



Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 12:29 PM JST

PDB ID : 9KQQ
EMDB ID : EMD-62512
Title : PSI-LHCI supercomplex binding with 8 Lhcas from *C. subellipsoidea*
Authors : Tsai, P.-C.; Kato, K.; Shen, J.-R.; Akita, F.
Deposited on : 2024-11-26
Resolution : 2.06 Å (reported)
Based on initial model : 6zzx

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

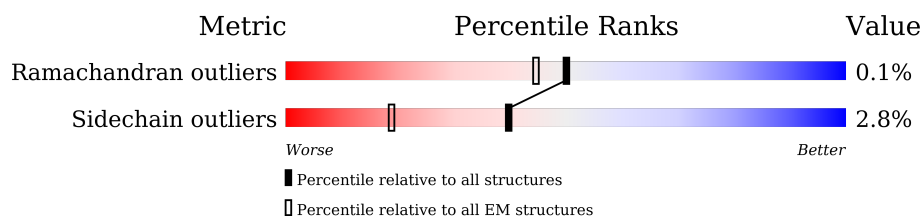
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.06 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.



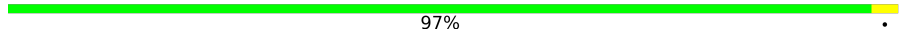







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	98% ..
2	B	734	98% .
3	C	81	99% .
4	D	192	73% . 26%
5	E	71	85% 15%
6	F	245	65% . 33%
7	G	138	7% 14% . 86%
8	I	36	89% . 8%
9	J	41	95% 5%

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Mol	Chain	Length	Quality of chain
10	K	131	
11	M	31	
12	a	229	
12	b	229	
13	3	246	
14	4	246	
15	5	274	
16	6	272	
17	7	259	
18	8	255	
19	L	210	

