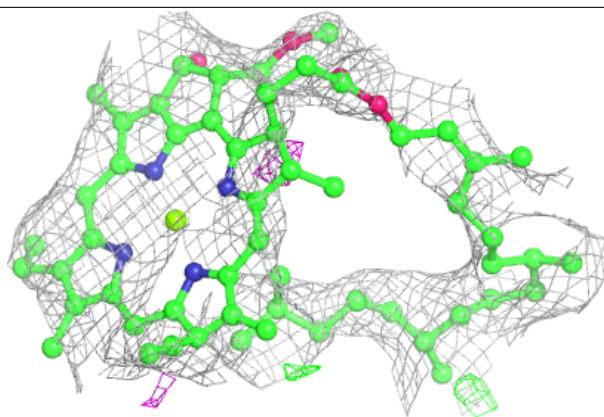
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





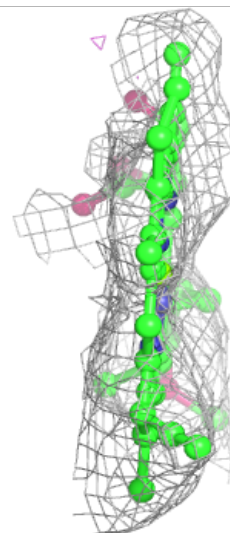
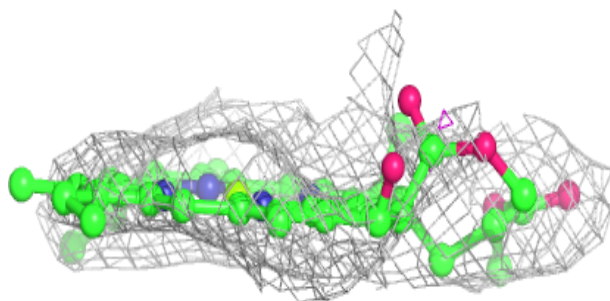
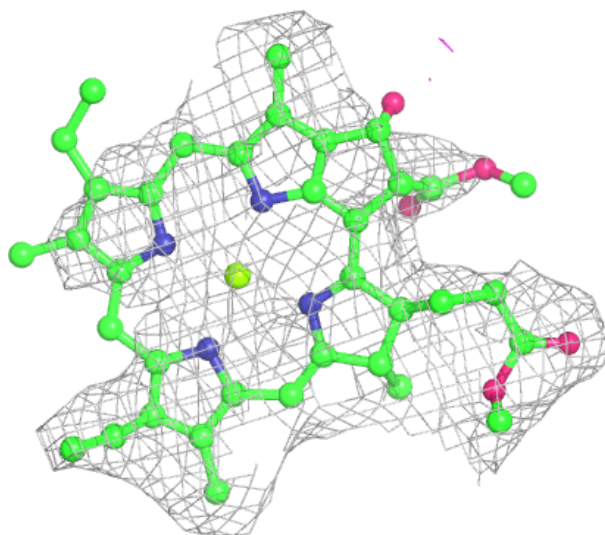
**Electron density around CLA A 1797:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



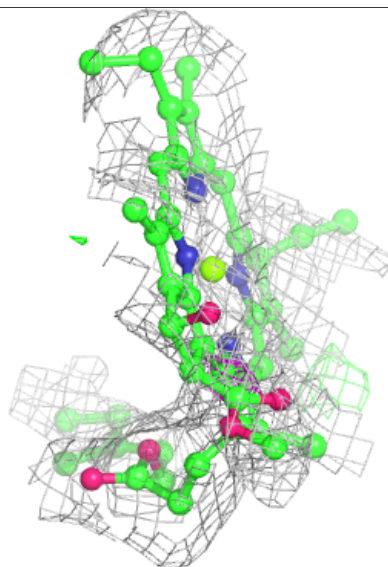
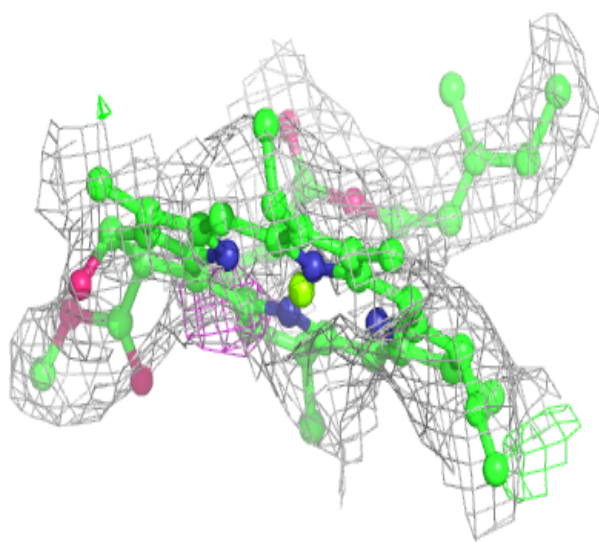
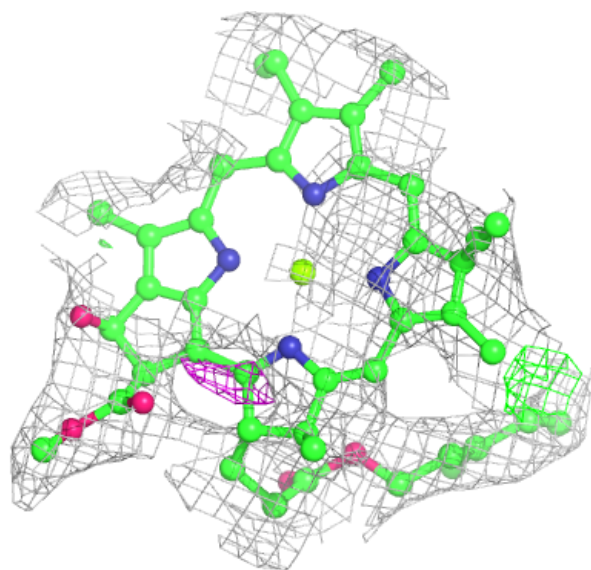
**Electron density around CLA B 1746:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



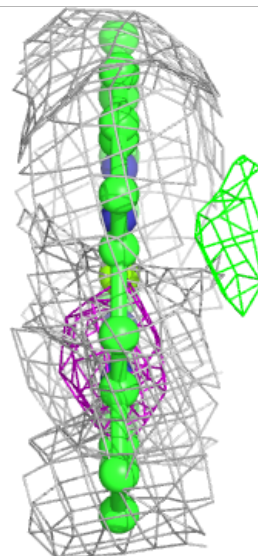
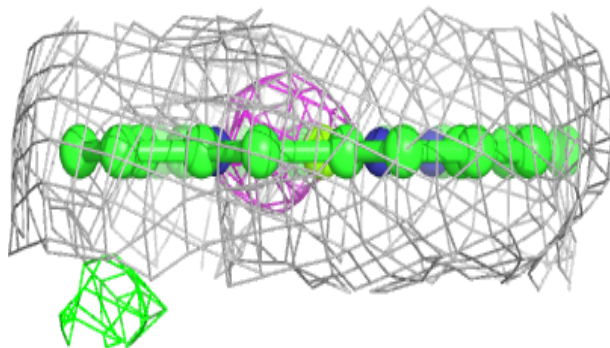
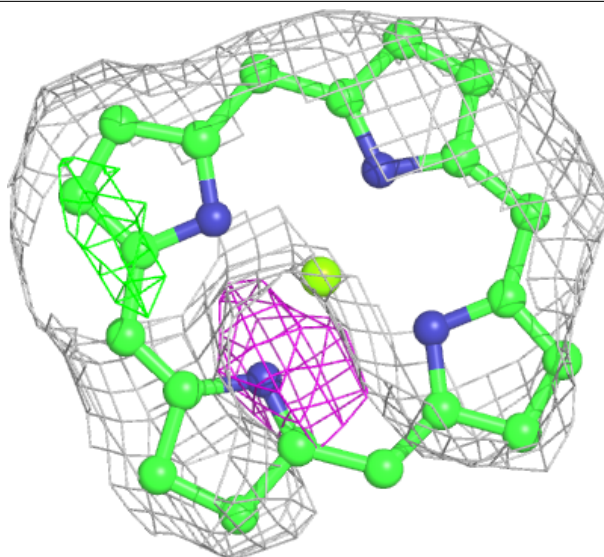
**Electron density around CLA B 1766:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



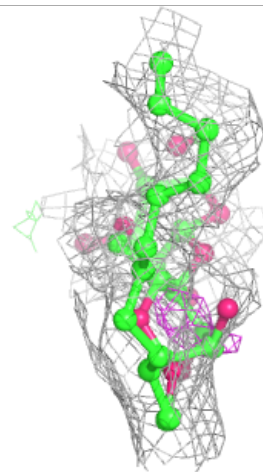
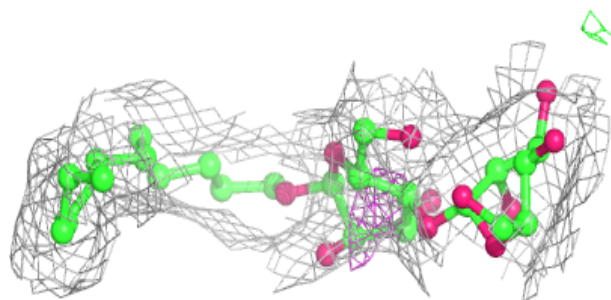
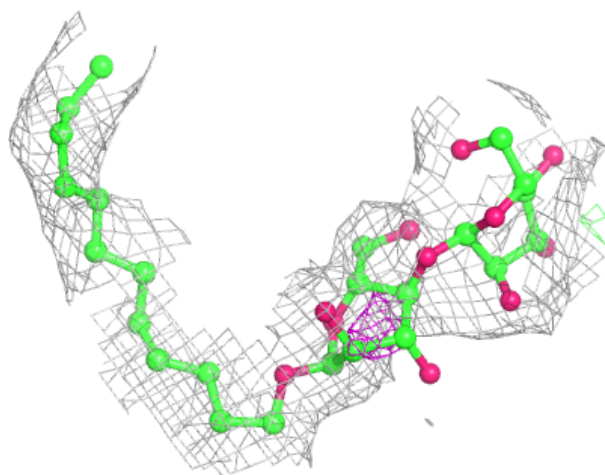
**Electron density around CLA 3 1214:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LMU A 7041:**

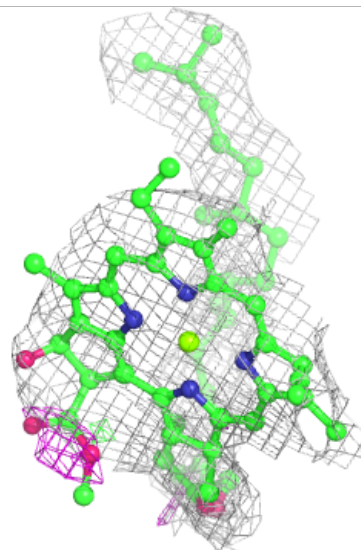
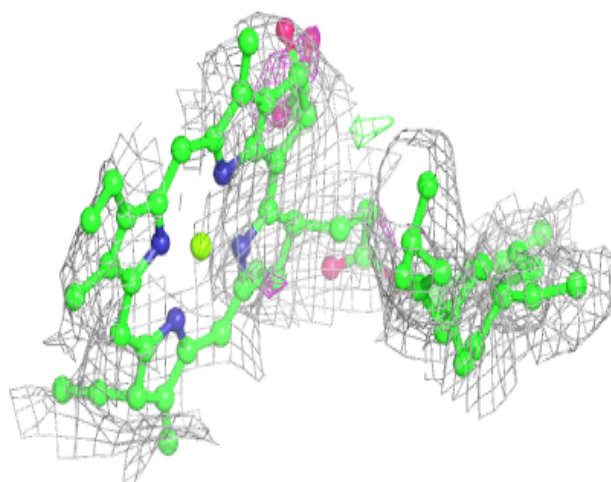
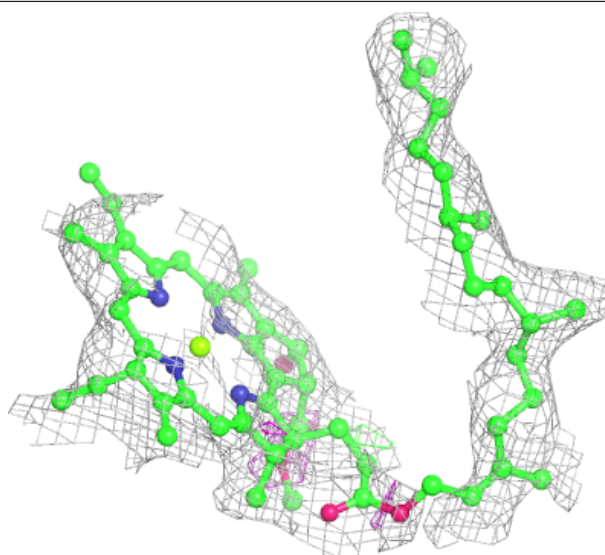
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





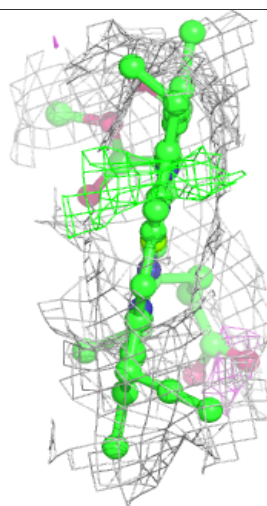
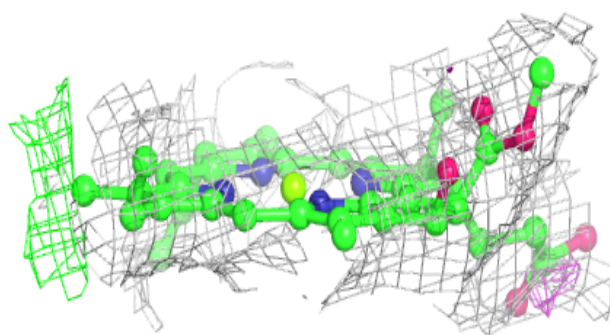
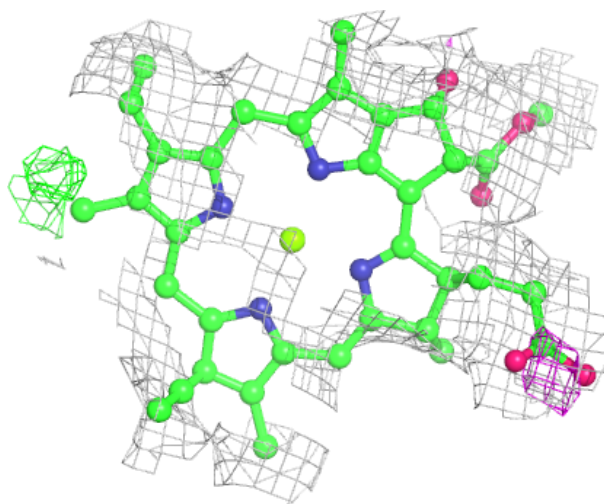
**Electron density around CLA 3 1219:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



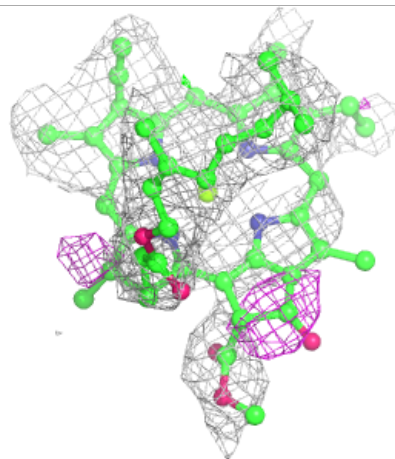
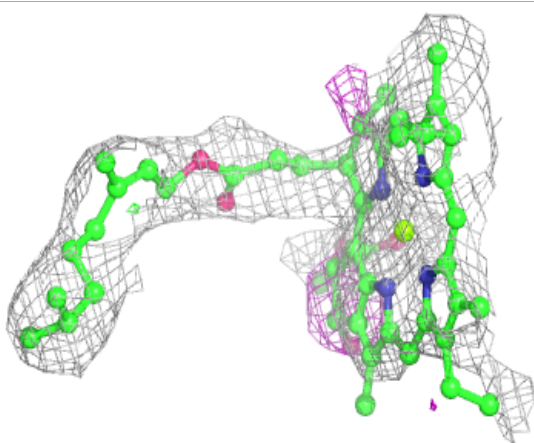
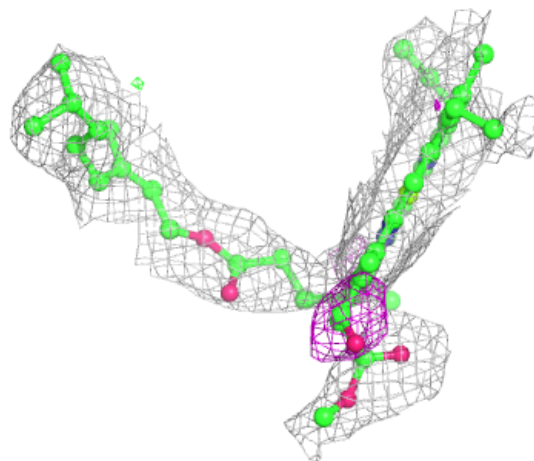
**Electron density around CLA K 1142:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 1801:**

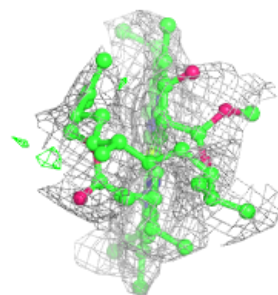
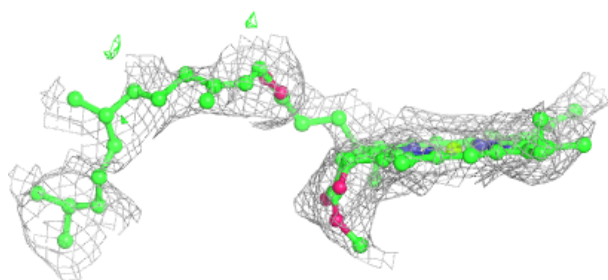
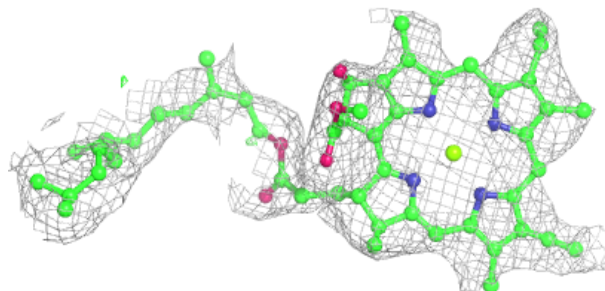
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



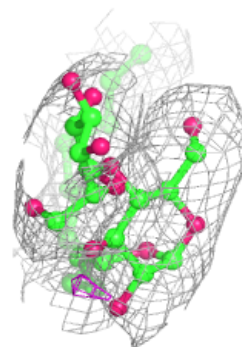
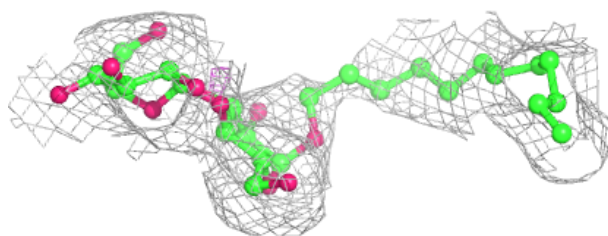
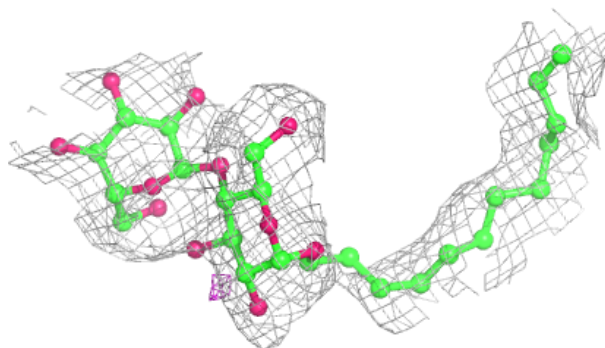


**Electron density around CLA B 1745:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

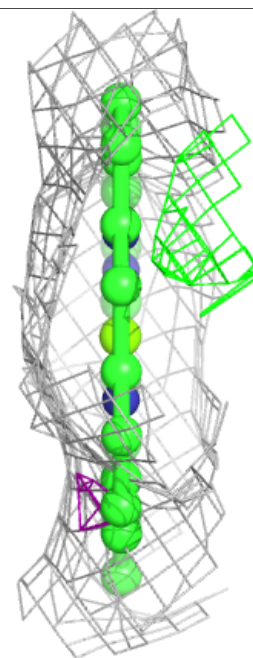
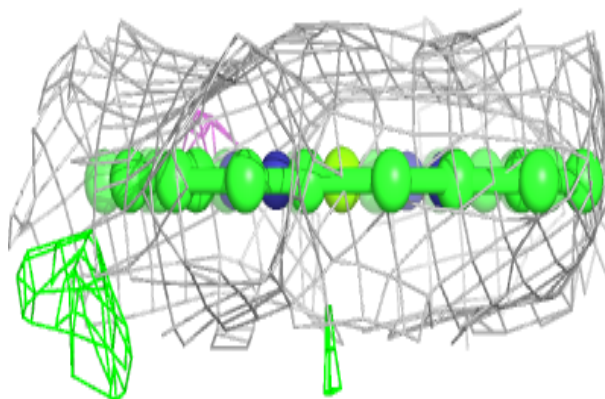
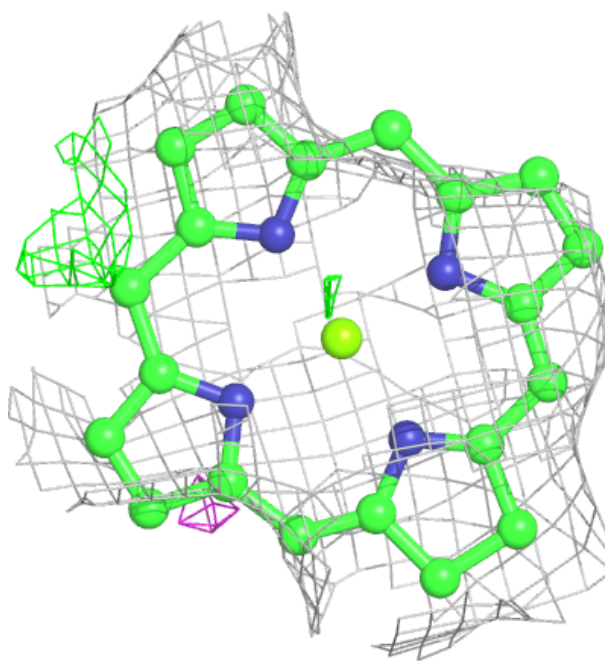
**Electron density around LMU 1 7004:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



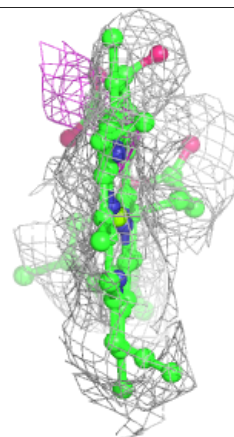
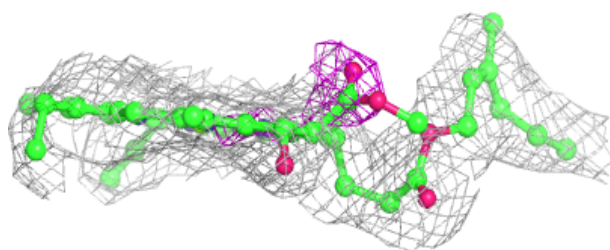
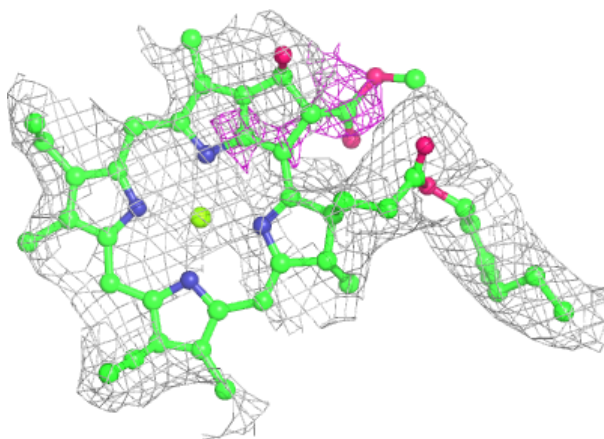
**Electron density around CLA 2 1216:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



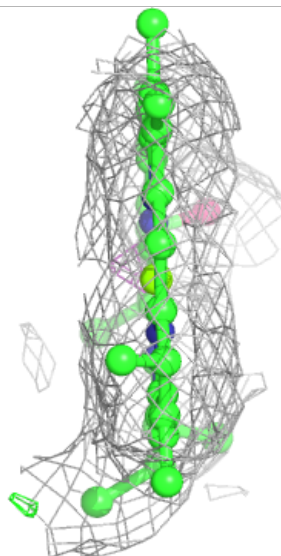
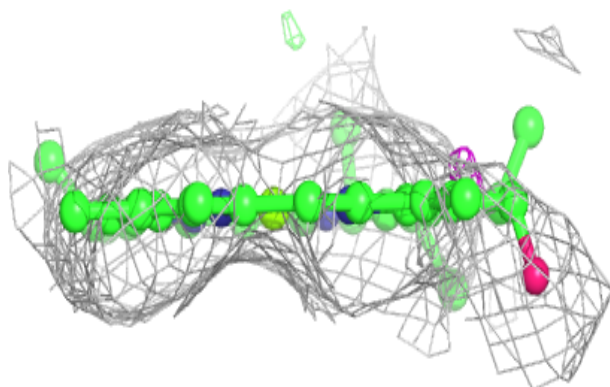
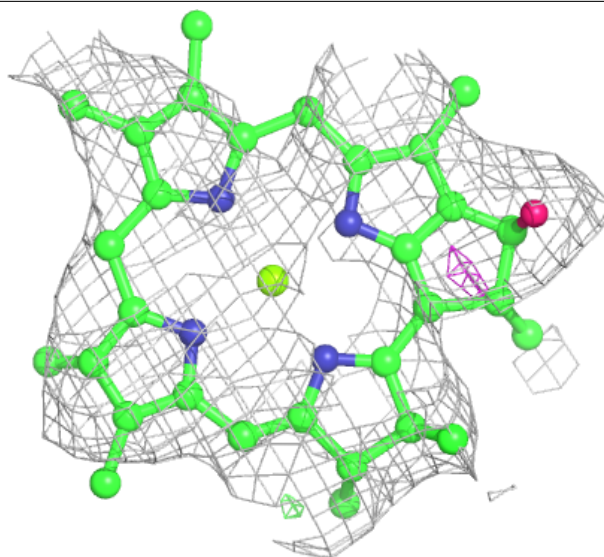
**Electron density around CLA 4 4007:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



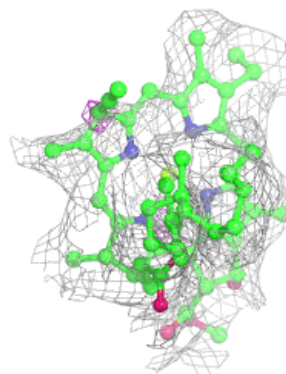
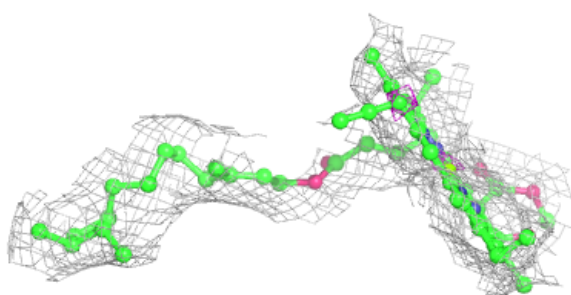
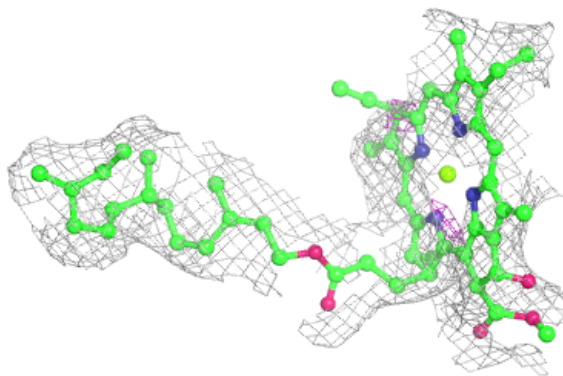
**Electron density around CLA 1 1191:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

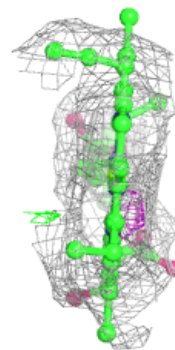
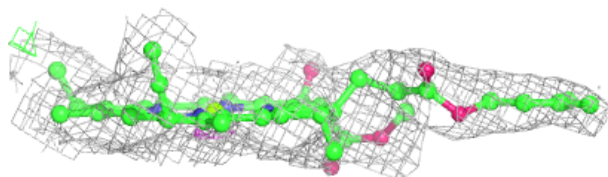
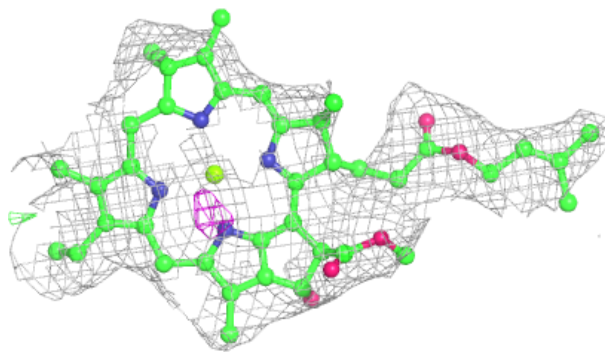


**Electron density around CLA J 1044:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 1799:**

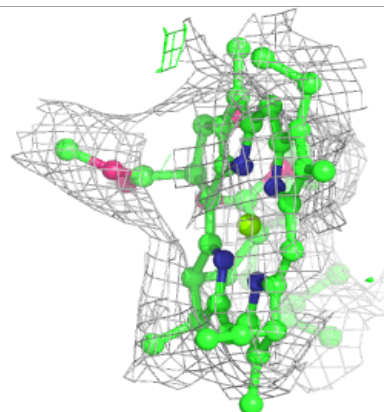
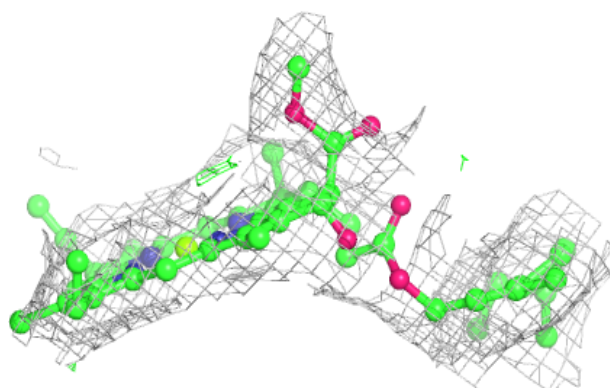
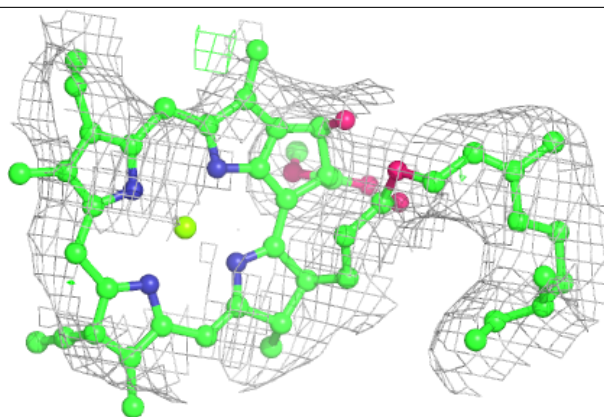
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



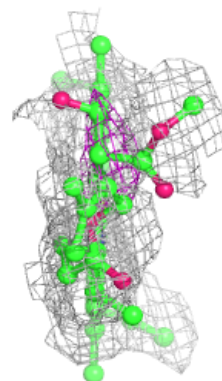
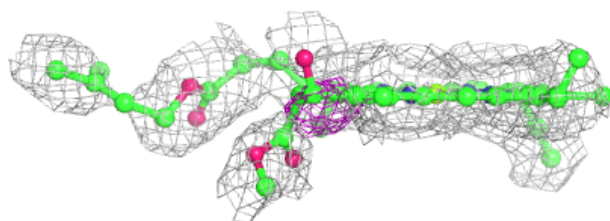
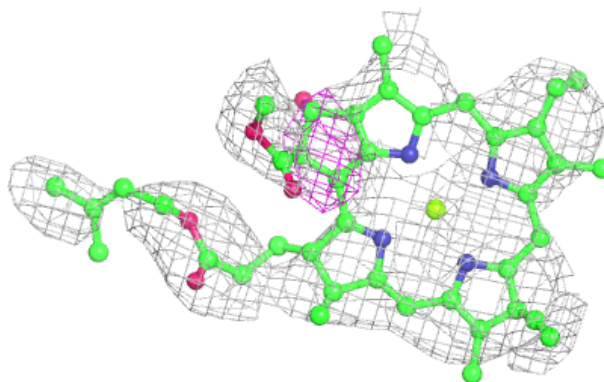


**Electron density around CLA 2 1220:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

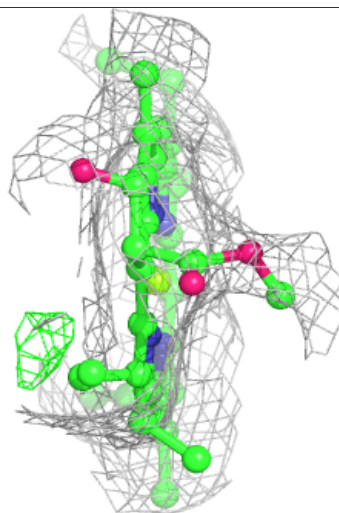
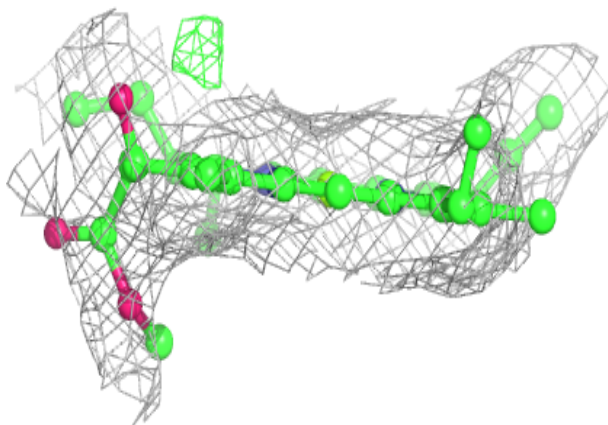
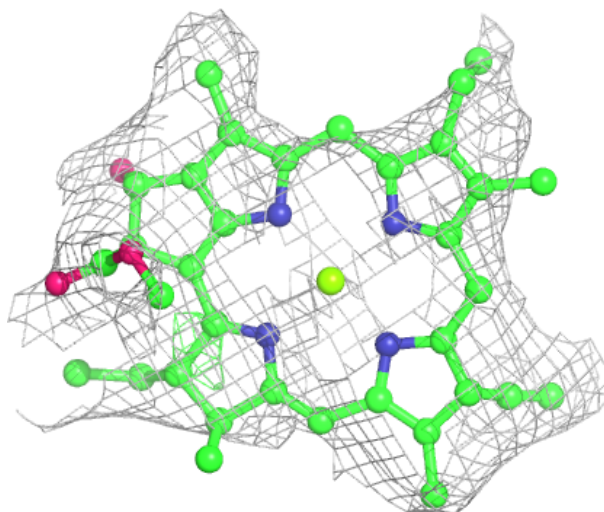
**Electron density around CLA 4 1200:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



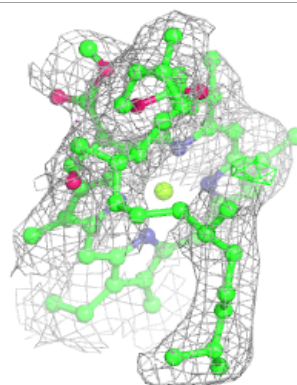
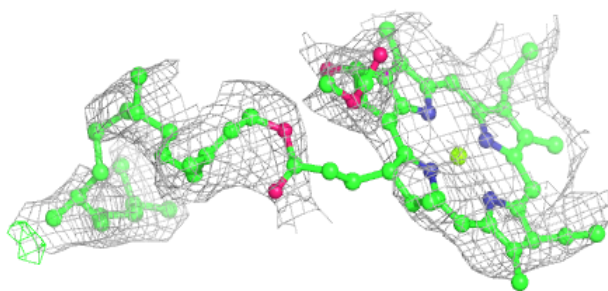
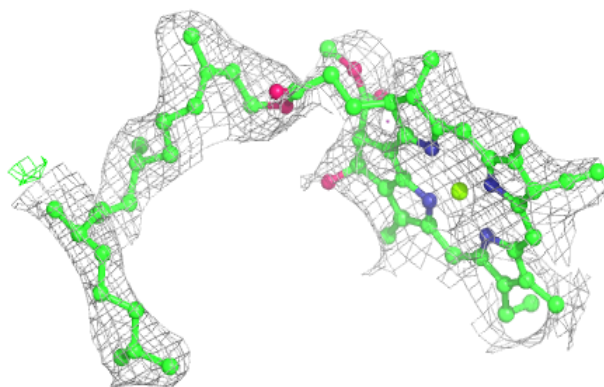
**Electron density around CLA 3 3007:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

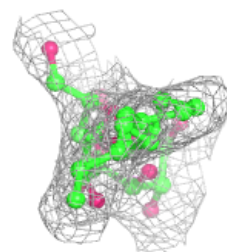
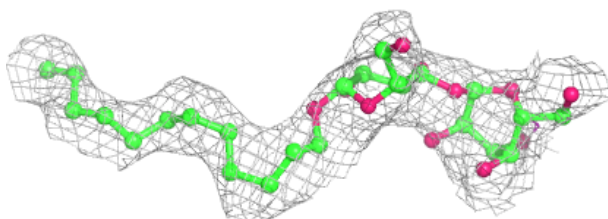
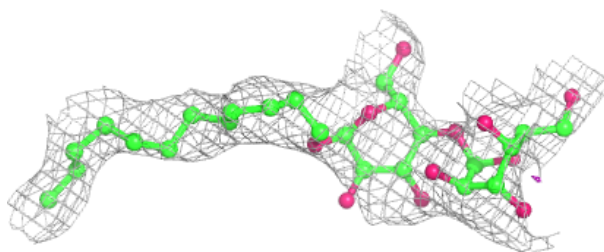


**Electron density around CLA K 3009:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMU A 7010:**

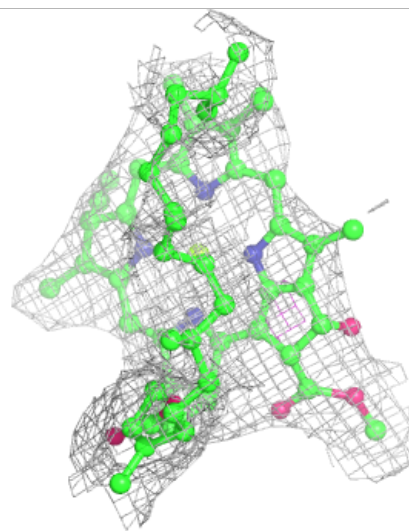
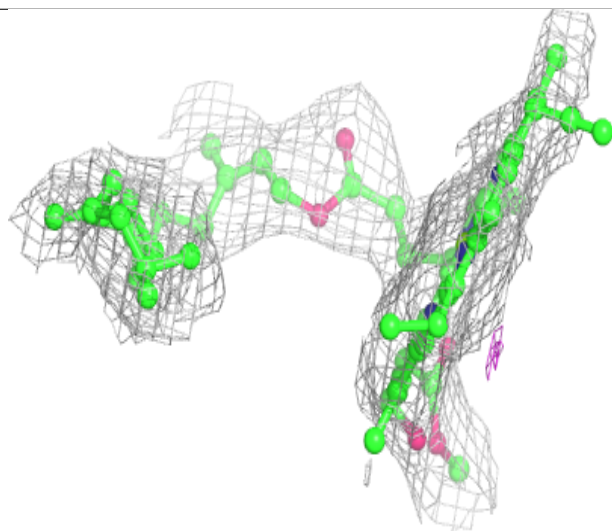
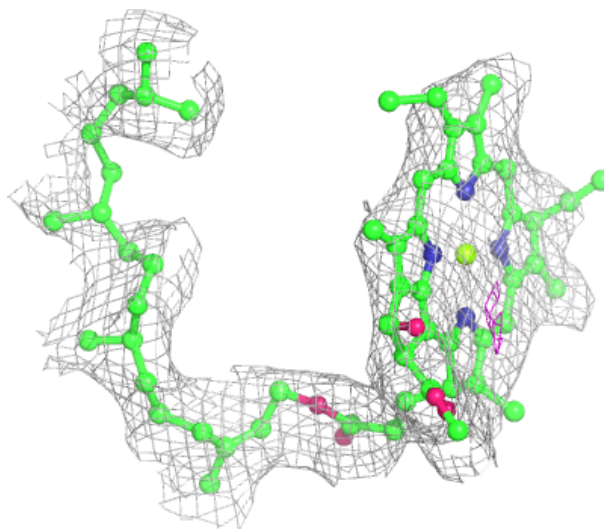
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





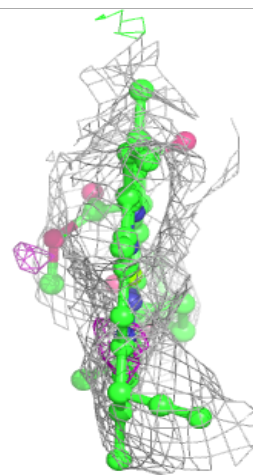
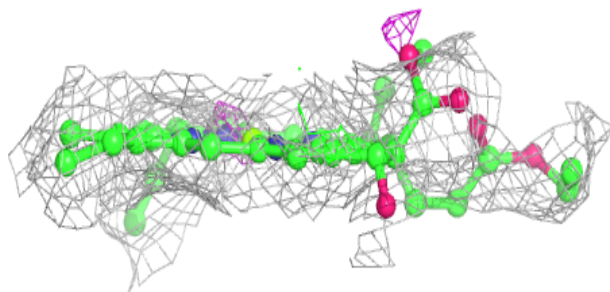
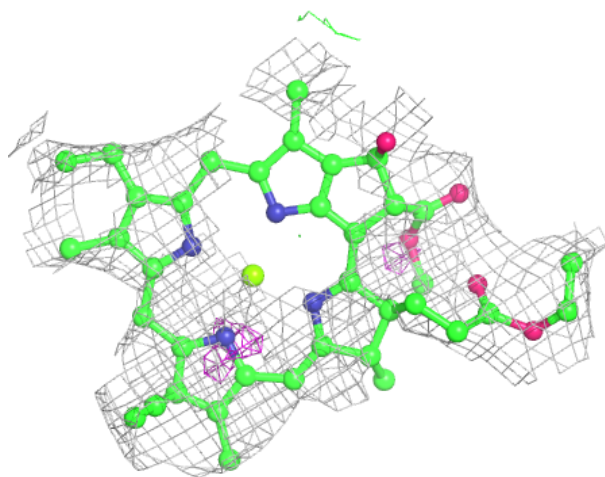
**Electron density around CLA 3 1218:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



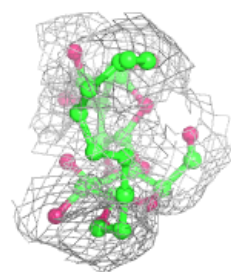
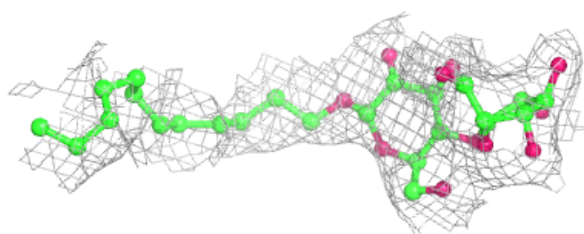
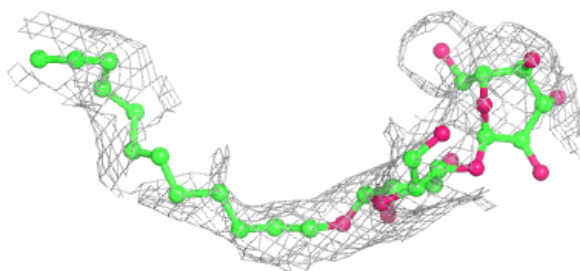
**Electron density around CLA 4 4014:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



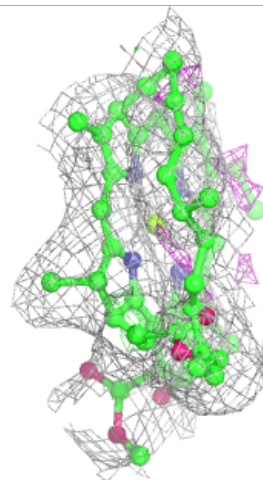
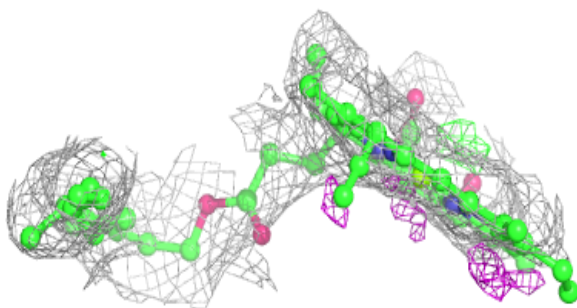
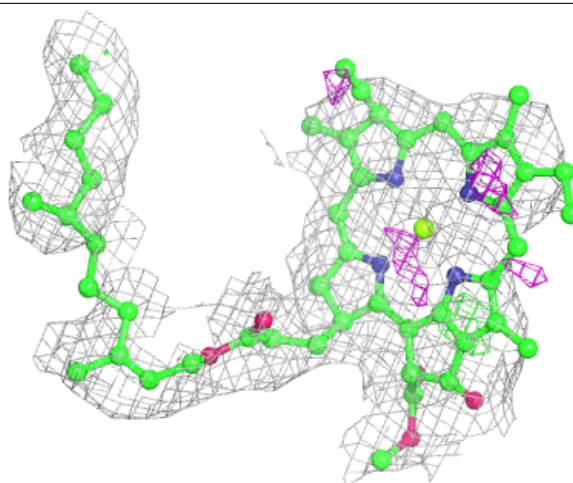
**Electron density around LMU A 7017:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



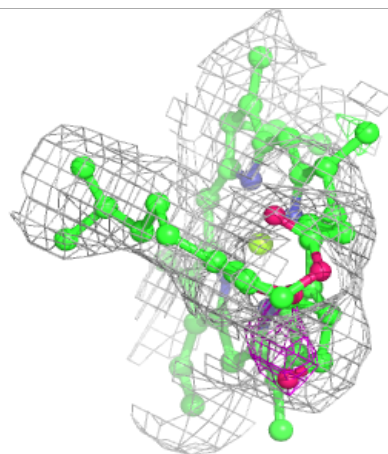
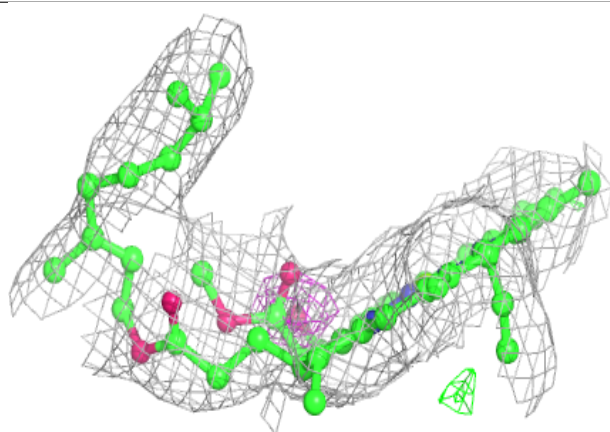
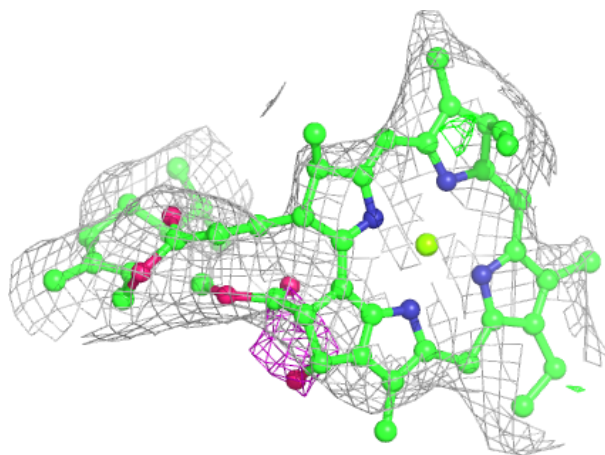
**Electron density around CLA B 1755:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



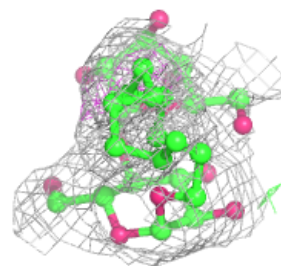
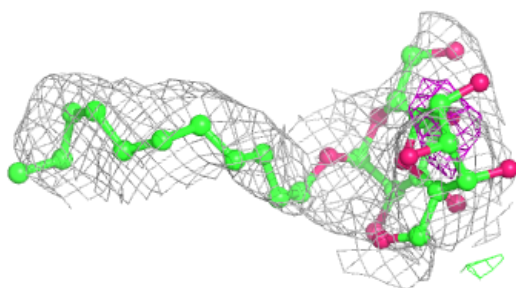
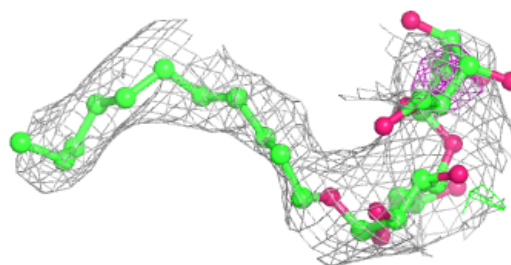
**Electron density around CLA A 1816:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



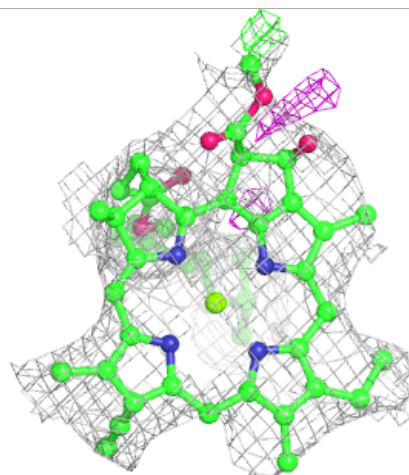
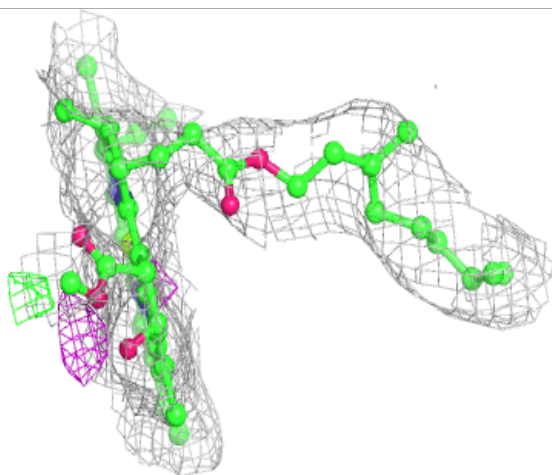
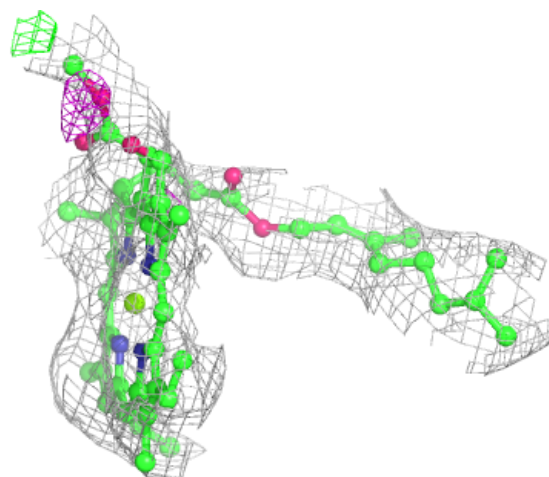
**Electron density around LMU A 7009:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 4 1196:**