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
26	CL0	A	815	X	-	-	-
27	CHL	3	308	X	-	-	-
27	CHL	3	309	X	-	-	-
27	CHL	3	310	X	-	-	-
27	CHL	3	311	X	-	-	-
27	CHL	3	312	X	-	-	-
27	CHL	3	313	X	-	-	-
27	CHL	3	314	X	-	-	-
27	CHL	3	315	X	-	-	-
27	CHL	3	316	X	-	-	-
27	CHL	3	317	X	-	-	-
27	CHL	3	318	X	-	-	-
27	CHL	3	319	X	-	-	-
27	CHL	3	320	X	-	-	-
27	CHL	3	321	X	-	-	-
27	CHL	4	304	X	-	-	-
27	CHL	4	305	X	-	-	-
27	CHL	4	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	4	307	X	-	-	-
27	CHL	4	308	X	-	-	-
27	CHL	4	309	X	-	-	-
27	CHL	4	310	X	-	-	-
27	CHL	4	311	X	-	-	-
27	CHL	4	312	X	-	-	-
27	CHL	4	313	X	-	-	-
27	CHL	4	314	X	-	-	-
27	CHL	4	315	X	-	-	-
27	CHL	4	316	X	-	-	-
27	CHL	4	317	X	-	-	-
27	CHL	4	318	X	-	-	-
27	CHL	4	319	X	-	-	-
27	CHL	4	320	X	-	-	-
27	CHL	5	307	X	-	-	-
27	CHL	5	308	X	-	-	-
27	CHL	5	309	X	-	-	-
27	CHL	5	310	X	-	-	-
27	CHL	5	311	X	-	-	-
27	CHL	5	312	X	-	-	-
27	CHL	5	313	X	-	-	-
27	CHL	5	314	X	-	-	-
27	CHL	5	315	X	-	-	-
27	CHL	5	316	X	-	-	-
27	CHL	5	317	X	-	-	-
27	CHL	5	318	X	-	-	-
27	CHL	5	319	X	-	-	-
27	CHL	5	320	X	-	-	-
27	CHL	5	321	X	-	-	-
27	CHL	5	322	X	-	-	-
27	CHL	5	323	X	-	-	-
27	CHL	5	325	X	-	-	-
27	CHL	6	305	X	-	-	-
27	CHL	6	306	X	-	-	-
27	CHL	6	307	X	-	-	-
27	CHL	6	308	X	-	-	-
27	CHL	6	309	X	-	-	-
27	CHL	6	310	X	-	-	-
27	CHL	6	311	X	-	-	-
27	CHL	6	312	X	-	-	-
27	CHL	6	313	X	-	-	-
27	CHL	6	314	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	6	315	X	-	-	-
27	CHL	6	316	X	-	-	-
27	CHL	6	317	X	-	-	-
27	CHL	6	318	X	-	-	-
27	CHL	6	319	X	-	-	-
27	CHL	6	320	X	-	-	-
27	CHL	7	311	X	-	-	-
27	CHL	7	312	X	-	-	-
27	CHL	7	313	X	-	-	-
27	CHL	7	314	X	-	-	-
27	CHL	7	315	X	-	-	-
27	CHL	7	316	X	-	-	-
27	CHL	7	317	X	-	-	-
27	CHL	7	318	X	-	-	-
27	CHL	7	319	X	-	-	-
27	CHL	7	320	X	-	-	-
27	CHL	7	321	X	-	-	-
27	CHL	7	322	X	-	-	-
27	CHL	7	323	X	-	-	-
27	CHL	7	324	X	-	-	-
27	CHL	8	311	X	-	-	-
27	CHL	8	312	X	-	-	-
27	CHL	8	313	X	-	-	-
27	CHL	8	314	X	-	-	-
27	CHL	8	315	X	-	-	-
27	CHL	8	316	X	-	-	-
27	CHL	8	317	X	-	-	-
27	CHL	8	318	X	-	-	-
27	CHL	8	319	X	-	-	-
27	CHL	8	320	X	-	-	-
27	CHL	8	321	X	-	-	-
27	CHL	8	322	X	-	-	-
27	CHL	8	323	X	-	-	-
27	CHL	8	324	X	-	-	-
27	CHL	8	325	X	-	-	-
27	CHL	8	326	X	-	-	-
27	CHL	A	816	X	-	-	-
27	CHL	A	817	X	-	-	-
27	CHL	A	818	X	-	-	-
27	CHL	A	819	X	-	-	-
27	CHL	A	820	X	-	-	-
27	CHL	A	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	A	822	X	-	-	-
27	CHL	A	823	X	-	-	-
27	CHL	A	824	X	-	-	-
27	CHL	A	825	X	-	-	-
27	CHL	A	826	X	-	-	-
27	CHL	A	827	X	-	-	-
27	CHL	A	828	X	-	-	-
27	CHL	A	829	X	-	-	-
27	CHL	A	830	X	-	-	-
27	CHL	A	831	X	-	-	-
27	CHL	A	832	X	-	-	-
27	CHL	A	833	X	-	-	-
27	CHL	A	834	X	-	-	-
27	CHL	A	835	X	-	-	-
27	CHL	A	836	X	-	-	-
27	CHL	A	837	X	-	-	-
27	CHL	A	838	X	-	-	-
27	CHL	A	839	X	-	-	-
27	CHL	A	840	X	-	-	-
27	CHL	A	841	X	-	-	-
27	CHL	A	842	X	-	-	-
27	CHL	A	843	X	-	-	-
27	CHL	A	844	X	-	-	-
27	CHL	A	845	X	-	-	-
27	CHL	A	846	X	-	-	-
27	CHL	A	847	X	-	-	-
27	CHL	A	848	X	-	-	-
27	CHL	A	849	X	-	-	-
27	CHL	A	850	X	-	-	-
27	CHL	A	851	X	-	-	-
27	CHL	A	852	X	-	-	-
27	CHL	A	853	X	-	-	-
27	CHL	A	854	X	-	-	-
27	CHL	A	855	X	-	-	-
27	CHL	A	856	X	-	-	-
27	CHL	A	857	X	-	-	-
27	CHL	A	858	X	-	-	-
27	CHL	A	859	X	-	-	-
27	CHL	B	811	X	-	-	-
27	CHL	B	812	X	-	-	-
27	CHL	B	813	X	-	-	-
27	CHL	B	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	B	815	X	-	-	-
27	CHL	B	816	X	-	-	-
27	CHL	B	817	X	-	-	-
27	CHL	B	818	X	-	-	-
27	CHL	B	819	X	-	-	-
27	CHL	B	820	X	-	-	-
27	CHL	B	821	X	-	-	-
27	CHL	B	822	X	-	-	-
27	CHL	B	823	X	-	-	-
27	CHL	B	824	X	-	-	-
27	CHL	B	825	X	-	-	-
27	CHL	B	826	X	-	-	-
27	CHL	B	827	X	-	-	-
27	CHL	B	828	X	-	-	-
27	CHL	B	829	X	-	-	-
27	CHL	B	830	X	-	-	-
27	CHL	B	831	X	-	-	-
27	CHL	B	832	X	-	-	-
27	CHL	B	833	X	-	-	-
27	CHL	B	834	X	-	-	-
27	CHL	B	835	X	-	-	-
27	CHL	B	836	X	-	-	-
27	CHL	B	837	X	-	-	-
27	CHL	B	838	X	-	-	-
27	CHL	B	839	X	-	-	-
27	CHL	B	840	X	-	-	-
27	CHL	B	841	X	-	-	-
27	CHL	B	842	X	-	-	-
27	CHL	B	843	X	-	-	-
27	CHL	B	844	X	-	-	-
27	CHL	B	845	X	-	-	-
27	CHL	B	846	X	-	-	-
27	CHL	B	847	X	-	-	-
27	CHL	B	848	X	-	-	-
27	CHL	B	849	X	-	-	-
27	CHL	B	850	X	-	-	-
27	CHL	B	851	X	-	-	-
27	CHL	F	308	X	-	-	-
27	CHL	F	309	X	-	-	-
27	CHL	J	106	X	-	-	-
27	CHL	K	204	X	-	-	-
27	CHL	K	205	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CHL	K	206	X	-	-	-
27	CHL	K	207	X	-	-	-
27	CHL	L	303	X	-	-	-
27	CHL	L	304	X	-	-	-
27	CHL	a	307	X	-	-	-
27	CHL	a	308	X	-	-	-
27	CHL	a	309	X	-	-	-
27	CHL	a	310	X	-	-	-
27	CHL	a	311	X	-	-	-
27	CHL	a	312	X	-	-	-
27	CHL	a	313	X	-	-	-
27	CHL	a	314	X	-	-	-
27	CHL	a	315	X	-	-	-
27	CHL	a	316	X	-	-	-
27	CHL	a	317	X	-	-	-
27	CHL	a	318	X	-	-	-
27	CHL	a	319	X	-	-	-
27	CHL	a	320	X	-	-	-
27	CHL	b	304	X	-	-	-
27	CHL	b	305	X	-	-	-
27	CHL	b	306	X	-	-	-
27	CHL	b	307	X	-	-	-
27	CHL	b	308	X	-	-	-
27	CHL	b	309	X	-	-	-
27	CHL	b	310	X	-	-	-
27	CHL	b	311	X	-	-	-
27	CHL	b	312	X	-	-	-
27	CHL	b	313	X	-	-	-
27	CHL	b	314	X	-	-	-
27	CHL	b	315	X	-	-	-
27	CHL	b	316	X	-	-	-
27	CHL	b	317	X	-	-	-
29	LUT	4	301	-	X	-	-
29	LUT	4	302	-	X	-	-
29	LUT	5	303	-	X	-	-
29	LUT	6	303	-	X	-	-
29	LUT	F	303	-	X	-	-
29	LUT	J	103	-	X	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 46812 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5823	3806	994	1005	18		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	3	0
			5832	3829	989	1001	13		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			596	365	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1110	711	193	203	3		