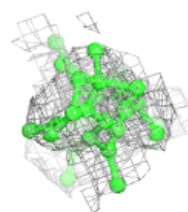
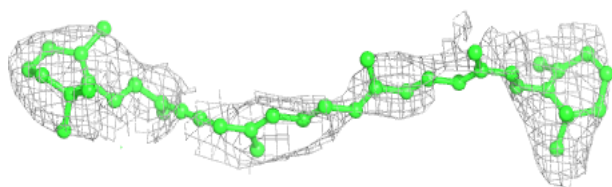
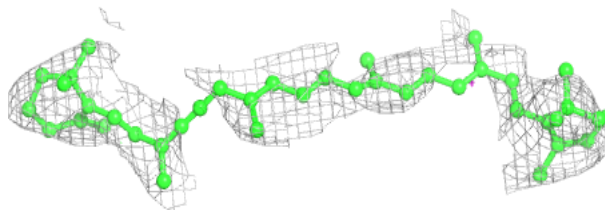
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



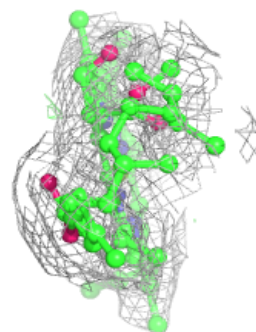
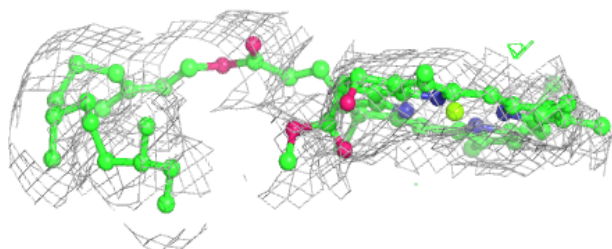
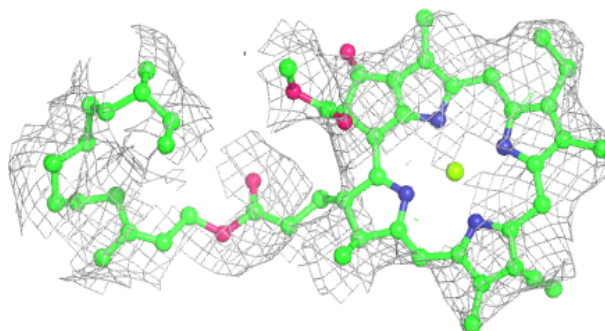


**Electron density around BCR A 1805:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA 1 1198:**

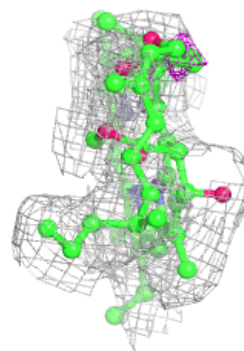
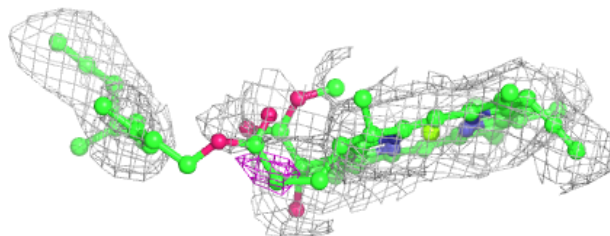
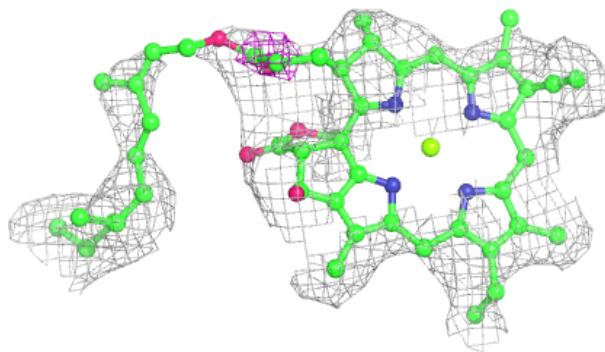
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





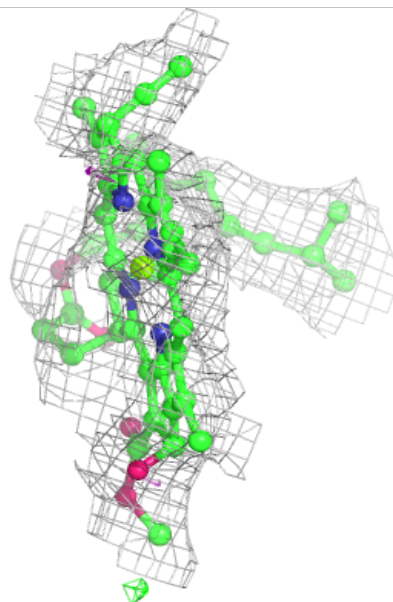
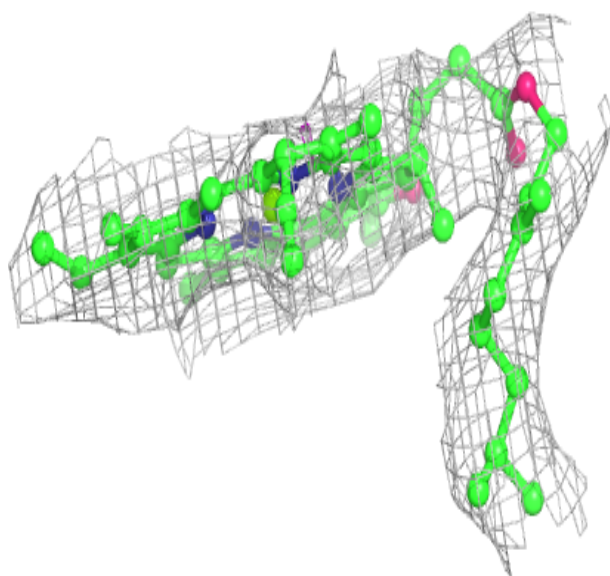
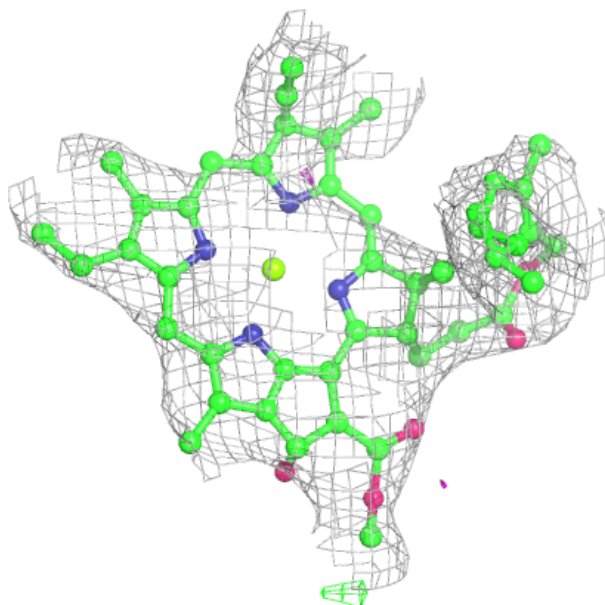
**Electron density around CLA R 1054:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



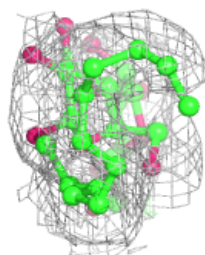
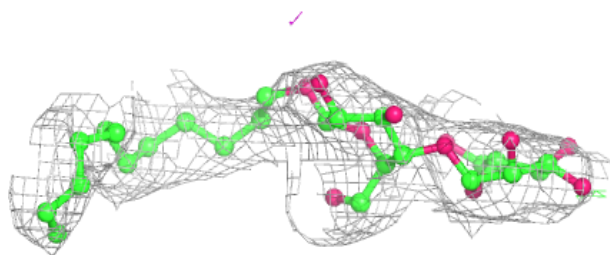
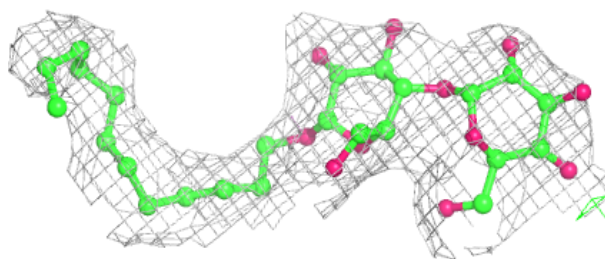
**Electron density around CLA A 1815:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

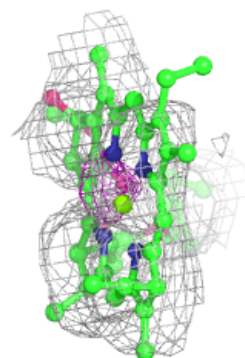
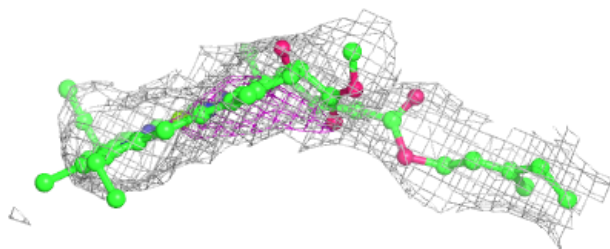
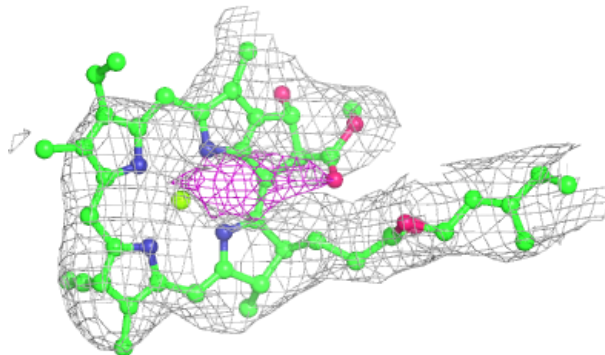


**Electron density around LMU A 7015:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

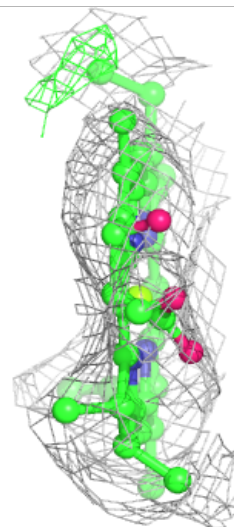
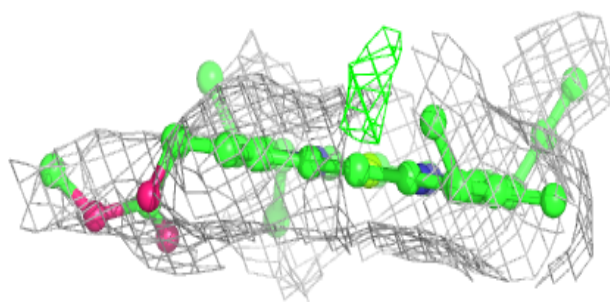
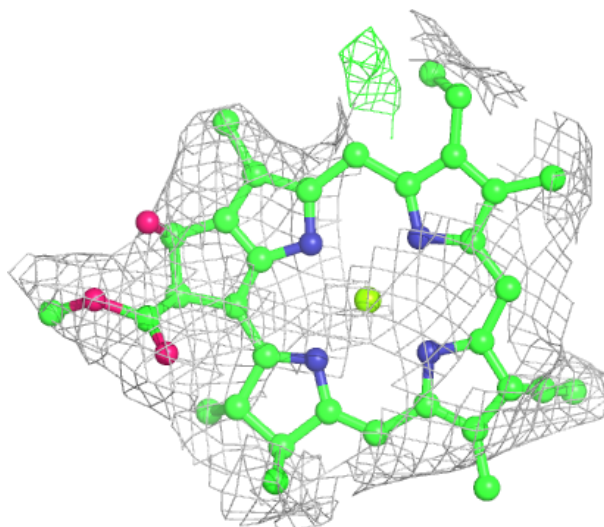
**Electron density around CLA 1 1197:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



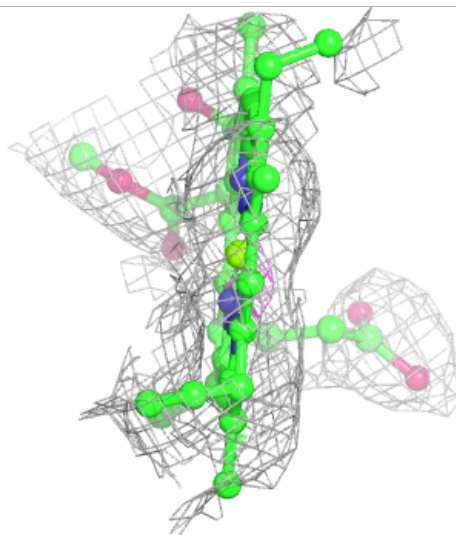
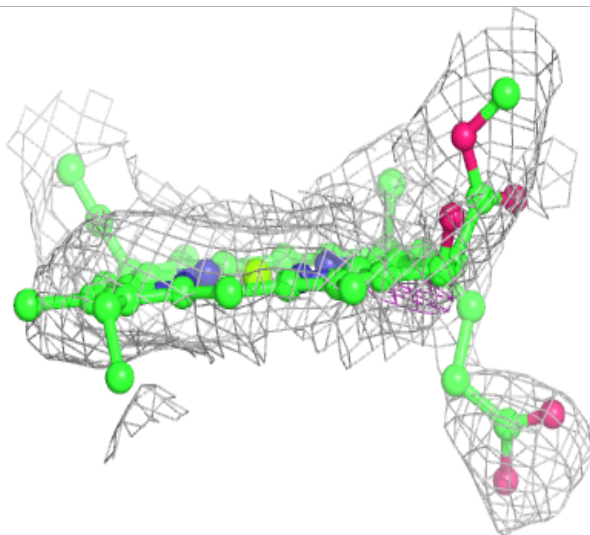
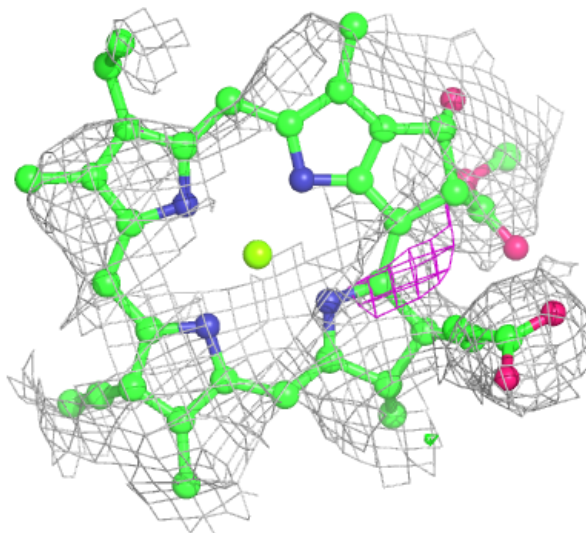
**Electron density around CLA F 1156:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1765:**

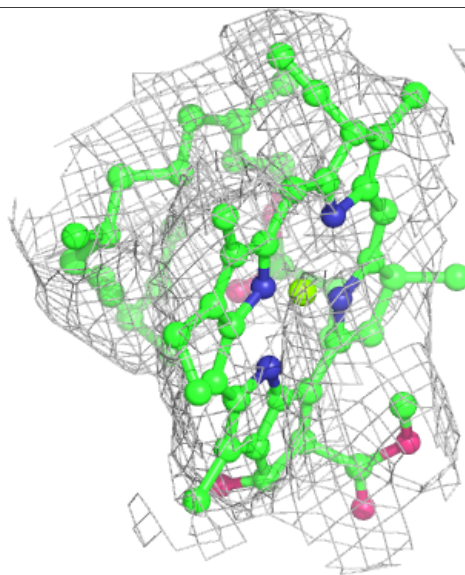
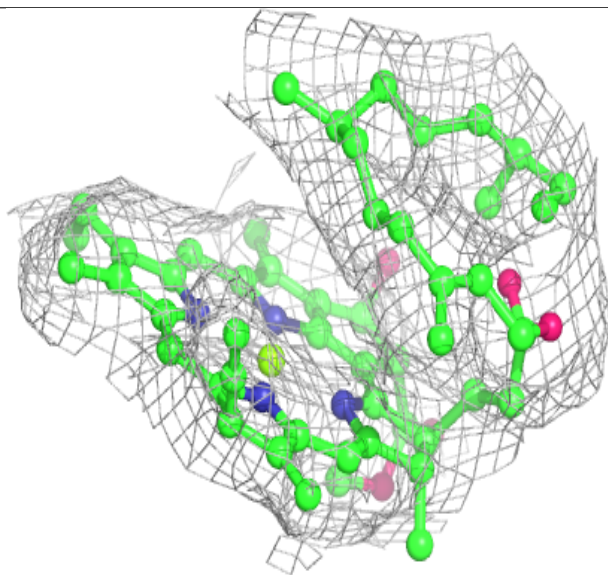
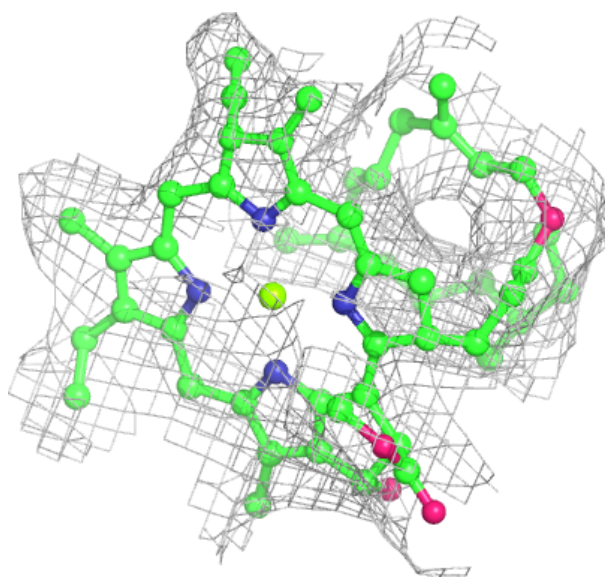
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





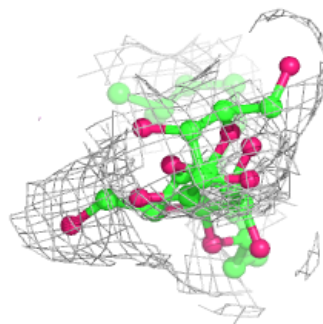
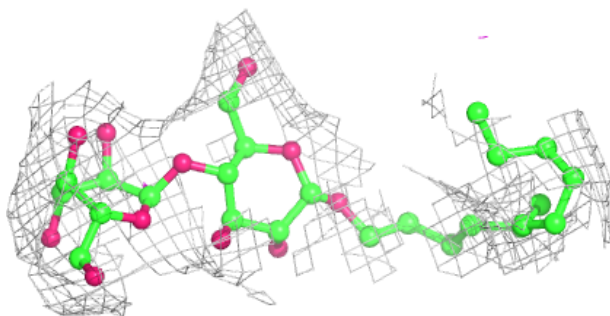
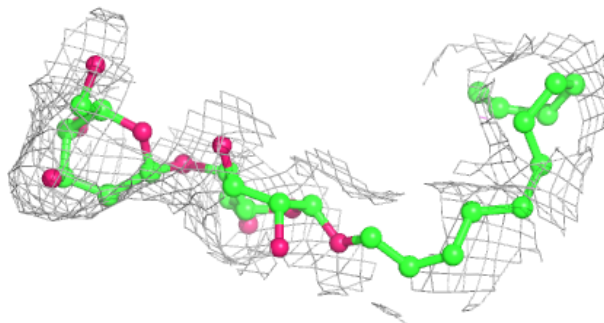
**Electron density around CLA J 1043:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

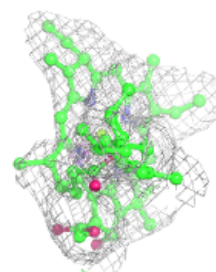
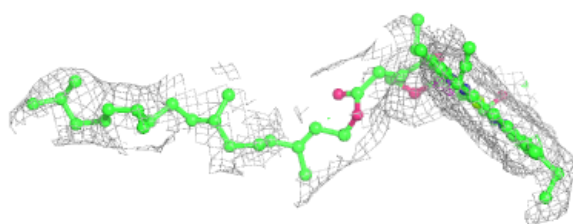
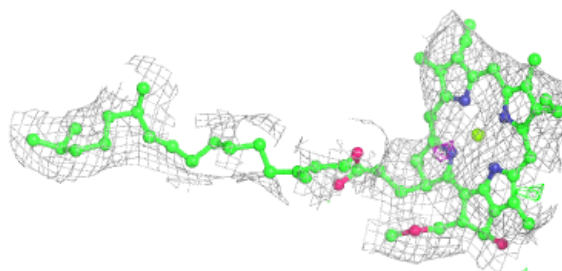


**Electron density around LMU A 7043:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

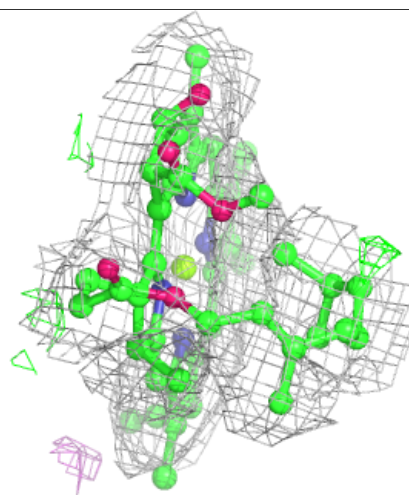
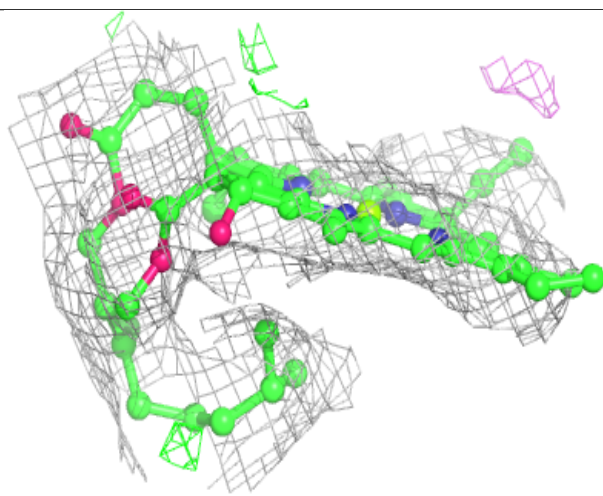
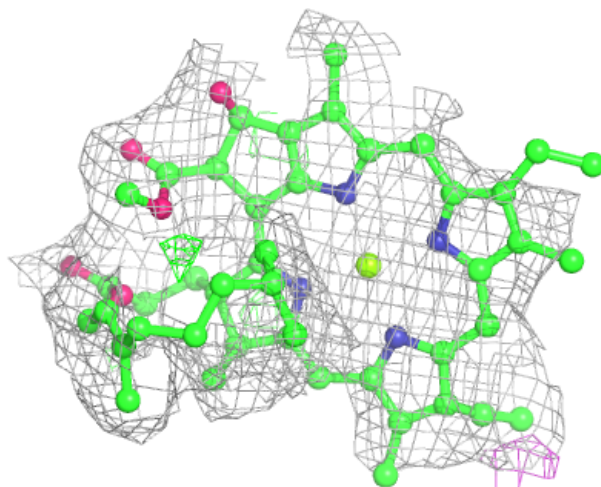
**Electron density around CLA 4 1198:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 4 1199:**

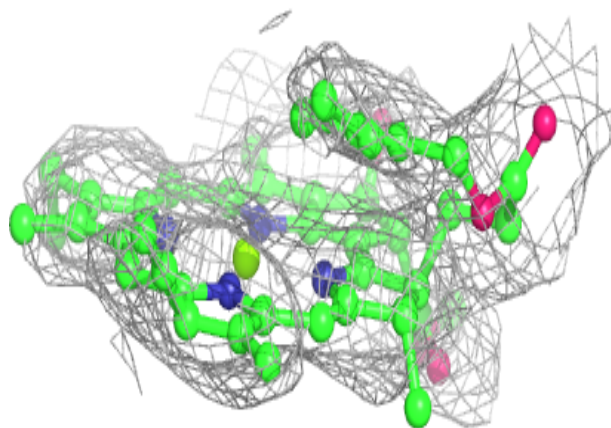
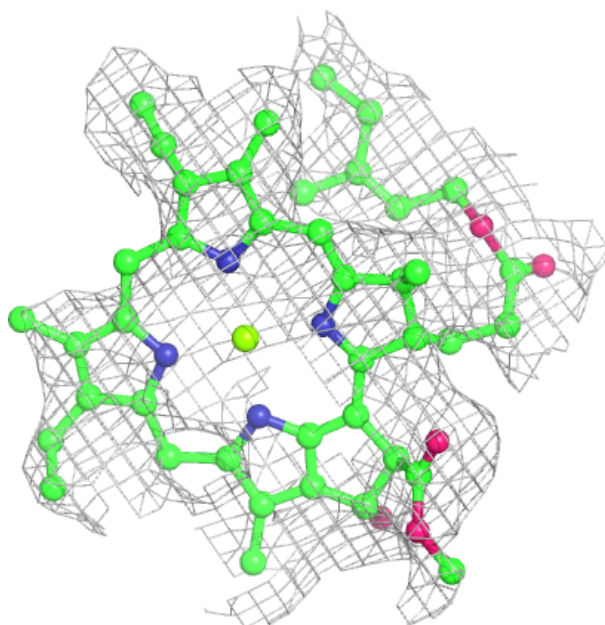
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





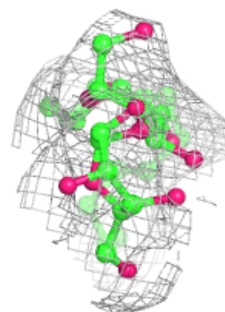
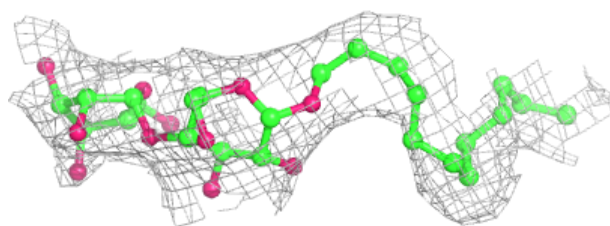
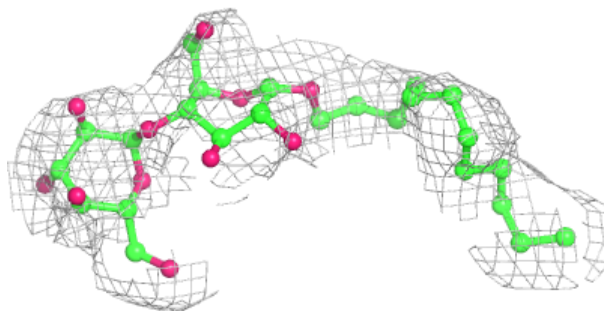
**Electron density around CLA G 1099:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

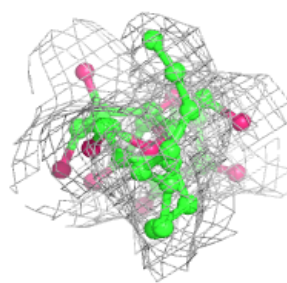
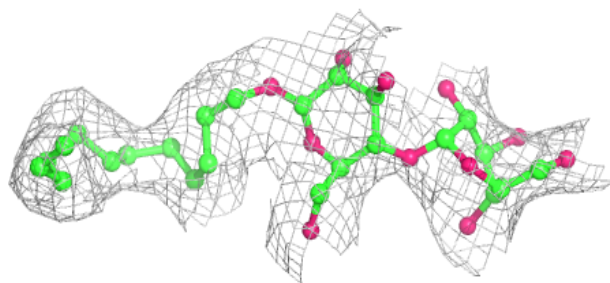
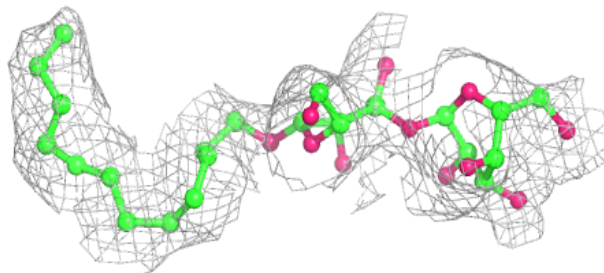


**Electron density around LMU A 7034:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

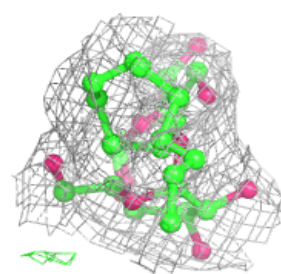
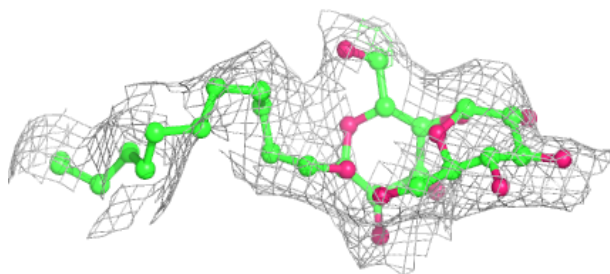
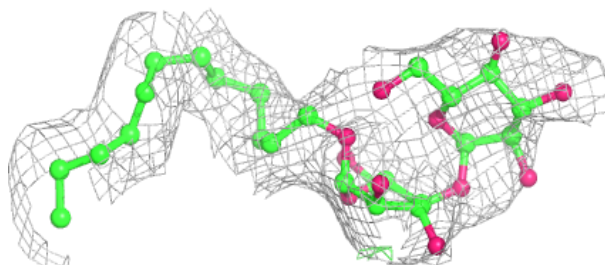
**Electron density around LMU A 1809:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

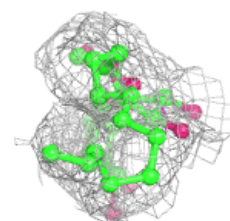
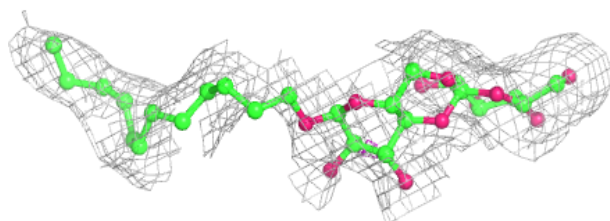
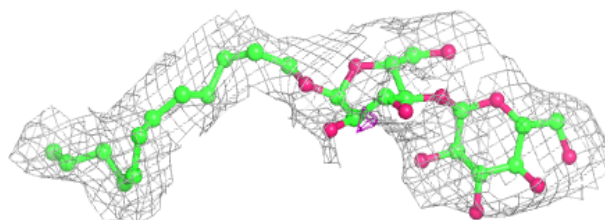


**Electron density around LMU A 1810:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

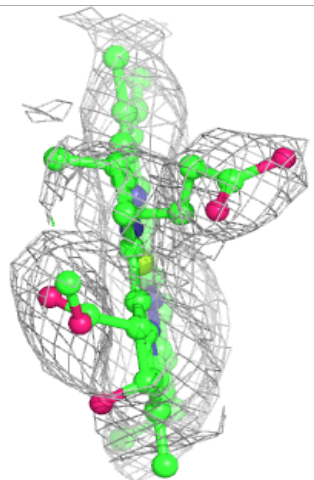
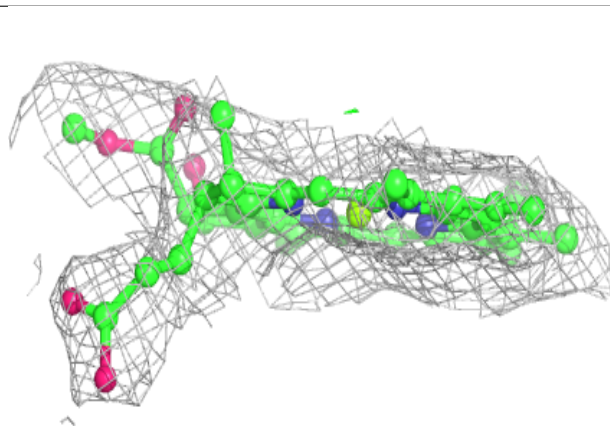
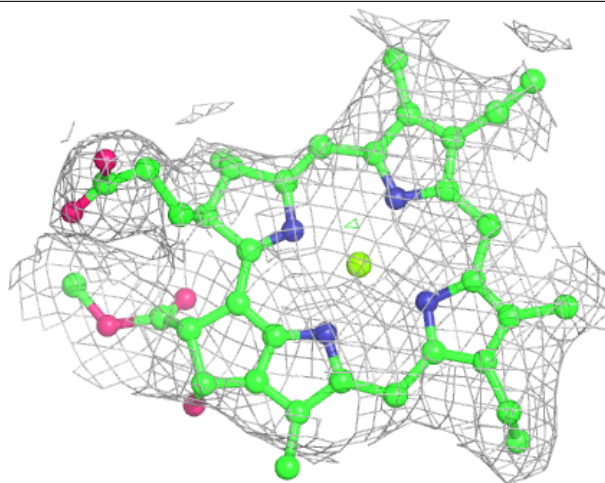
**Electron density around LMU A 7038:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



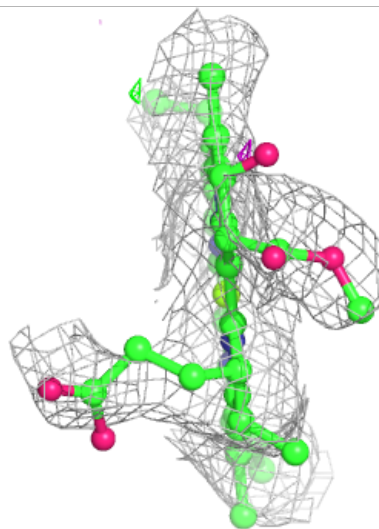
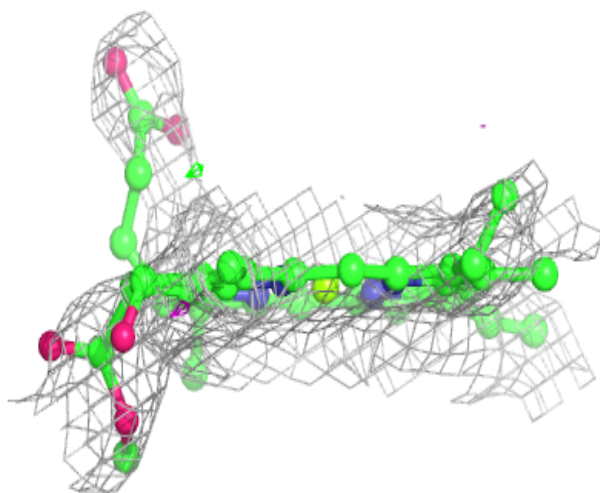
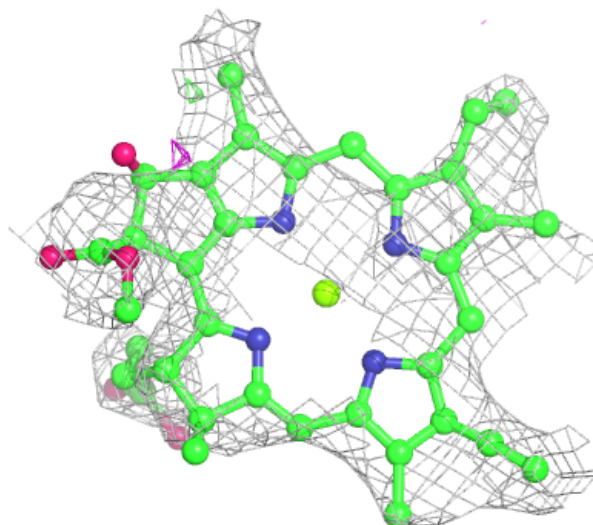
**Electron density around CLA A 1766:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 1770:**

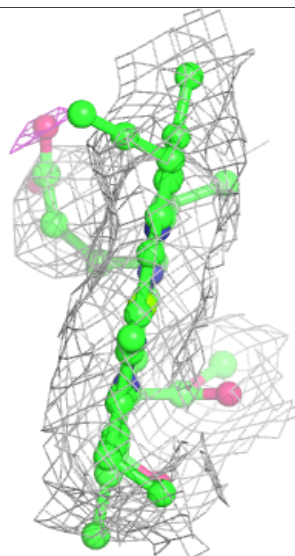
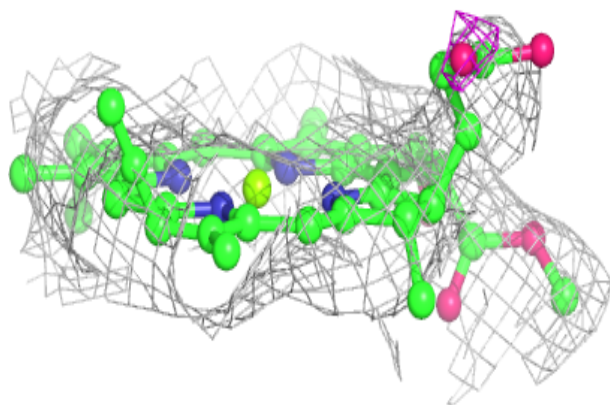
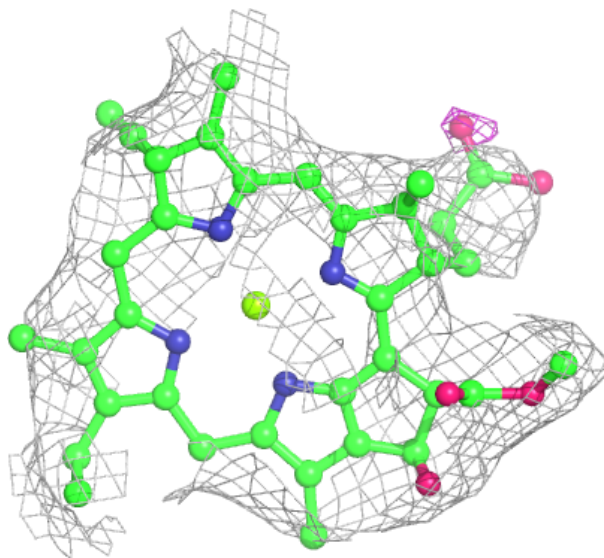
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





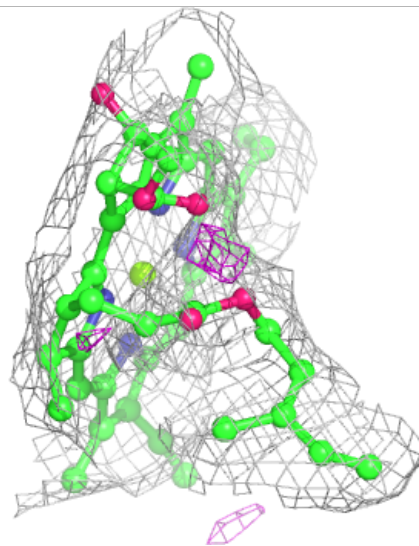
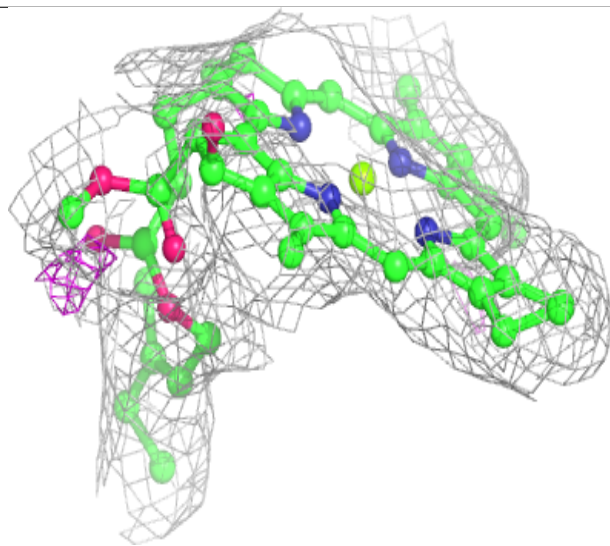
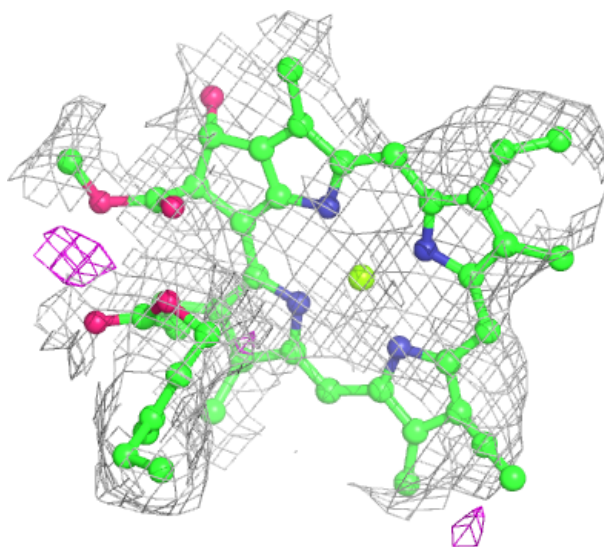
**Electron density around CLA A 1791:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



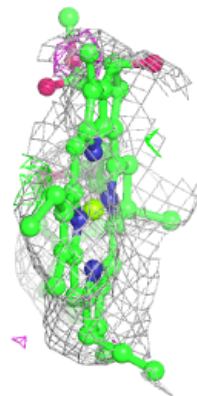
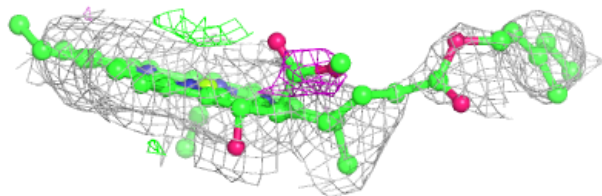
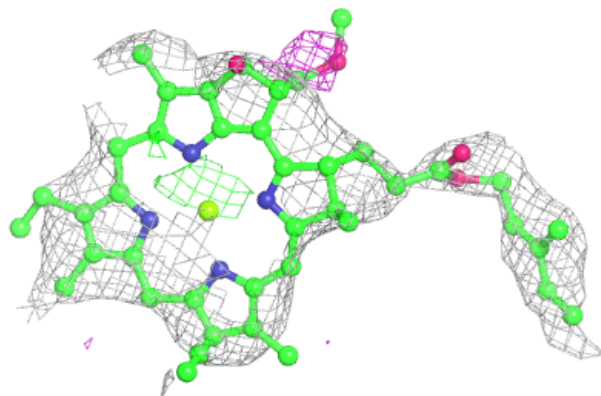
**Electron density around CLA 1 1193:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

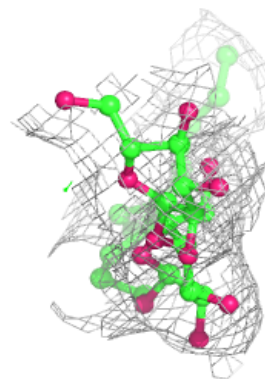
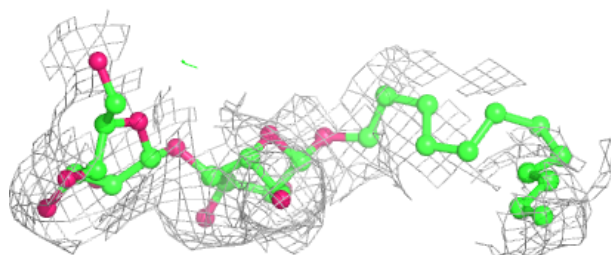
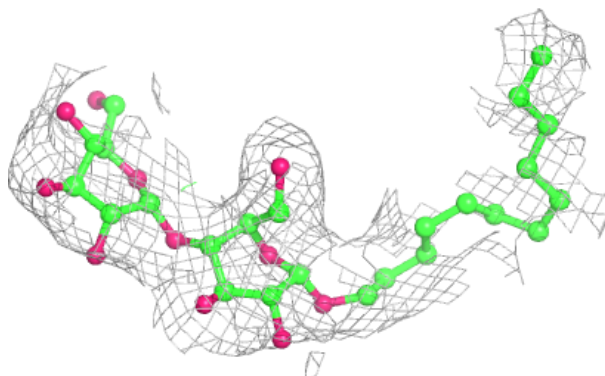


**Electron density around CLA 1 1200:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMU A 7030:**

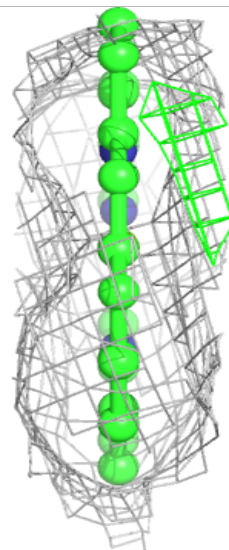
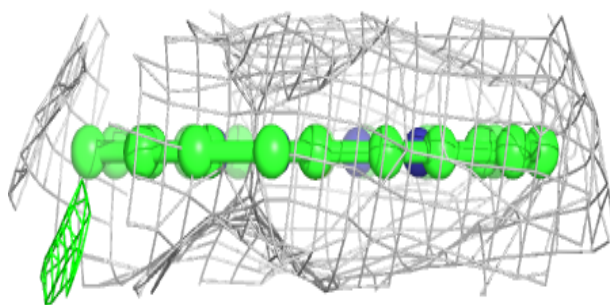
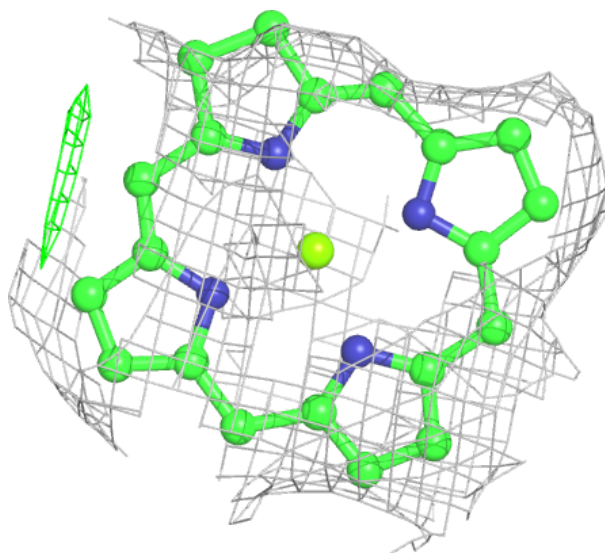
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





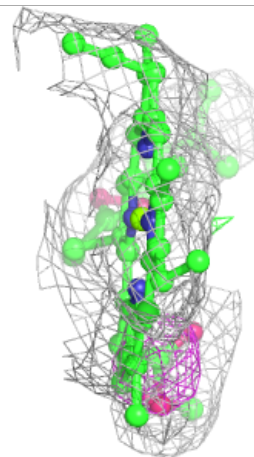
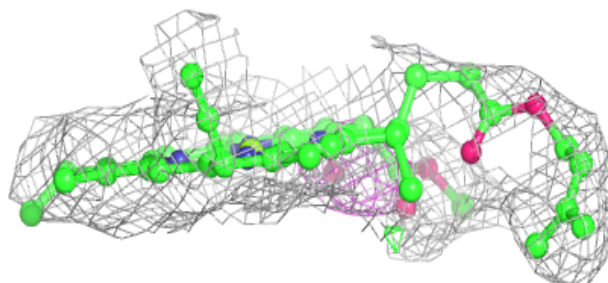
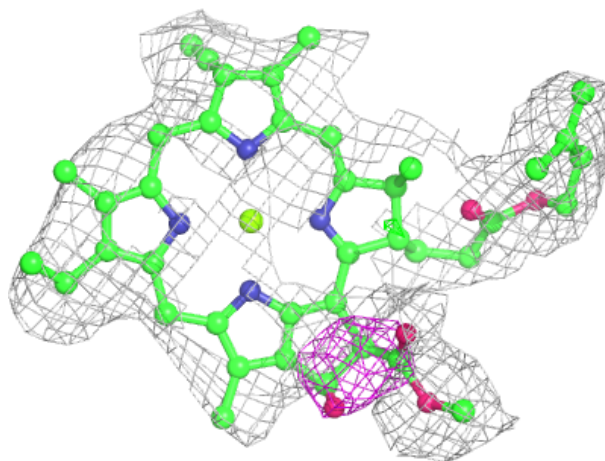
**Electron density around CLA 3 1213:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



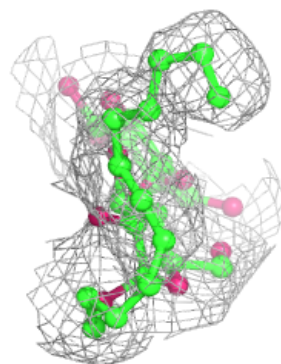
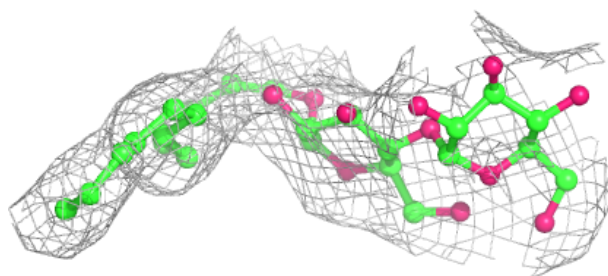
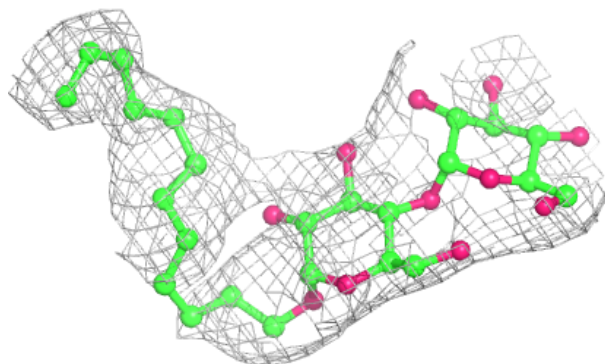
**Electron density around CLA K 1146:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

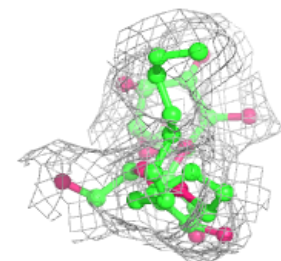
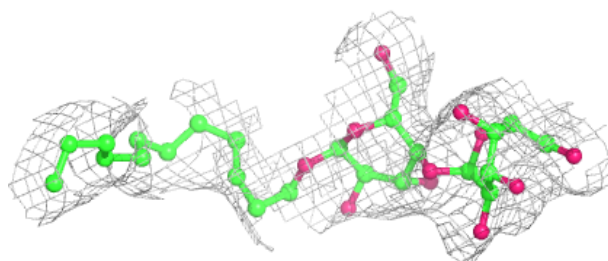
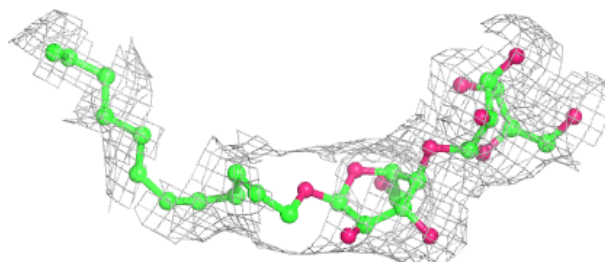