- Molecule 5 is a protein called Photosystem I reaction centre subunit IV/PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	60	Total	C	N	O	S	0	0
			490	316	83	90	1		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1264	805	223	234	2		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	20	Total	C	N	O	0	0
			159	107	23	29		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	33	Total	C	N	O	S	0	0
			248	171	34	41	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	41	Total	C	N	O	S	0	0
			336	232	48	55	1		

- Molecule 10 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	82	Total	C	N	O	S	0	0
			571	365	97	108	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			237	160	35	41	1		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	195	Total	C	N	O	S	0	0
			1458	944	245	267	2		
12	b	192	Total	C	N	O	S	0	0
			1441	933	242	264	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	220	Total	C	N	O	S	0	0
			1707	1117	275	312	3		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	207	Total	C	N	O	S	0	0
			1603	1045	264	290	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	231	Total	C	N	O	S	0	0
			1779	1160	306	309	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	234	Total	C	N	O	S	0	0
			1774	1159	296	311	8		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	7	216	Total	C	N	O	S	0	0
			1650	1070	280	298	2		

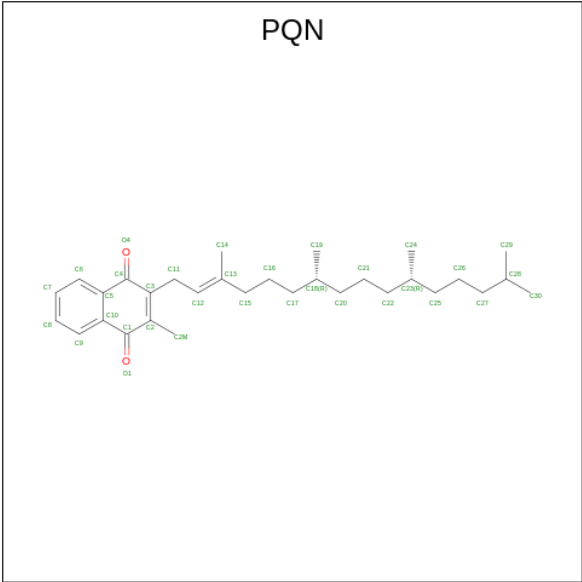
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	8	222	Total	C	N	O	S	0	0
			1701	1112	276	310	3		

- Molecule 19 is a protein called PSI subunit V.

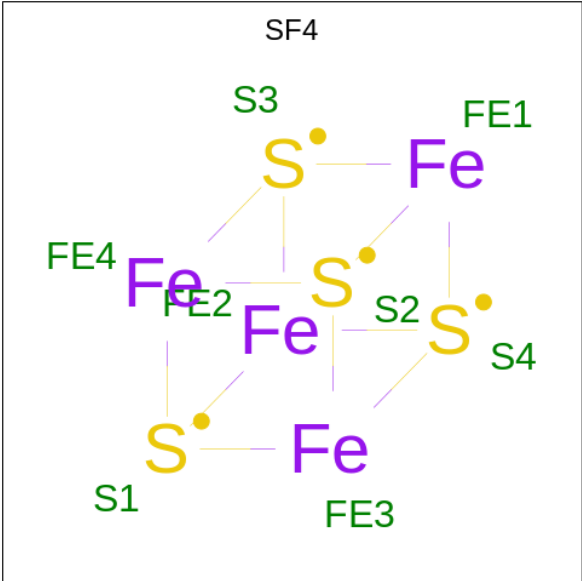
Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	122	Total	C	N	O	S	0	0
			890	585	148	155	2		

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



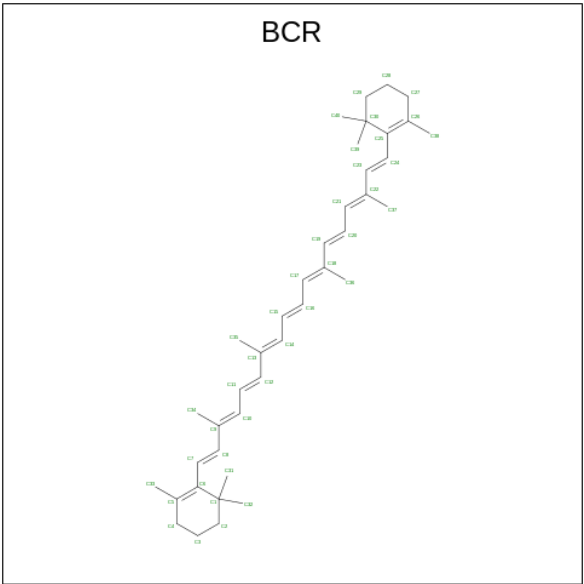
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
21	C	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



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

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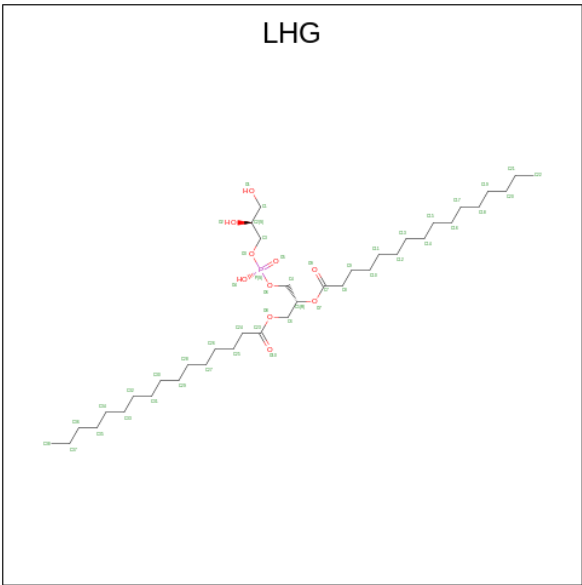
Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	M	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	5	1	Total C 40 40	0
22	6	1	Total C 40 40	0
22	7	1	Total C 40 40	0
22	8	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 40 40	0

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total 35	C 24	O 11	0
23	A	1	Total 35	C 24	O 11	0
23	B	1	Total 35	C 24	O 11	0
23	F	1	Total 29	C 18	O 11	0
23	5	1	Total 30	C 19	O 11	0
23	5	1	Total 35	C 24	O 11	0
23	7	1	Total 35	C 24	O 11	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).

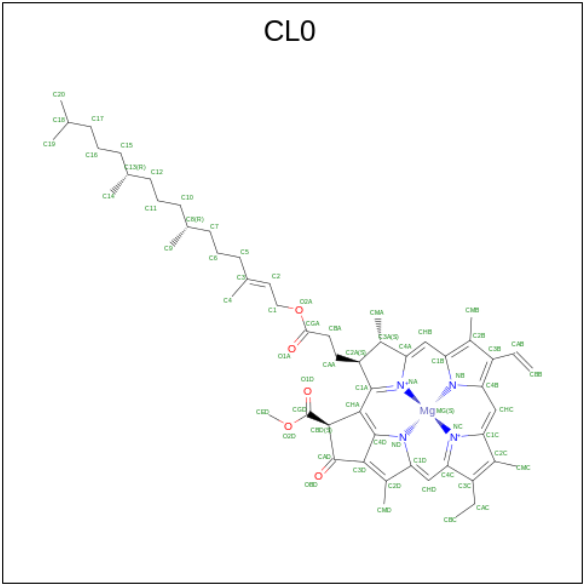


Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			42	31	10	1	
24	A	1	Total	C	O	P	0
			42	31	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	B	1	Total	C	O	P	0
			32	21	10	1	
24	a	1	Total	C	O	P	0
			49	38	10	1	
24	4	1	Total	C	O	P	0
			49	38	10	1	
24	5	1	Total	C	O	P	0
			35	24	10	1	
24	5	1	Total	C	O	P	0
			32	21	10	1	
24	7	1	Total	C	O	P	0
			49	38	10	1	
24	7	1	Total	C	O	P	0
			44	33	10	1	
24	8	1	Total	C	O	P	0
			49	38	10	1	
24	b	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 25 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