**Electron density around LMU A 7025:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

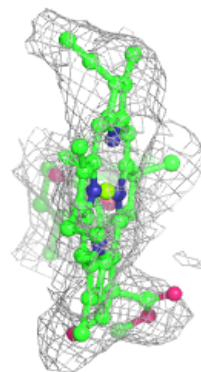
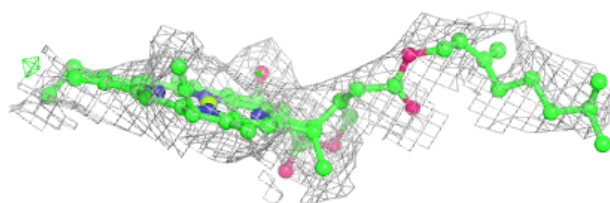
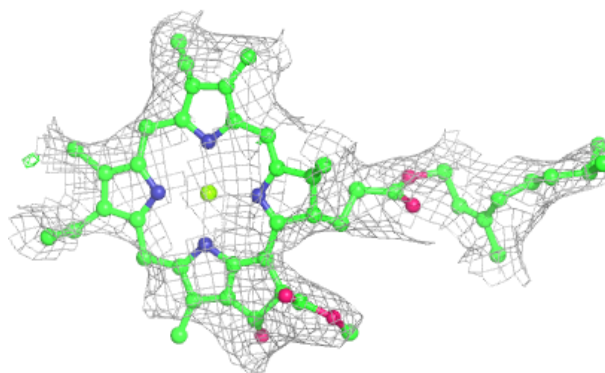
**Electron density around LMU A 7027:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

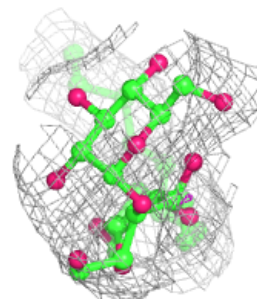
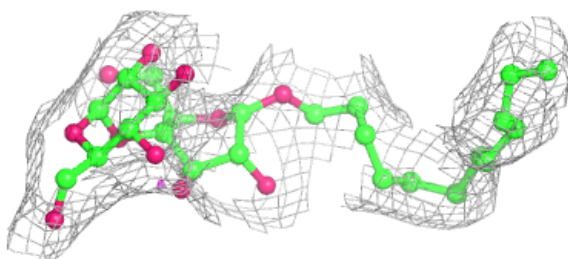
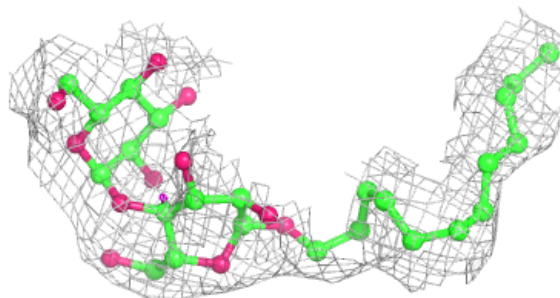


**Electron density around CLA A 1798:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

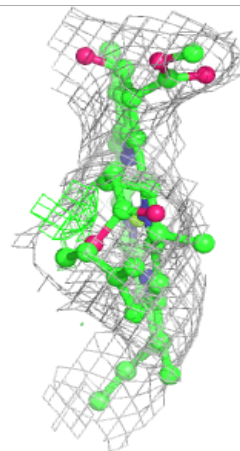
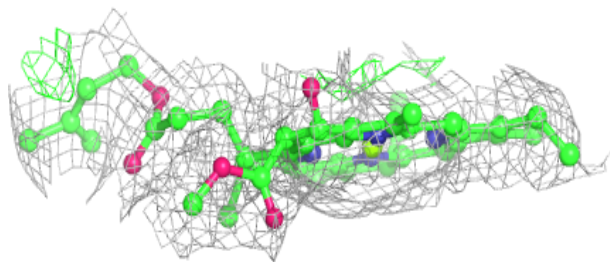
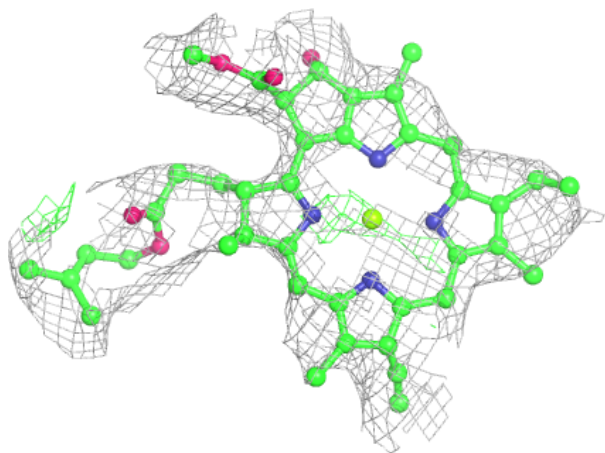
**Electron density around LMU A 7031:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 2 1215:**

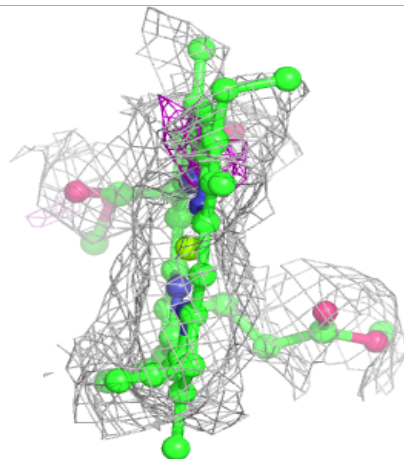
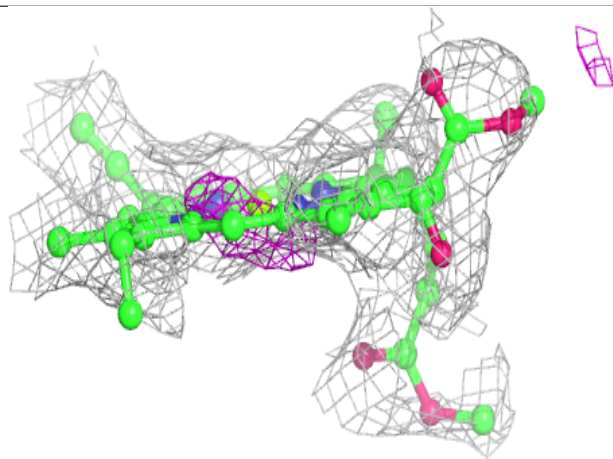
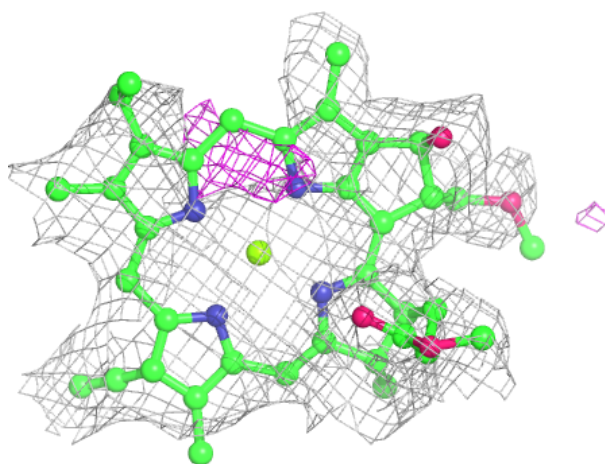
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





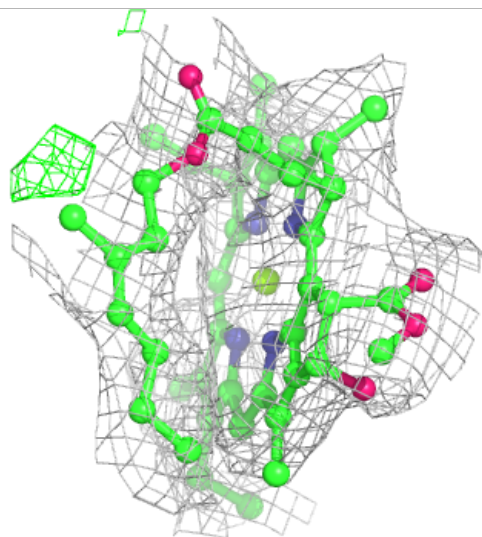
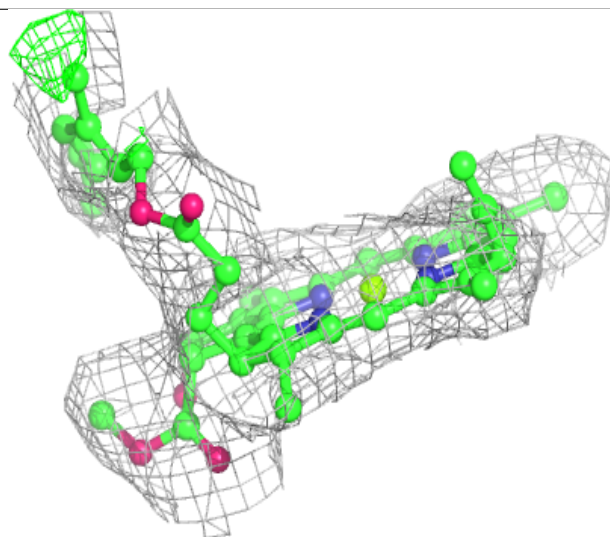
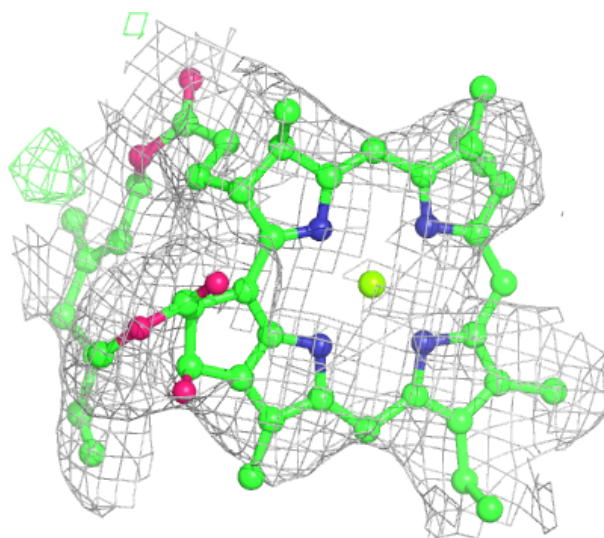
**Electron density around CLA A 1763:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



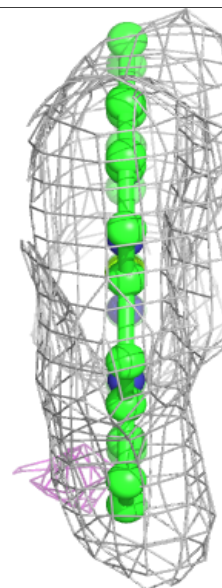
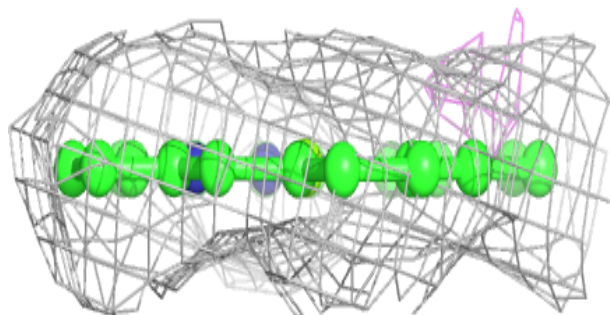
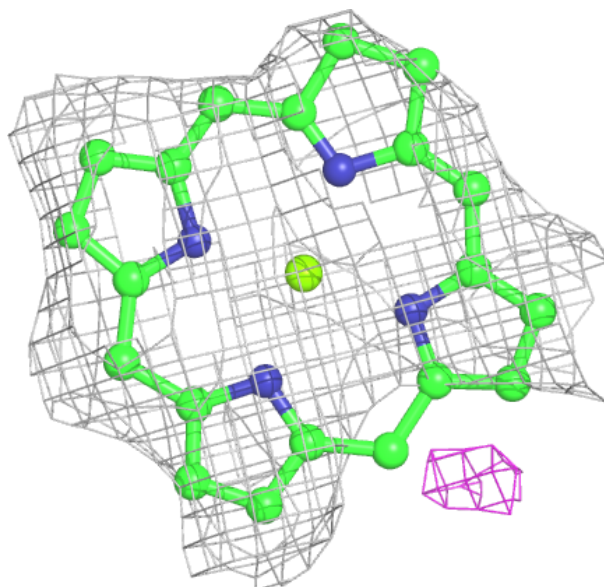
**Electron density around CLA F 1157:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 3 3001:**

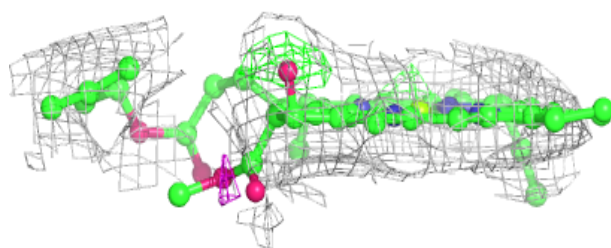
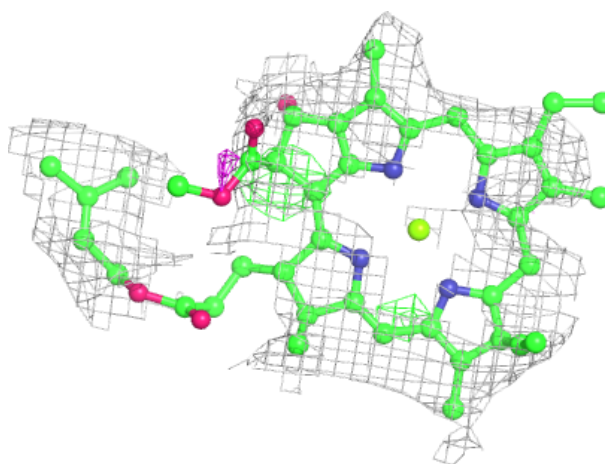
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





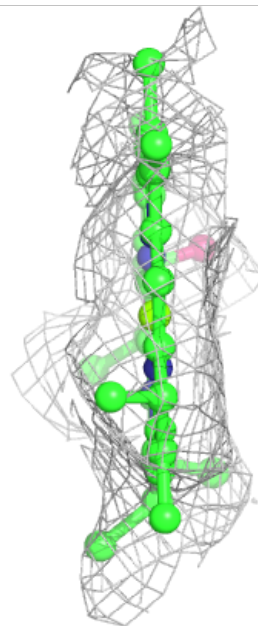
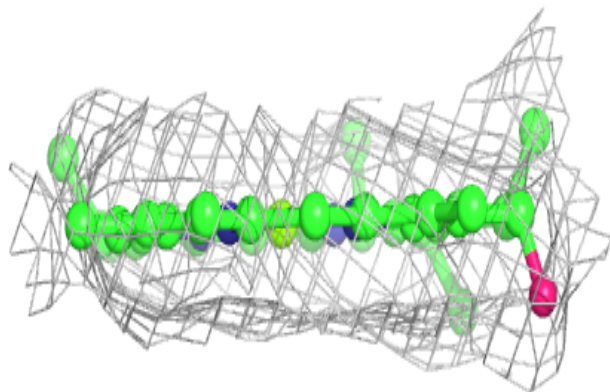
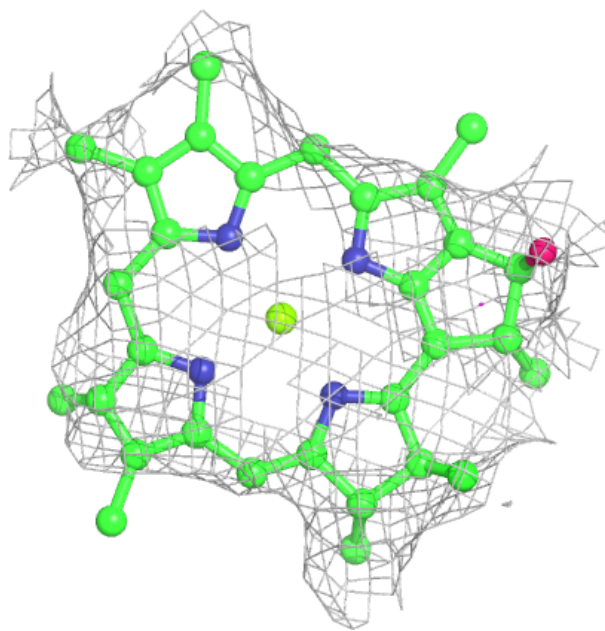
**Electron density around CLA 2 1223:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



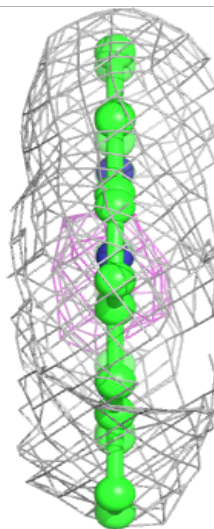
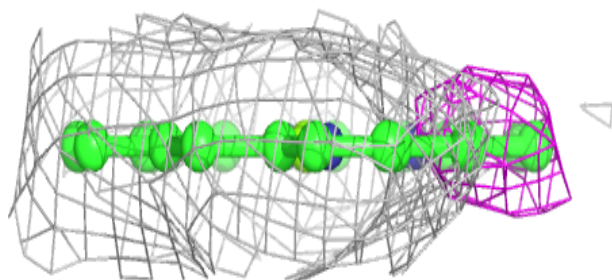
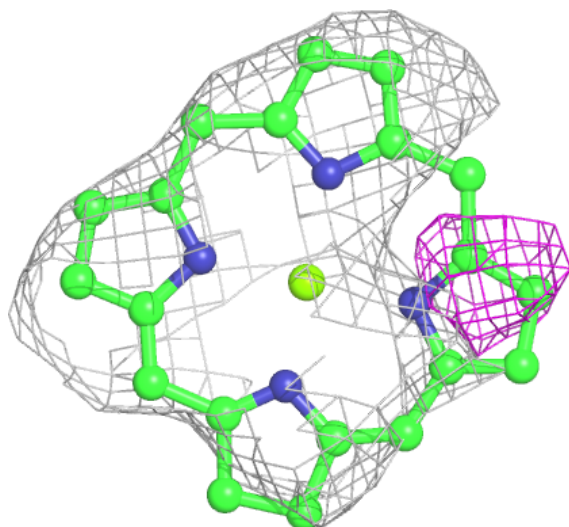
**Electron density around CLA A 1775:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



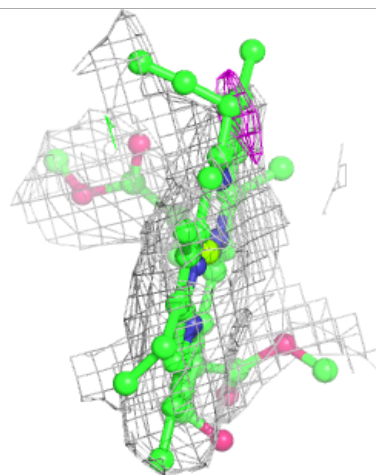
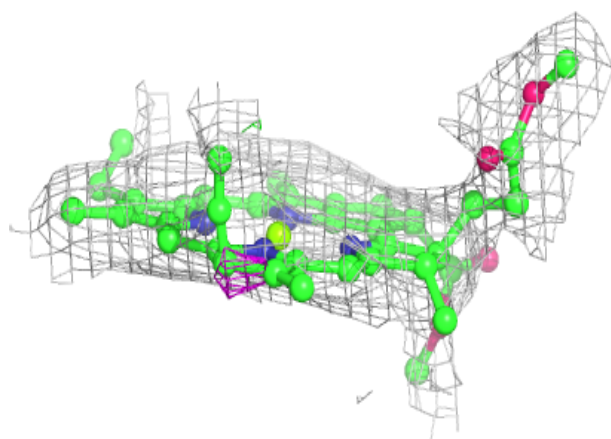
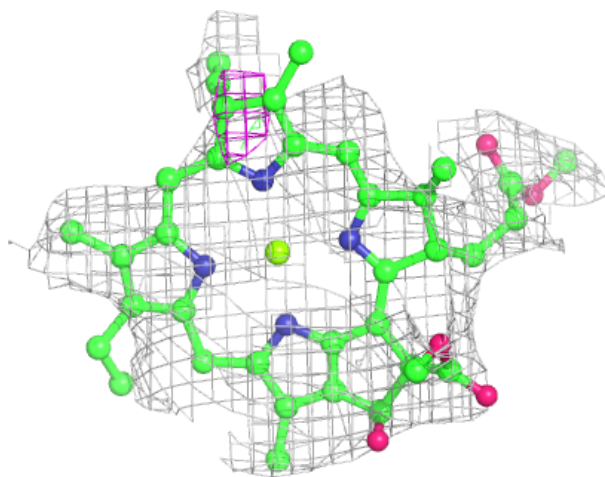
**Electron density around CLA 3 3014:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



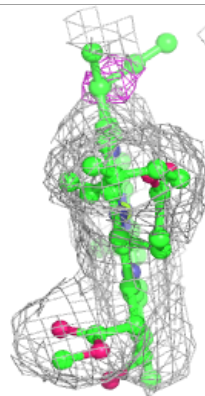
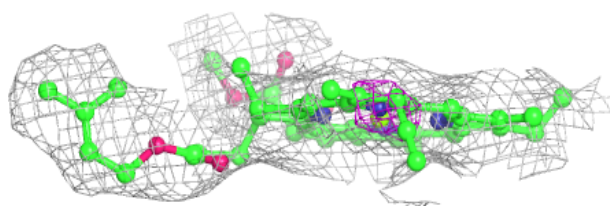
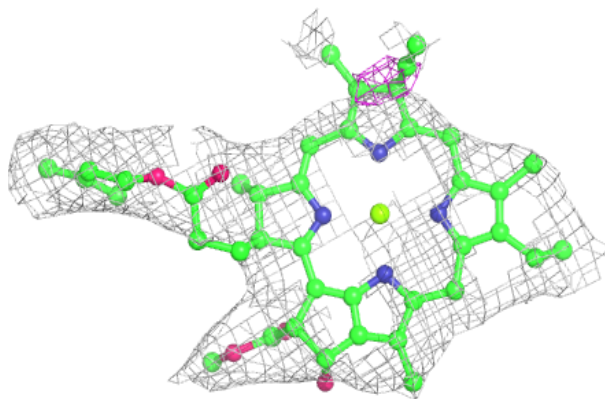
**Electron density around CLA B 1751:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

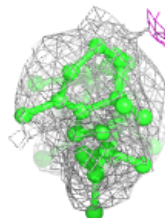
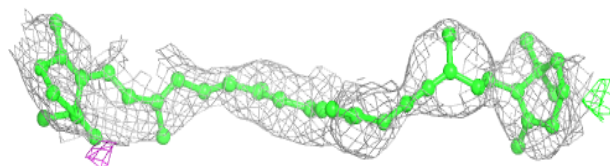
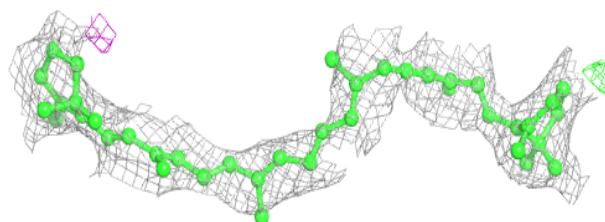


**Electron density around CLA K 1085:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

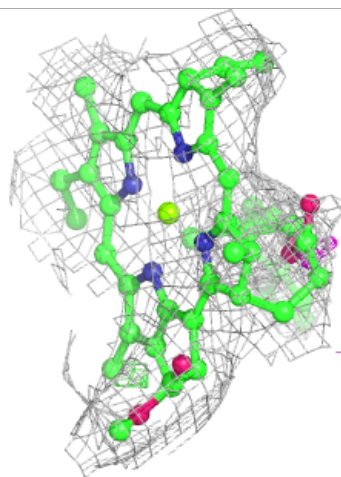
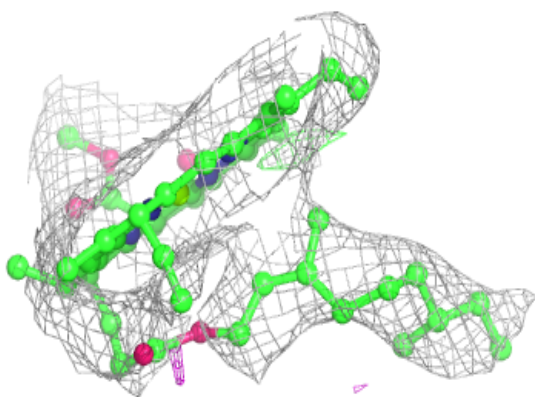
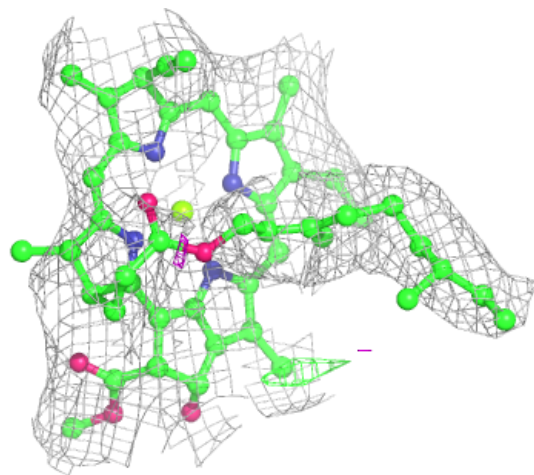
**Electron density around BCR I 1032:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 2 1213:**

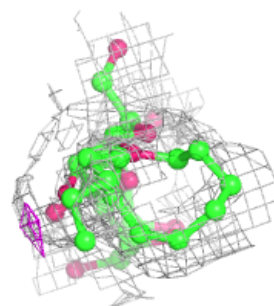
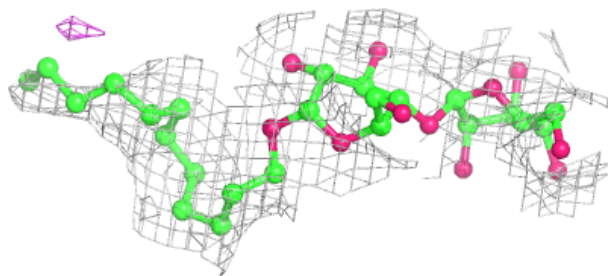
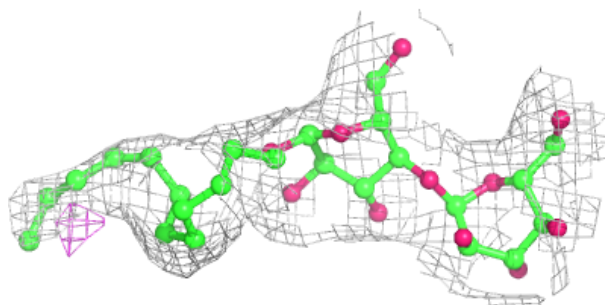
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



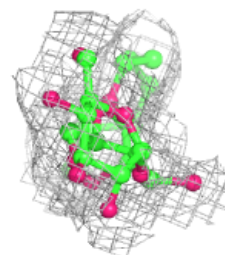
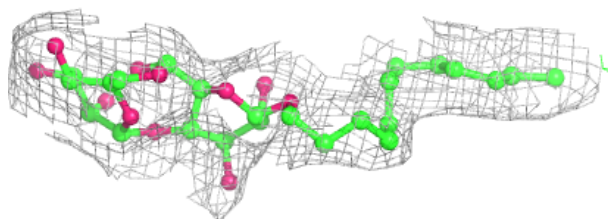
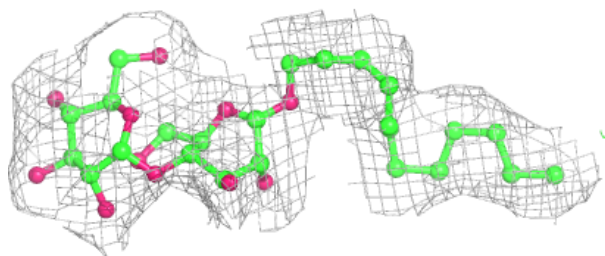


**Electron density around LMU 3 7005:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

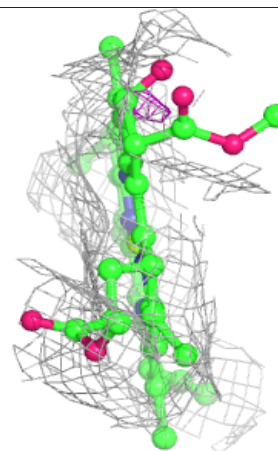
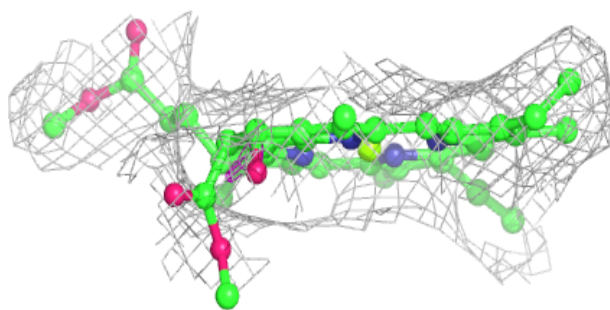
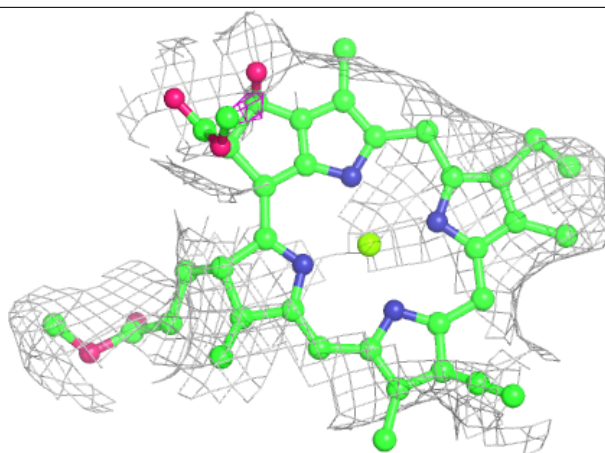
**Electron density around LMU A 7020:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

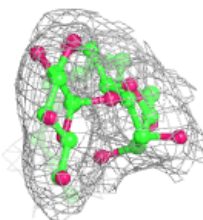
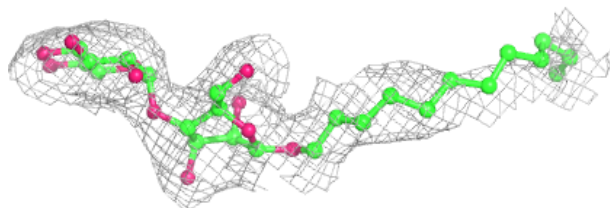
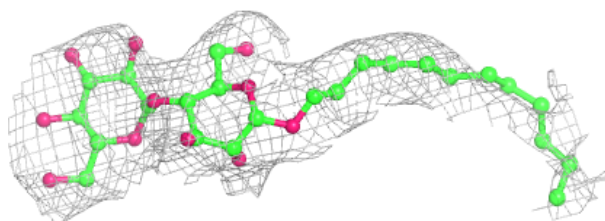


**Electron density around CLA 1 1187:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMU A 7047:**

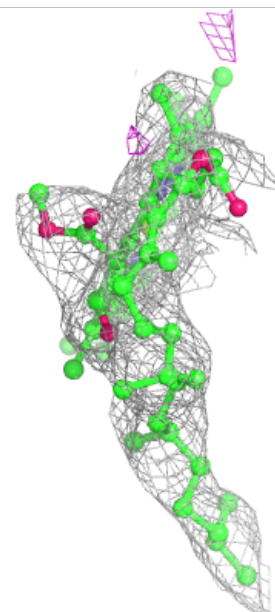
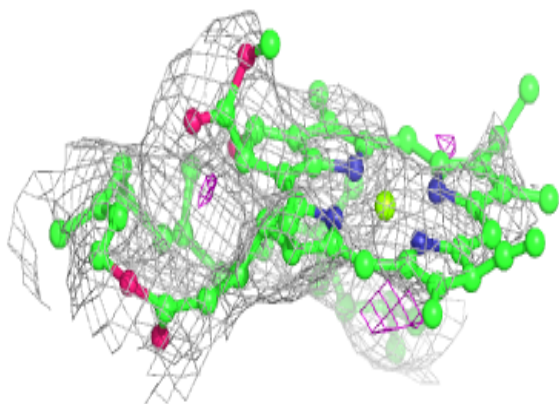
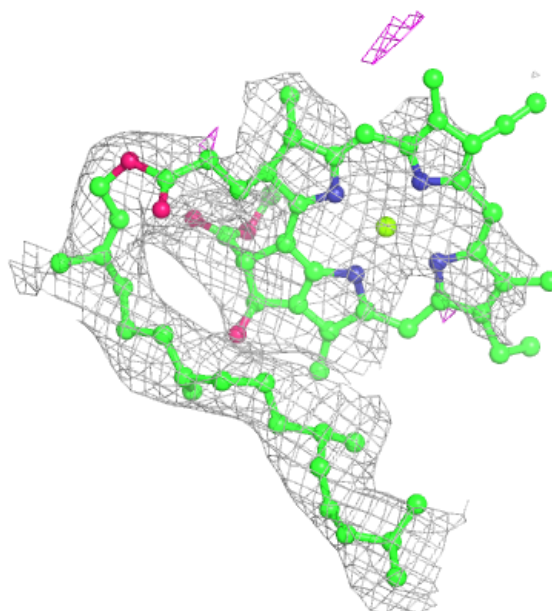
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





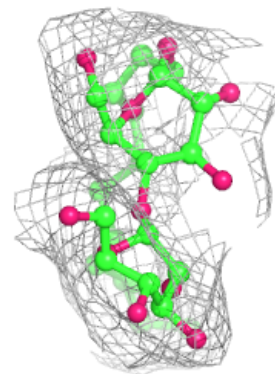
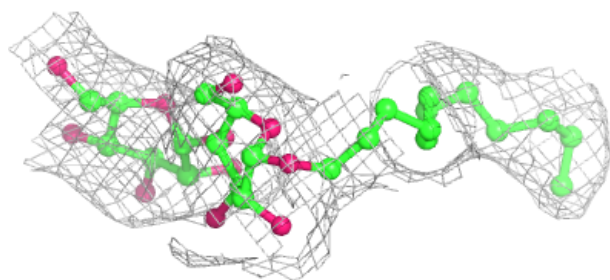
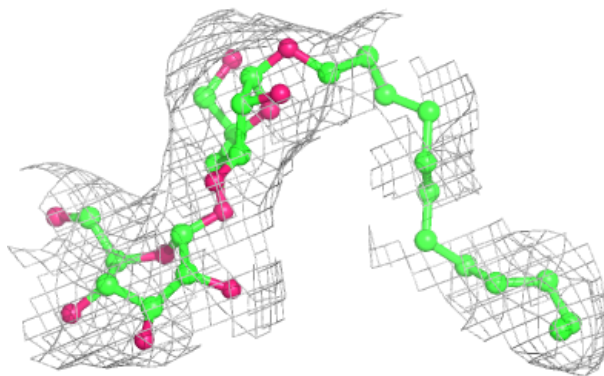
**Electron density around CLA A 1780:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



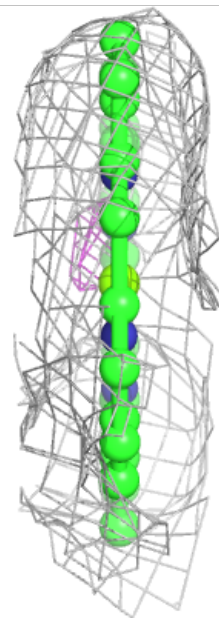
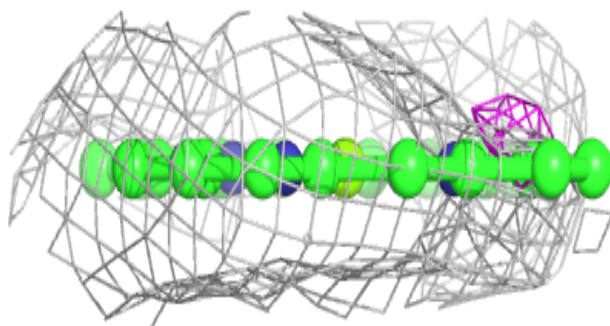
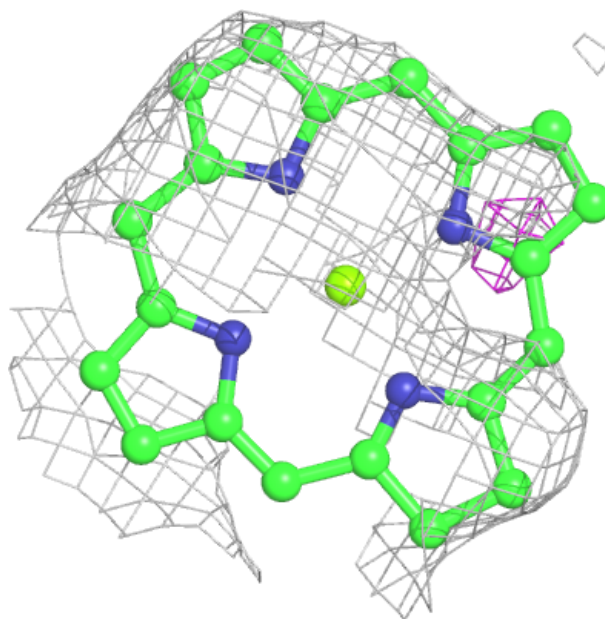
**Electron density around LMU A 7028:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



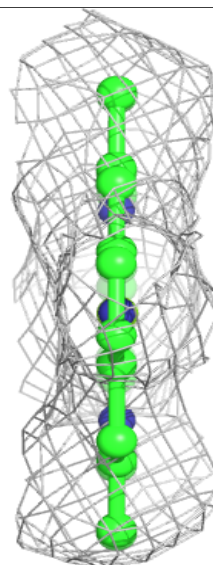
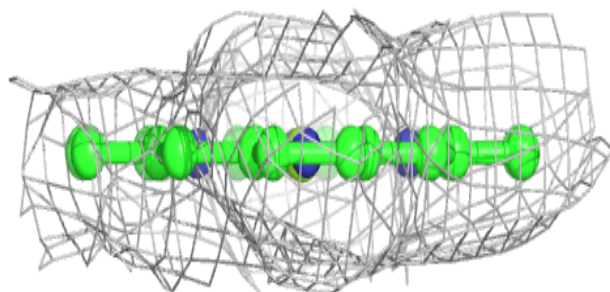
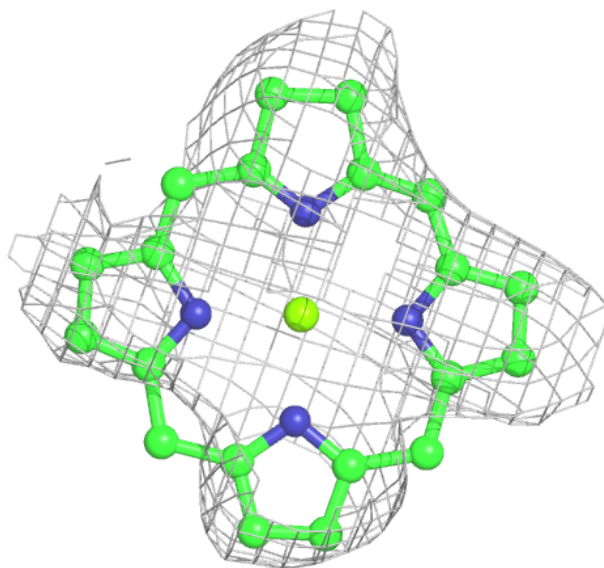
**Electron density around CLA 3 1215:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



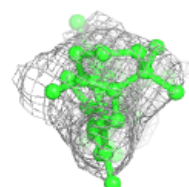
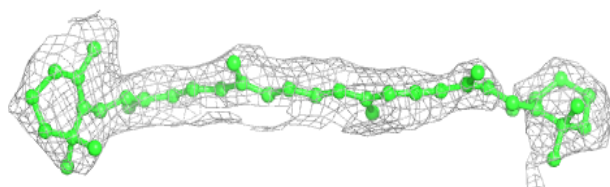
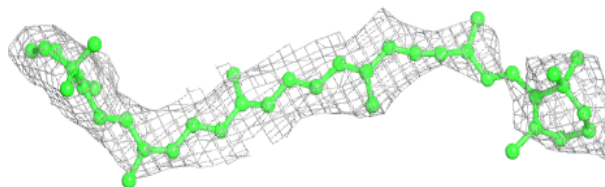
**Electron density around CLA 3 3002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

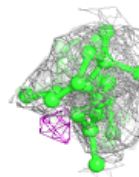
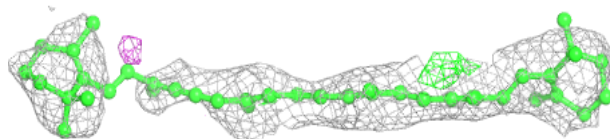
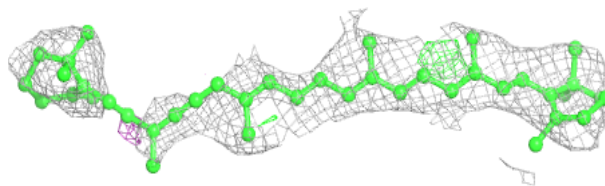


**Electron density around BCR B 1776:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

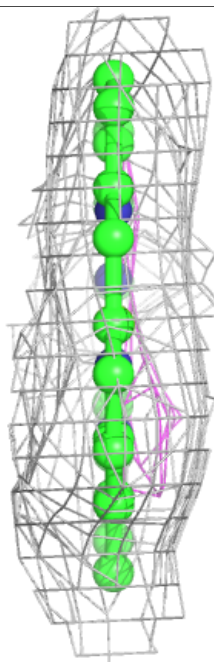
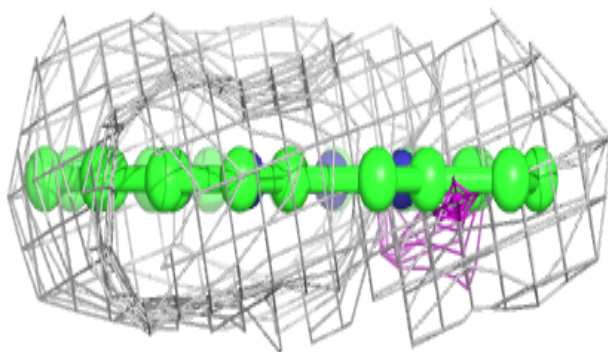
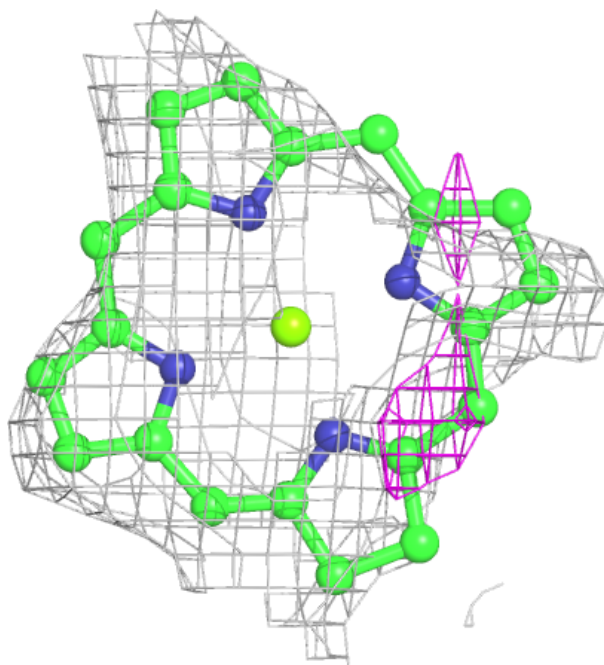
**Electron density around BCR B 1780:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 2 1227:**

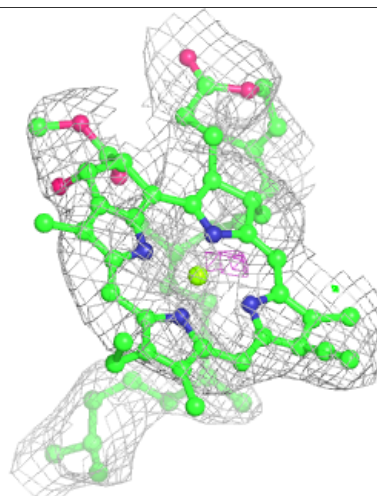
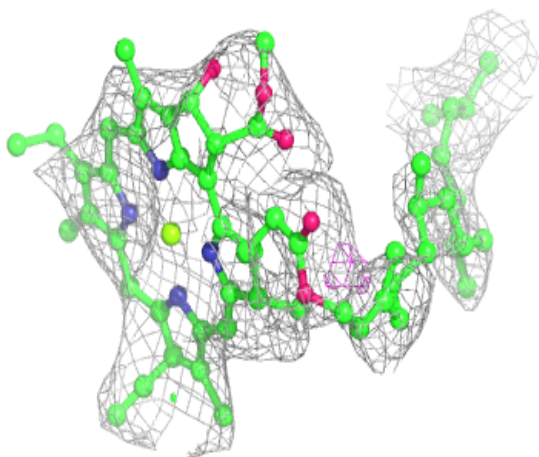
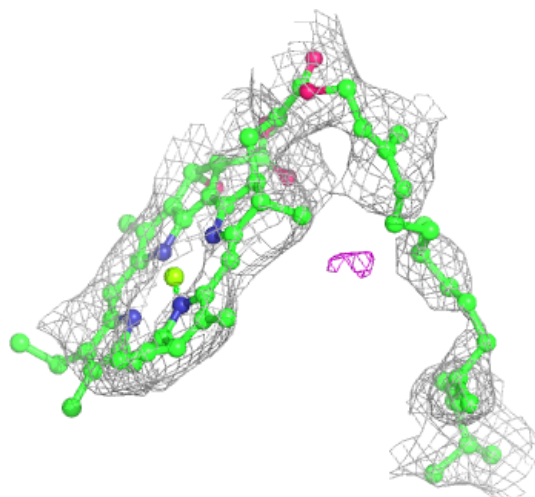
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





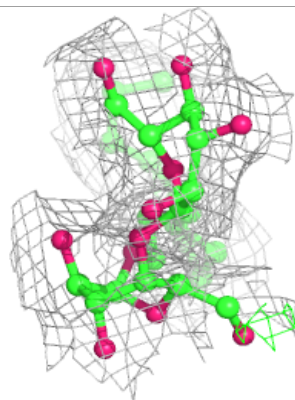
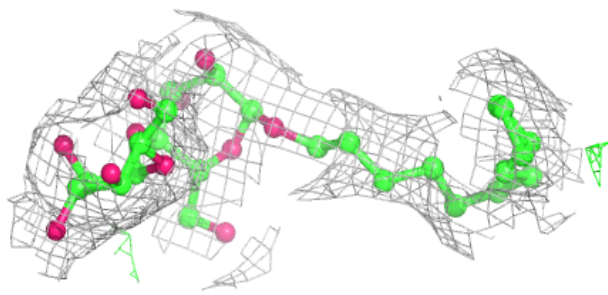
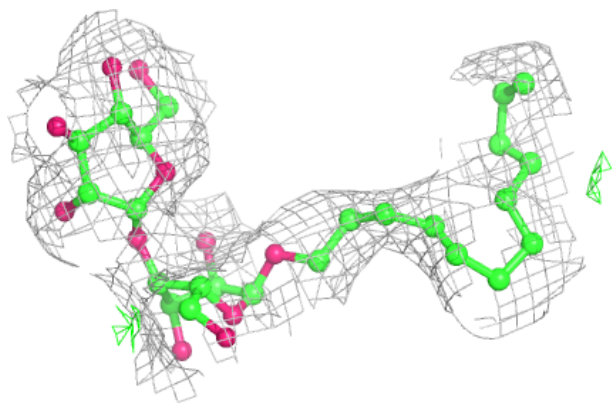
**Electron density around CLA 2 1217:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

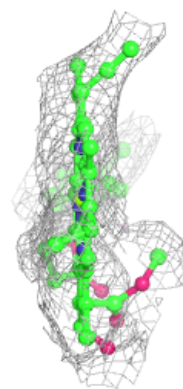
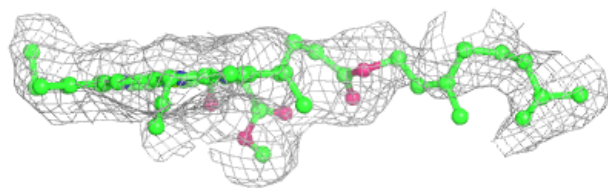
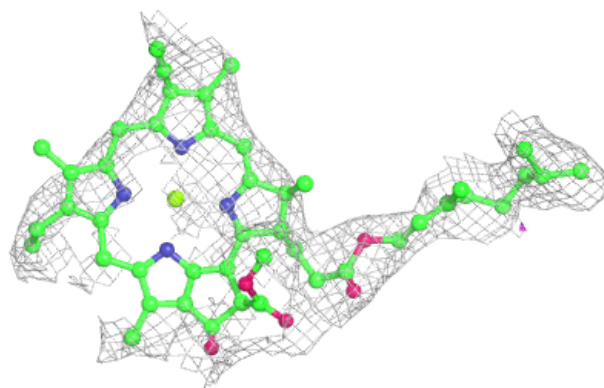


**Electron density around LMU K 1086:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA 4 1204:**

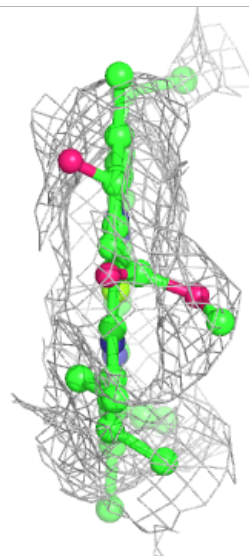
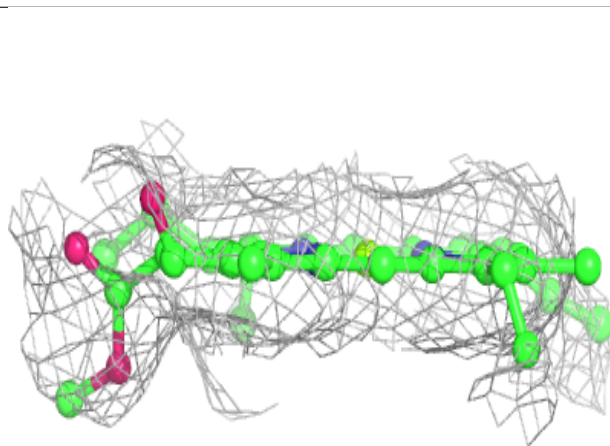
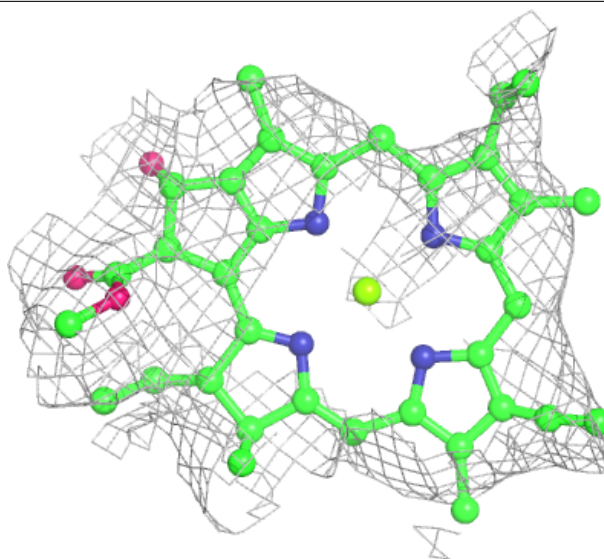
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





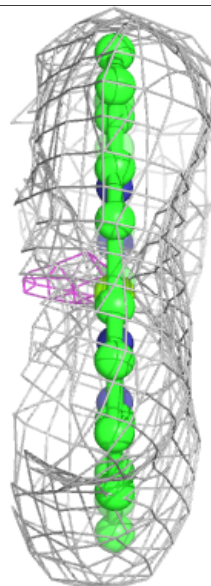
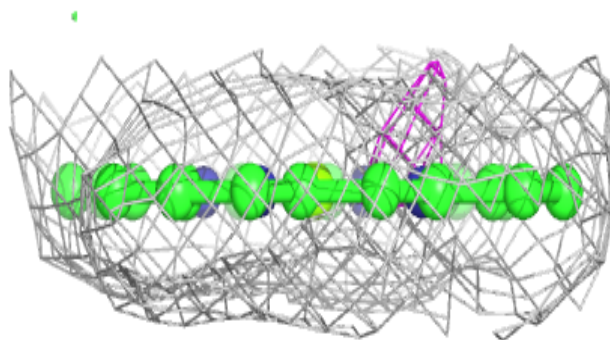
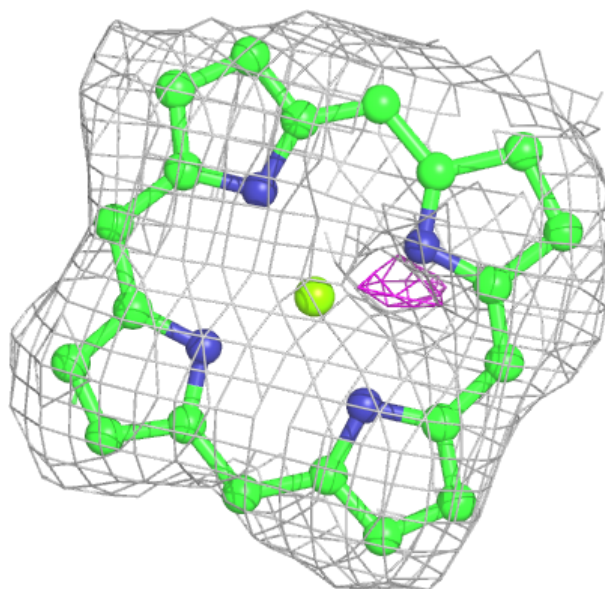
**Electron density around CLA A 1778:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



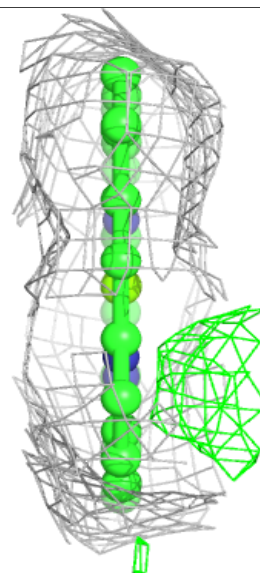
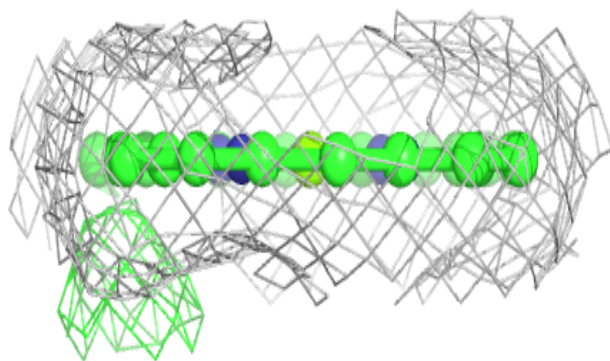
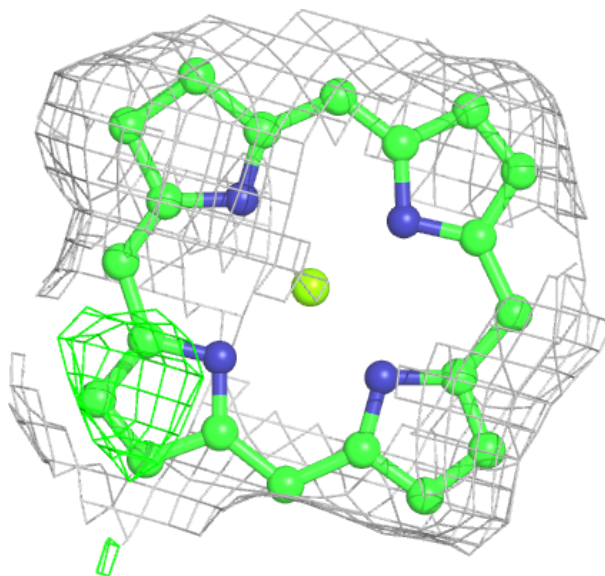
**Electron density around CLA 4 1208:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



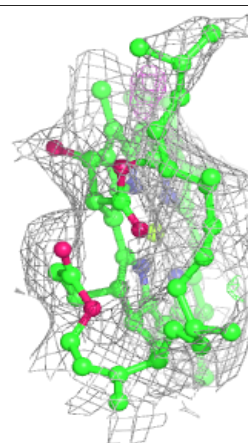
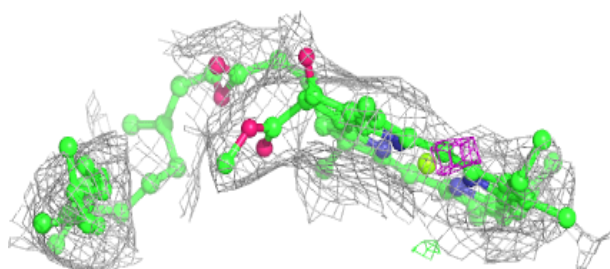
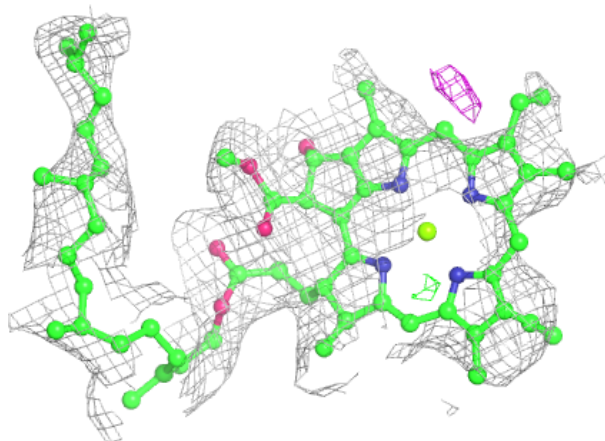
**Electron density around CLA 1 1194:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

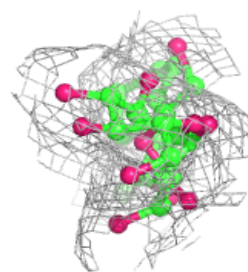
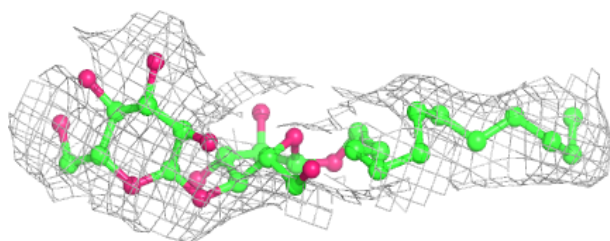
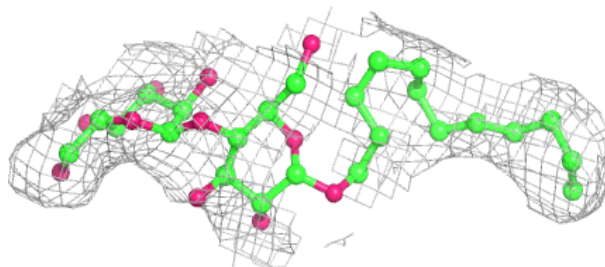


**Electron density around CLA R 1055:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

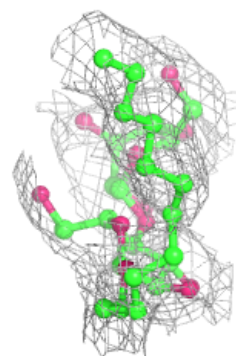
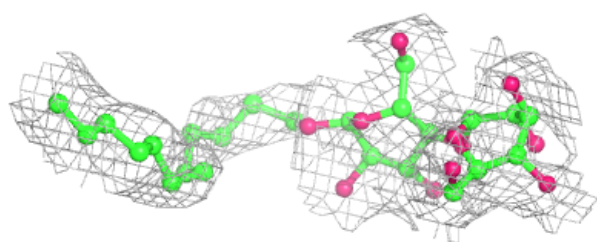
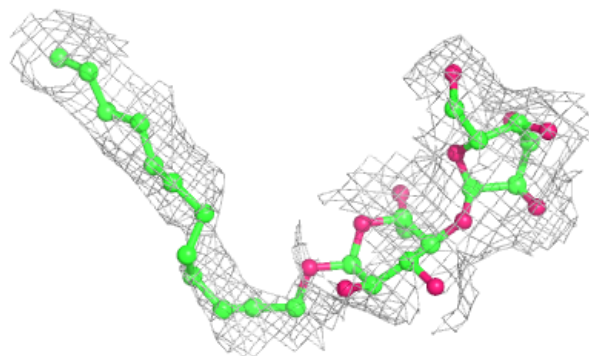
**Electron density around LMU A 7042:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

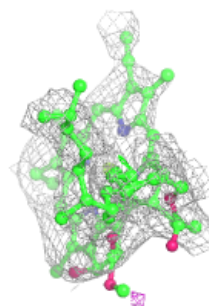
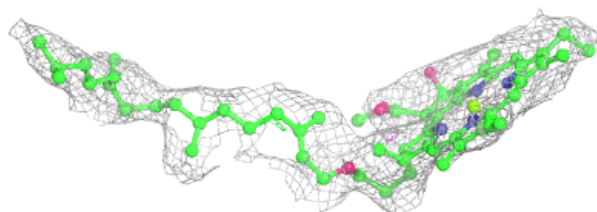
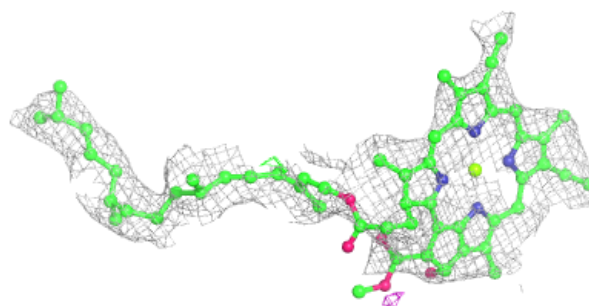


**Electron density around LMU 1 1202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA H 1079:**

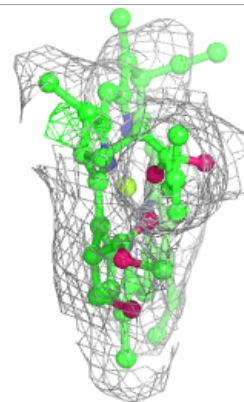
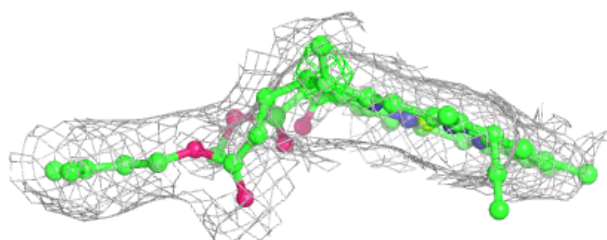
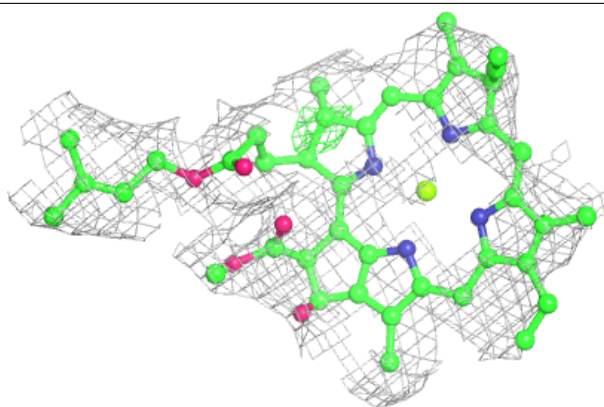
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



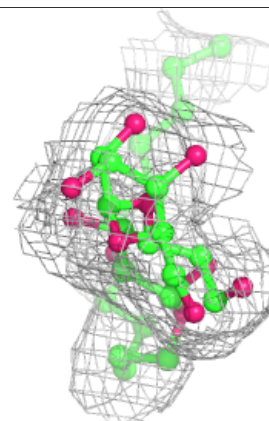
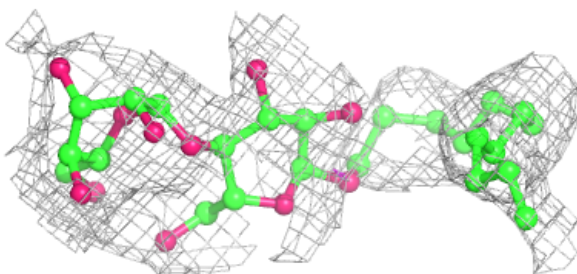
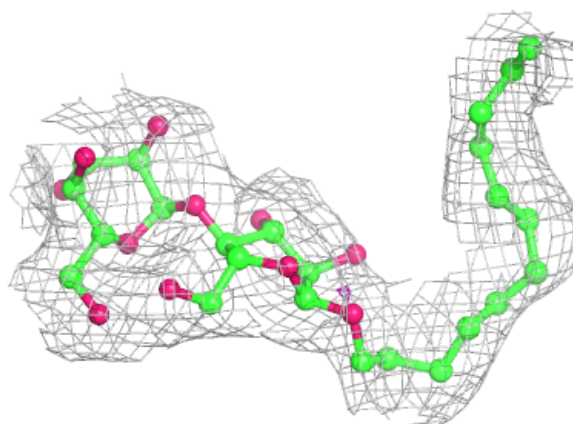


**Electron density around CLA L 1168:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

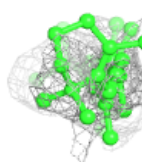
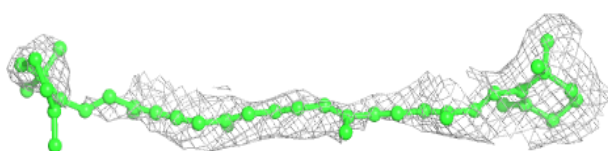
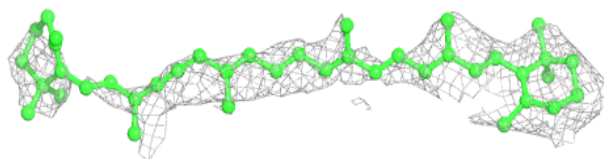
**Electron density around LMU 2 7003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

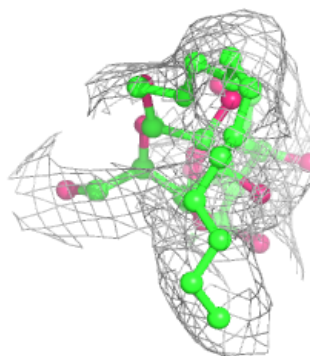
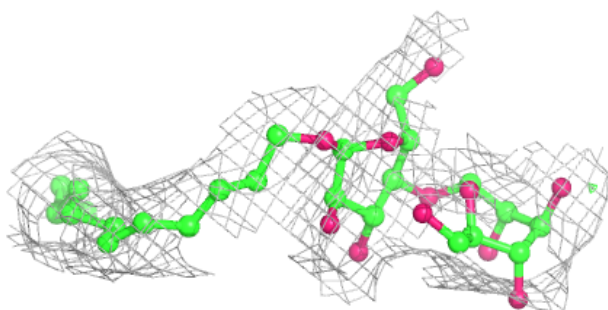
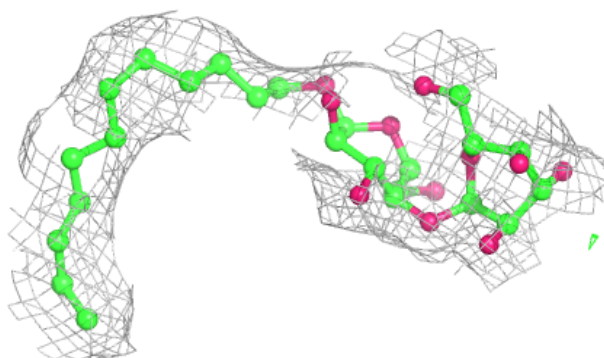


**Electron density around BCR A 1806:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

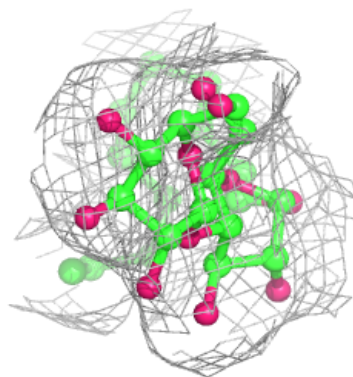
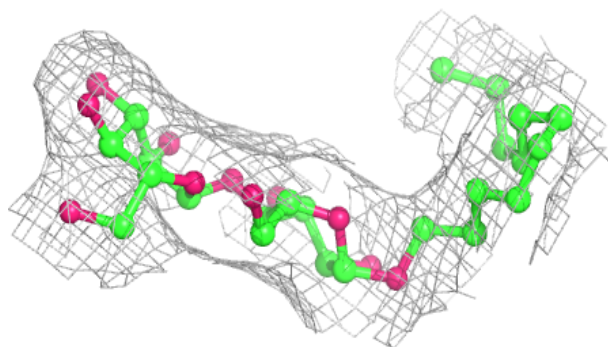
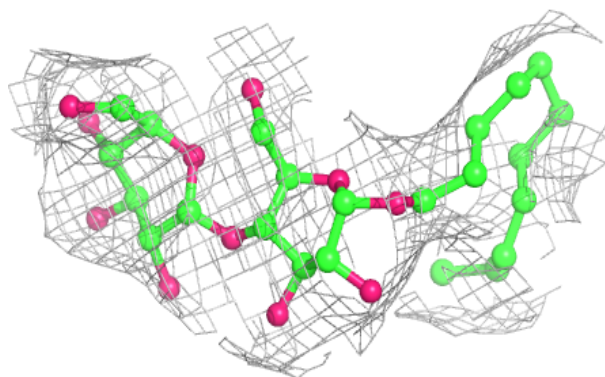
**Electron density around LMU 2 7006:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LMU A 7036:**

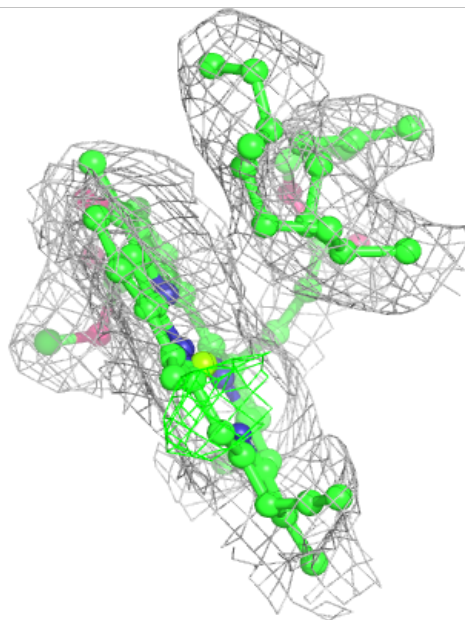
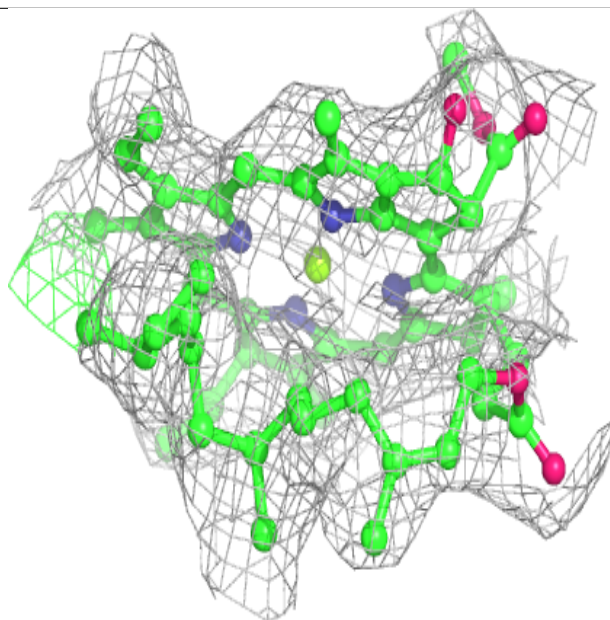
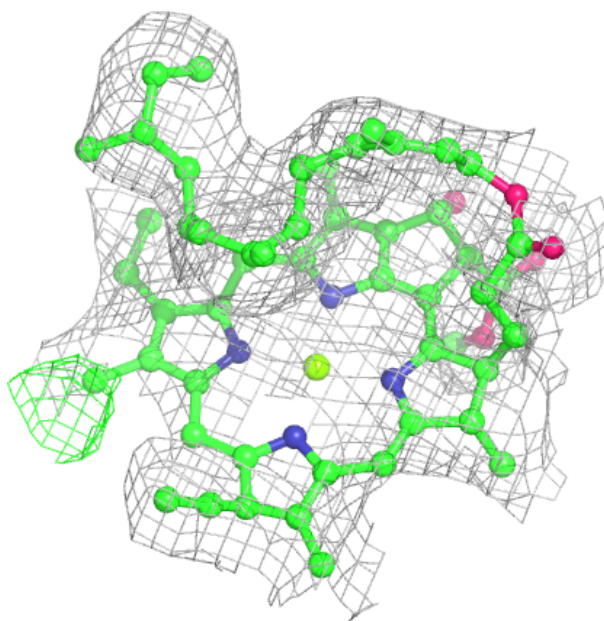
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





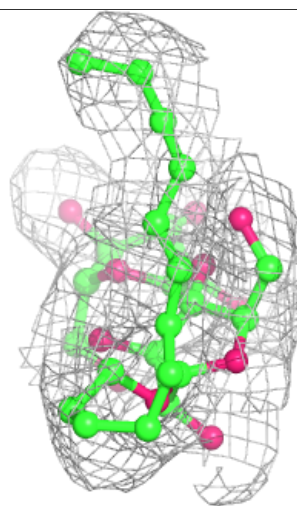
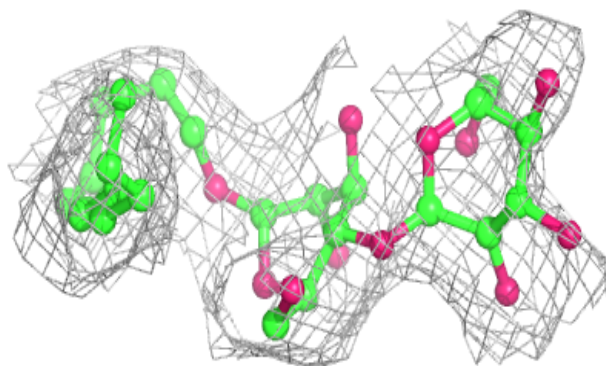
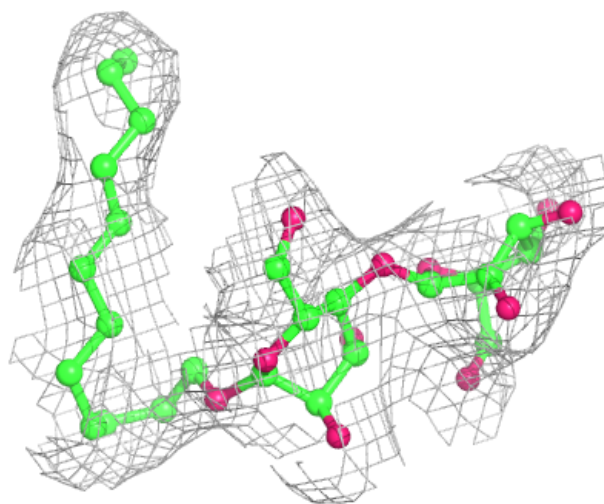
**Electron density around CLA 1 1192:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



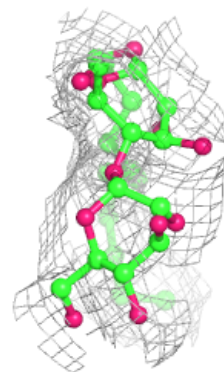
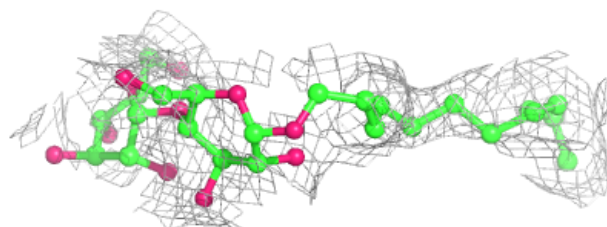
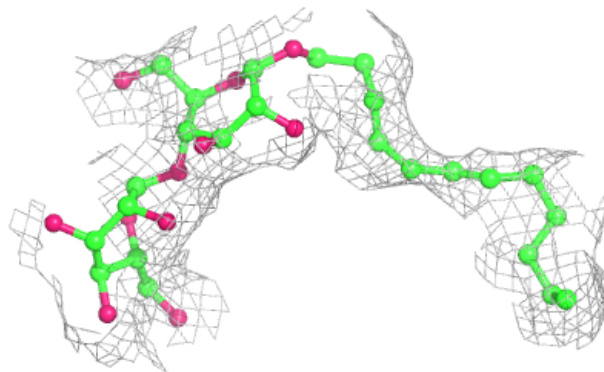
**Electron density around LMU R 1057:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



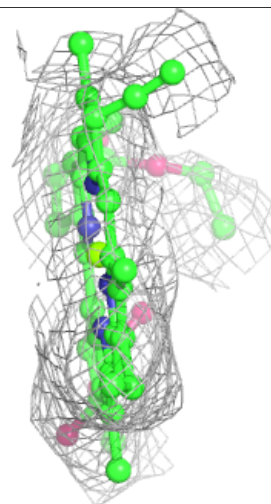
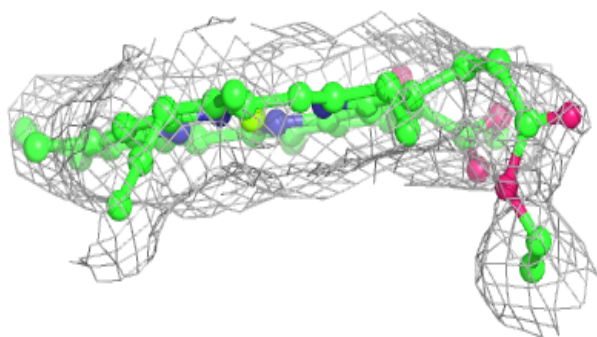
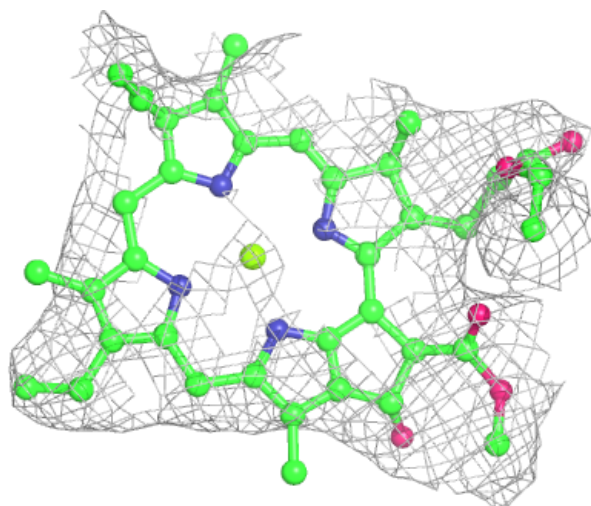
**Electron density around LMU A 7019:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



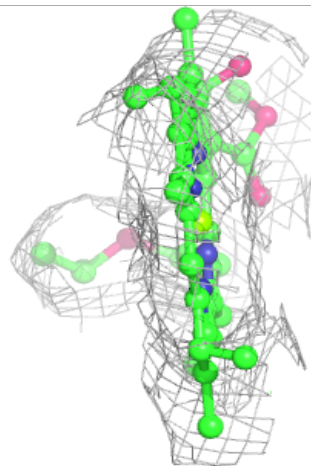
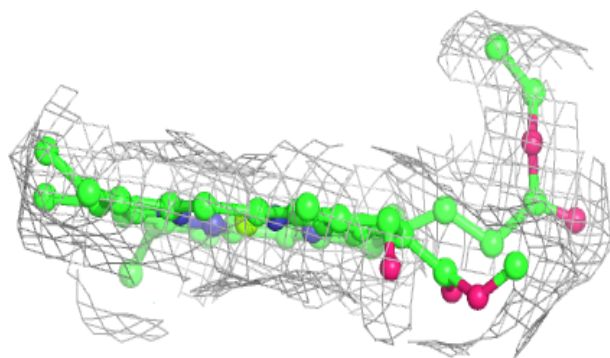
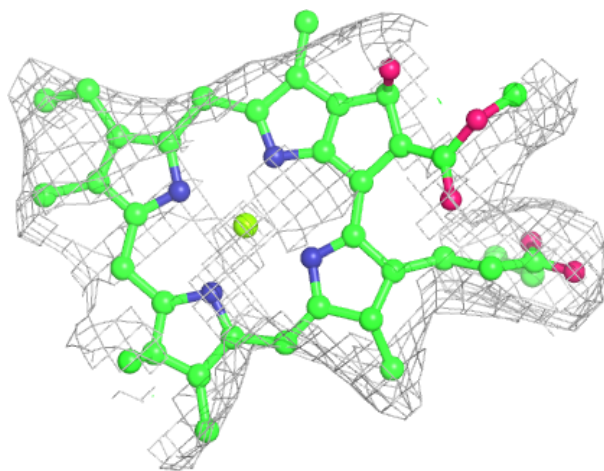
**Electron density around CLA 1 1188:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 1817:**

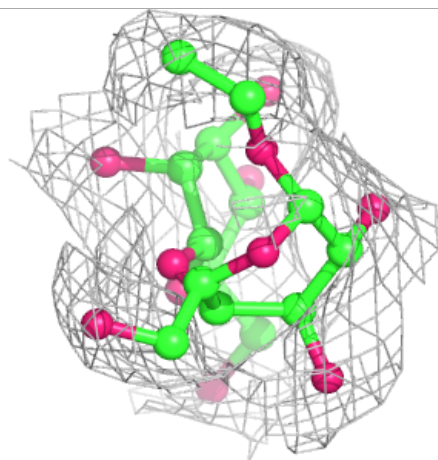
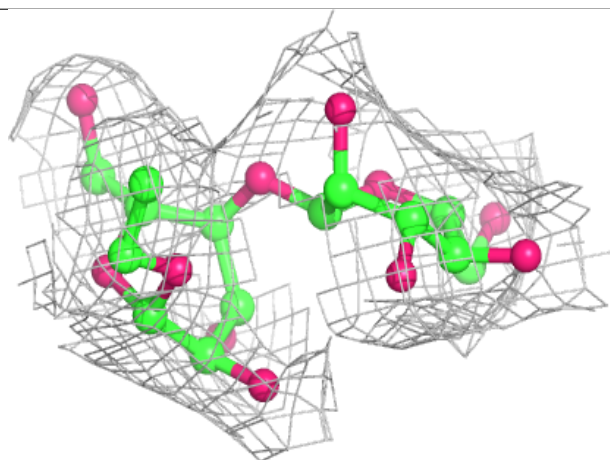
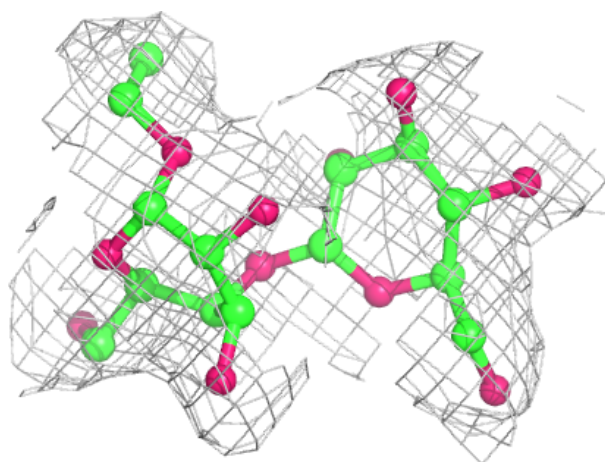
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





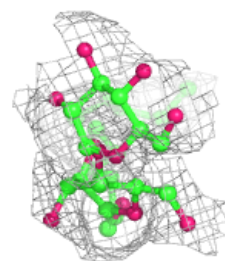
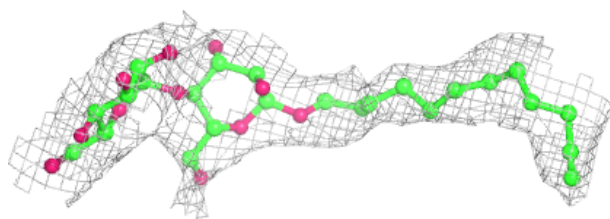
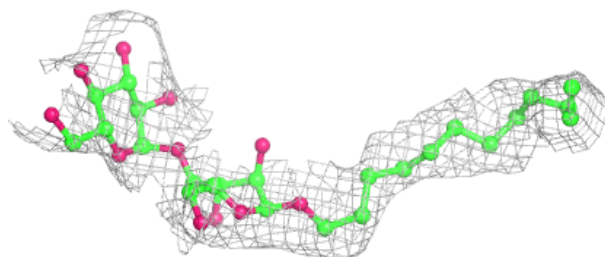
**Electron density around LMU B 1782:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



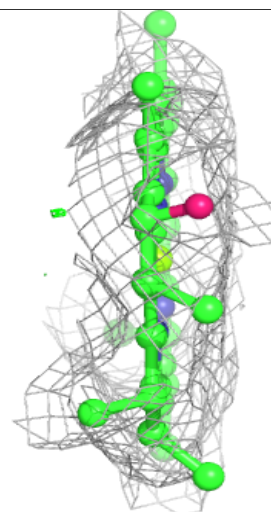
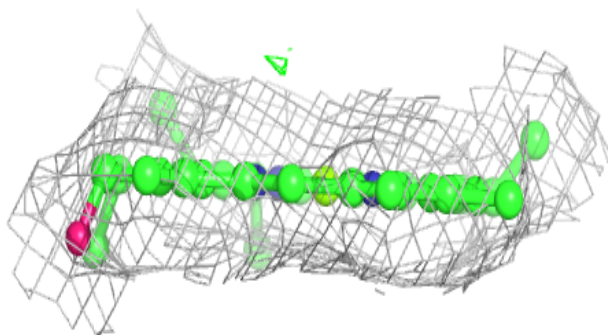
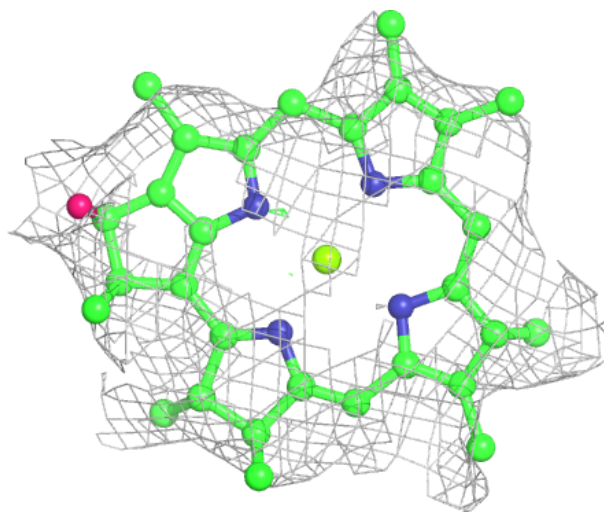
**Electron density around LMU 4 1210:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 3 1212:**

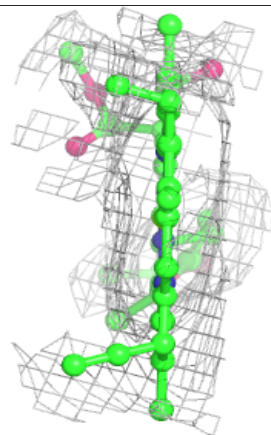
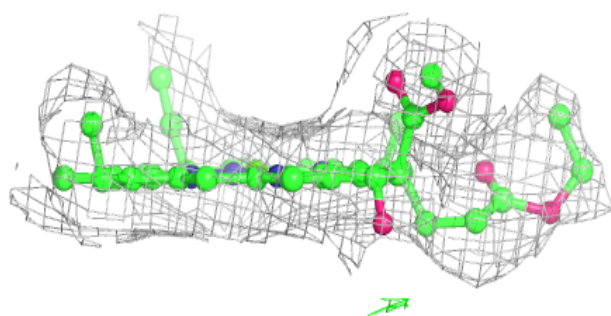
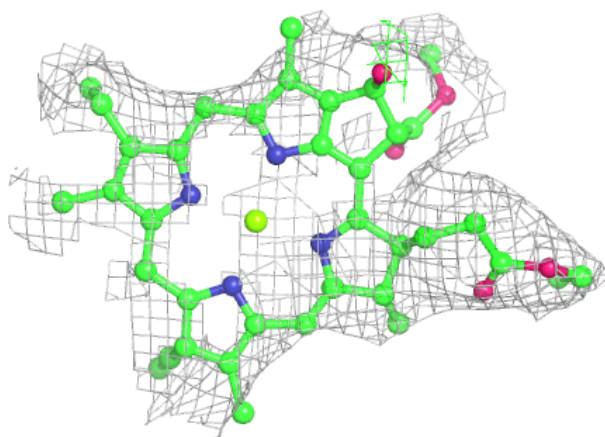
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



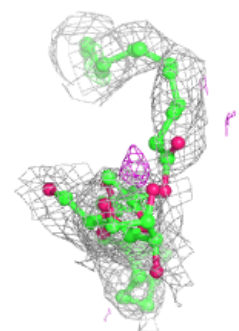
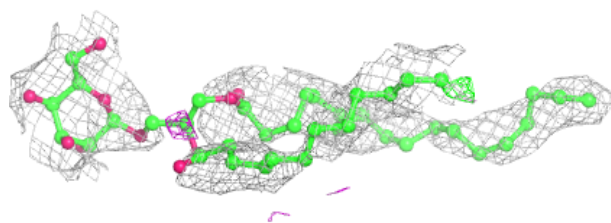
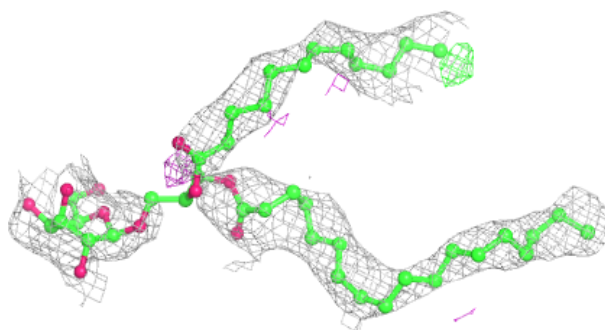


**Electron density around CLA 1 1189:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

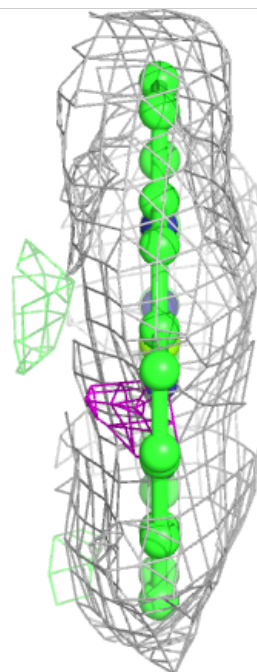
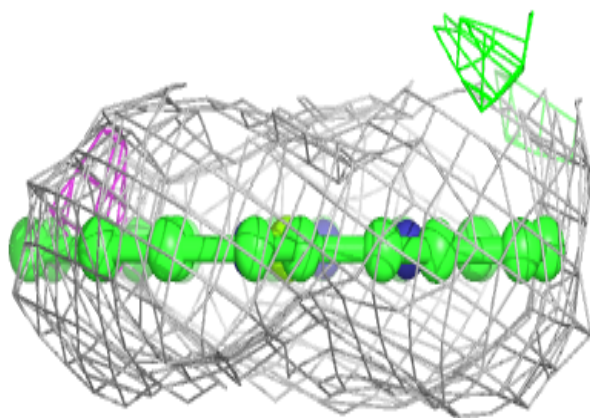
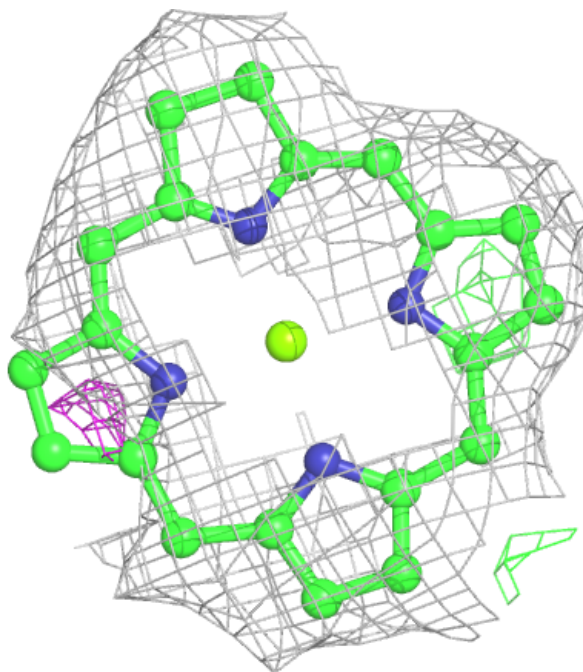
**Electron density around LMG B 1783:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



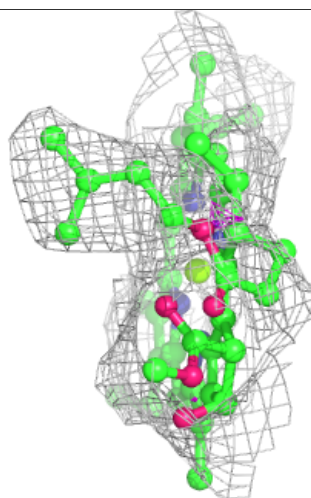
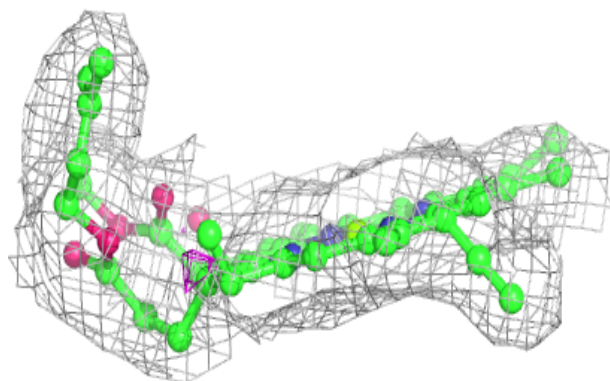
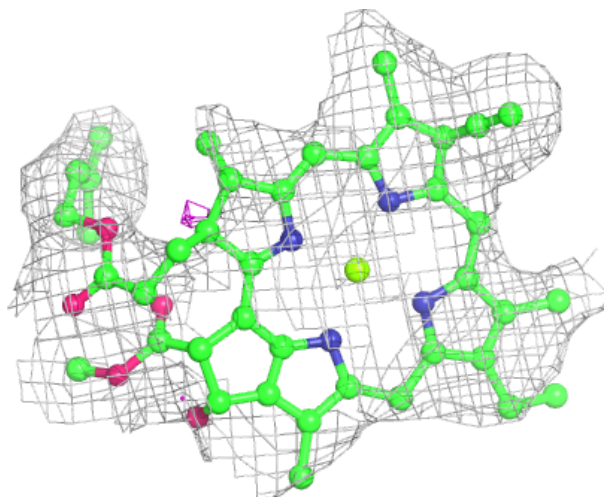
**Electron density around CLA 4 1203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



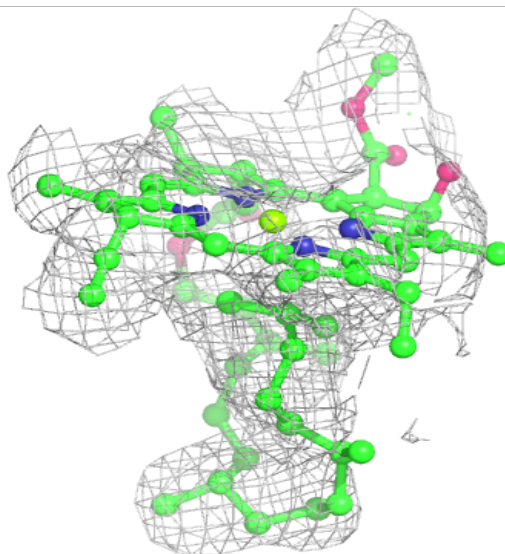
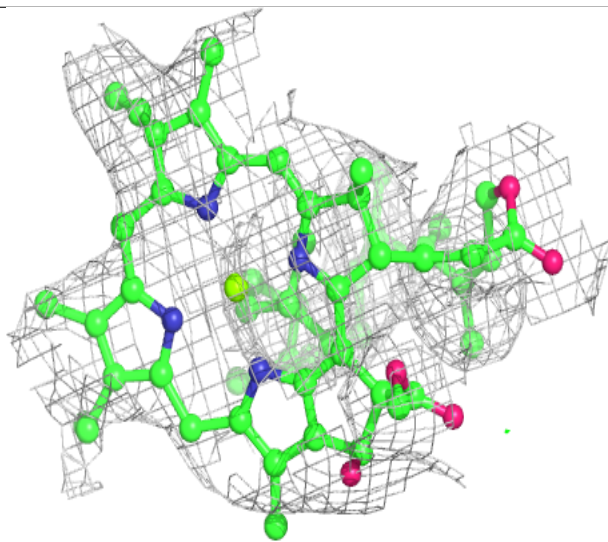
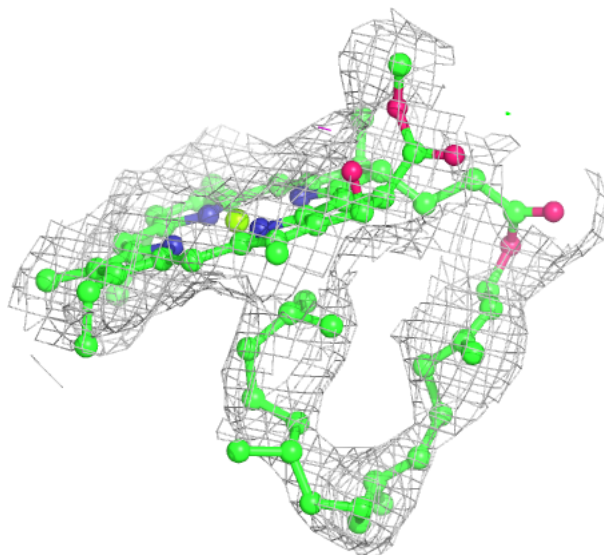
**Electron density around CLA 3 3008:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 2 1224:**

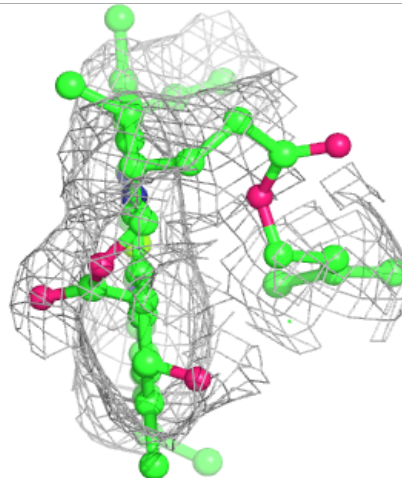
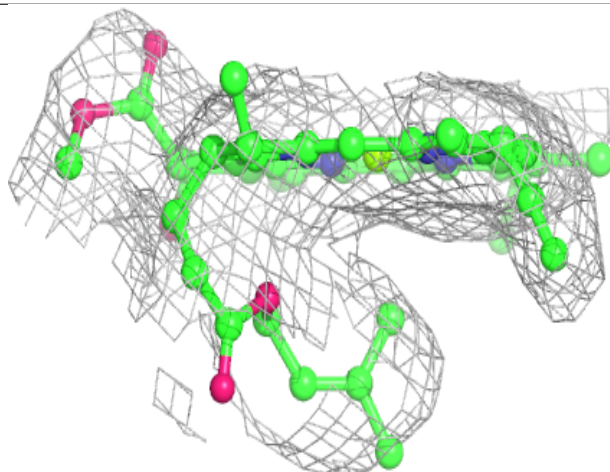
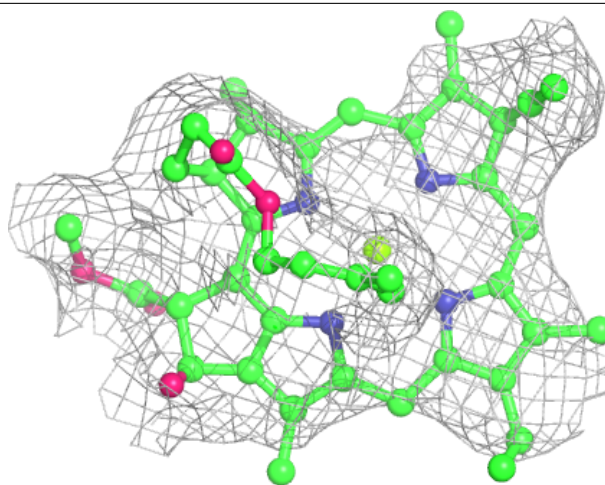
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





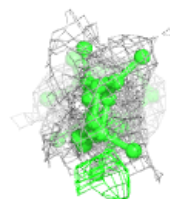
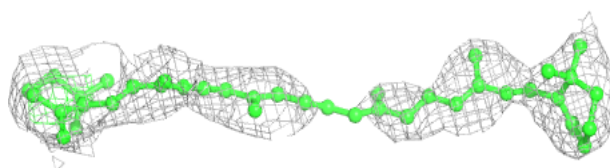
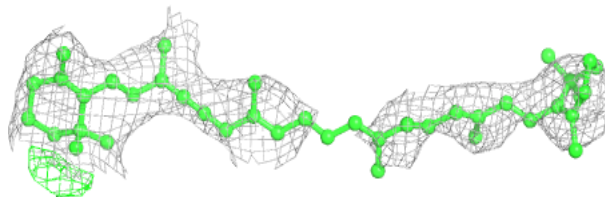
**Electron density around CLA L 1166:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