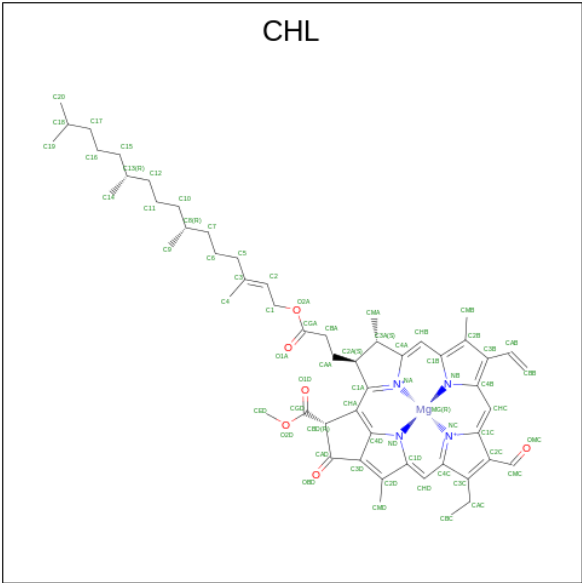
Mol	Chain	Residues	Atoms	AltConf
25	A	3	Total C 43 43	0
25	F	4	Total C 66 66	0
25	J	1	Total C 14 14	0
25	K	1	Total C 18 18	0
25	M	1	Total C 18 18	0
25	a	1	Total C 18 18	0
25	3	2	Total C 32 32	0
25	4	1	Total C 18 18	0
25	6	1	Total C 18 18	0
25	7	3	Total C 43 43	0
25	8	3	Total C 46 46	0

- Molecule 26 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 27 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	K	1	Total 47	C 36	Mg 1	N 4	O 6	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	a	1	Total 61	C 50	Mg 1	N 4	O 6	0
27	a	1	Total 48	C 37	Mg 1	N 4	O 6	0
27	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	a	1	Total 48	C 37	Mg 1	N 4	O 6	0
27	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	3	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
27	3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
27	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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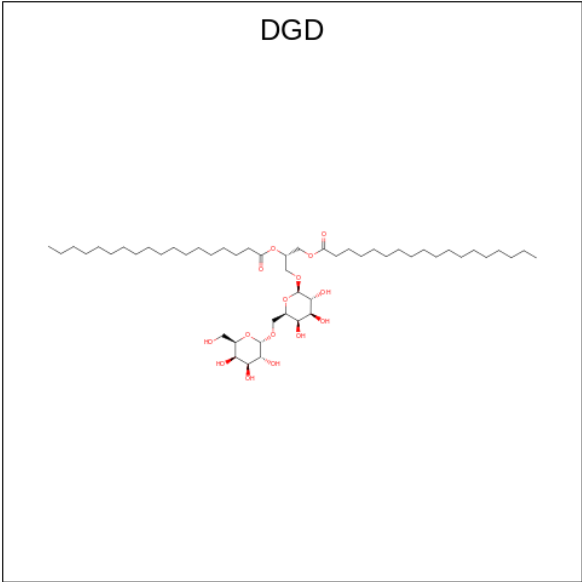
Mol	Chain	Residues	Atoms					AltConf
27	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
27	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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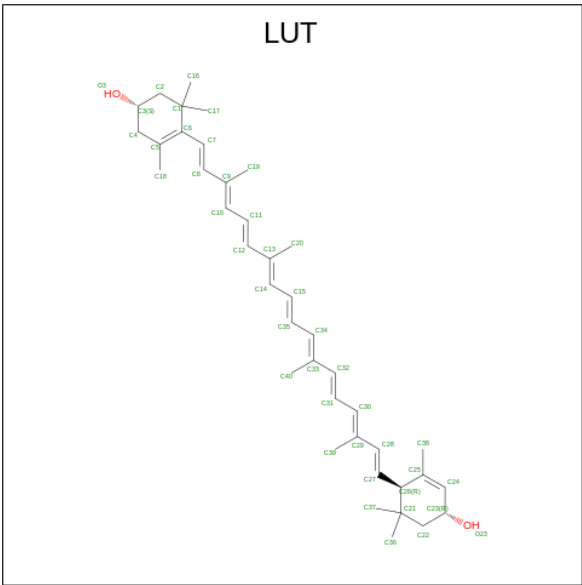
Mol	Chain	Residues	Atoms					AltConf
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	b	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			61	46	15	
28	7	1	Total	C	O	0
			66	51	15	