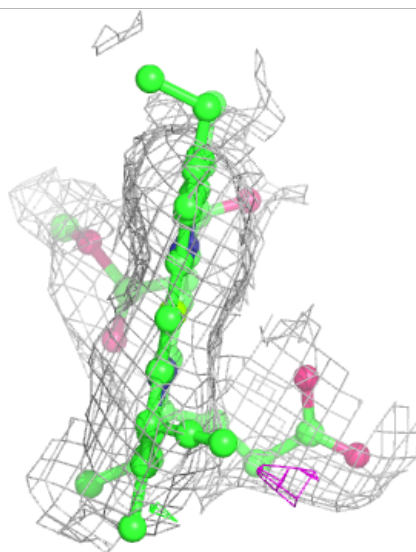
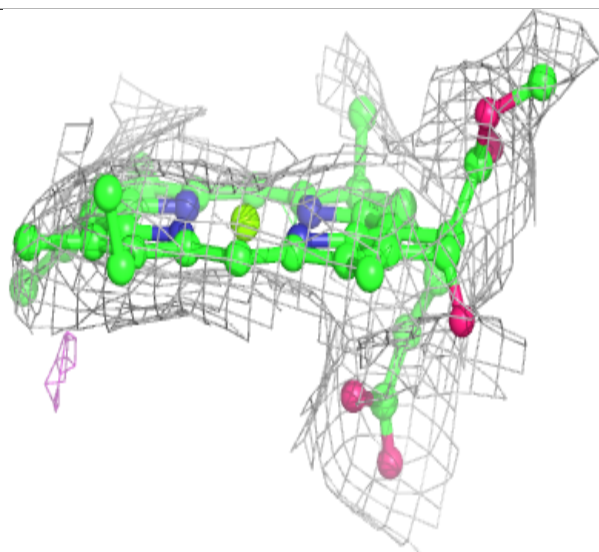
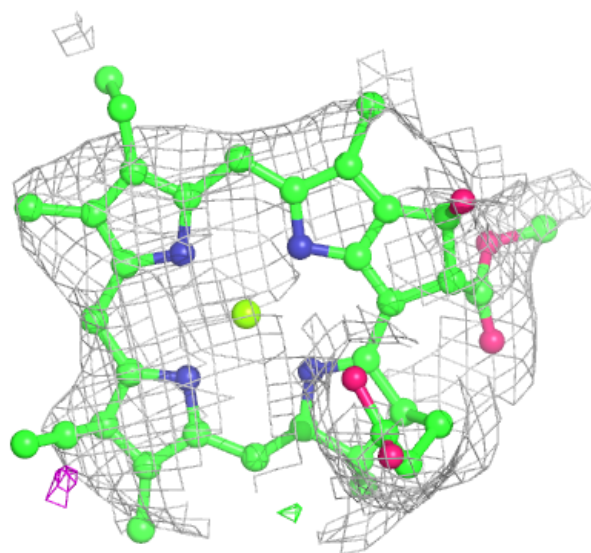
**Electron density around BCR A 1804:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



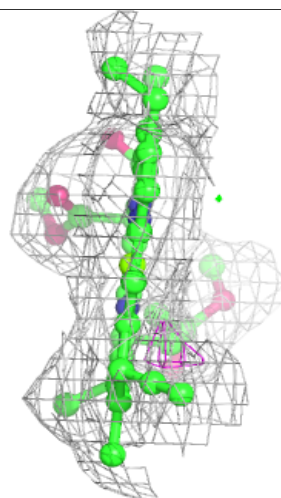
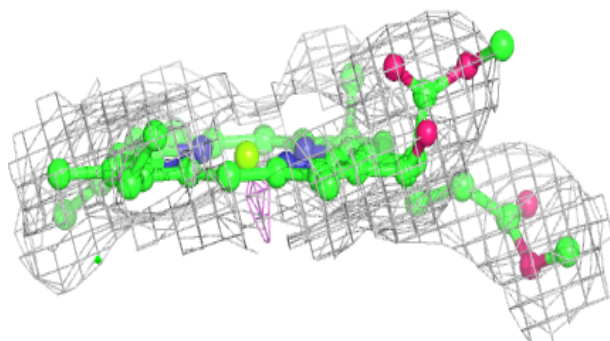
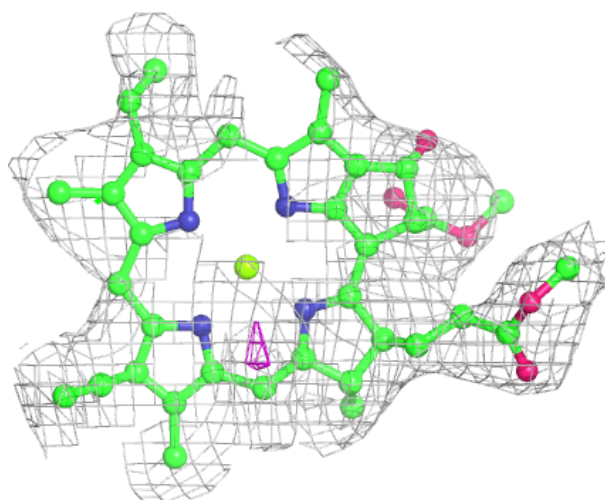
**Electron density around CLA B 1764:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 4 1209:**

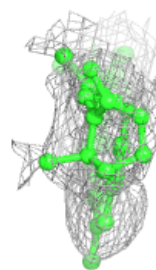
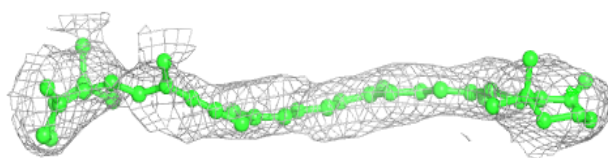
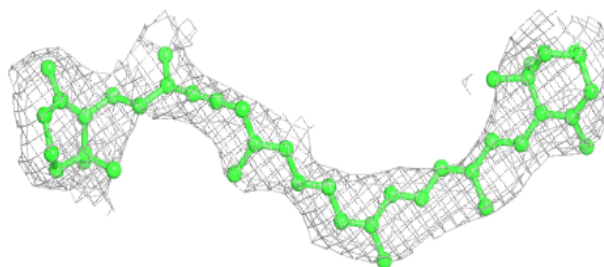
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



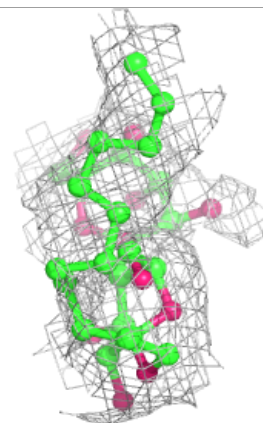
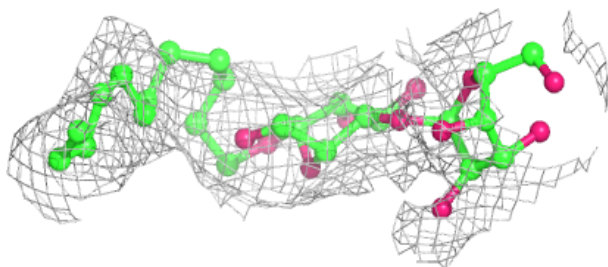
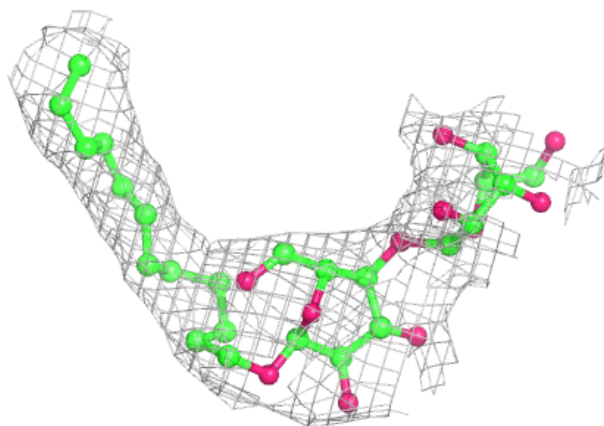


**Electron density around BCR A 1807:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

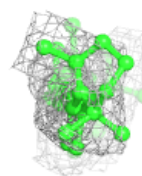
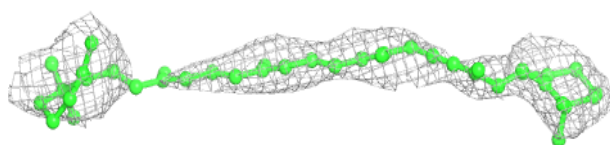
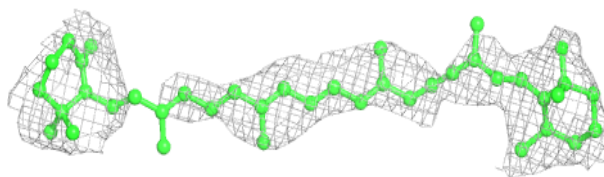
**Electron density around LMU A 7021:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

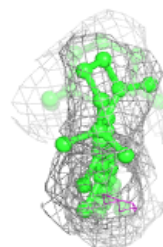
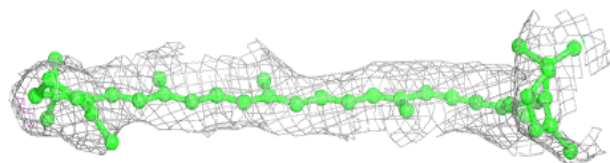
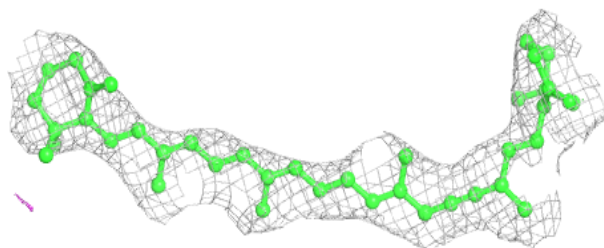


**Electron density around BCR B 1774:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

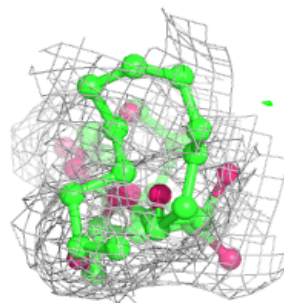
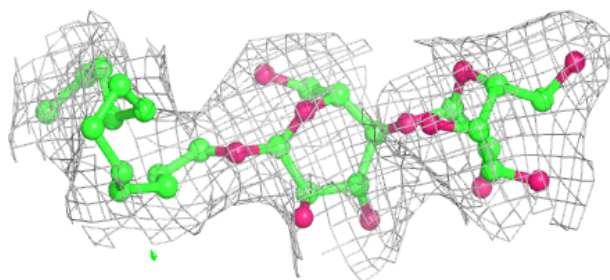
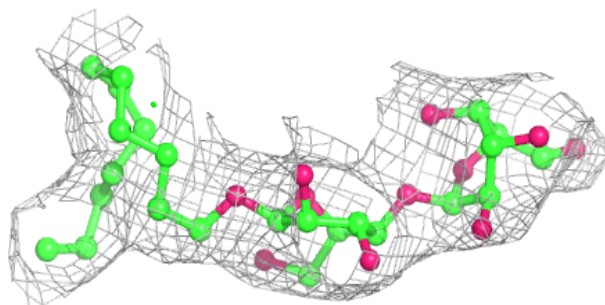
**Electron density around BCR B 1775:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

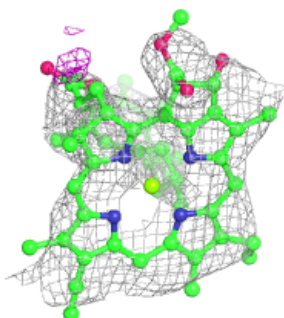
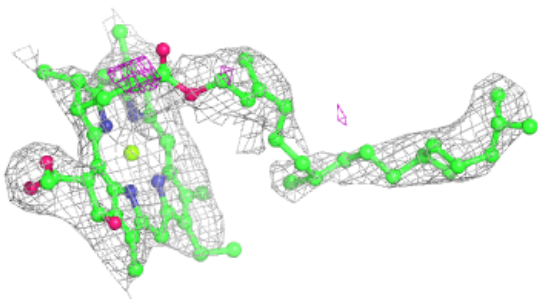
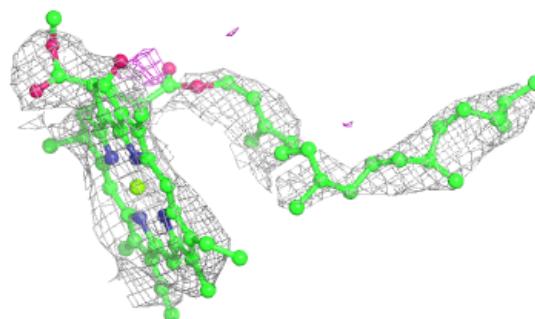


**Electron density around LMU A 7023:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

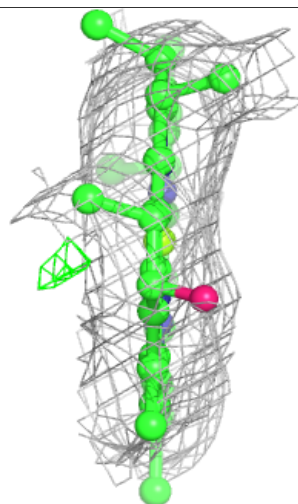
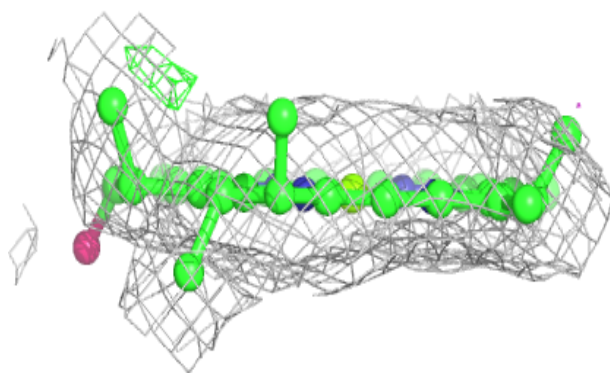
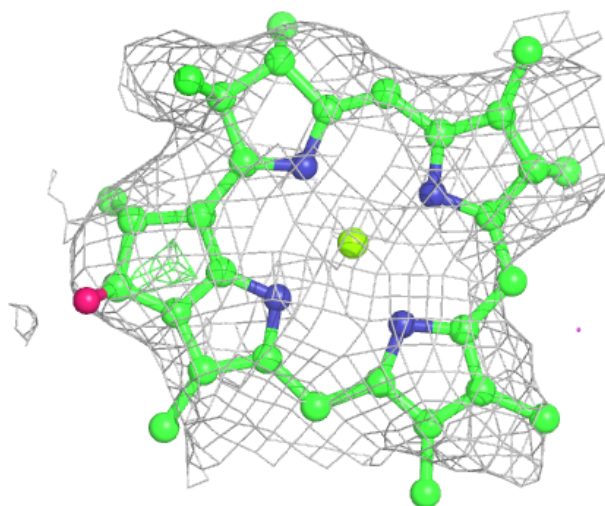
**Electron density around CLA A 1767:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



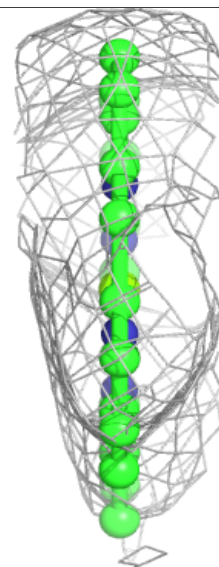
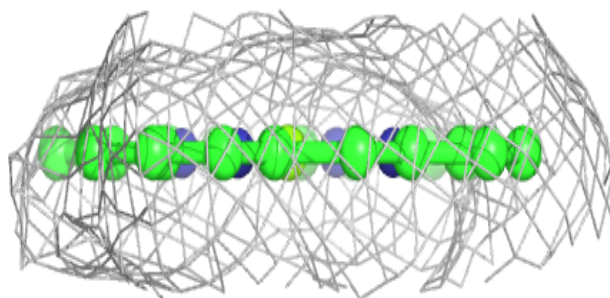
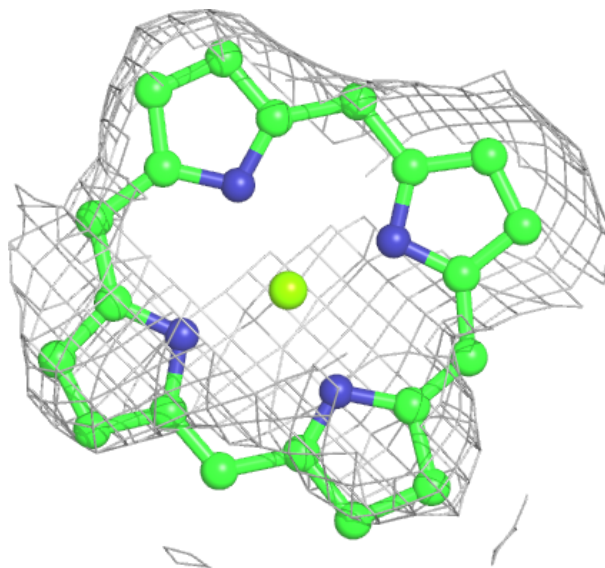
**Electron density around CLA B 1772:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



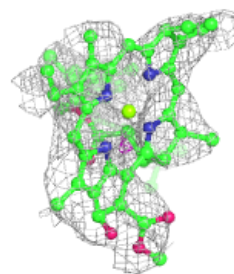
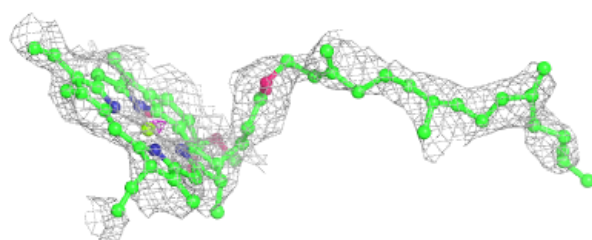
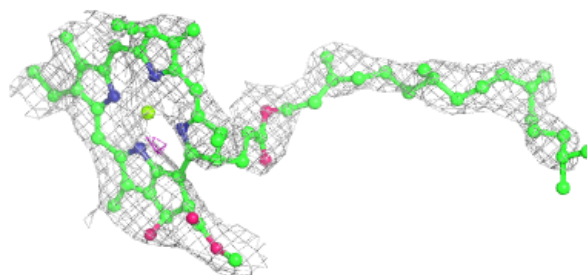
**Electron density around CLA 4 1202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 1776:**

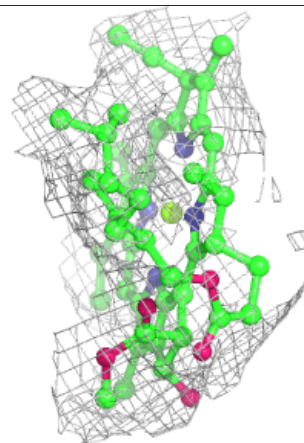
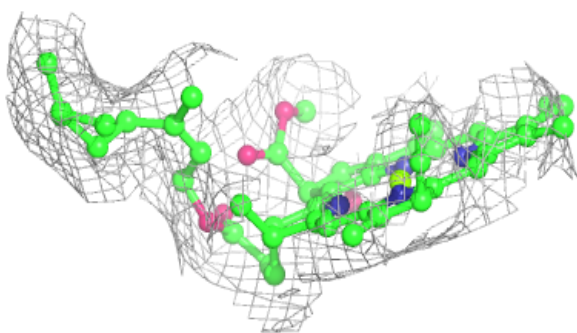
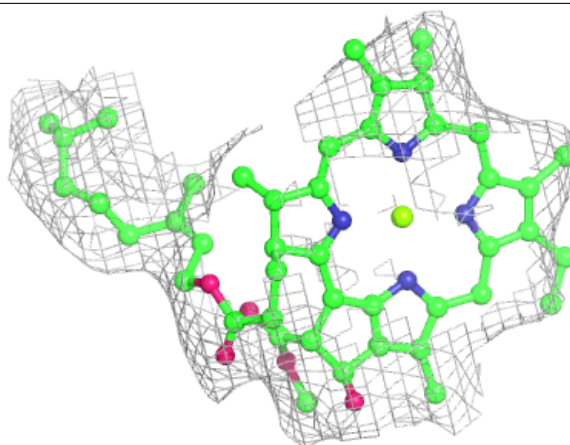
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





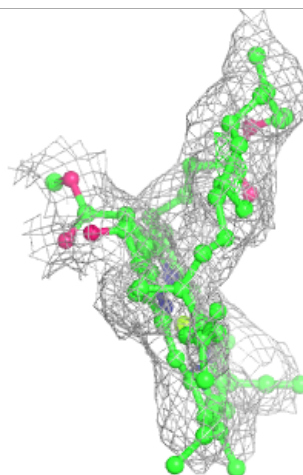
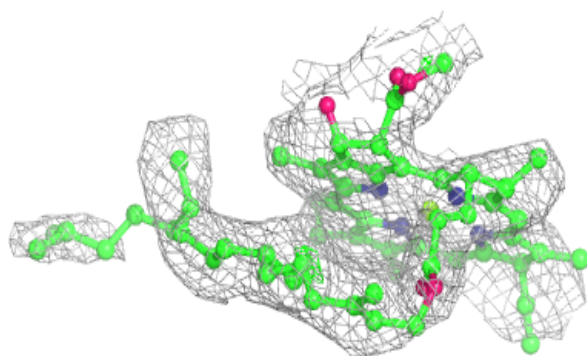
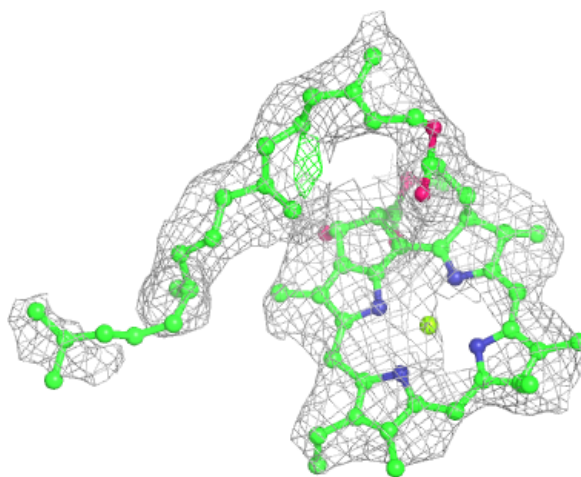
**Electron density around CLA J 1045:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1762:**

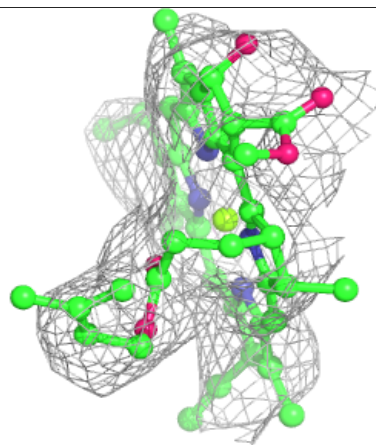
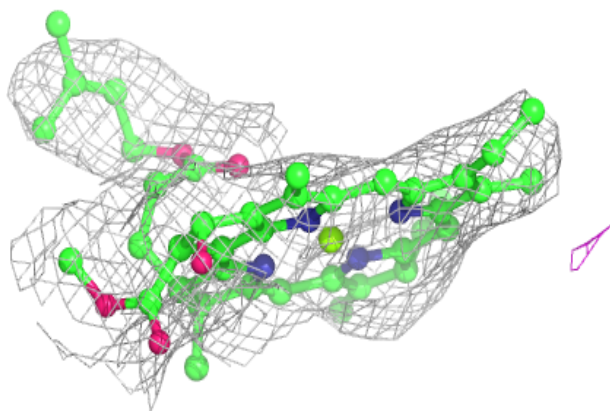
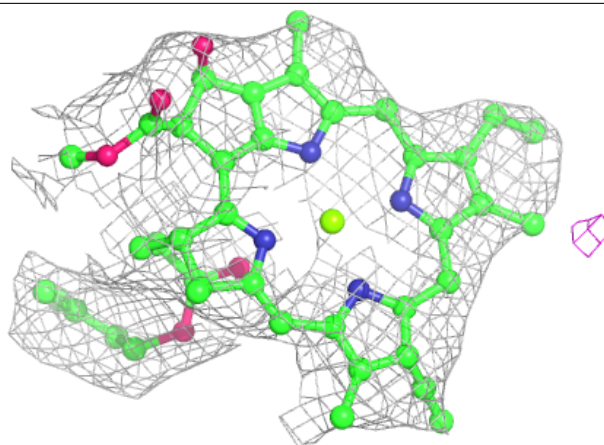
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





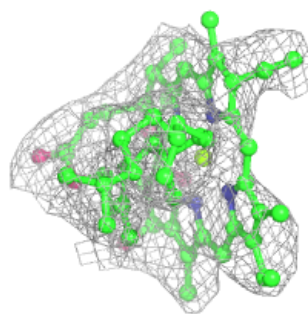
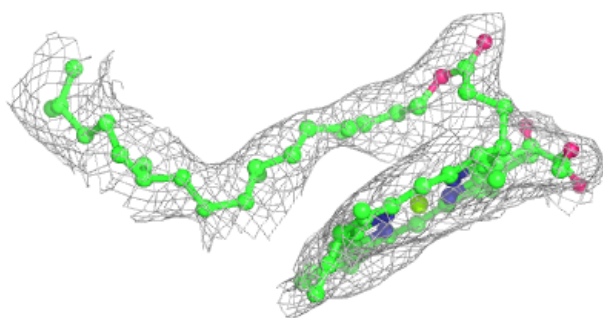
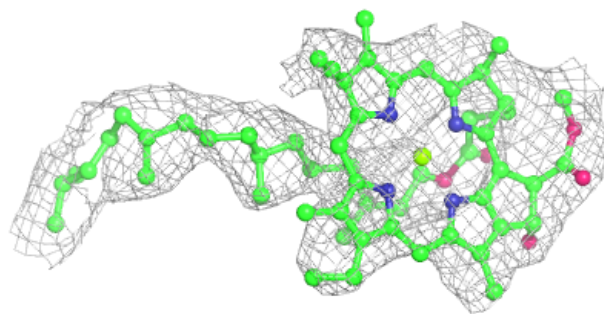
**Electron density around CLA A 1771:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

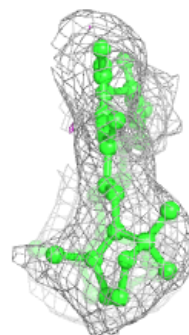
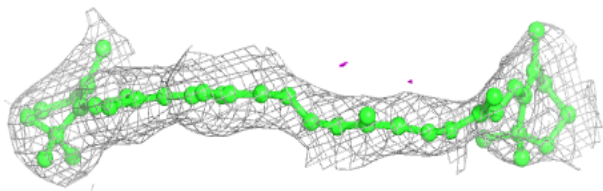
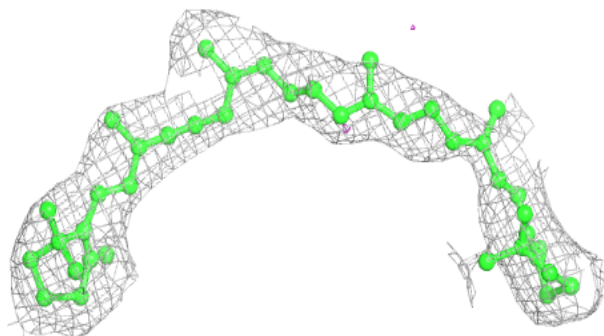


**Electron density around CLA A 1772:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

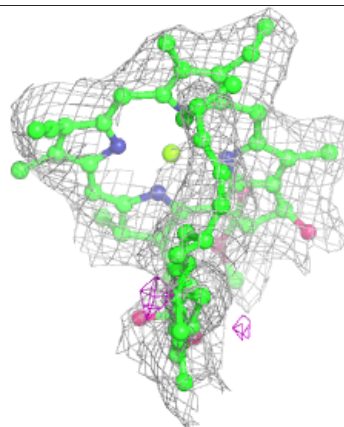
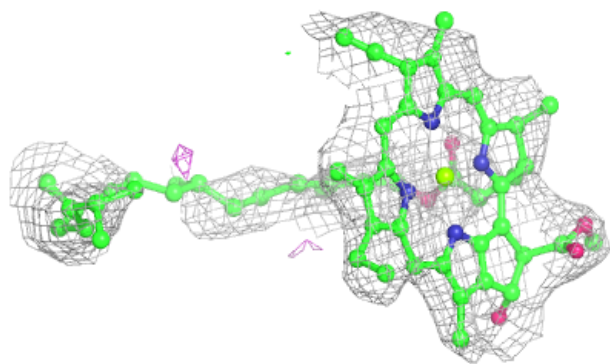
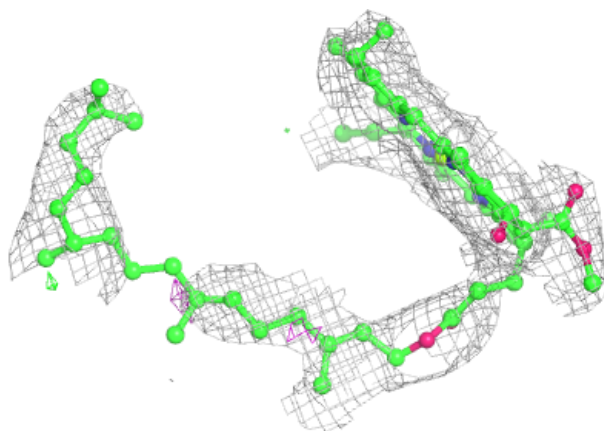
**Electron density around BCR B 1779:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



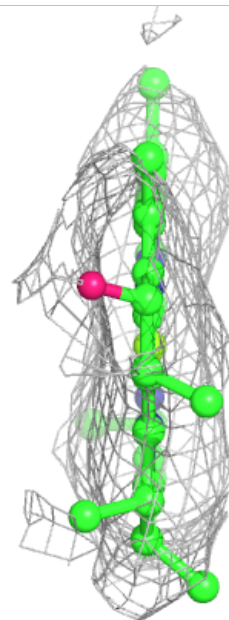
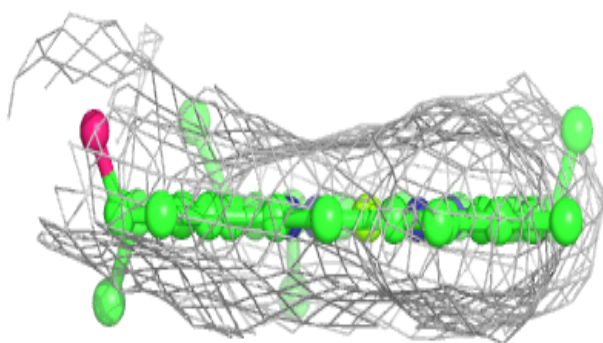
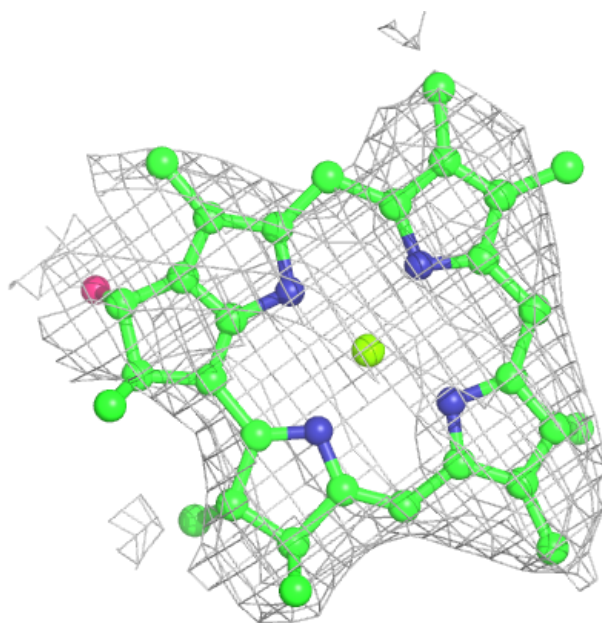
**Electron density around CLA A 1787:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



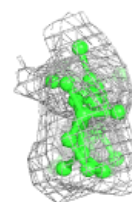
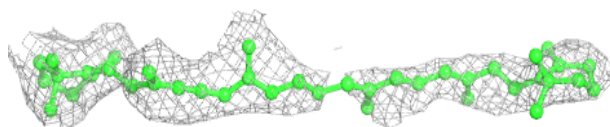
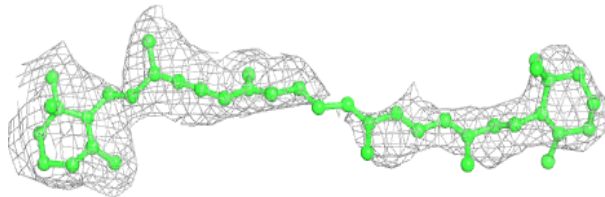
**Electron density around CLA 1 1195:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

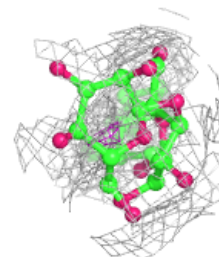
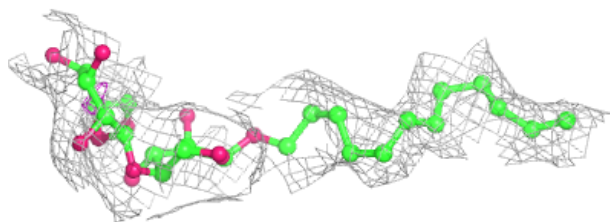
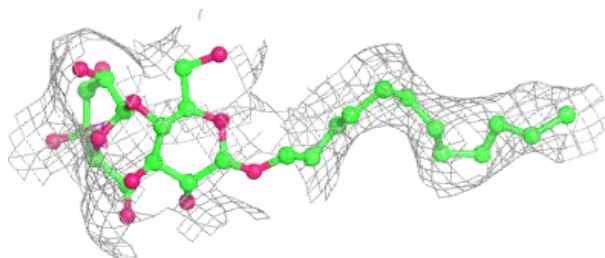


**Electron density around BCR L 1169:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMU A 7033:**

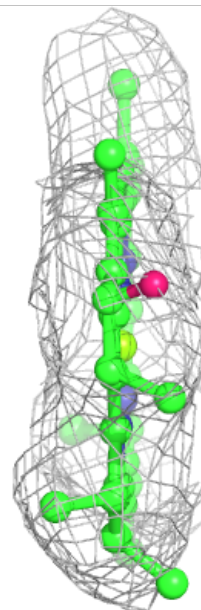
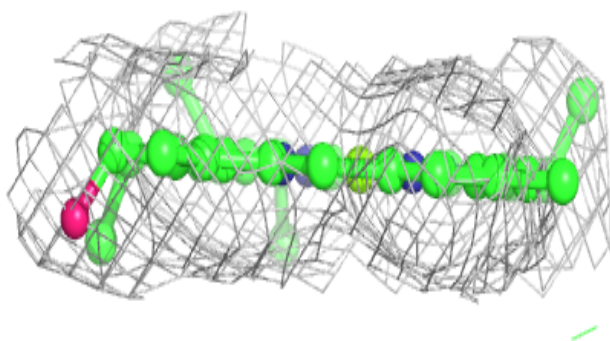
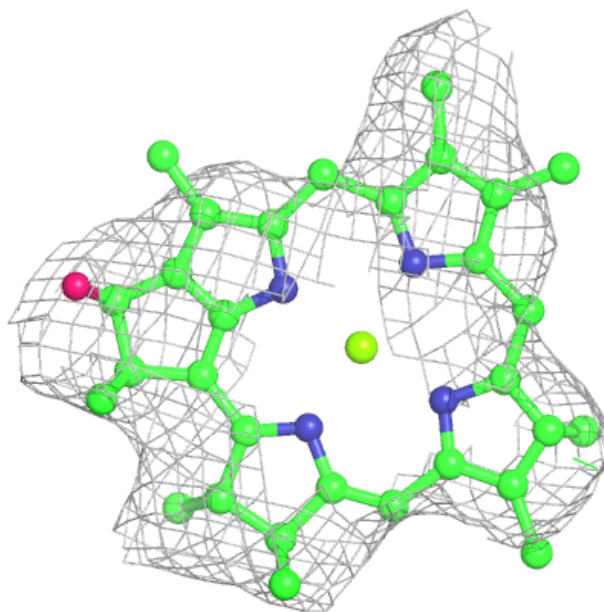
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





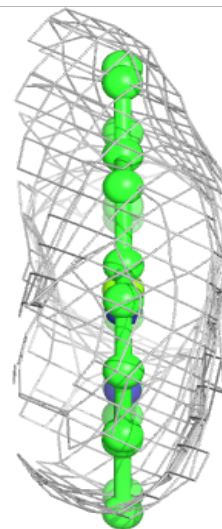
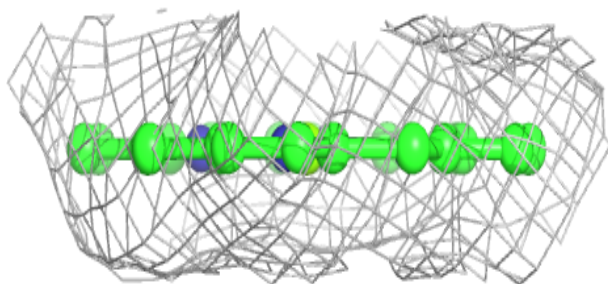
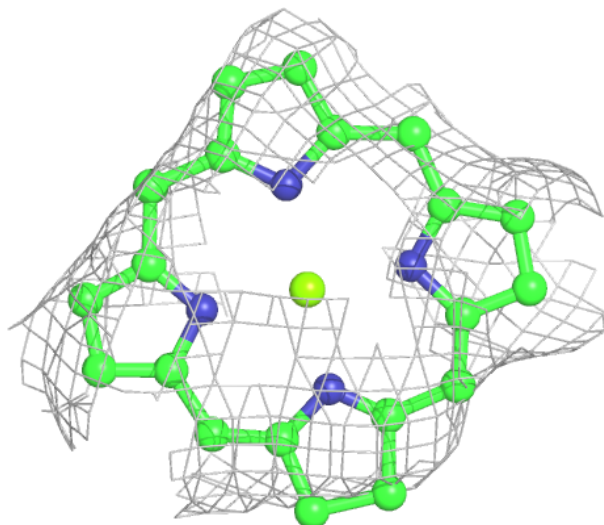
**Electron density around CLA 1 1196:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



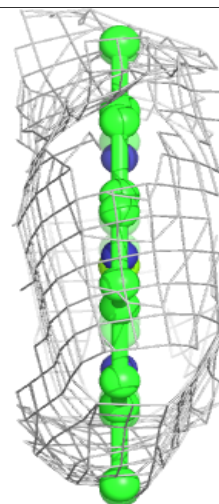
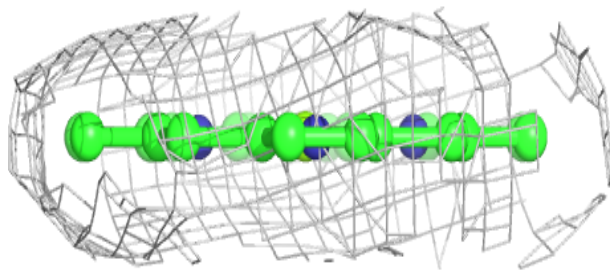
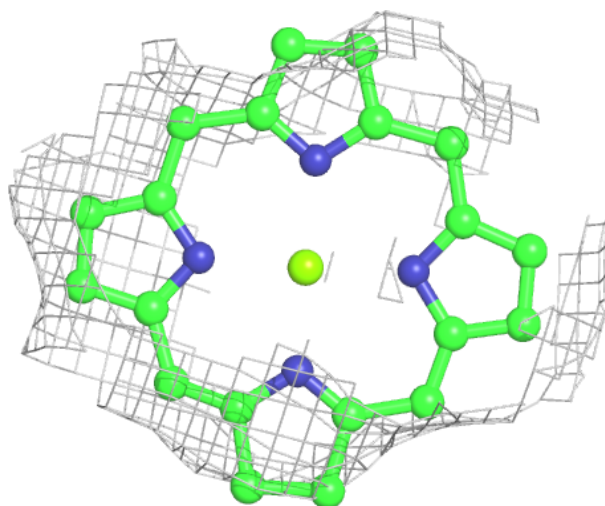
**Electron density around CLA 1 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 2 1219:**

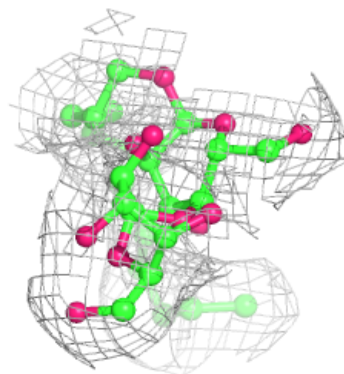
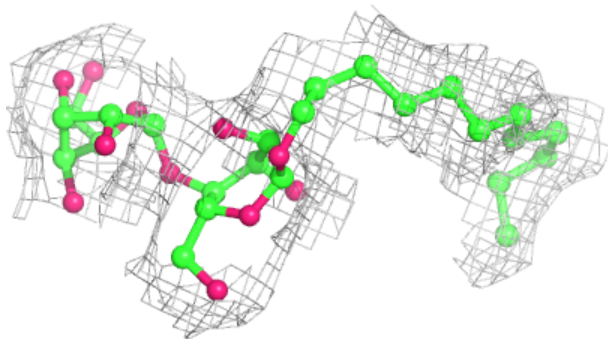
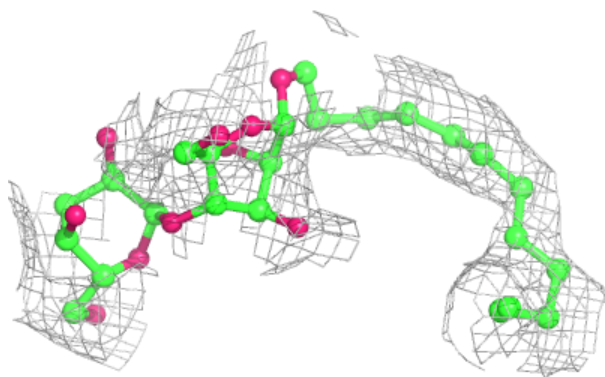
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



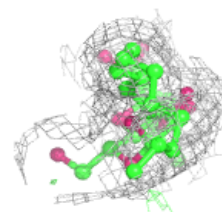
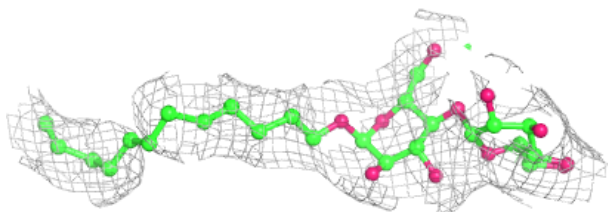
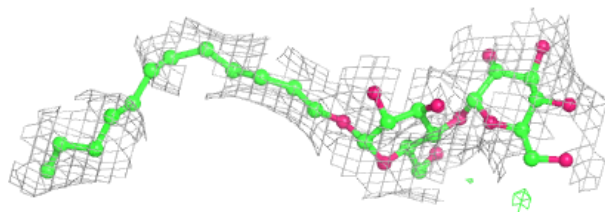


**Electron density around LMU A 7022:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

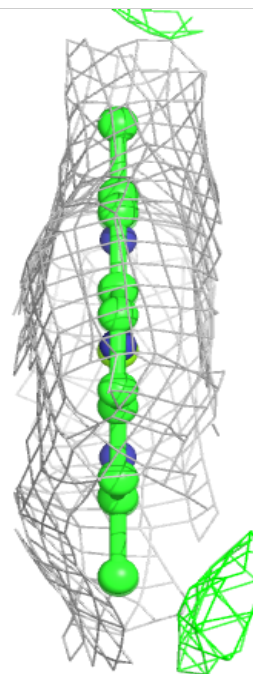
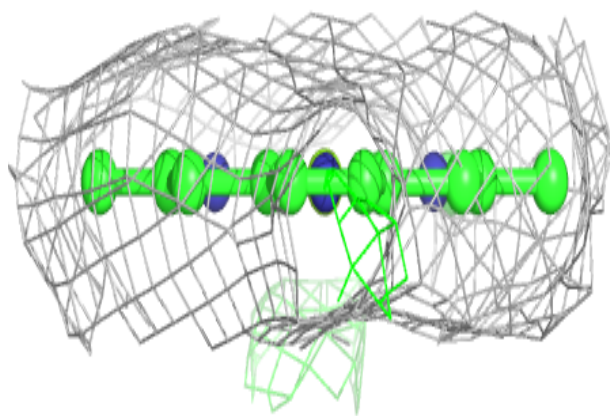
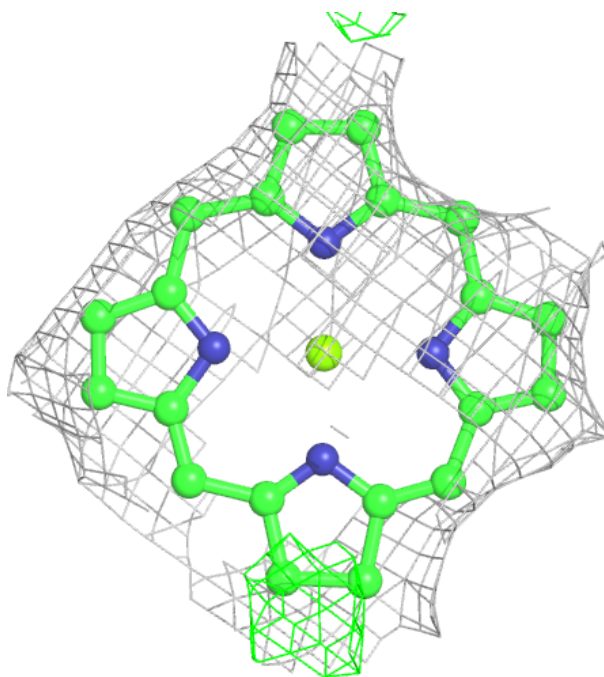
**Electron density around LMU A 7040:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



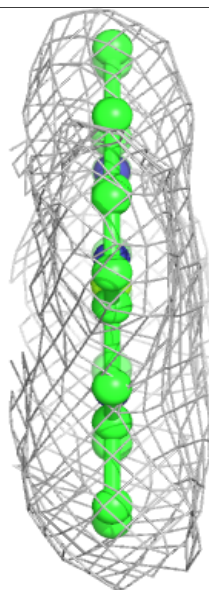
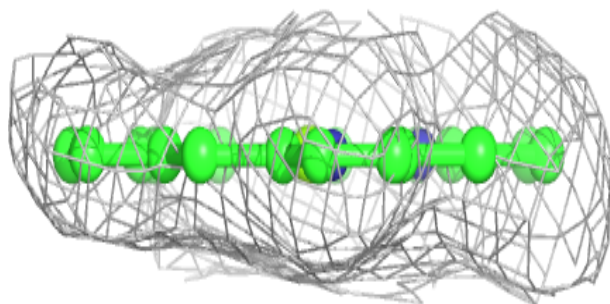
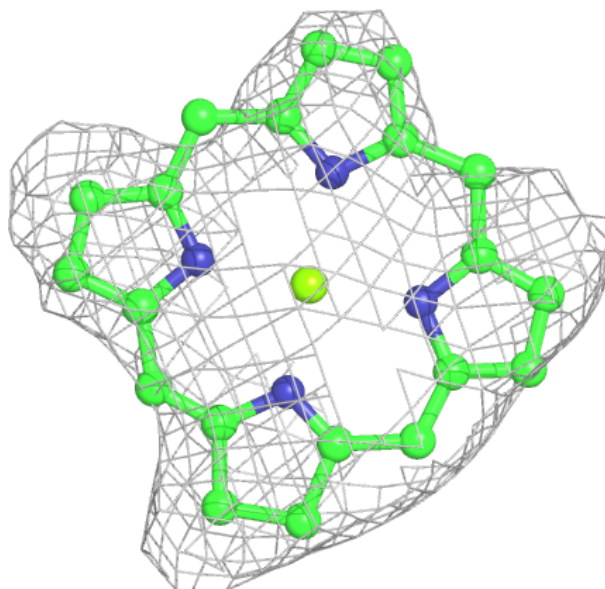
**Electron density around CLA 3 1216:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



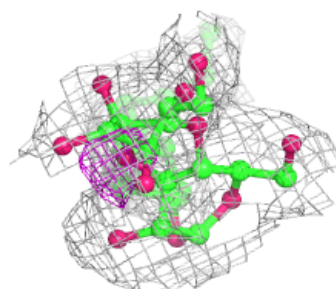
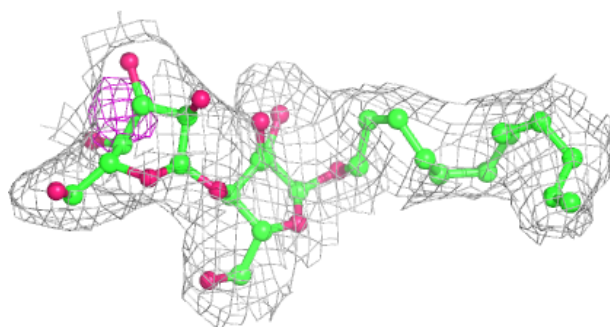
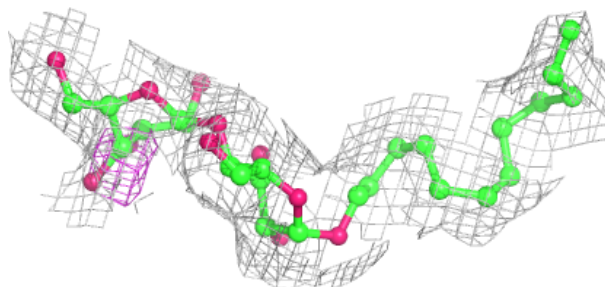
**Electron density around CLA 2 2010:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

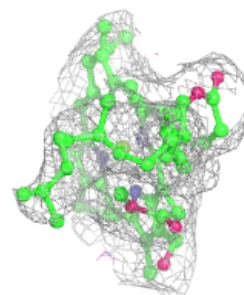
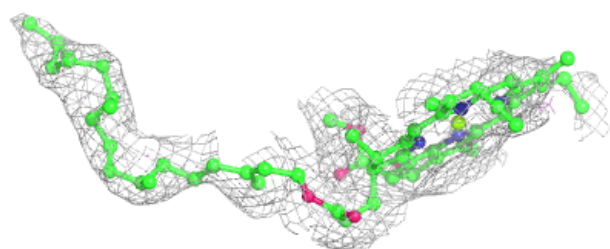
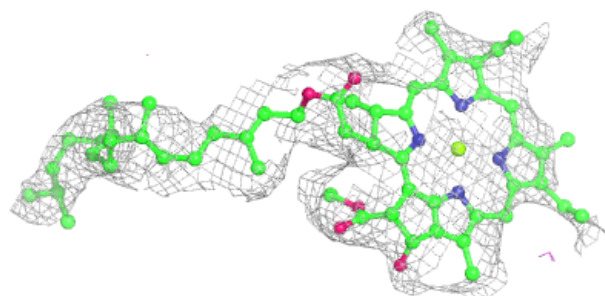


**Electron density around LMU A 7026:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

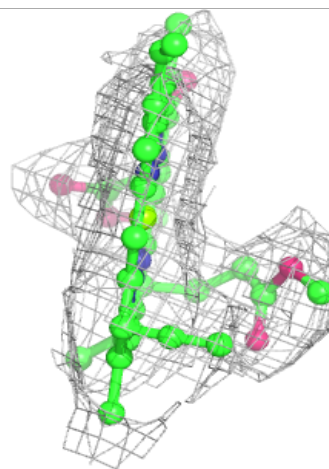
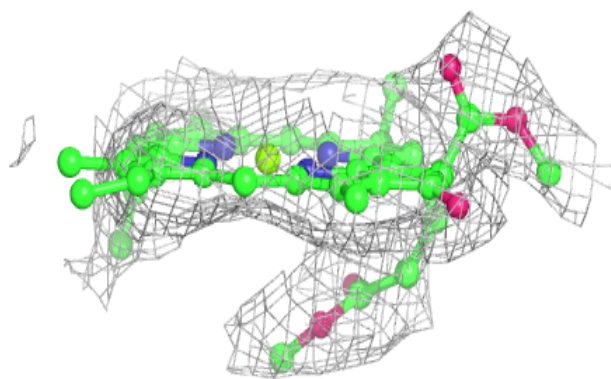
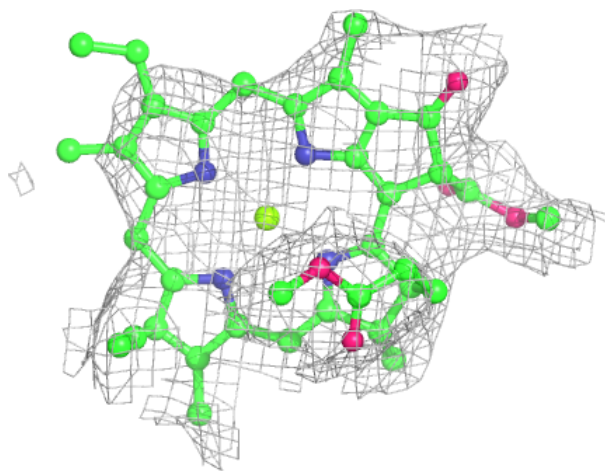
**Electron density around CLA 3 3011:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 1 1190:**

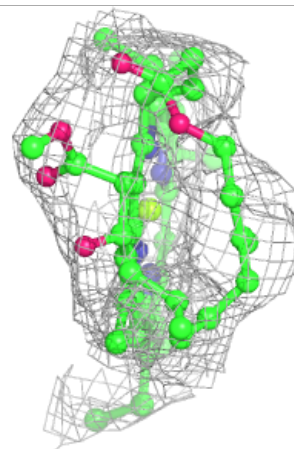
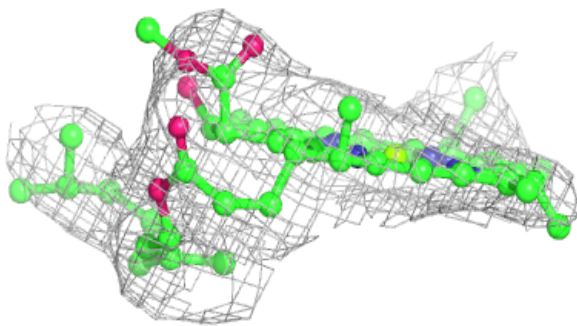
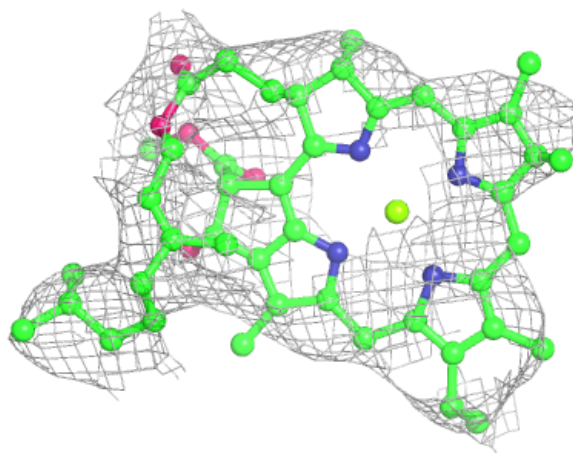
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





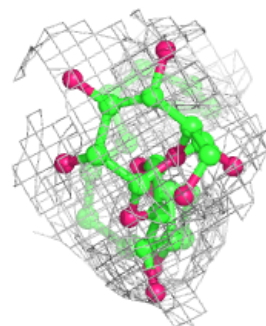
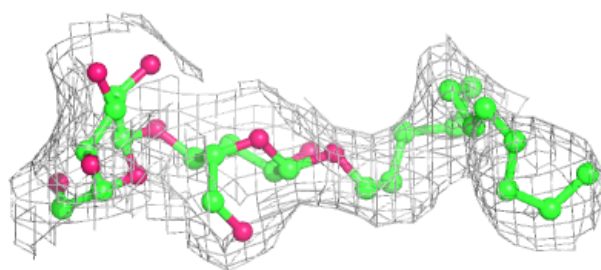
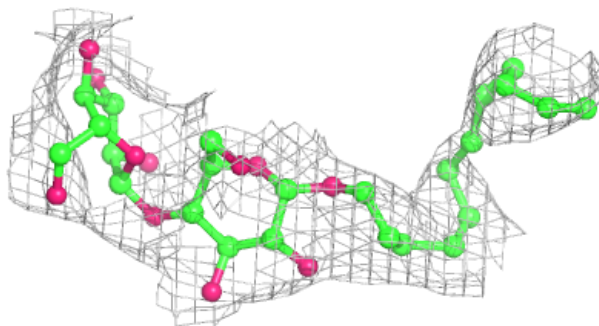
**Electron density around CLA B 1741:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



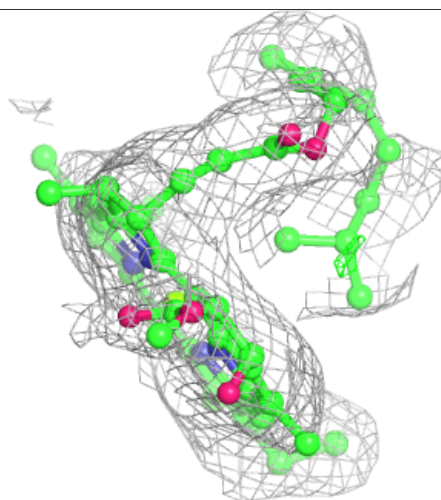
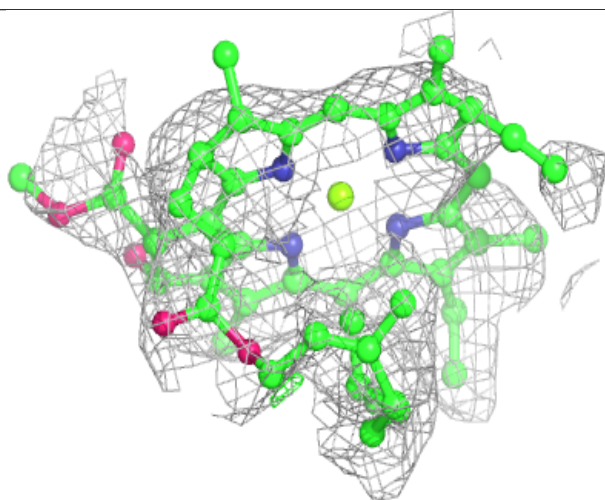
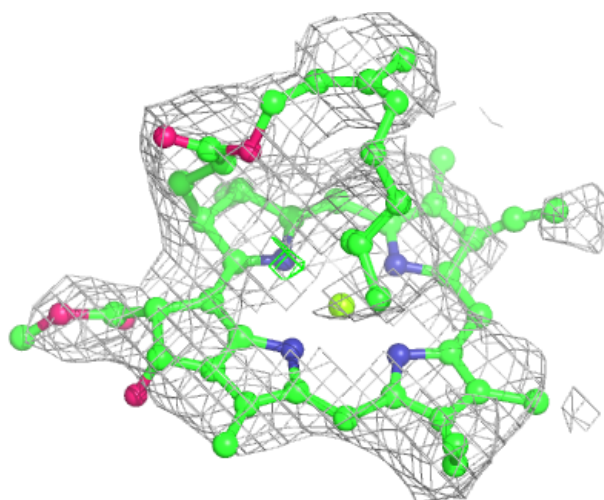
**Electron density around LMU R 1056:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1742:**

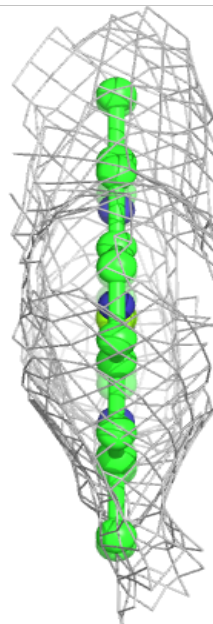
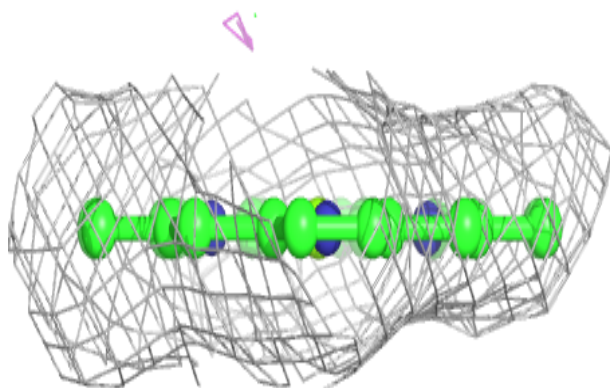
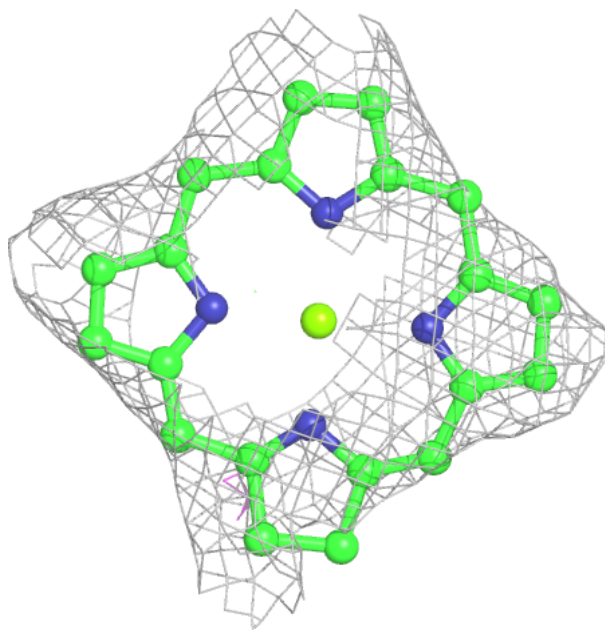
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





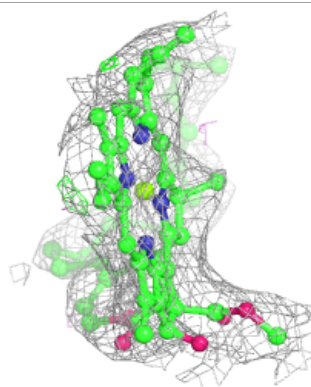
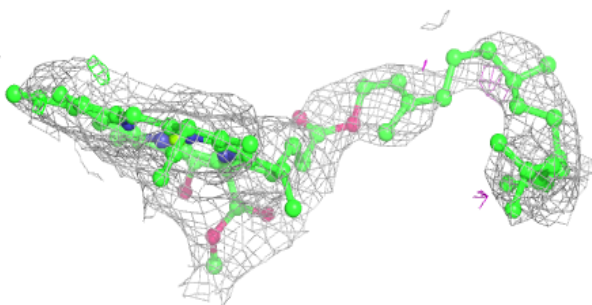
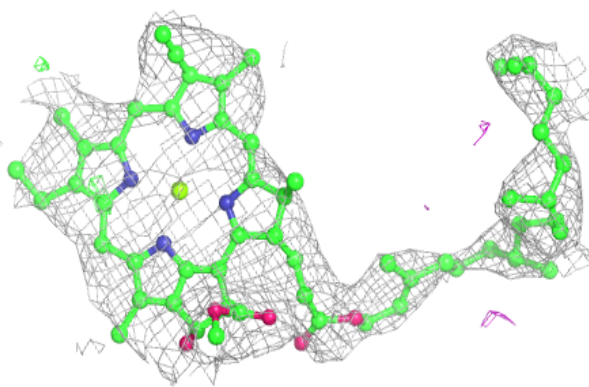
**Electron density around CLA 3 3015:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



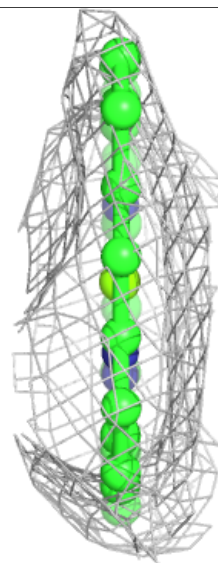
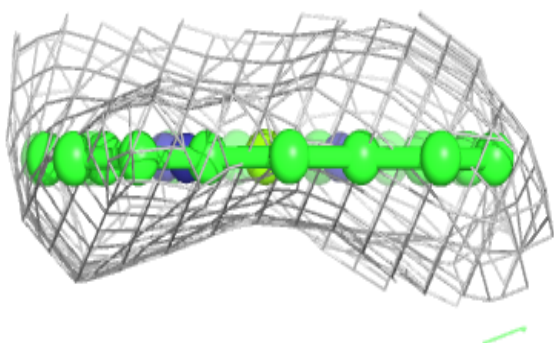
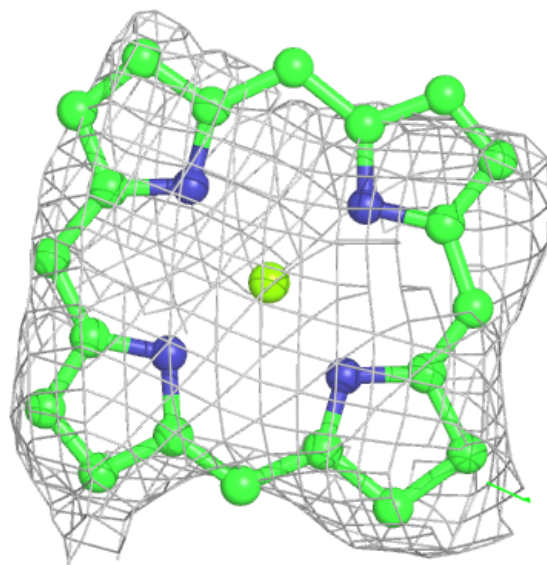
**Electron density around CLA A 1782:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



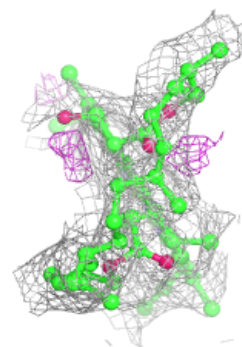
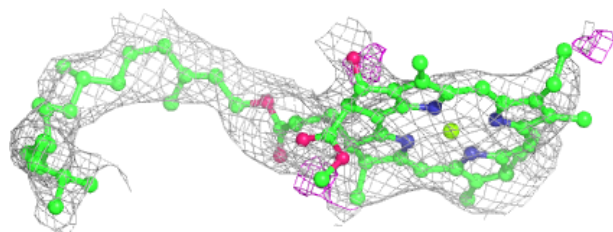
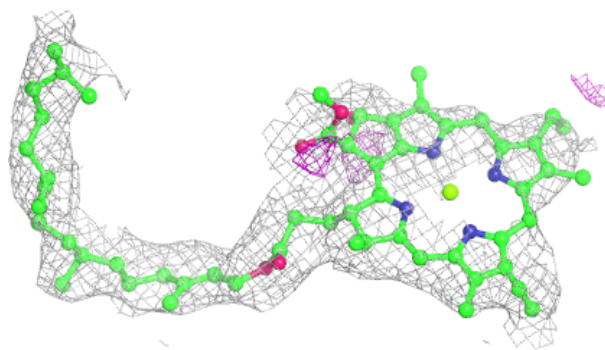
**Electron density around CLA 2 1221:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



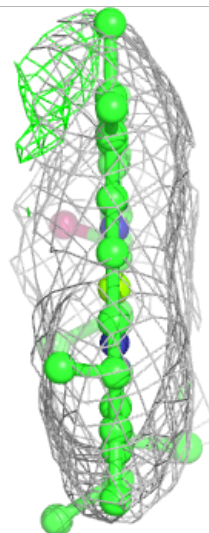
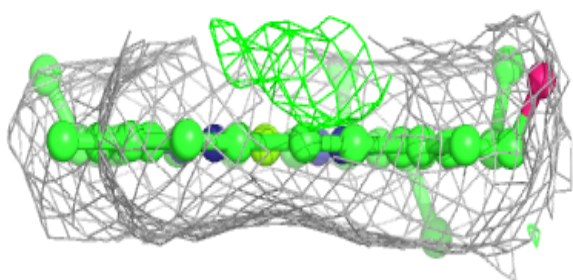
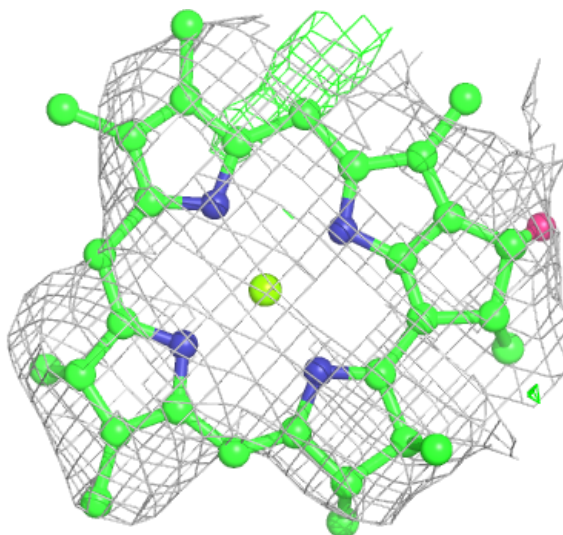
**Electron density around CLA B 1756:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



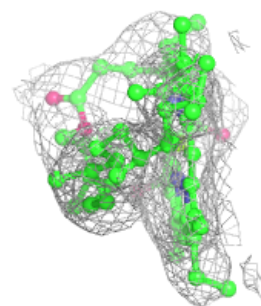
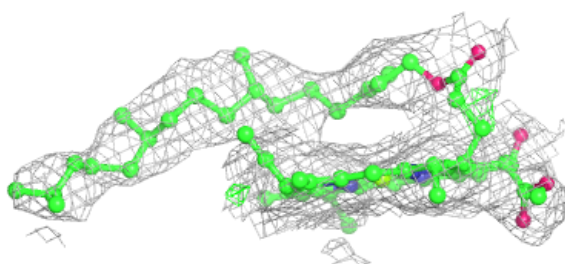
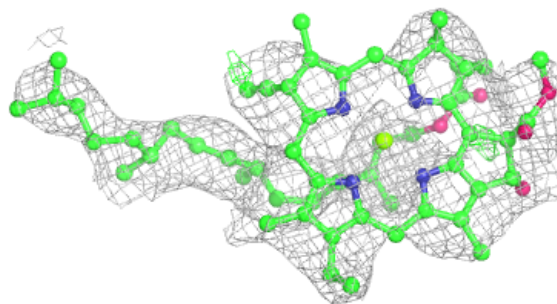
**Electron density around CLA 4 1197:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1735:**

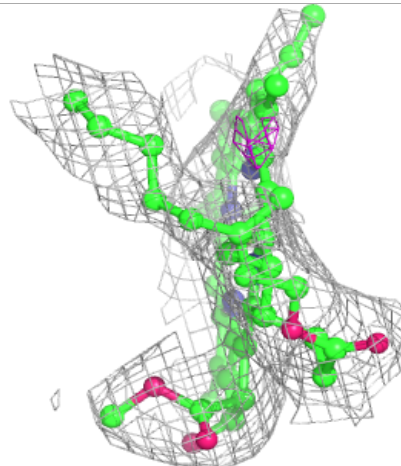
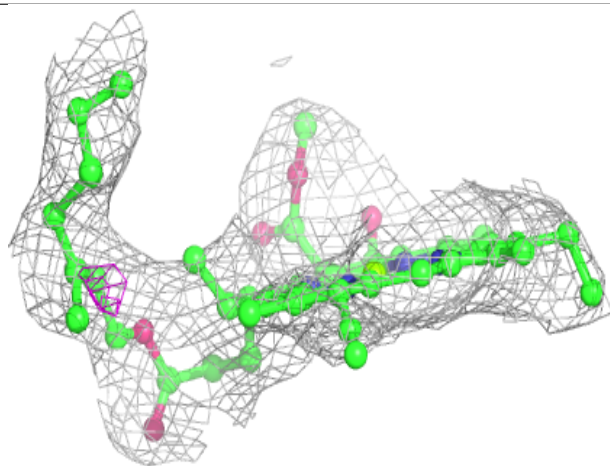
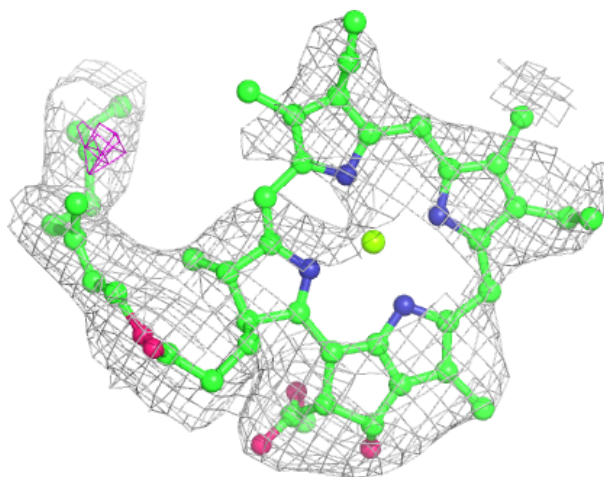
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





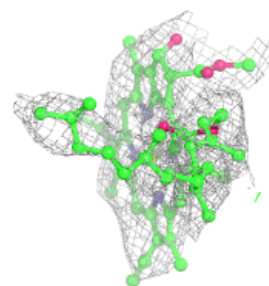
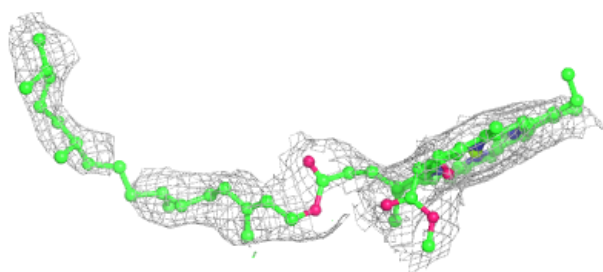
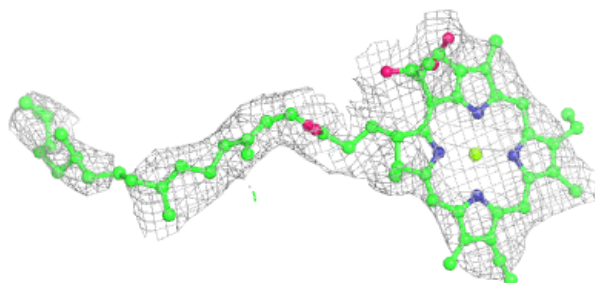
**Electron density around CLA A 1769:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

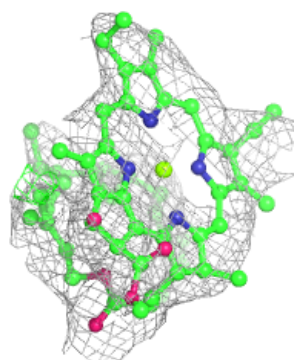
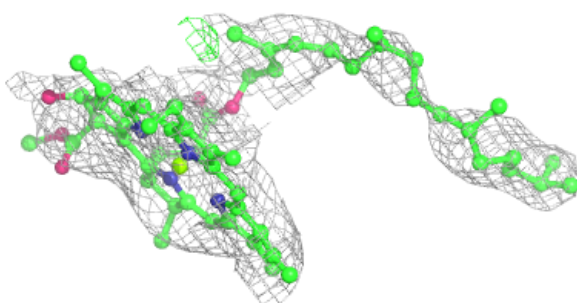
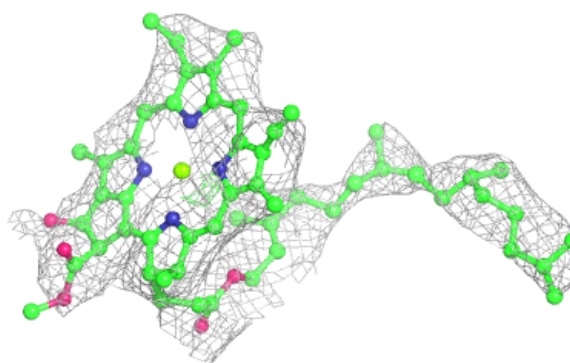


**Electron density around CLA A 1761:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 1744:**

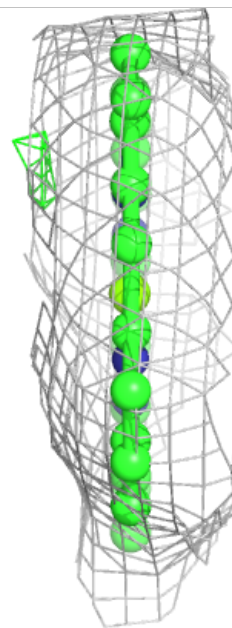
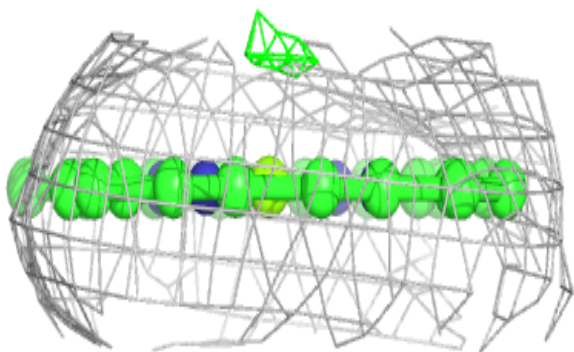
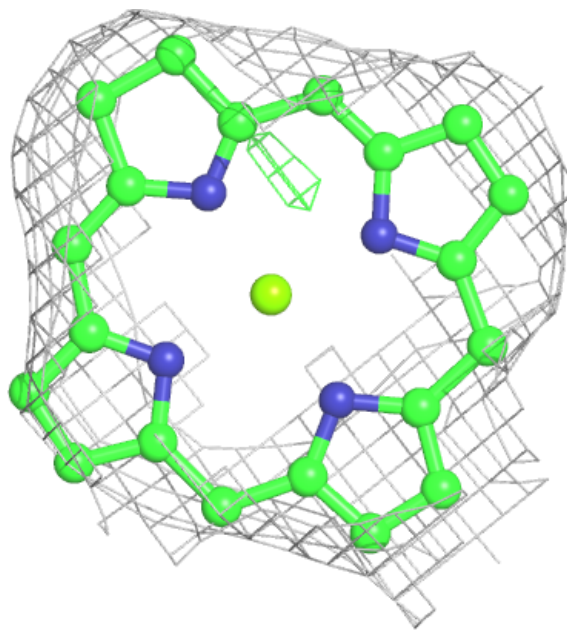
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





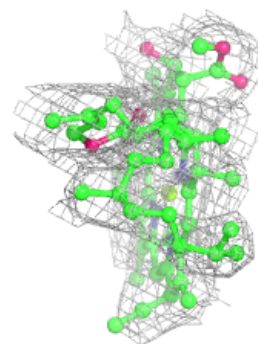
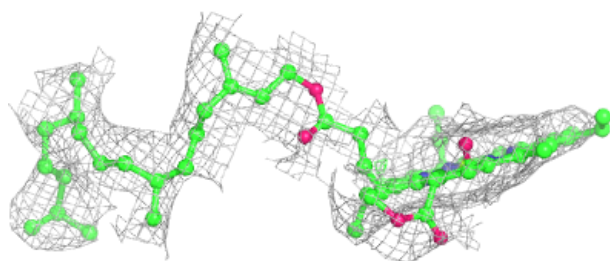
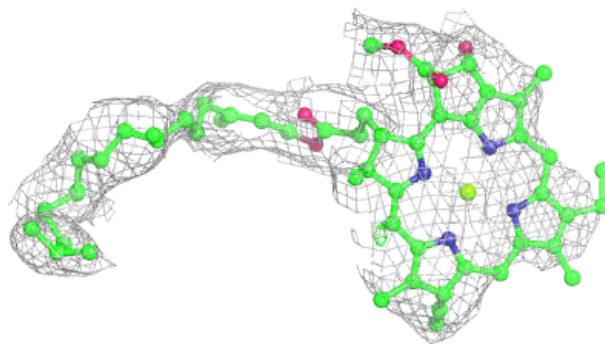
**Electron density around CLA 4 1205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



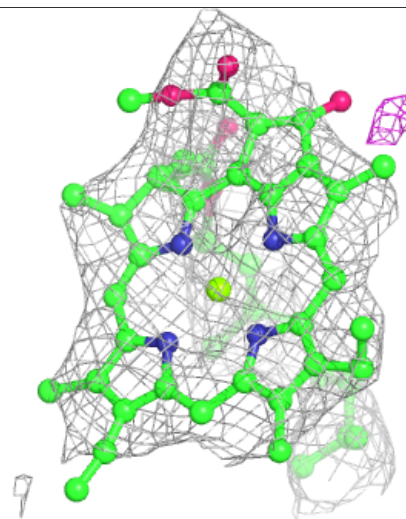
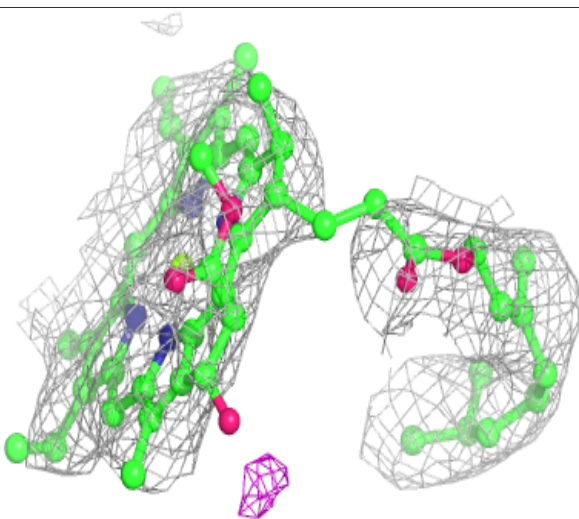
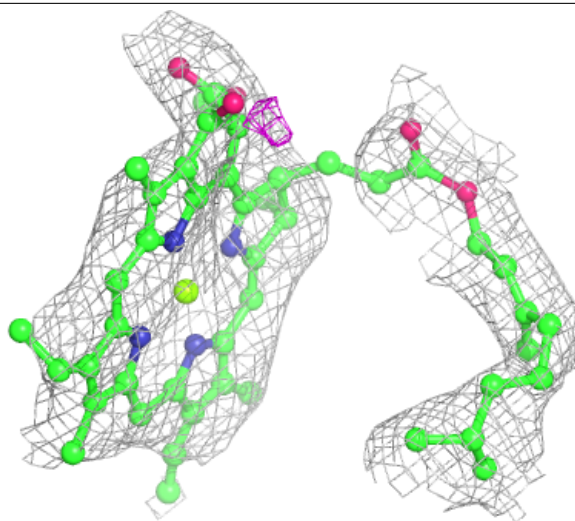
**Electron density around CLA A 1781:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



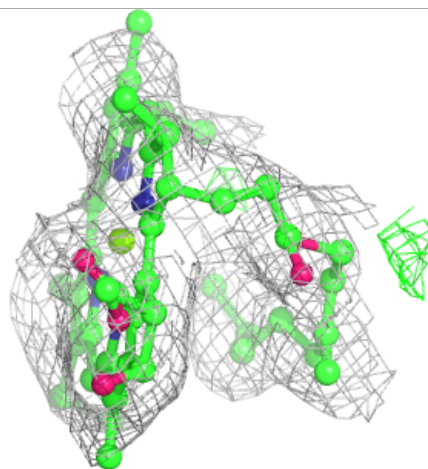
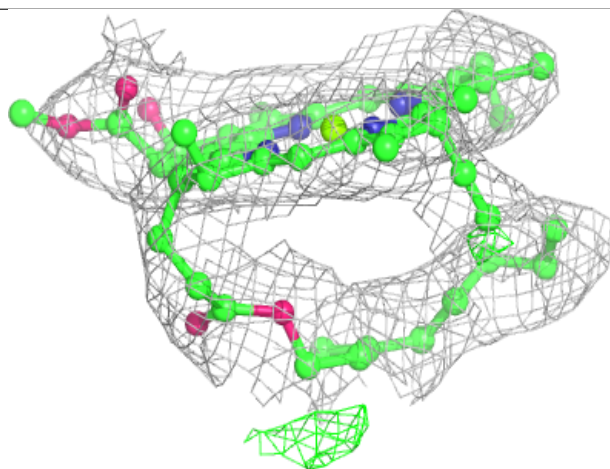
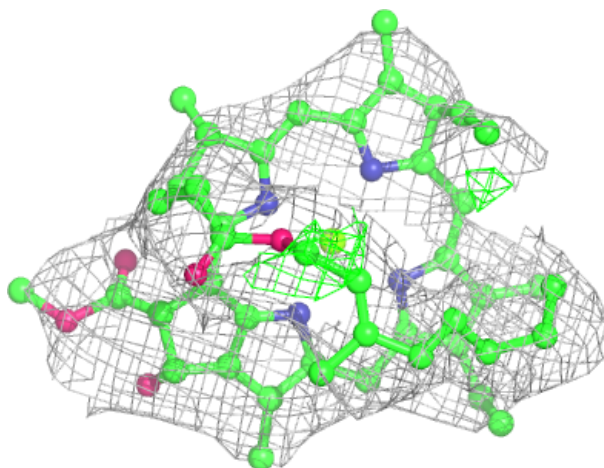
**Electron density around CLA A 1760:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



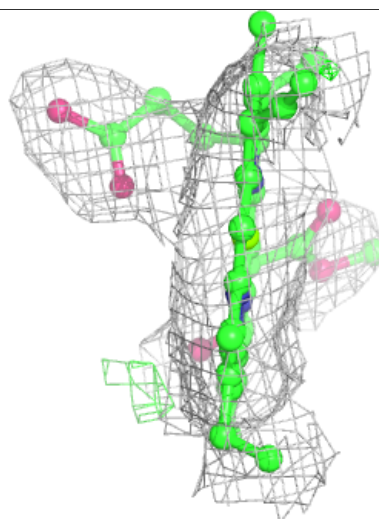
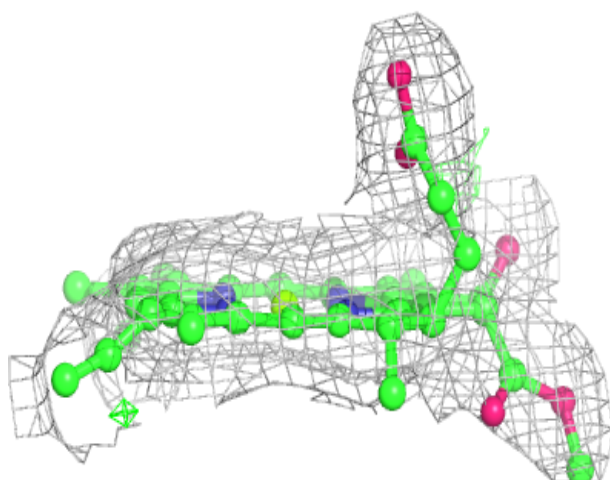
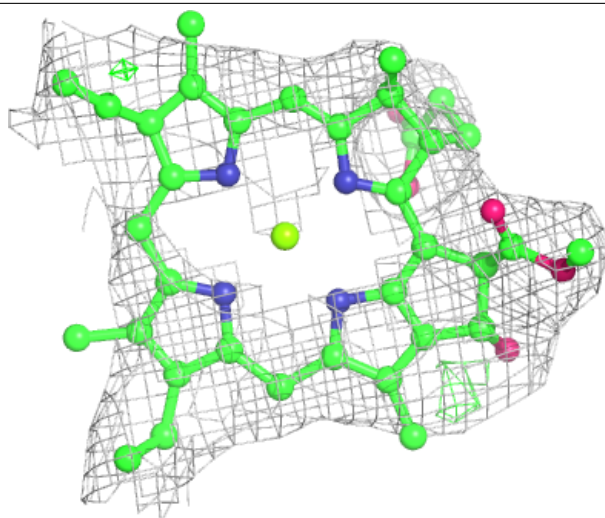
**Electron density around CLA A 1768:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1736:**

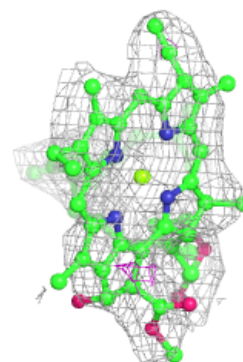
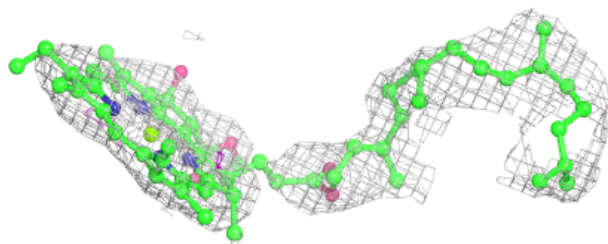
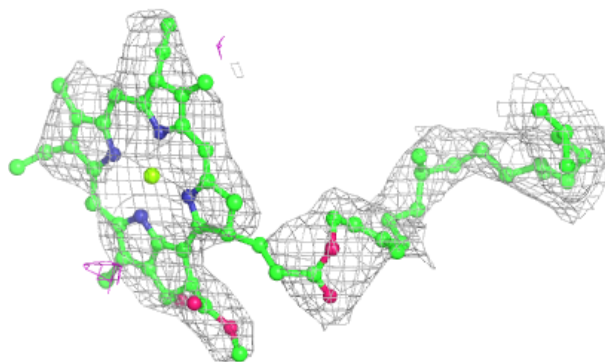
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



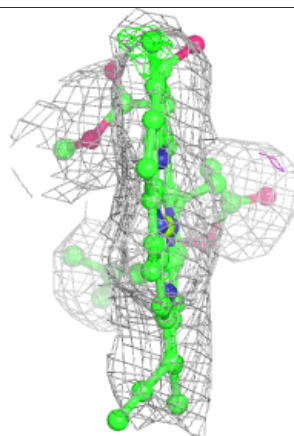
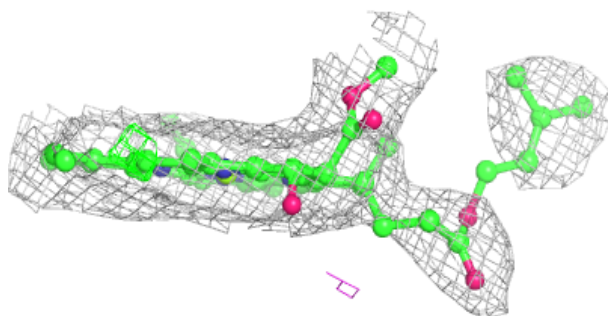
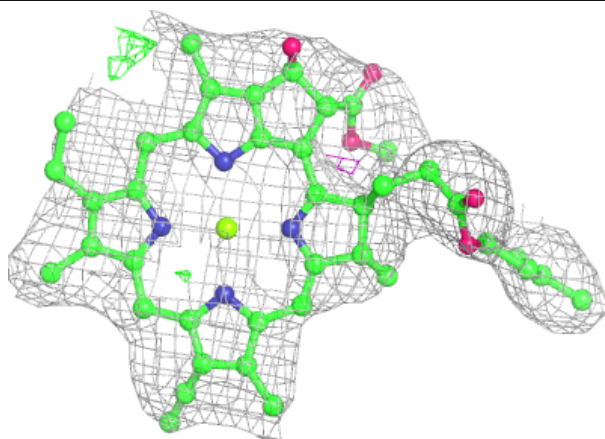


**Electron density around CLA B 1740:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

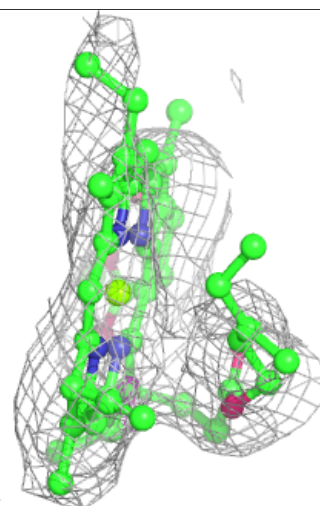
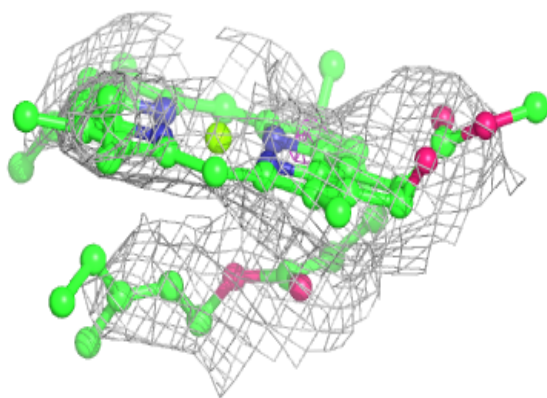
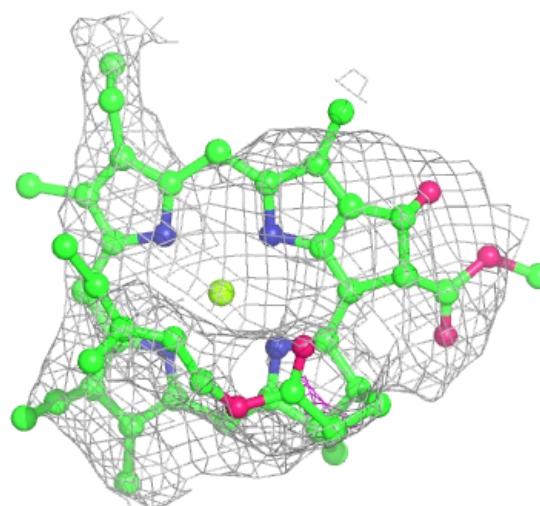
**Electron density around CLA B 1761:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



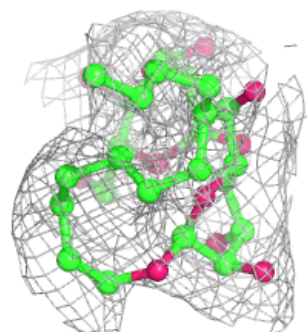
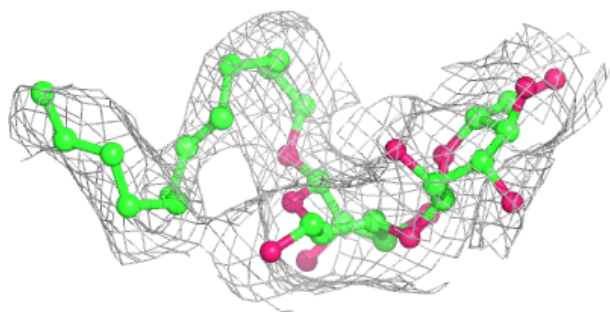
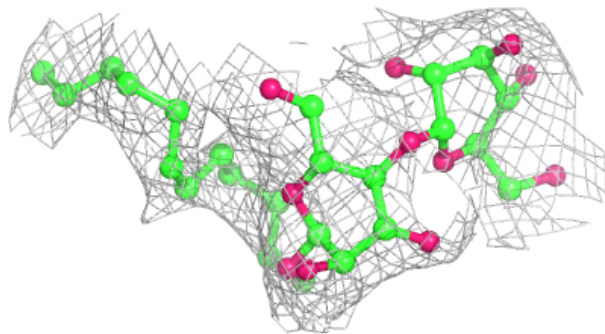
**Electron density around CLA A 1777:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

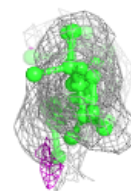
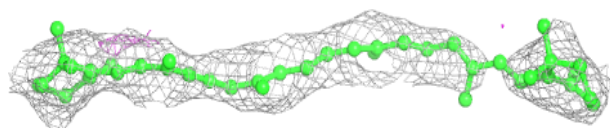
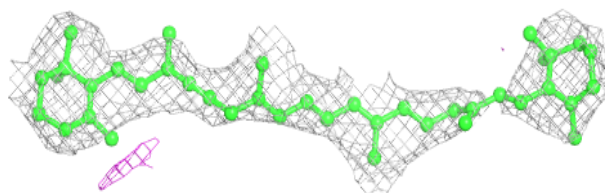


**Electron density around LMU L 1171:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCR B 1777:**

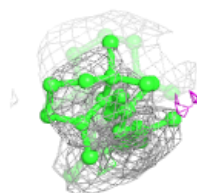
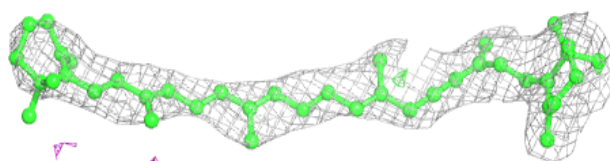
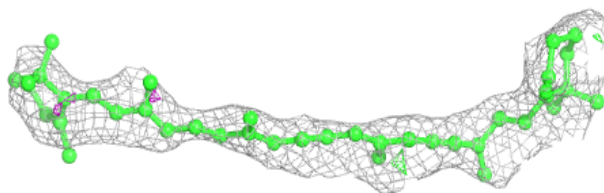
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



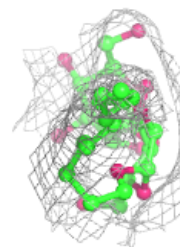
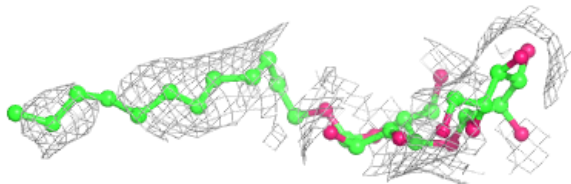
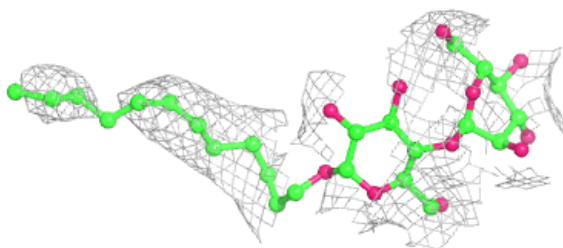


**Electron density around BCR B 1778:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

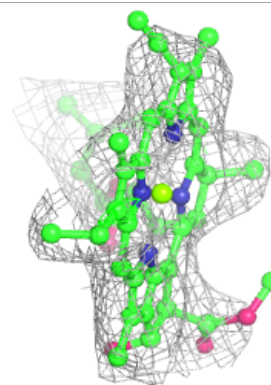
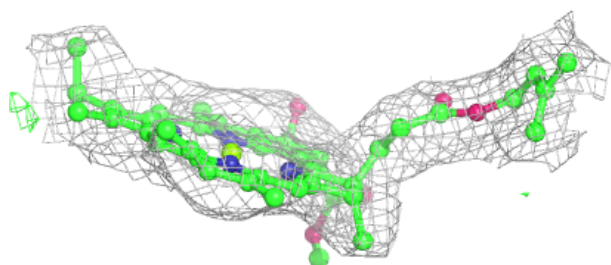
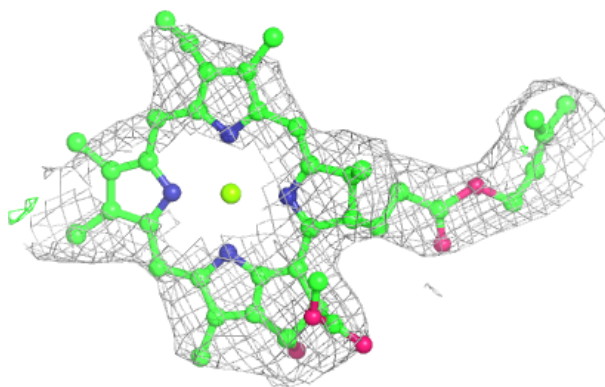
**Electron density around LMU A 7035:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

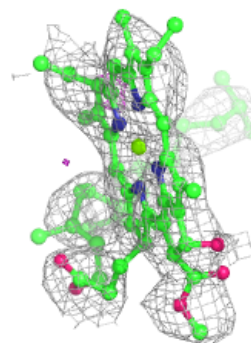
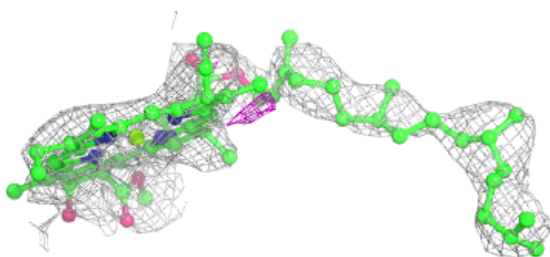
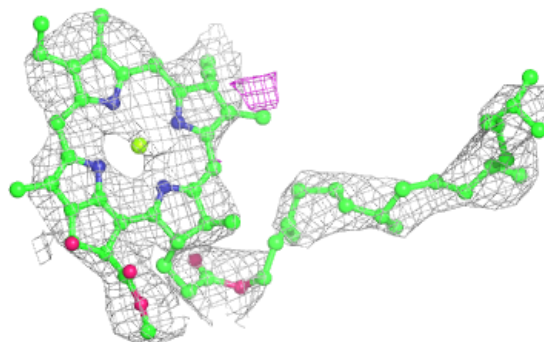


**Electron density around CLA B 1763:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

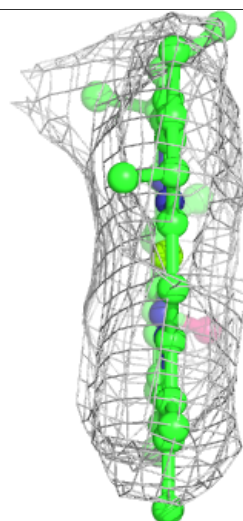
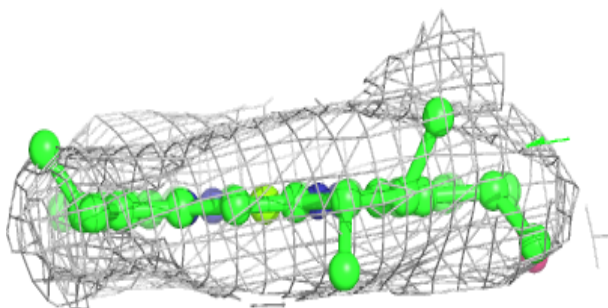
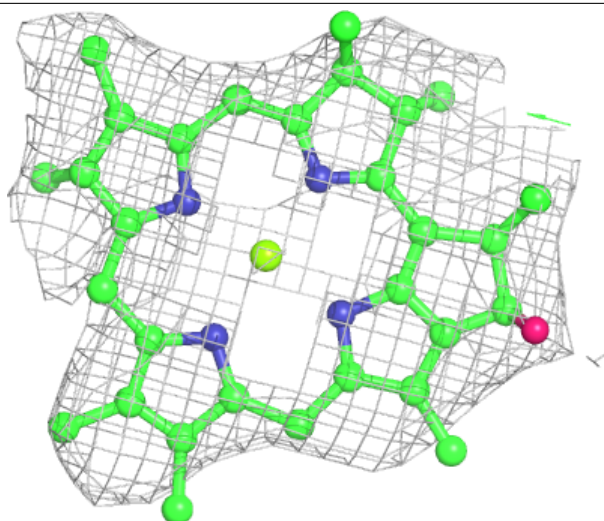
**Electron density around CLA A 1813:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



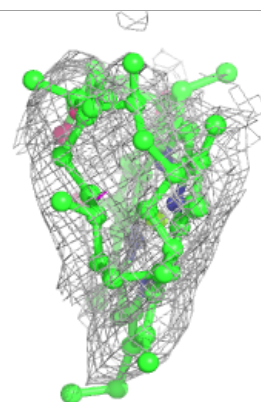
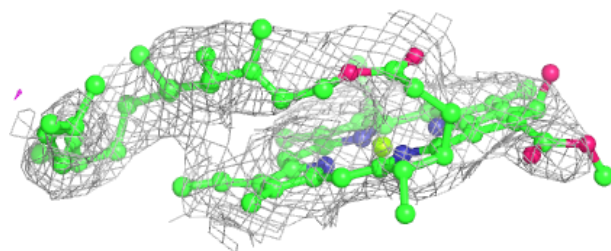
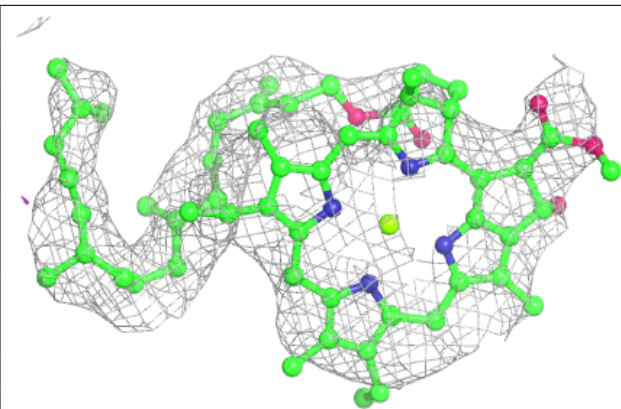
**Electron density around CLA 4 1207:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