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



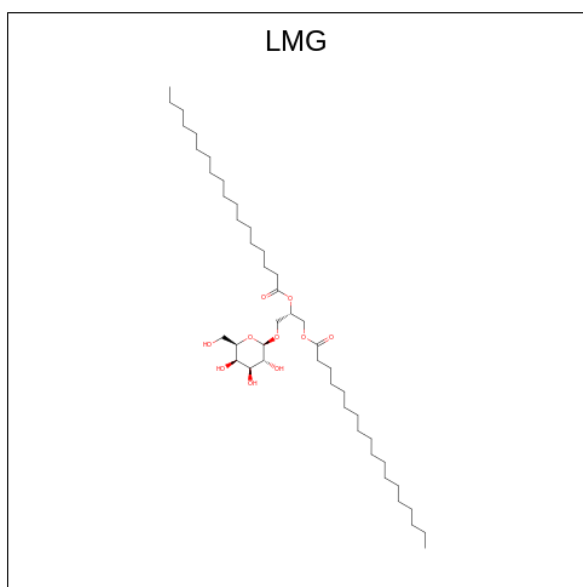
Mol	Chain	Residues	Atoms			AltConf
29	F	1	Total	C	O	0
			42	40	2	

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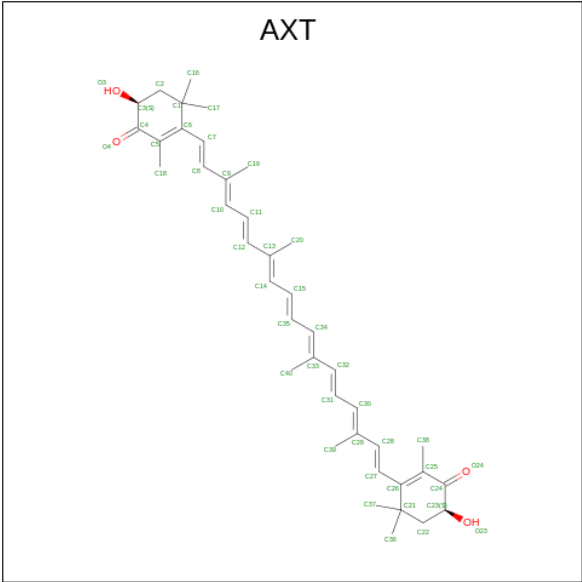
Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



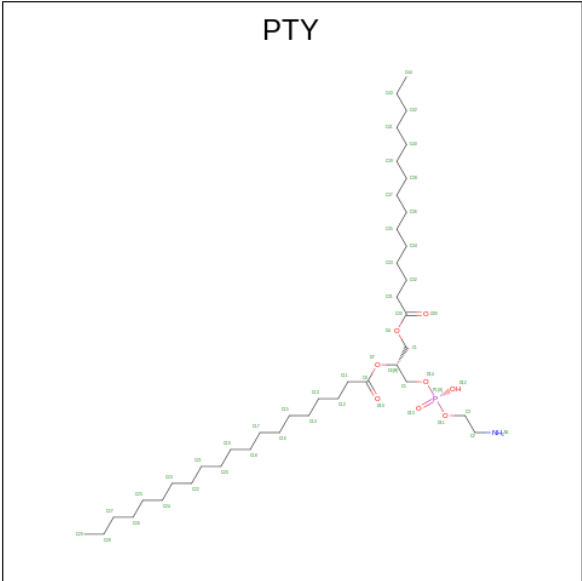
Mol	Chain	Residues	Atoms			AltConf
30	J	1	Total	C	O	0
			49	39	10	
30	J	1	Total	C	O	0
			29	19	10	
30	a	1	Total	C	O	0
			44	34	10	
30	7	1	Total	C	O	0
			41	31	10	
30	8	1	Total	C	O	0
			32	22	10	

- Molecule 31 is ASTAXANTHIN (three-letter code: AXT) (formula: $C_{40}H_{52}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			43	40	3	