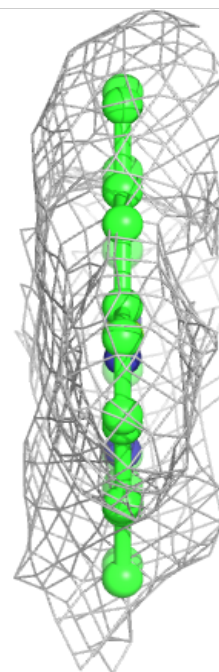
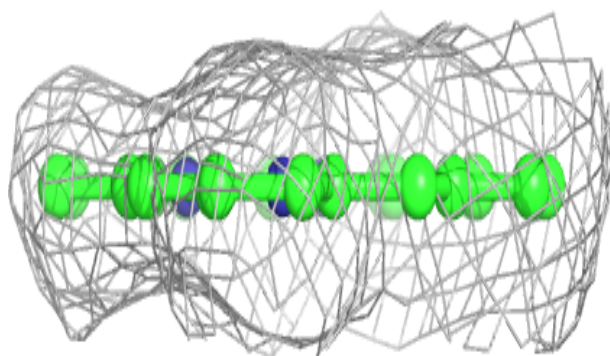
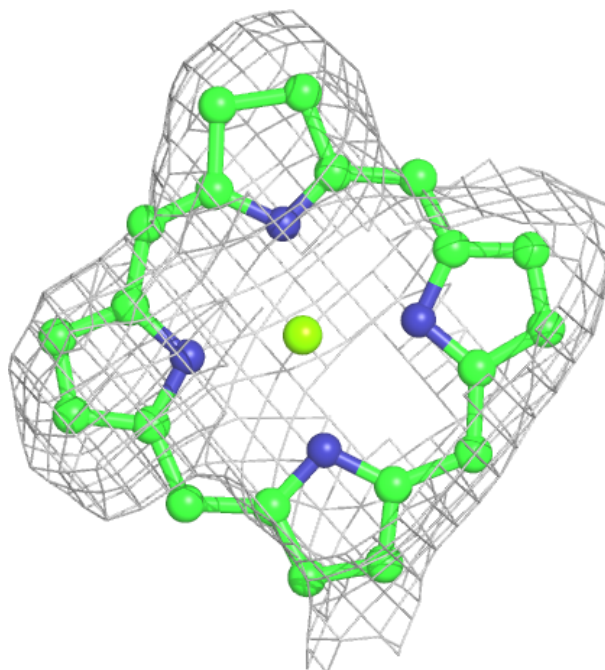
**Electron density around CLA A 1774:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 2 1214:**

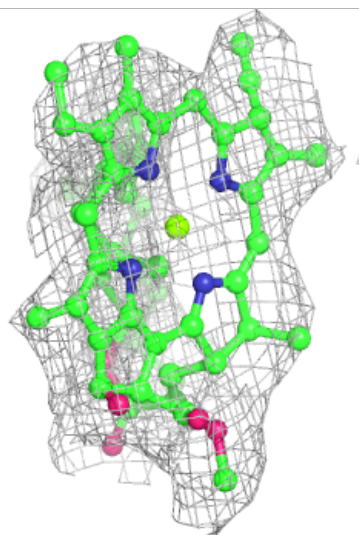
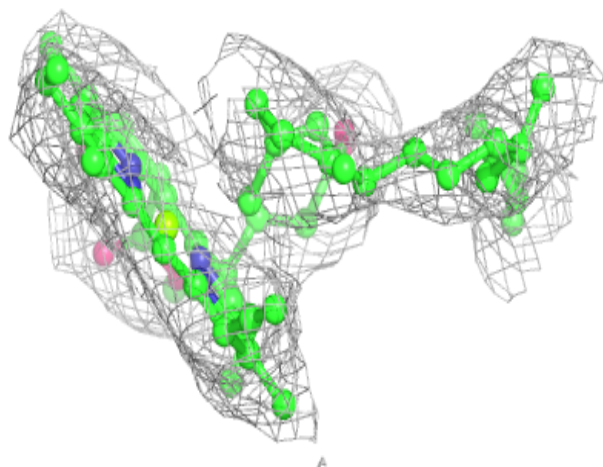
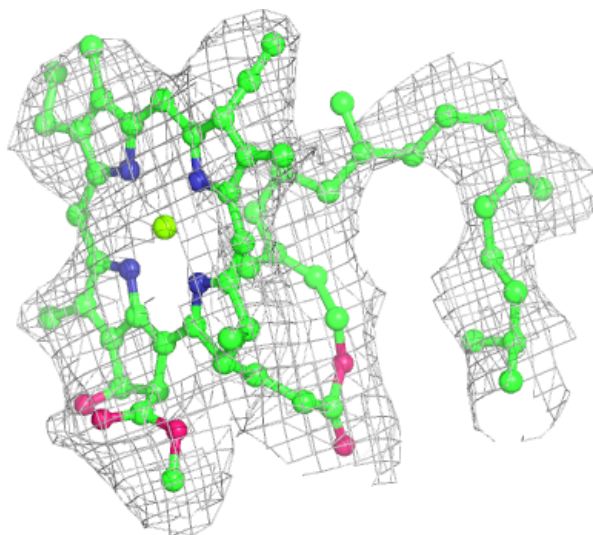
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





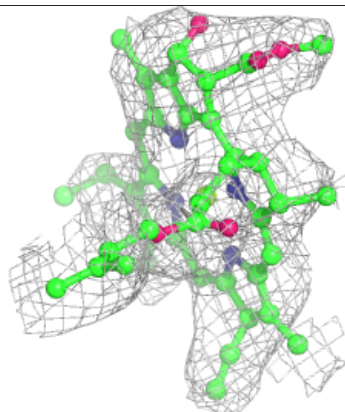
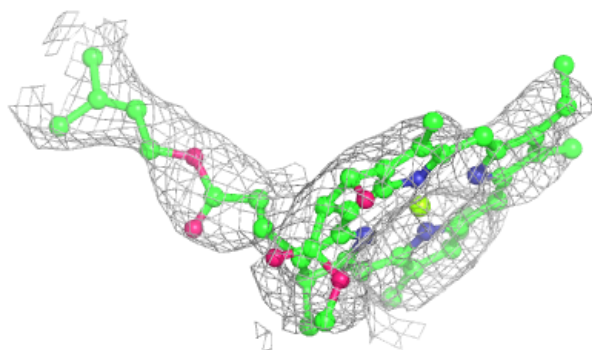
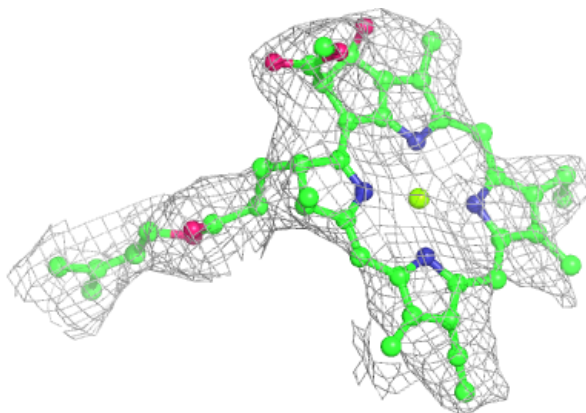
**Electron density around CLA B 1753:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

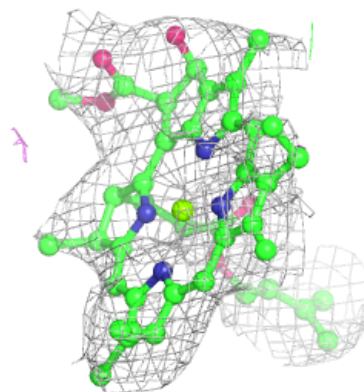
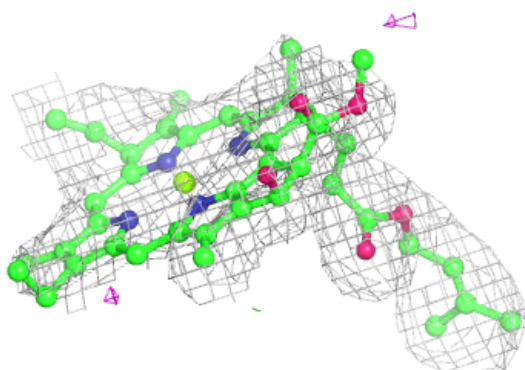
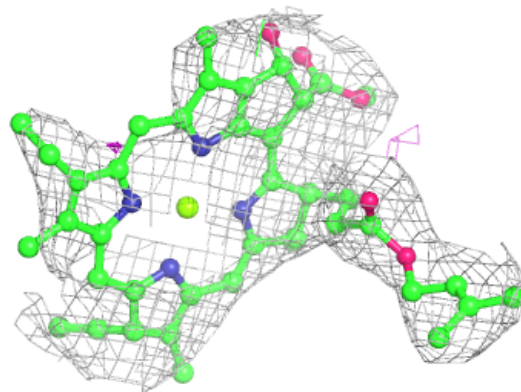


**Electron density around CLA A 1786:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

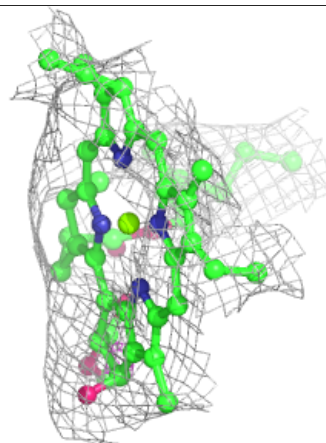
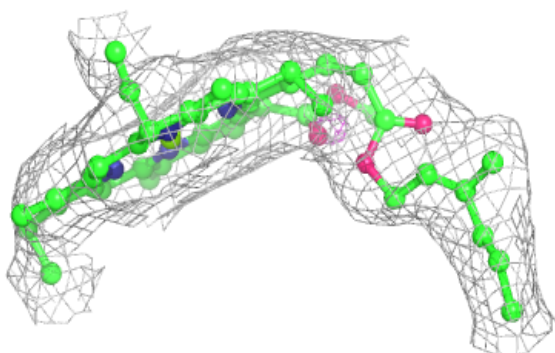
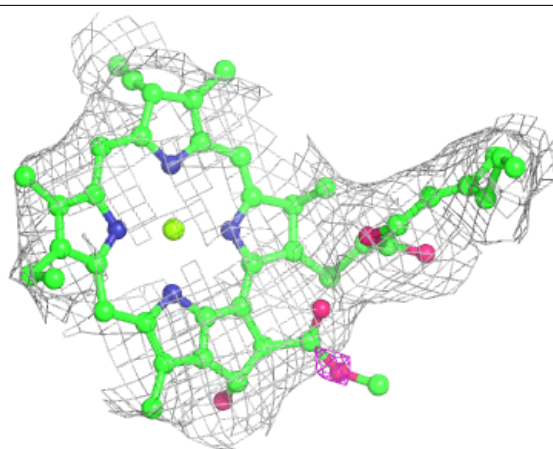
**Electron density around CLA 2 1222:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

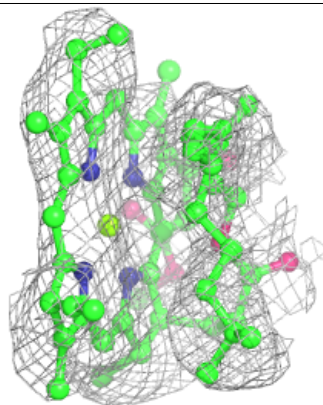
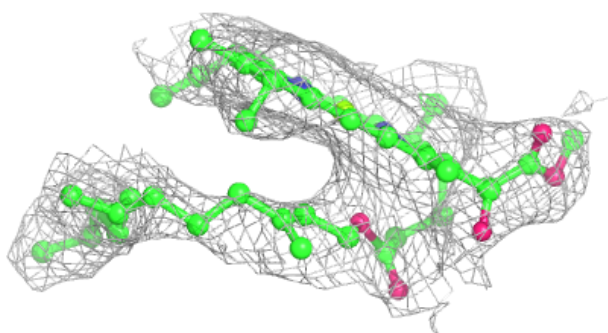
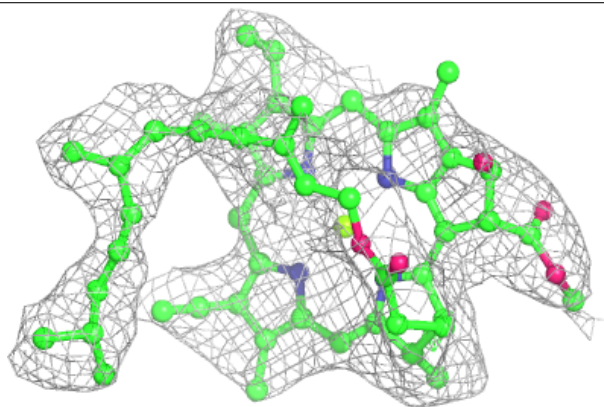


**Electron density around CLA 4 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA I 1031:**

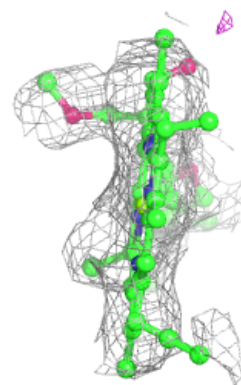
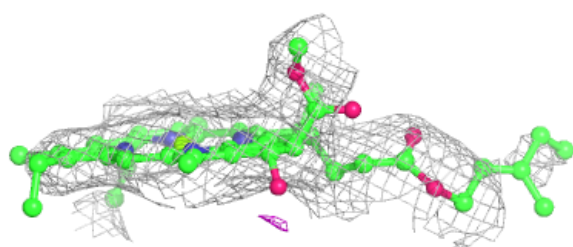
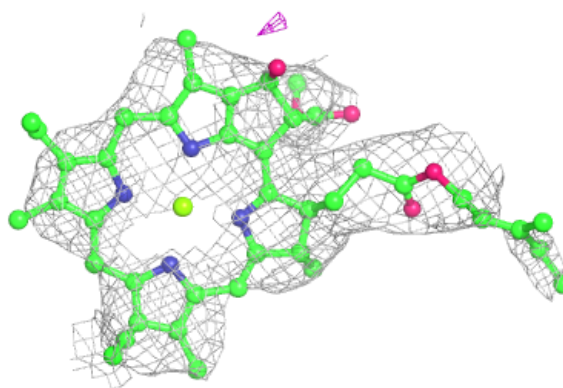
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



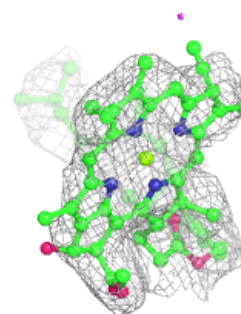
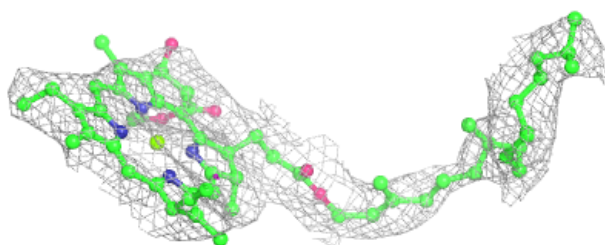
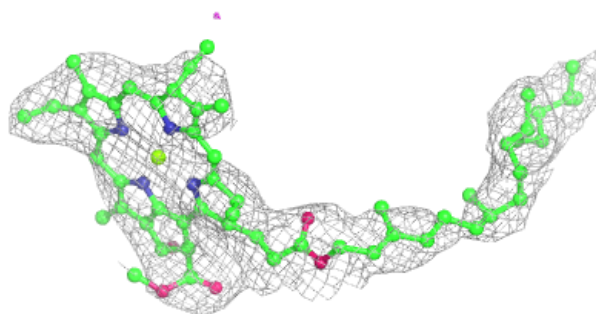


**Electron density around CLA A 1792:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

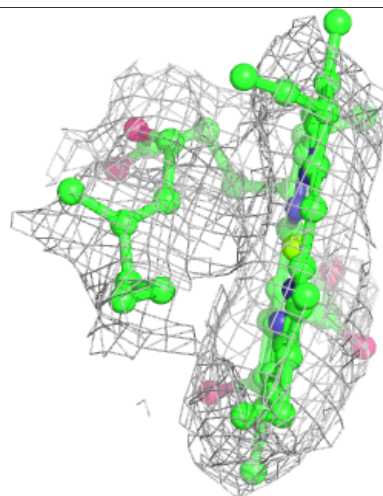
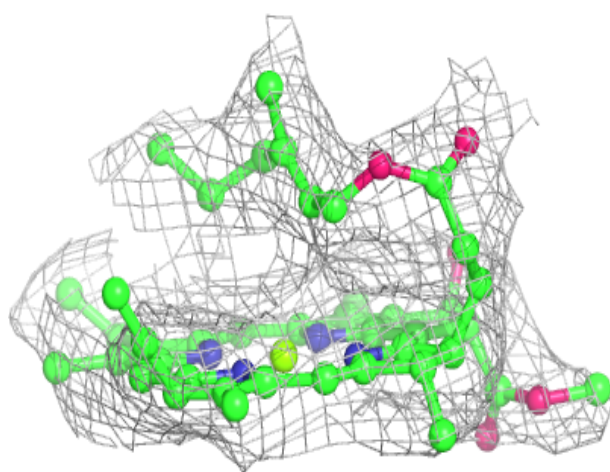
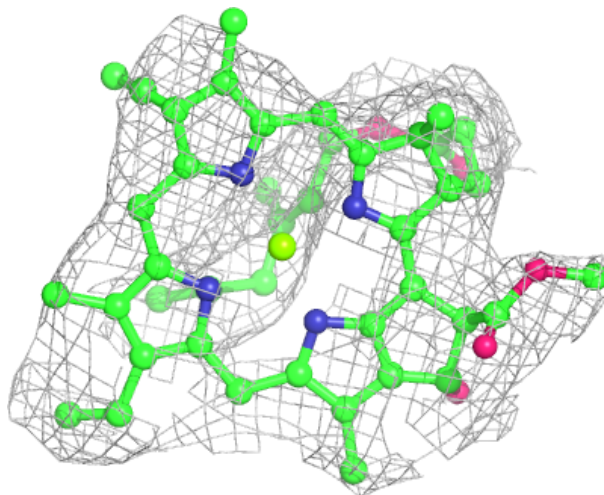
**Electron density around CLA A 1812:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



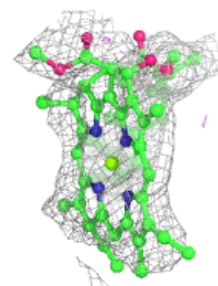
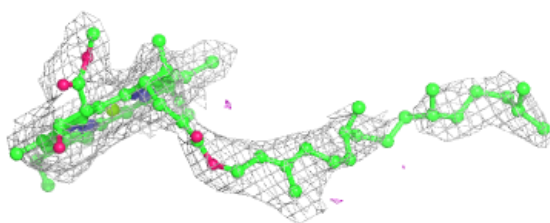
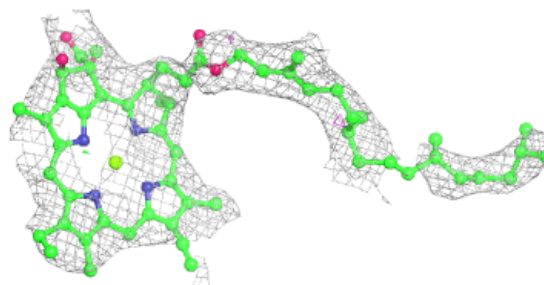
**Electron density around CLA A 1773:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



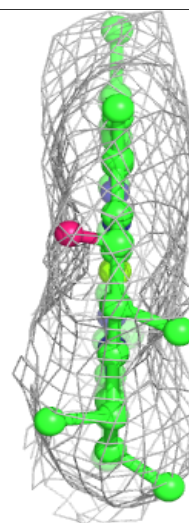
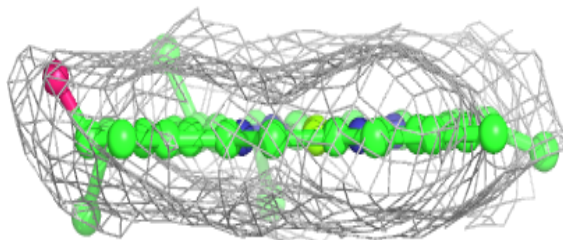
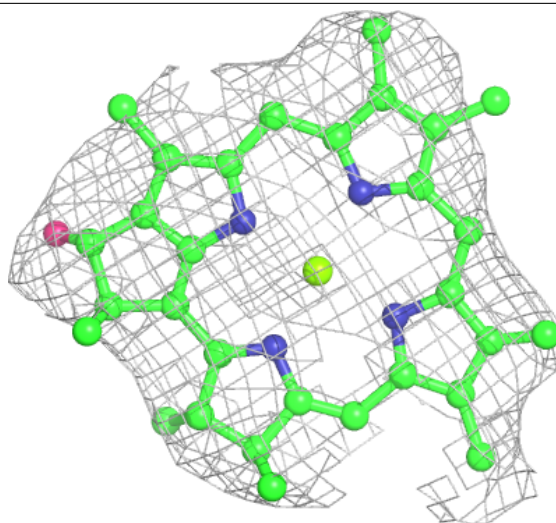
**Electron density around CLA A 1789:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



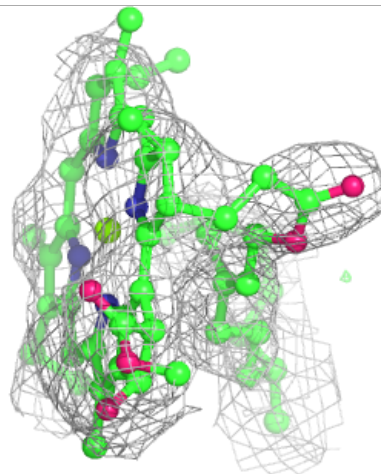
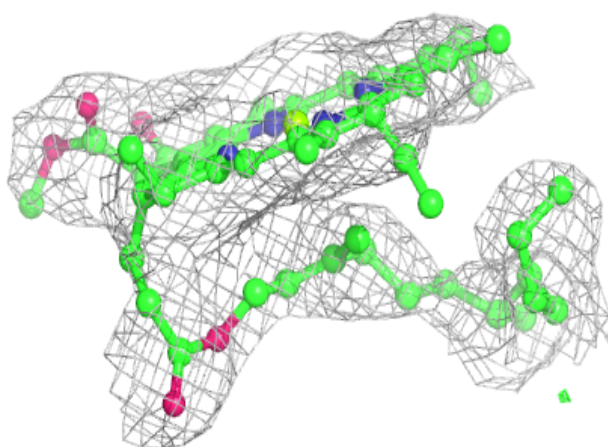
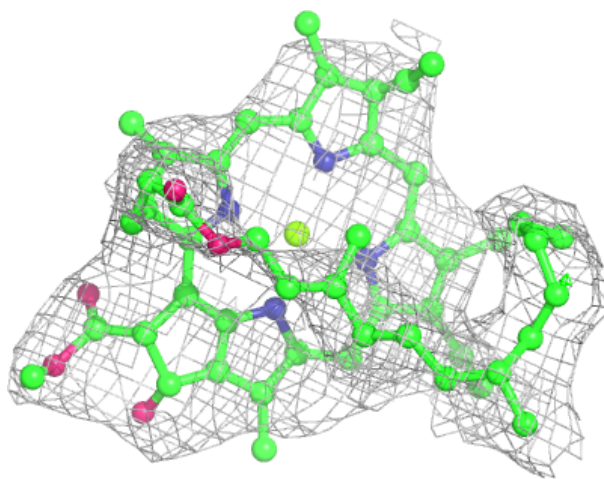
**Electron density around CLA F 1155:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1747:**

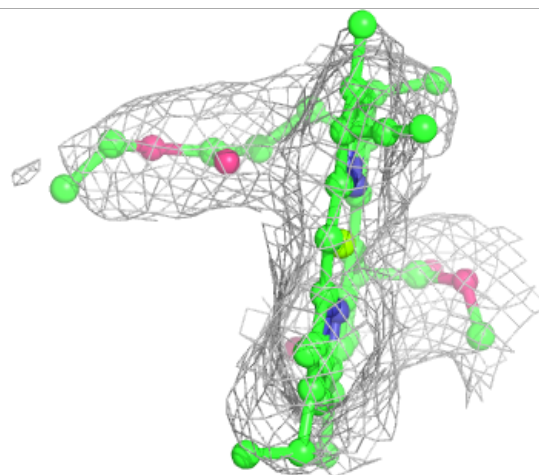
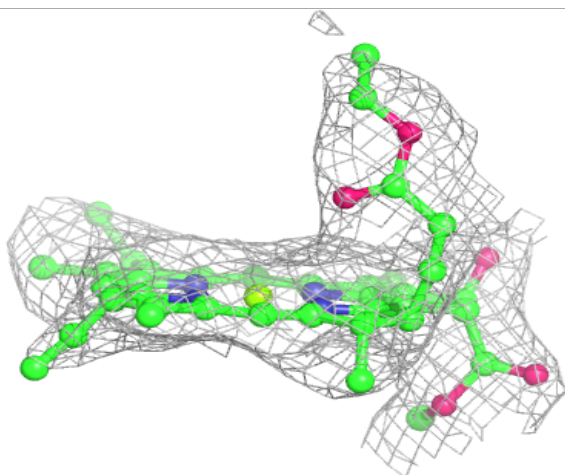
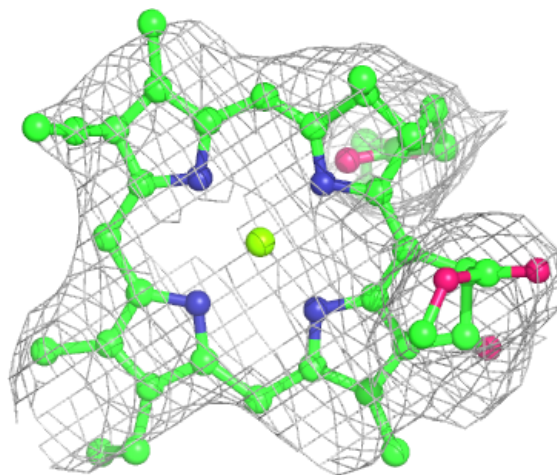
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





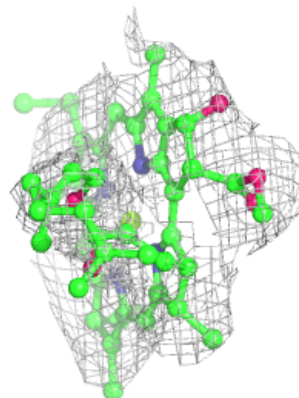
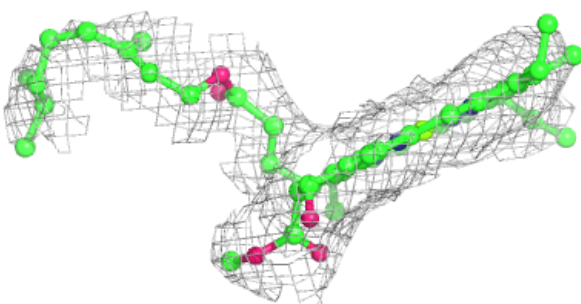
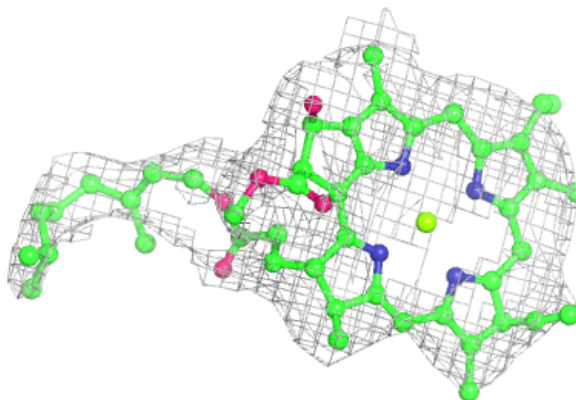
**Electron density around CLA L 1167:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

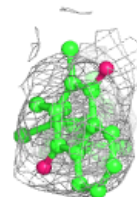
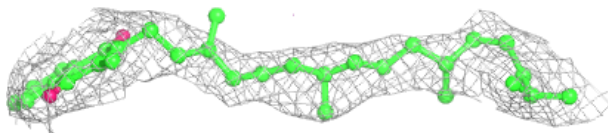
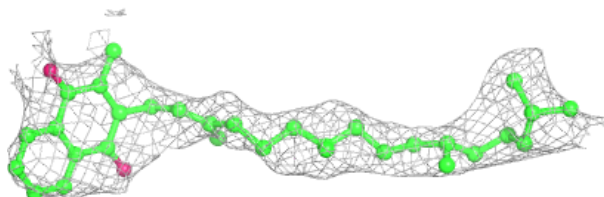


**Electron density around CLA A 1765:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

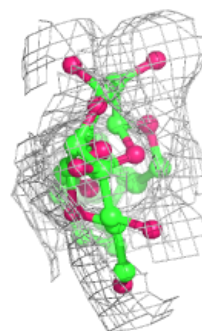
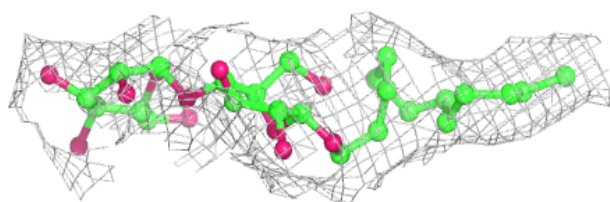
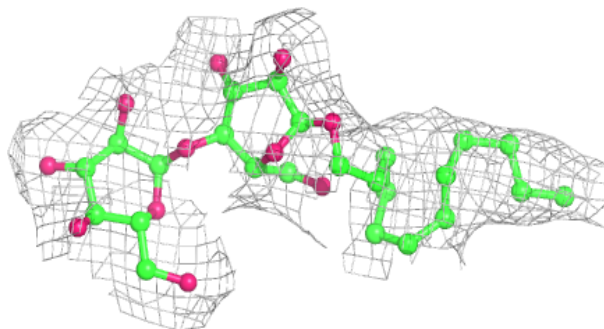
**Electron density around PQN A 1802:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LMU A 7016:**

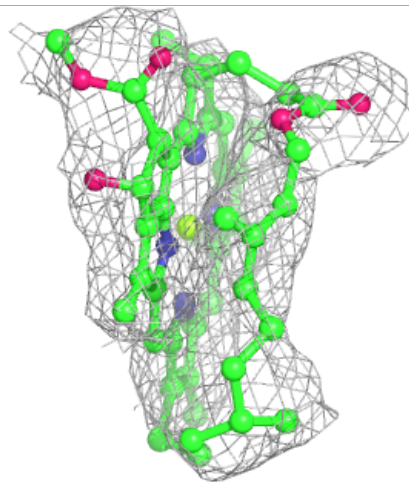
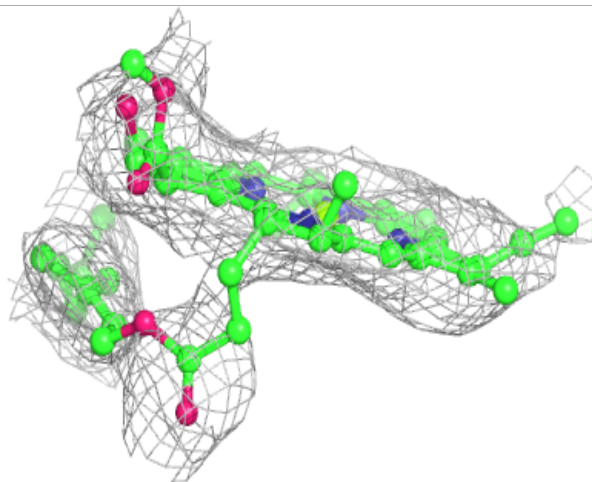
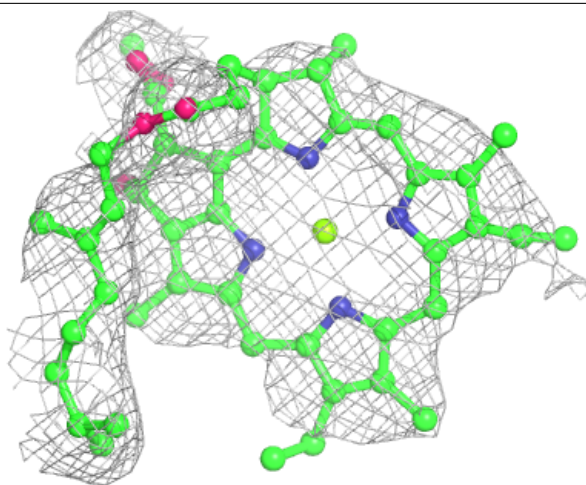
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





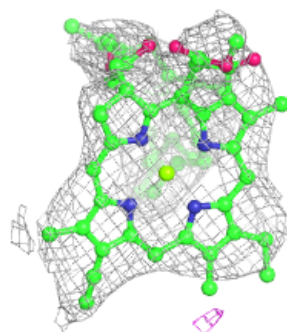
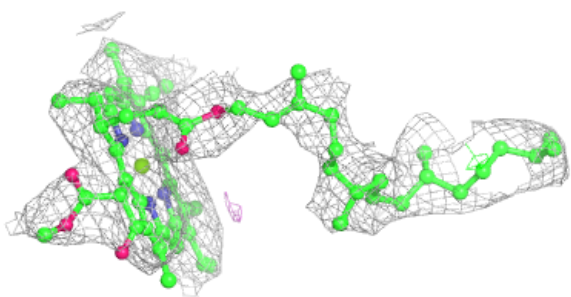
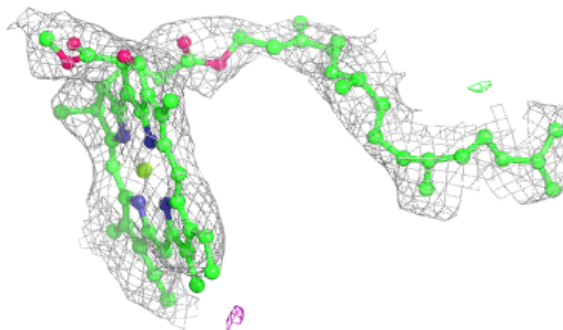
**Electron density around CLA A 1784:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

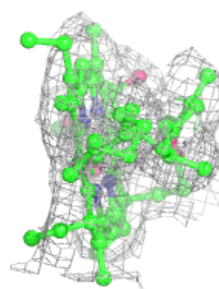
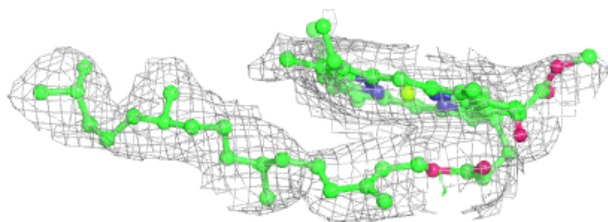
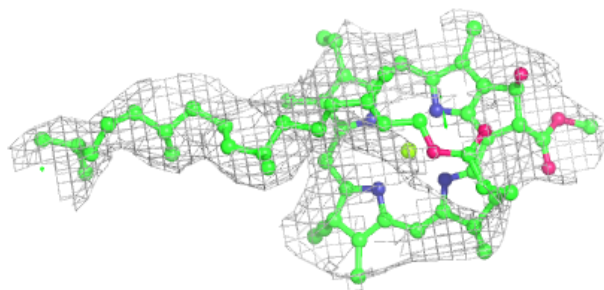


**Electron density around CLA B 1759:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

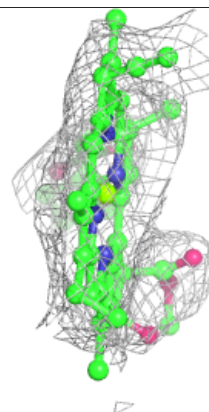
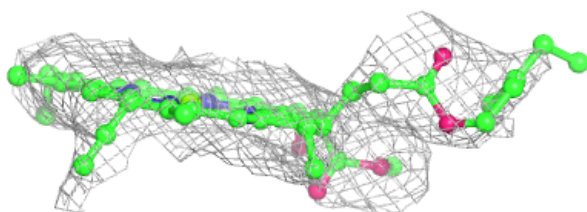
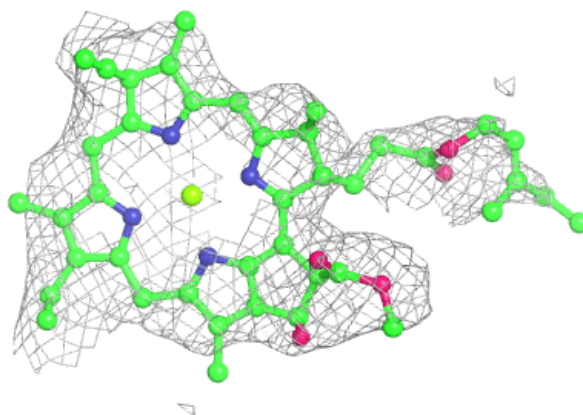
**Electron density around CLA A 1793:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

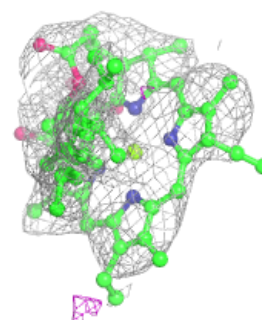
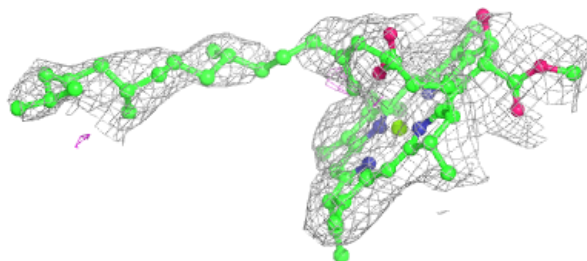
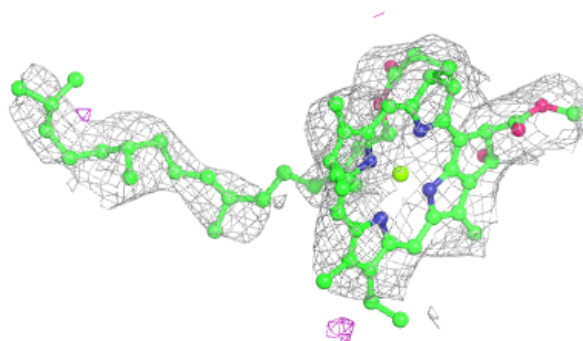


**Electron density around CLA A 1795:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

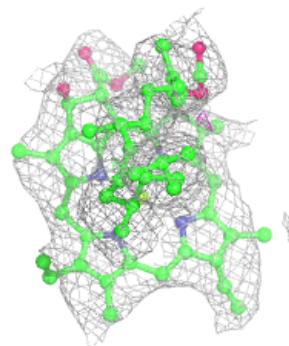
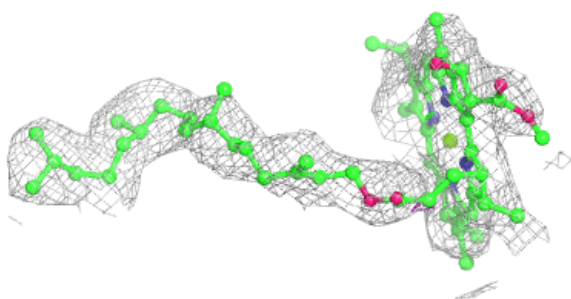
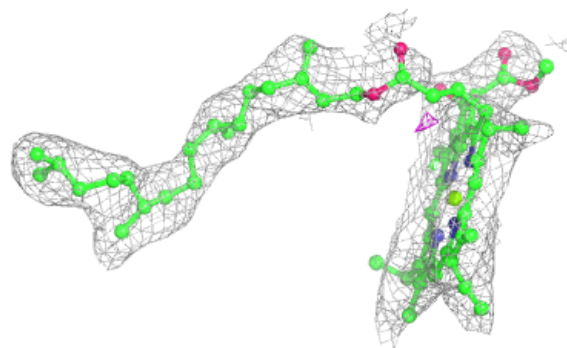
**Electron density around CLA A 1796:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



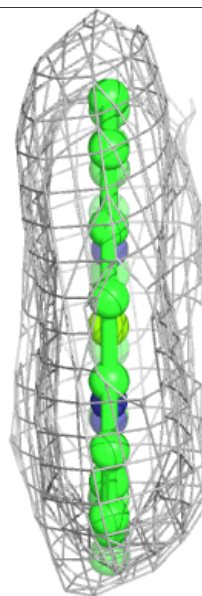
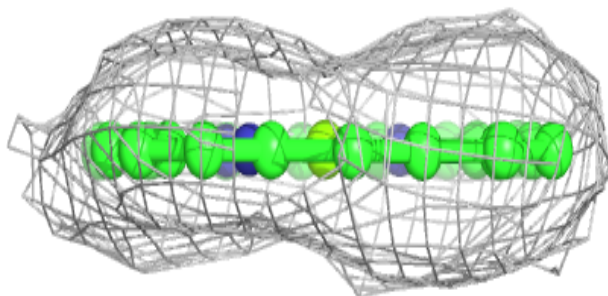
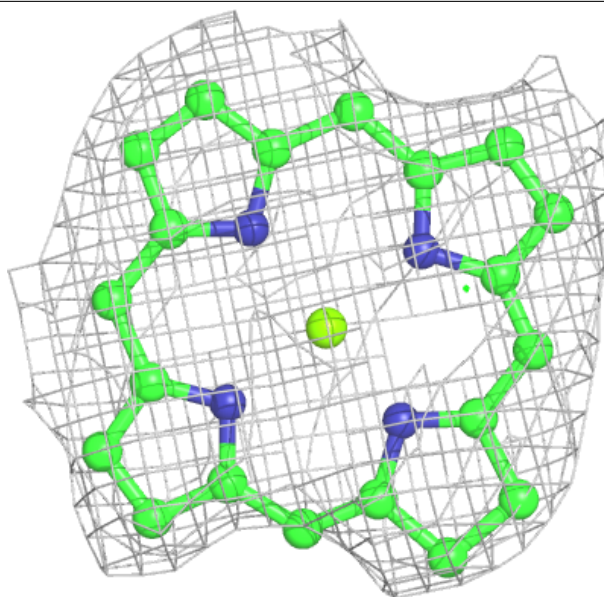
**Electron density around CLA A 1785:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 4 1206:**

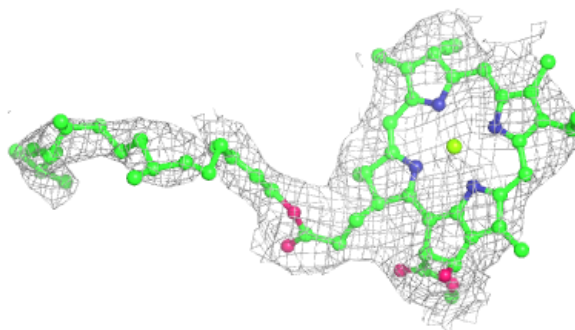
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



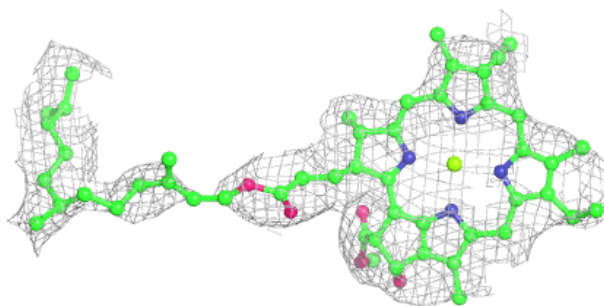


**Electron density around CLA B 1743:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

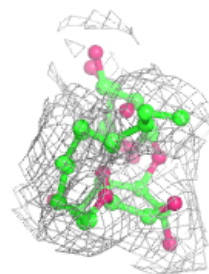
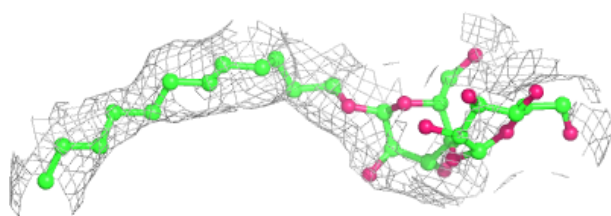
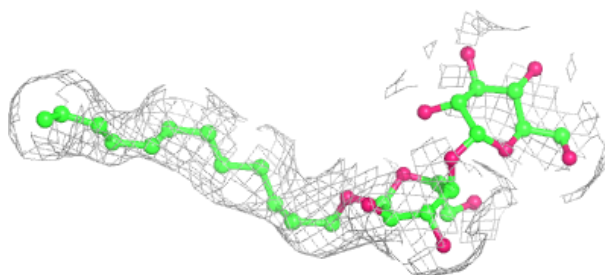
**Electron density around CLA B 1767:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

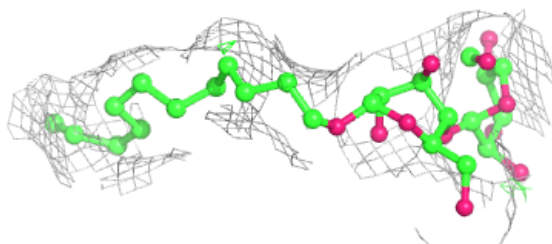
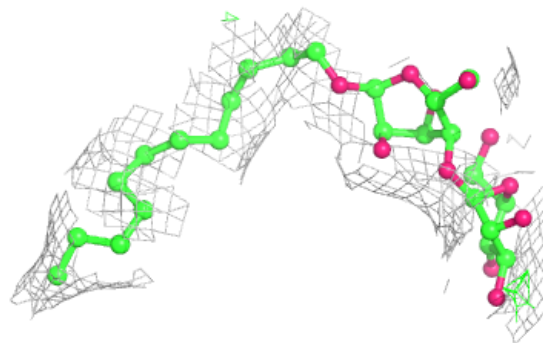


**Electron density around LMU A 7024:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

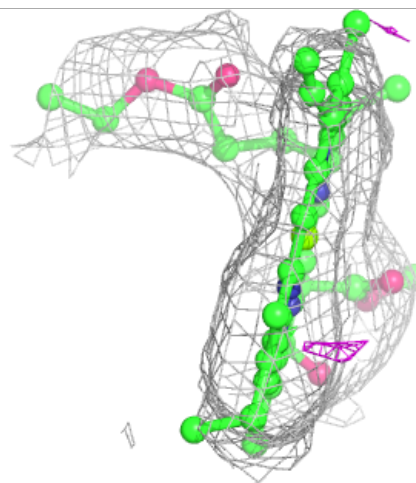
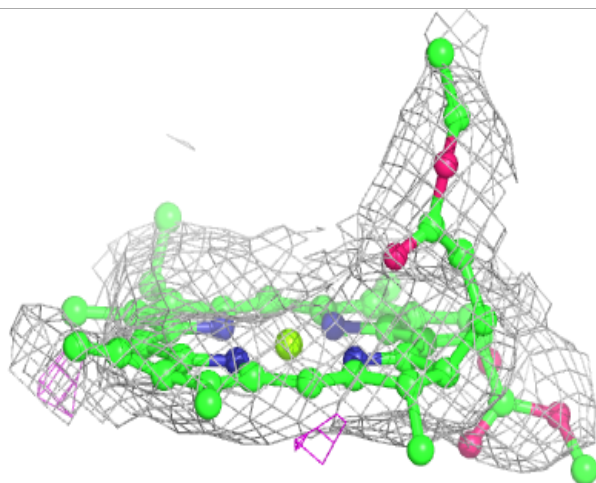
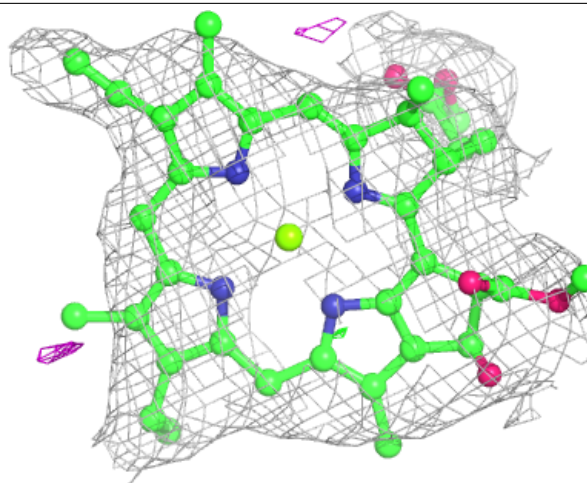
**Electron density around LMU A 7039:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1769:**

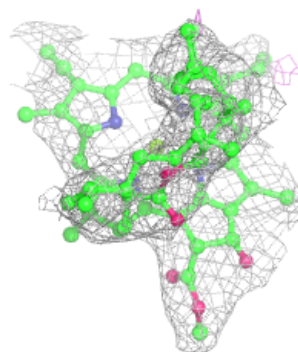
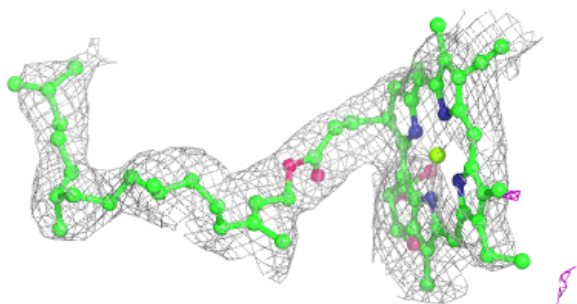
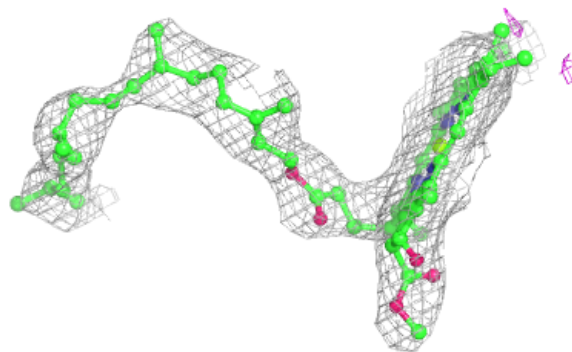
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





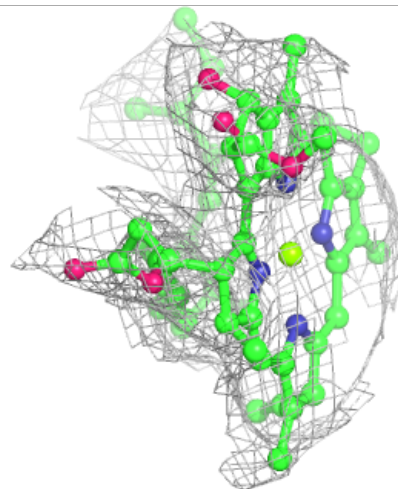
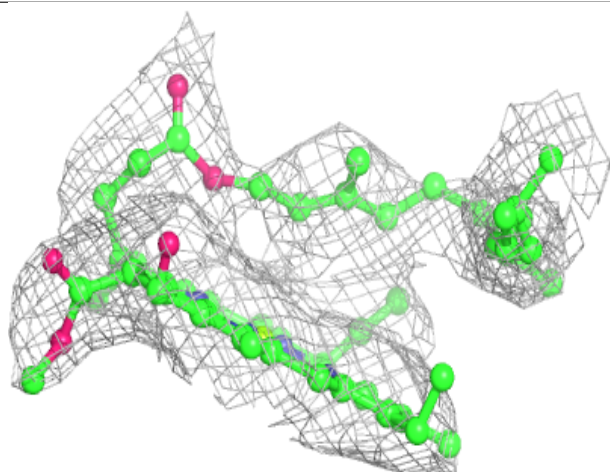
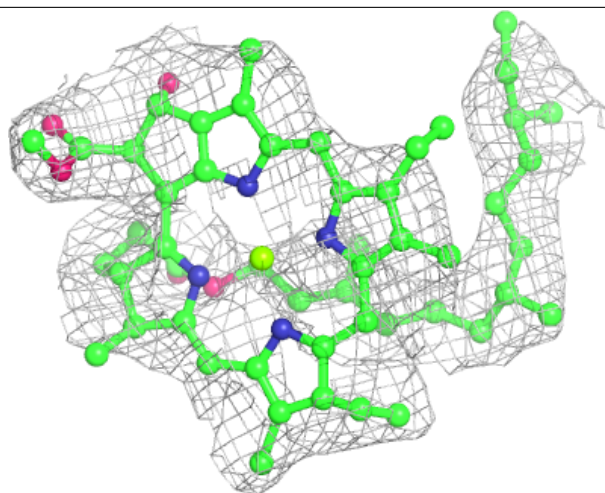
**Electron density around CLA B 1770:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



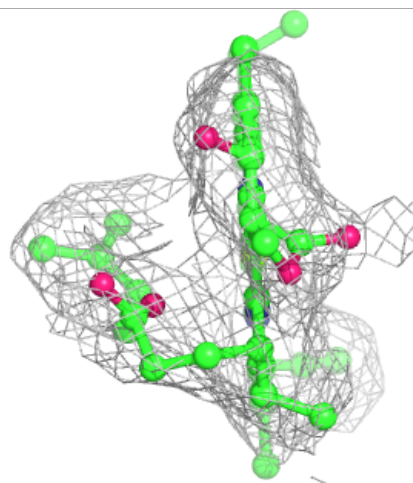
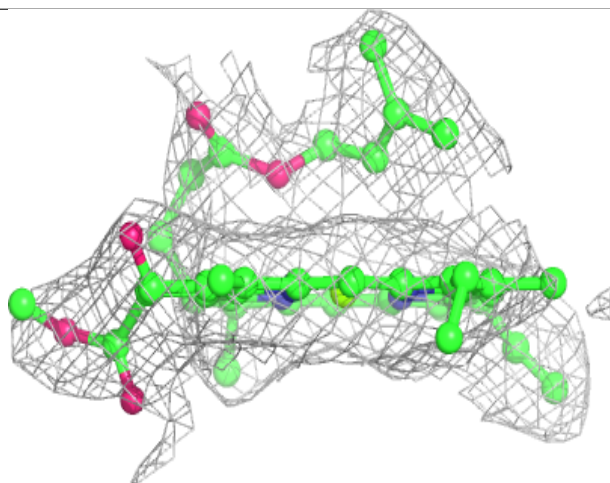
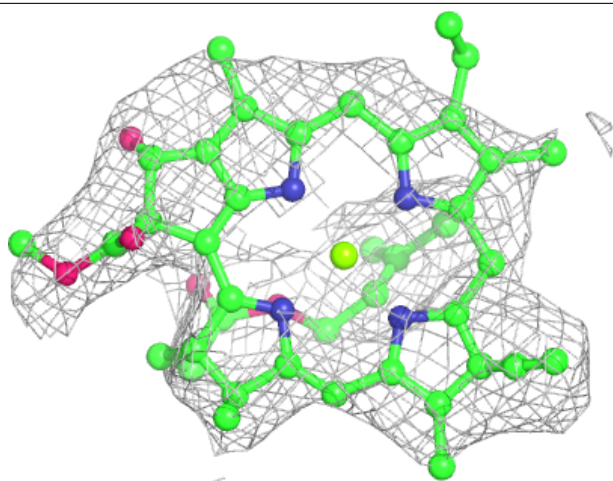
**Electron density around CLA B 1749:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



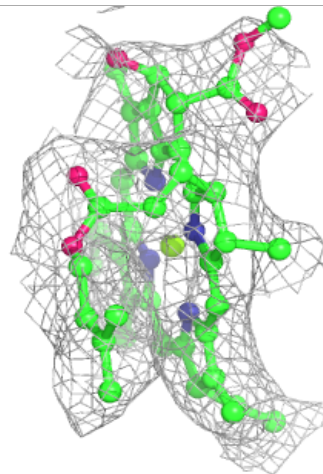
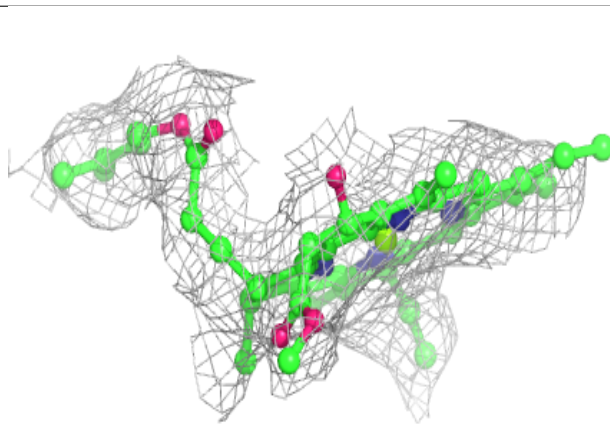
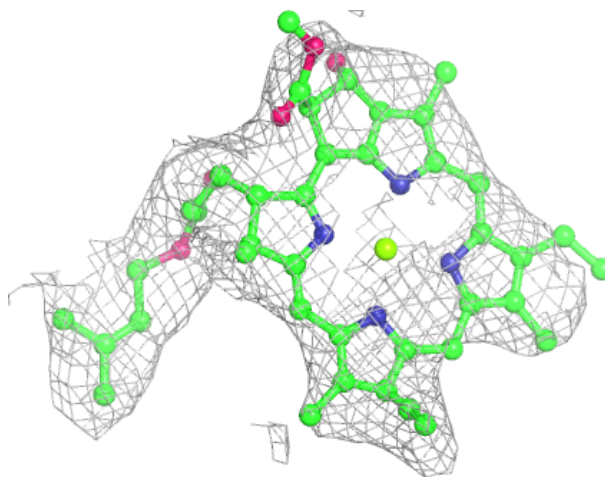
**Electron density around CLA B 1750:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



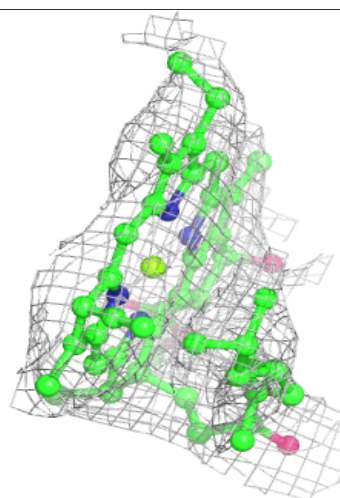
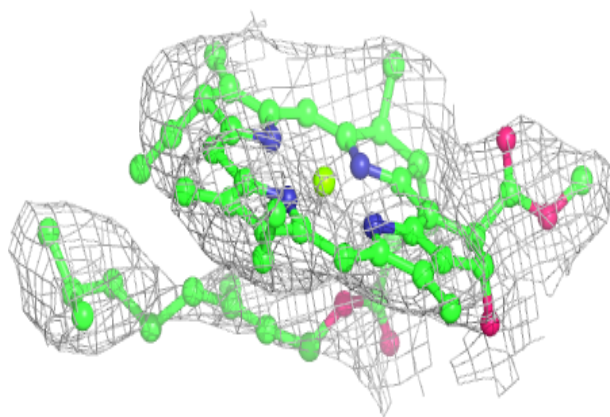
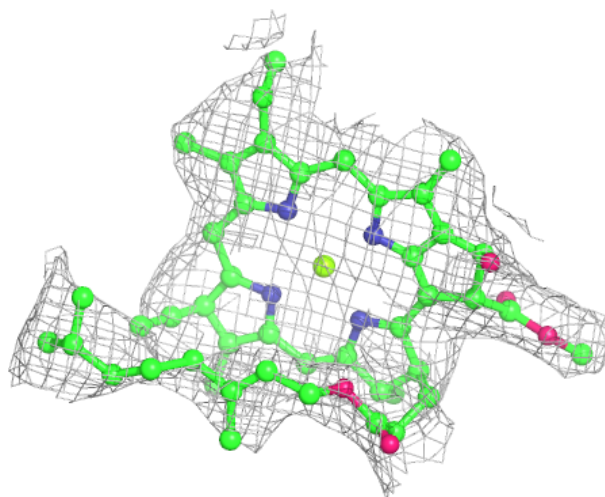
**Electron density around CLA A 1790:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1752:**

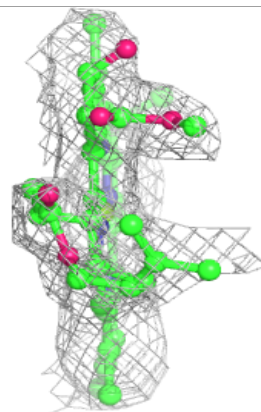
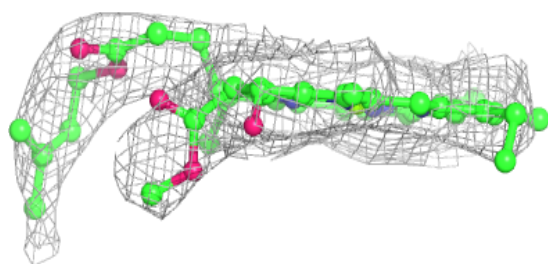
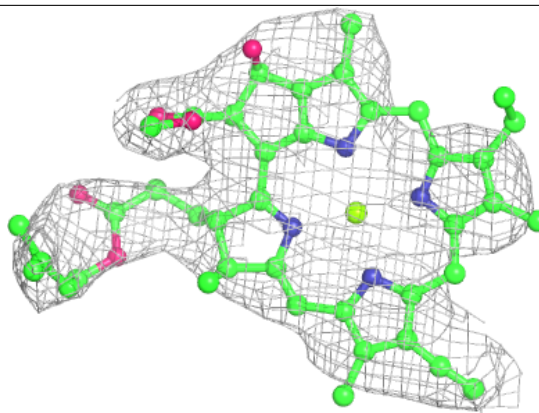
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



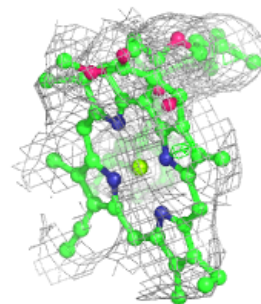
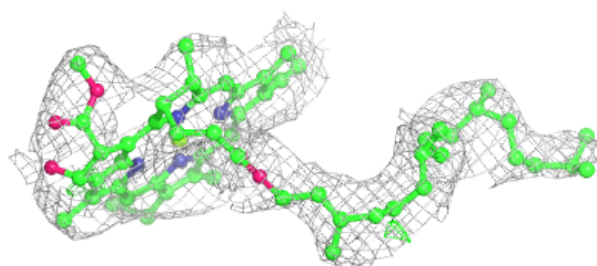
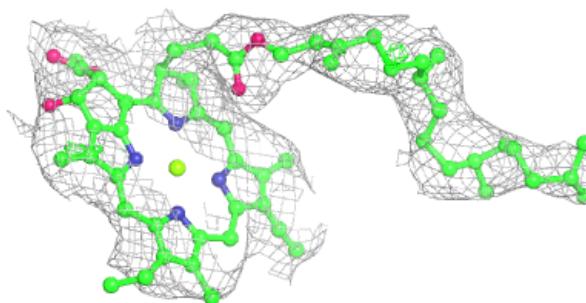


**Electron density around CLA A 1759:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

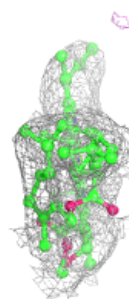
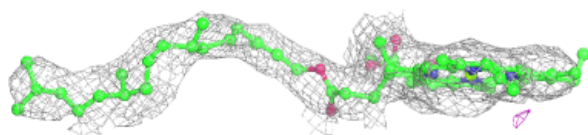
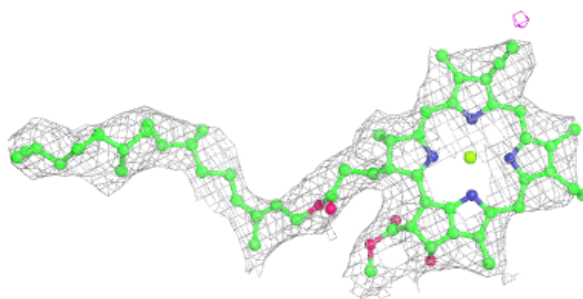
**Electron density around CLA A 1764:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

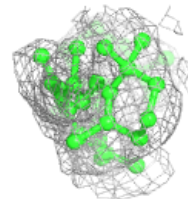
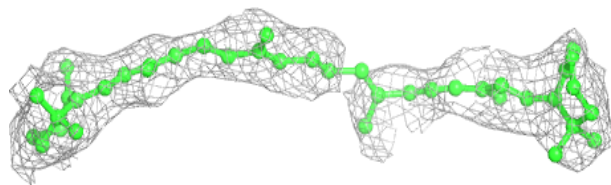
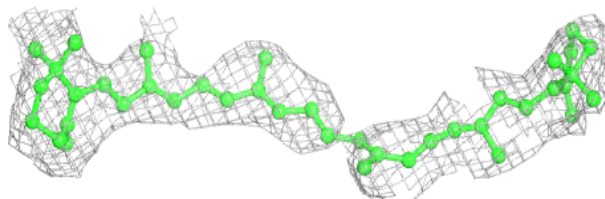


**Electron density around CLA A 1788:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

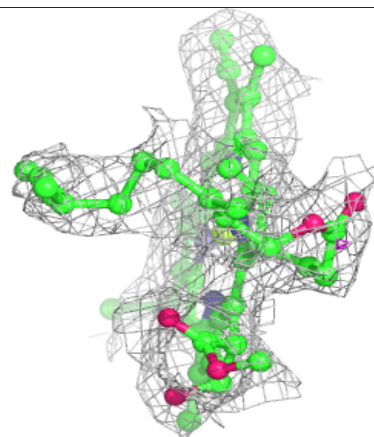
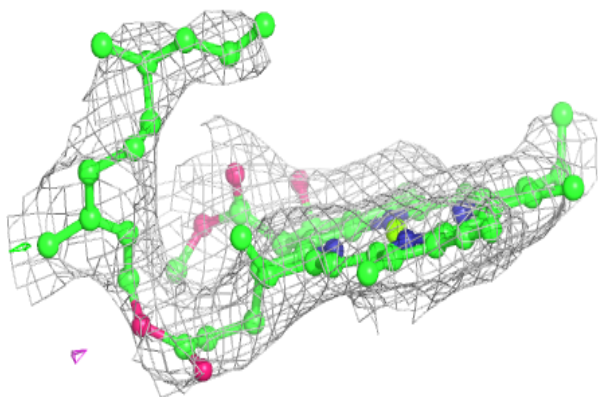
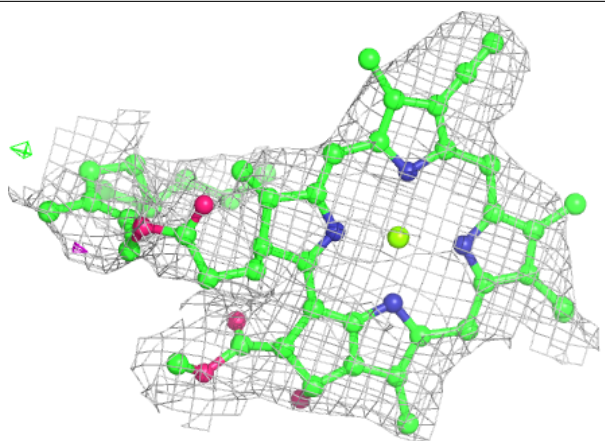
**Electron density around BCR B 1781:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 1762:**

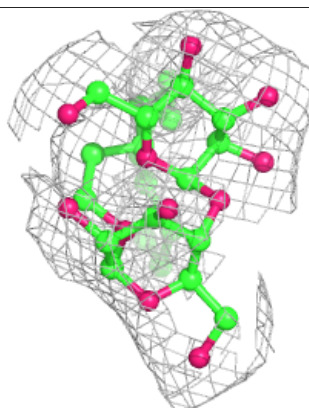
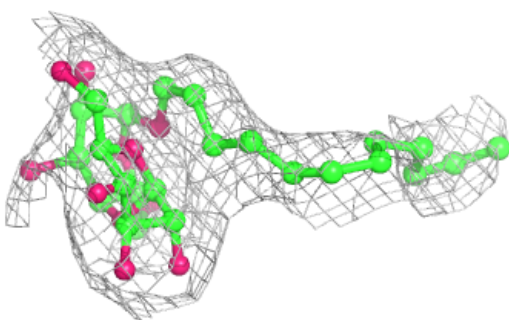
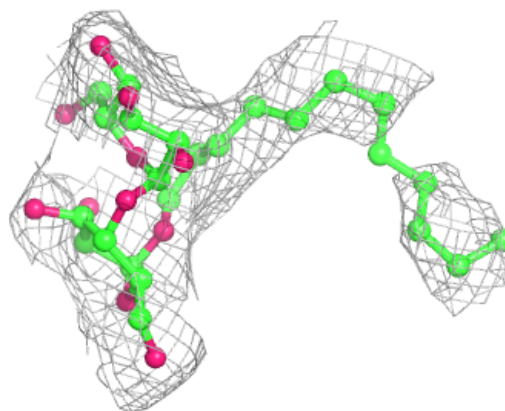
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



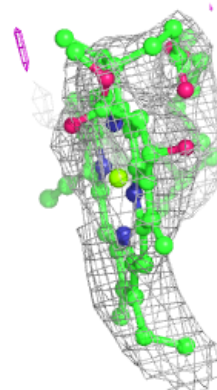
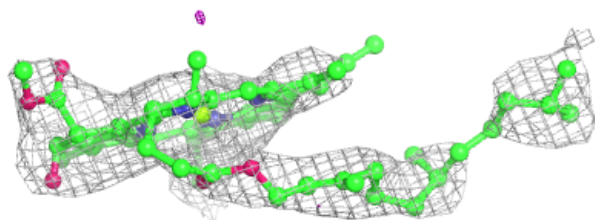
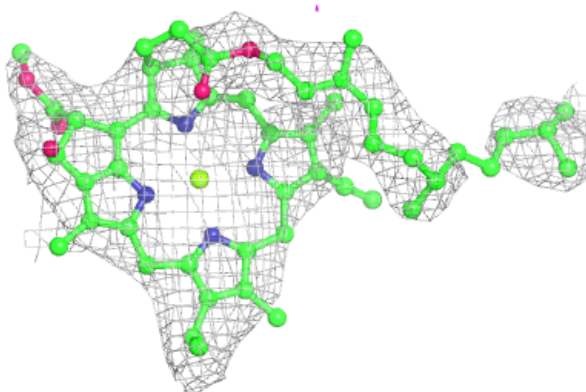


**Electron density around LMU A 7032:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

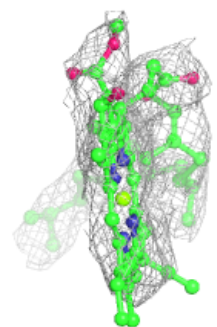
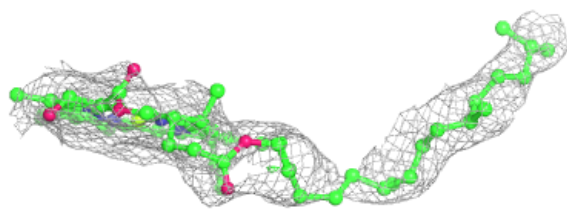
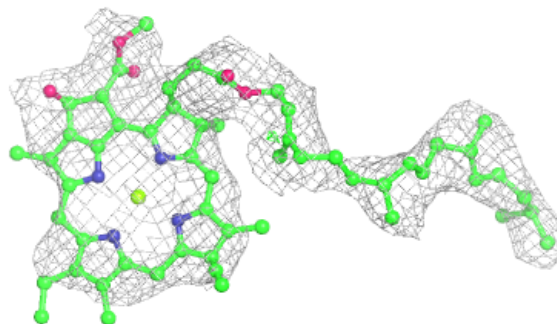
**Electron density around CLA B 1748:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

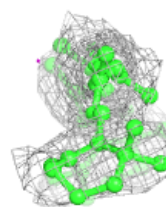
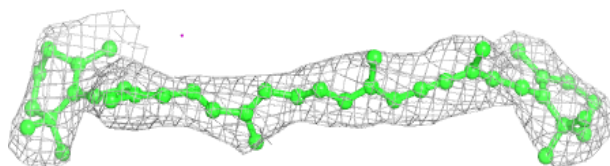
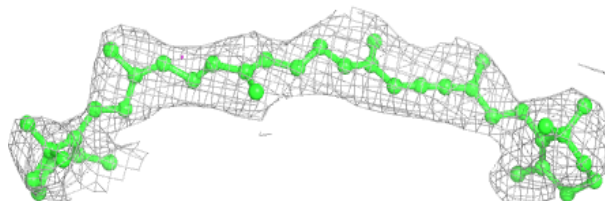


**Electron density around CLA B 1787:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

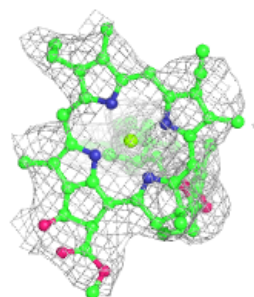
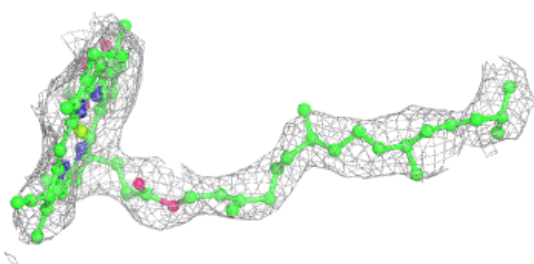
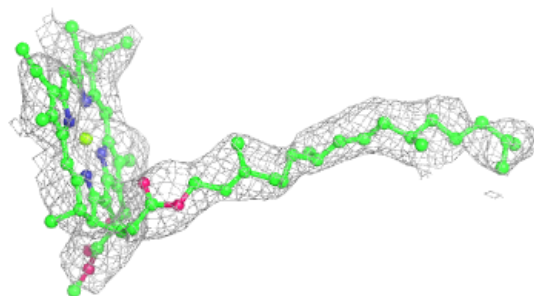
**Electron density around BCR L 1170:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

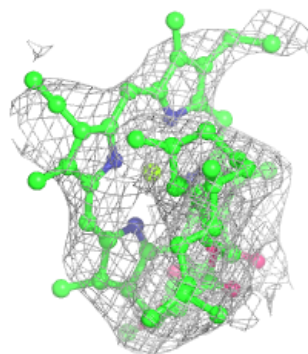
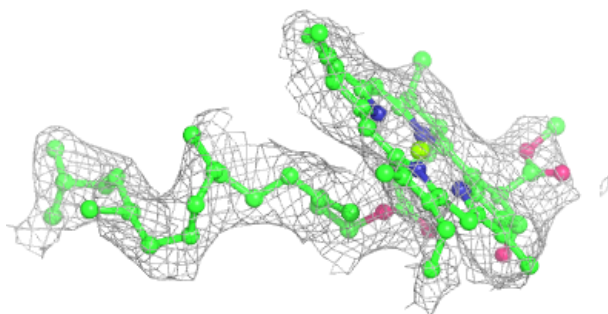
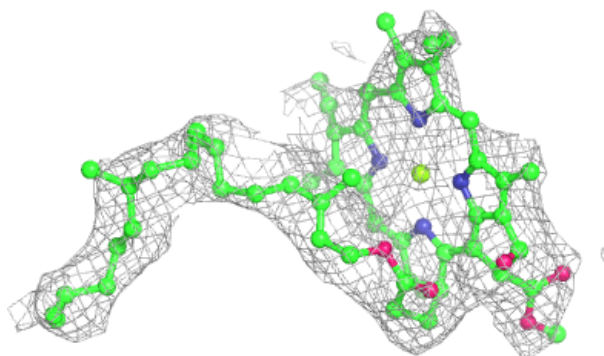


**Electron density around CLA B 1758:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

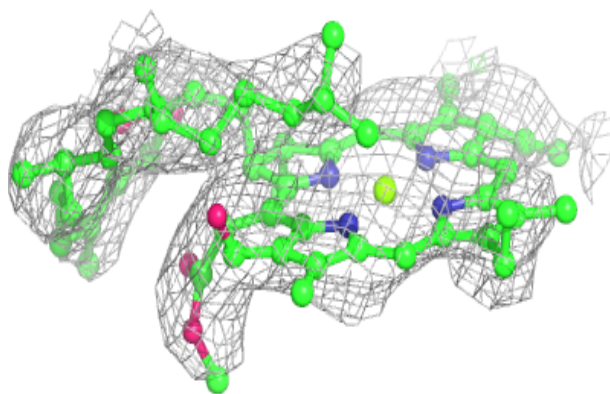
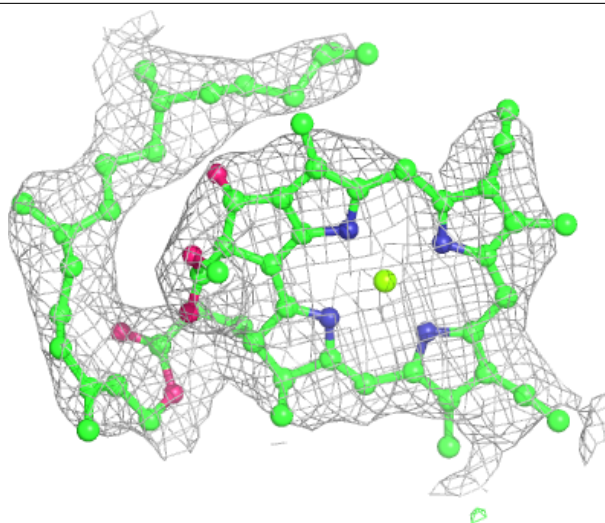
**Electron density around CLA A 1800:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1737:**

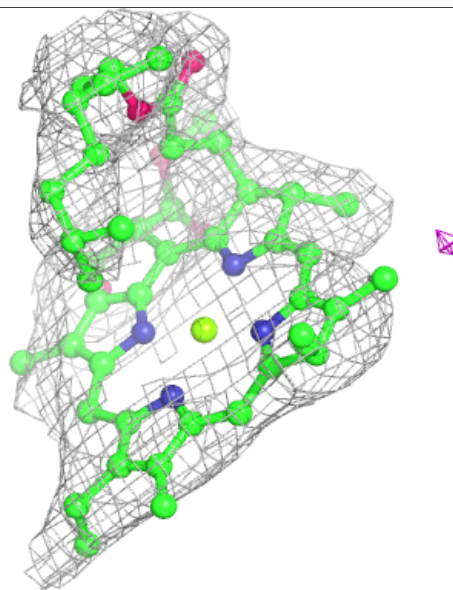
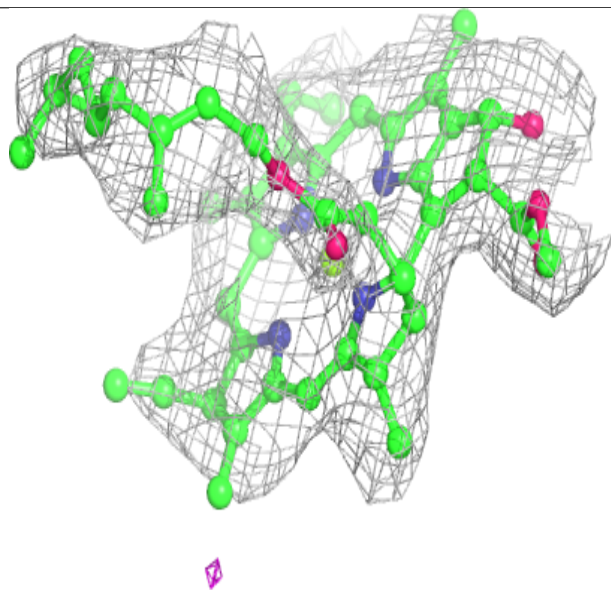
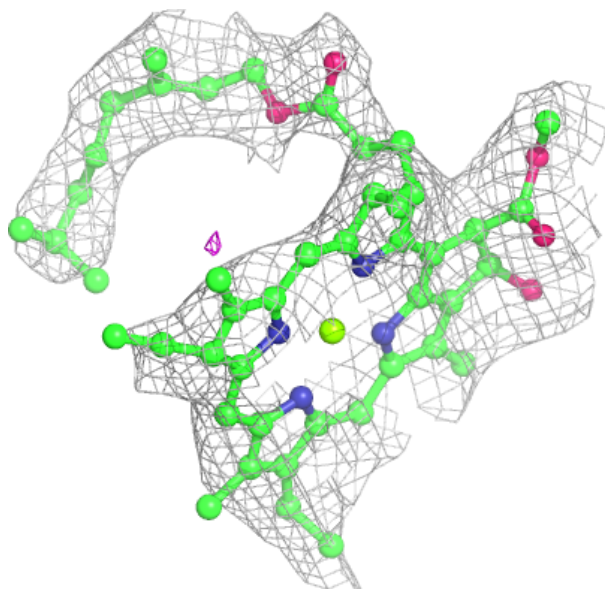
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





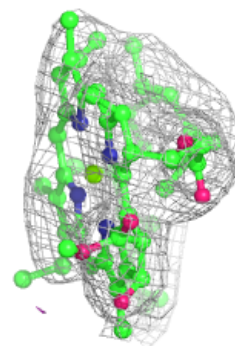
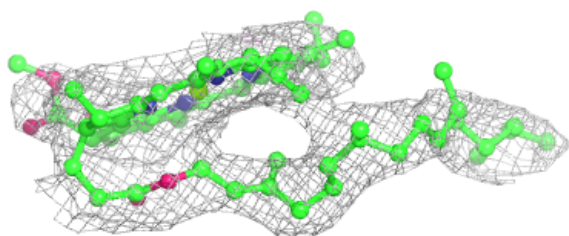
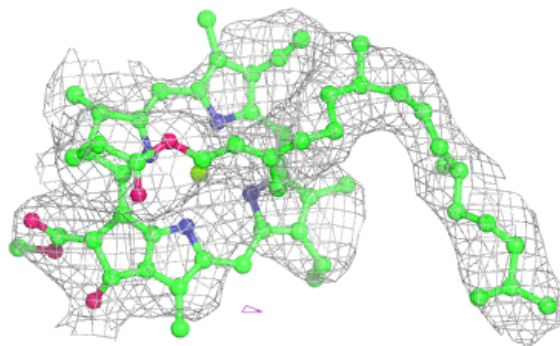
**Electron density around CLA A 1779:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

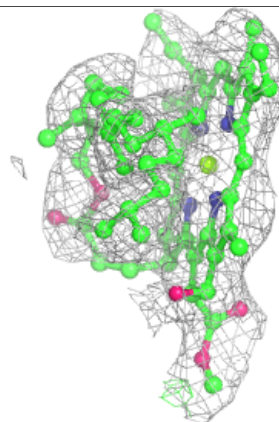
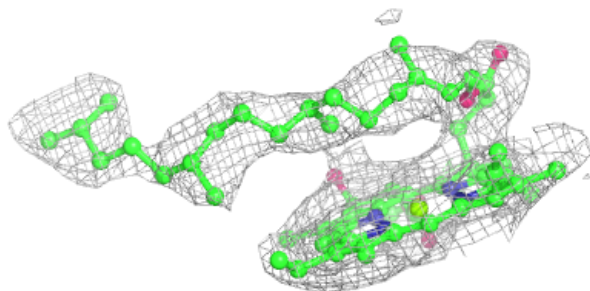
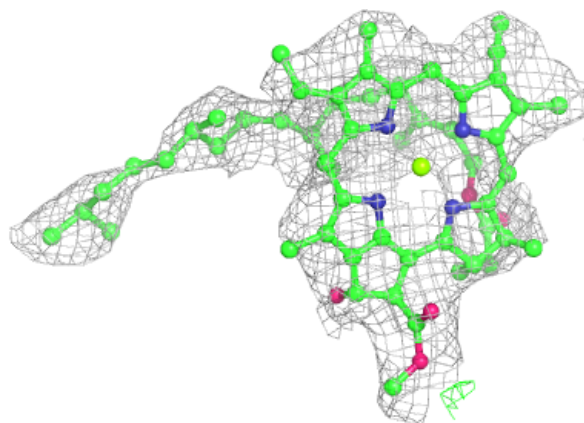


**Electron density around CLA B 1768:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

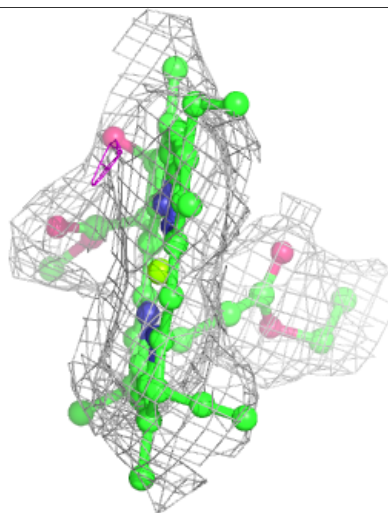
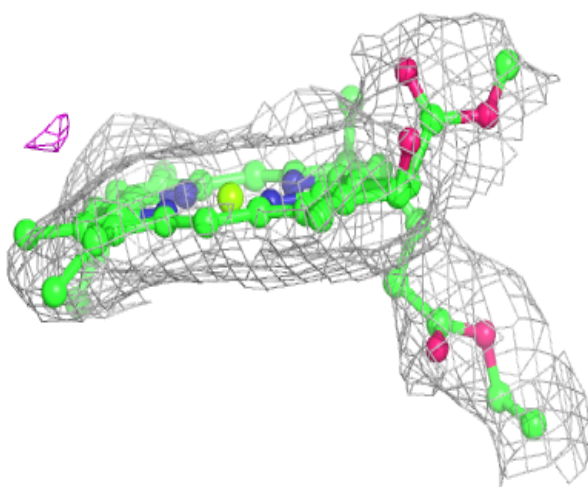
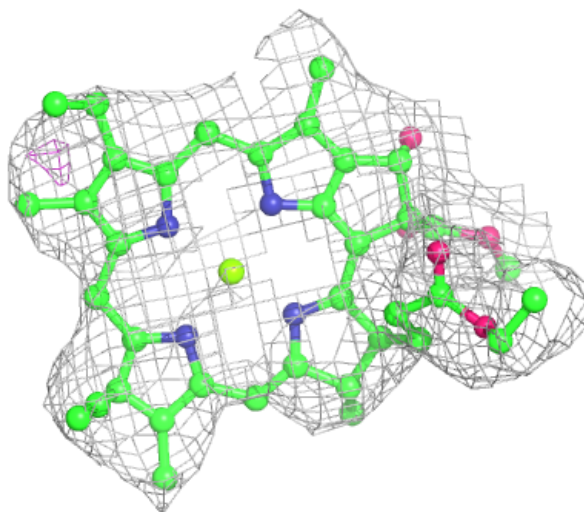
**Electron density around CLA B 1757:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



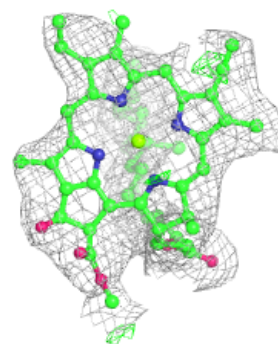
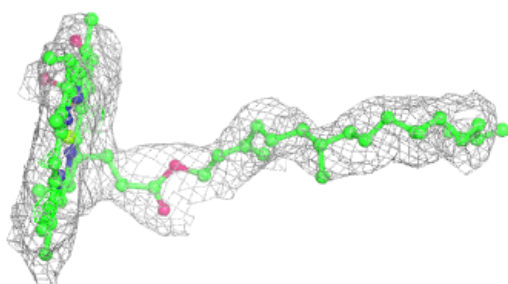
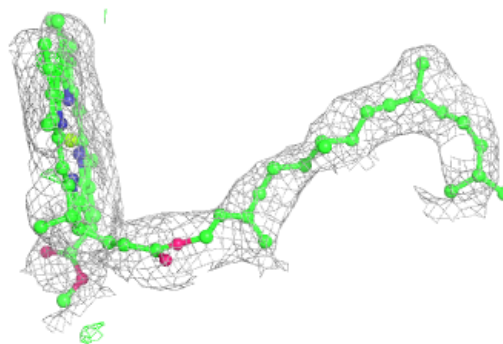
**Electron density around CLA A 1794:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1771:**

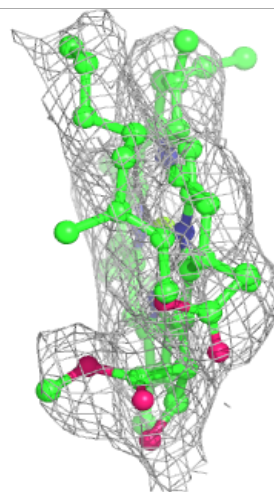
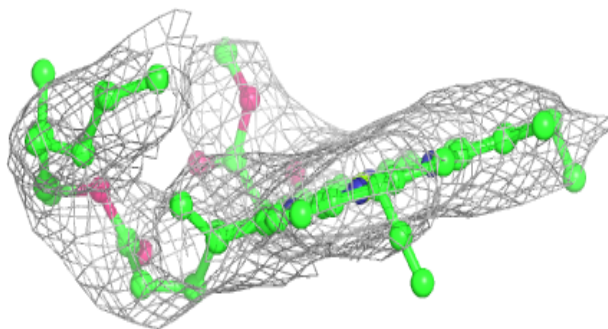
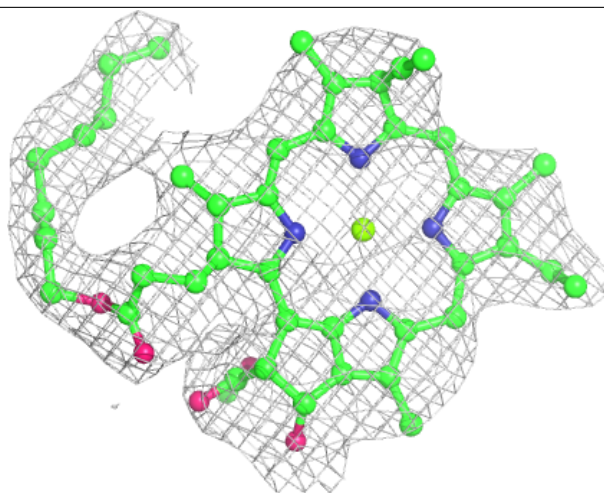
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





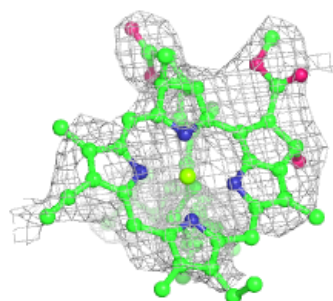
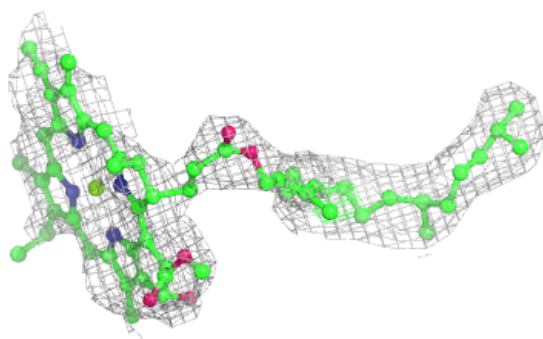
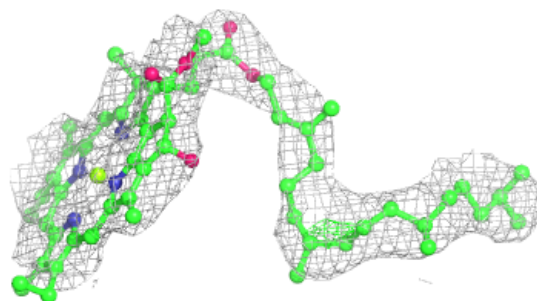
**Electron density around CLA B 1754:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

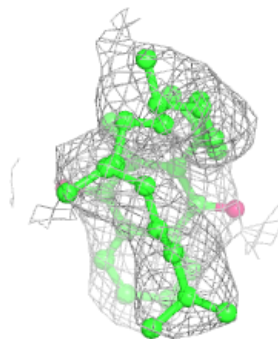
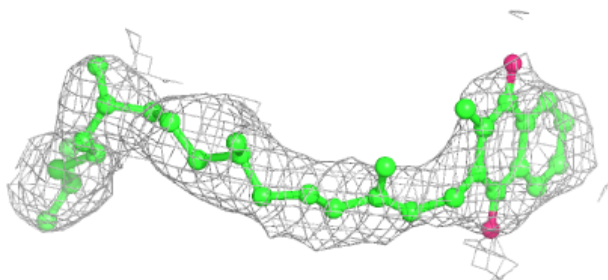
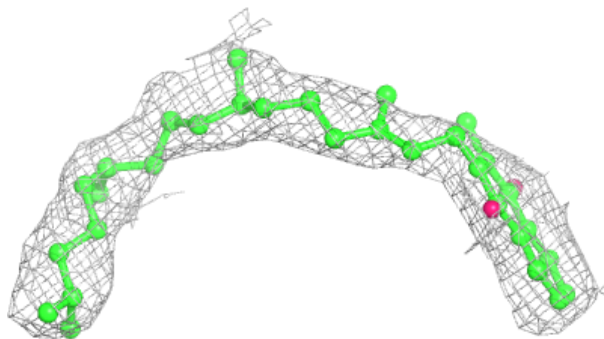


**Electron density around CLA B 1785:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

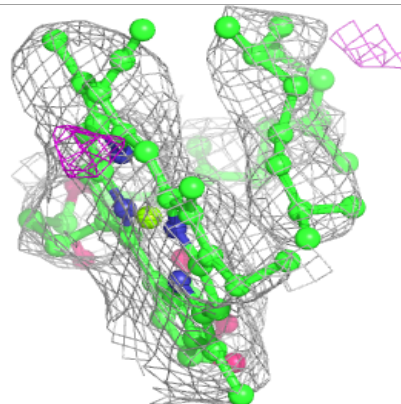
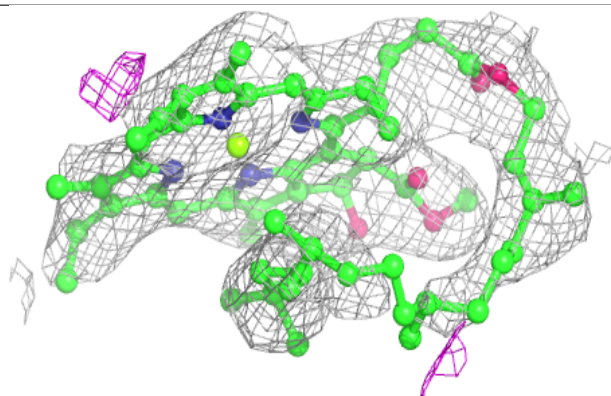
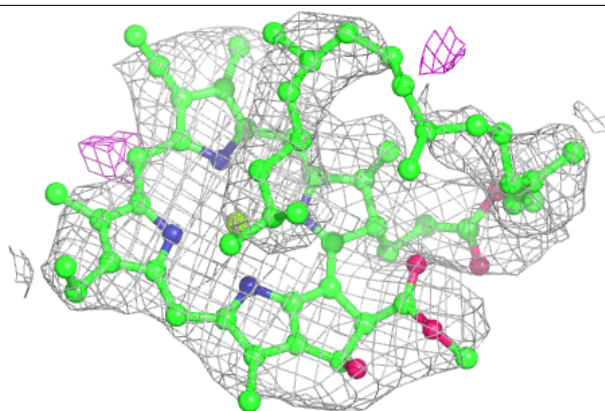
**Electron density around PQN B 1773:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

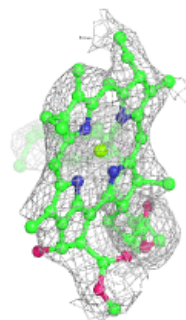
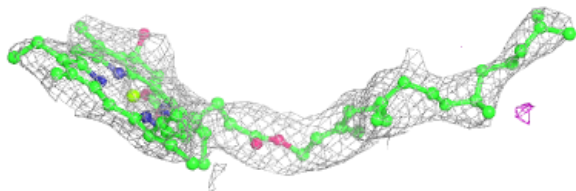
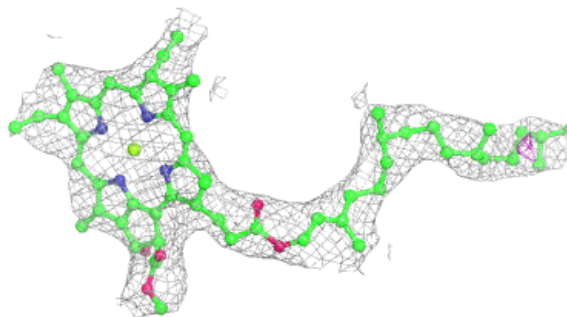


**Electron density around CLA B 1738:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

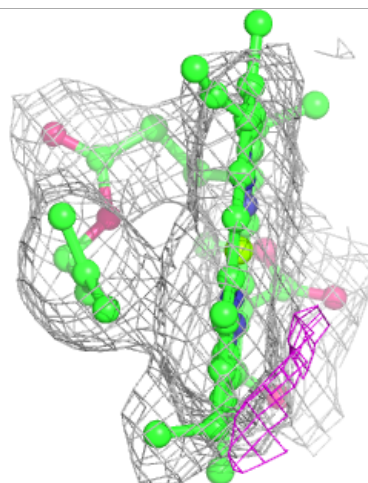
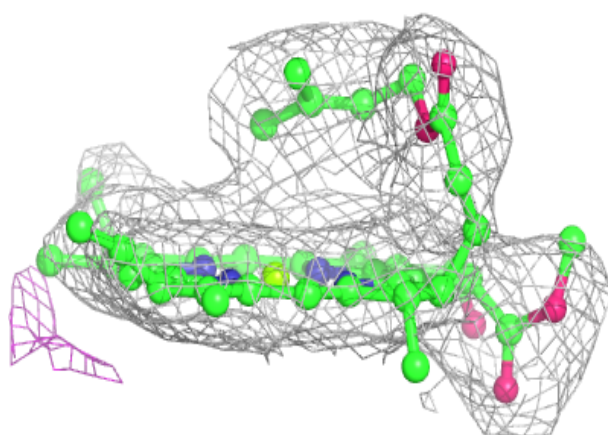
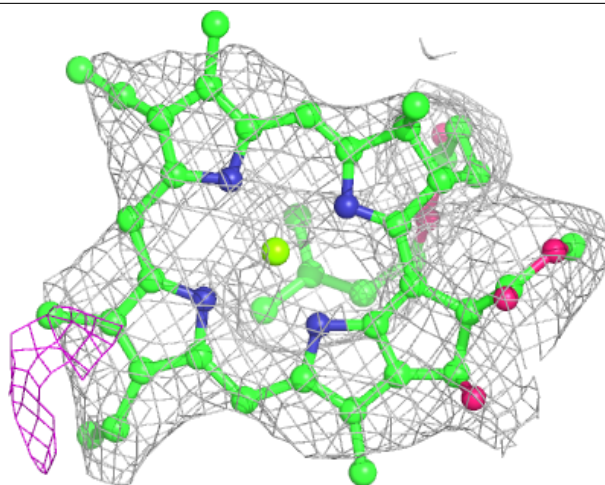
**Electron density around CLA B 1786:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1760:**

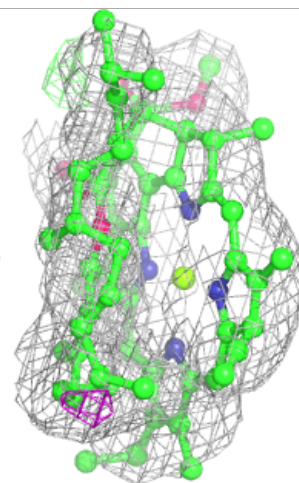
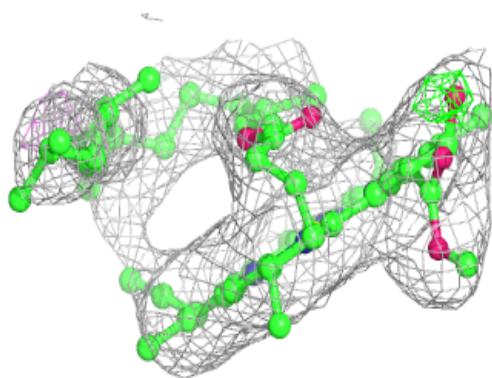
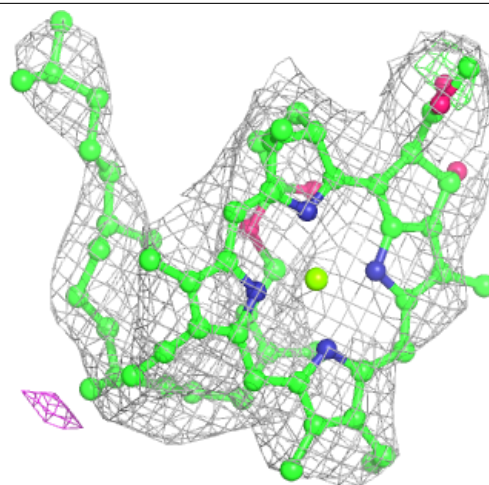
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





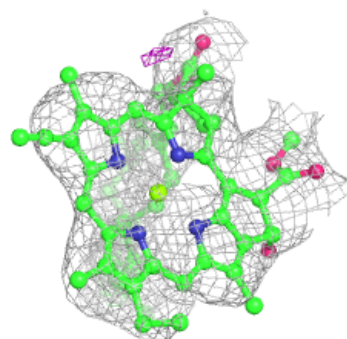
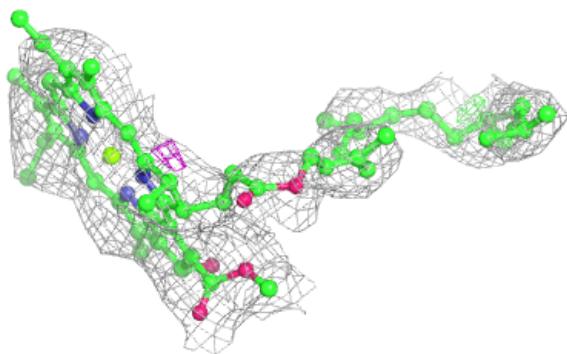
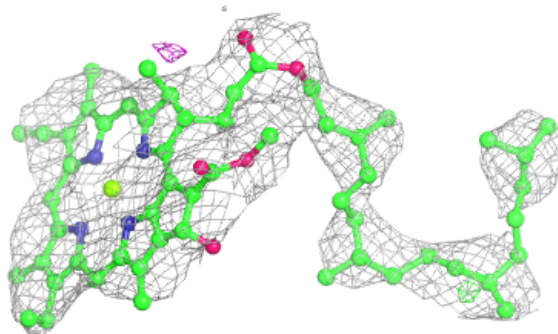
**Electron density around CLA B 1739:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

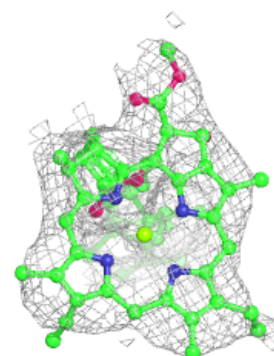
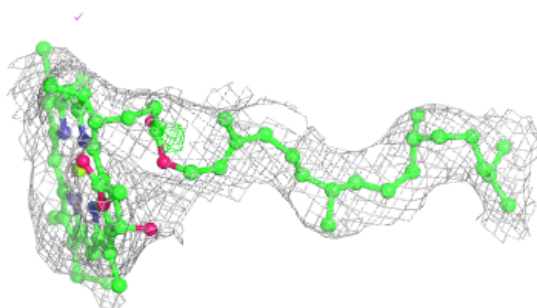
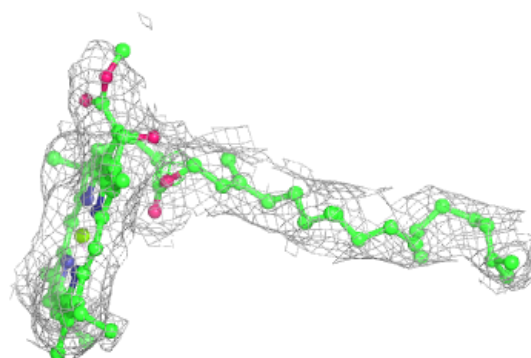


**Electron density around CLA A 1811:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA A 1783:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.