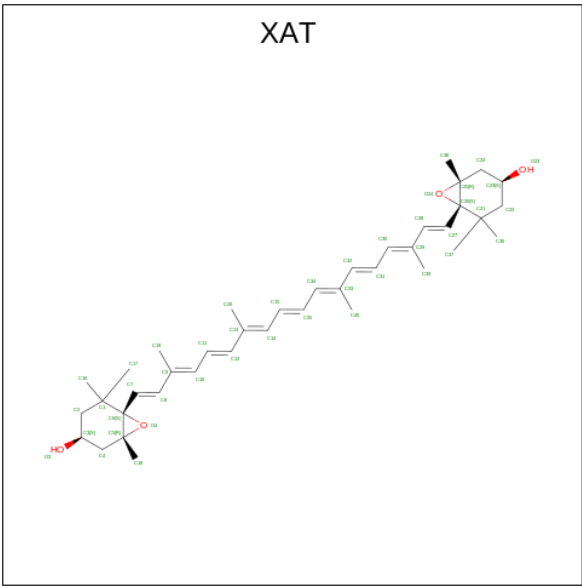
- Molecule 32 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

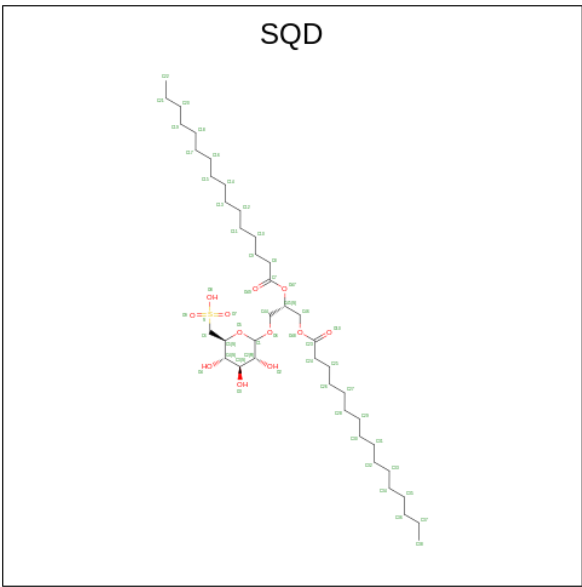
- Molecule 33 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as

"Ligand of Interest" by depositor).



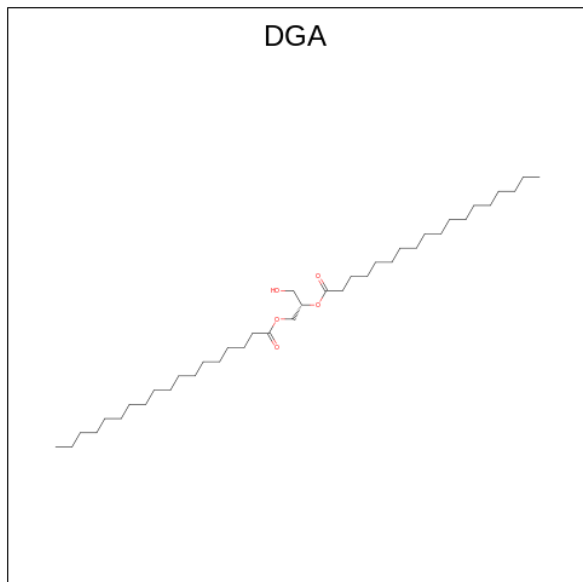
Mol	Chain	Residues	Atoms			AltConf
33	7	1	Total	C	O	0
			44	40	4	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
34	8	1	Total	C	O	S	0
			35	22	12	1	

- Molecule 35 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	8	1	Total	C	O	0
			28	23	5	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	189	Total	O	0
			189	189	
36	B	174	Total	O	0
			174	174	
36	C	37	Total	O	0
			37	37	
36	D	26	Total	O	0
			26	26	
36	E	9	Total	O	0
			9	9	
36	F	30	Total	O	0
			30	30	
36	I	1	Total	O	0
			1	1	
36	J	5	Total	O	0
			5	5	
36	K	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
36	a	13	Total 13	O 13	0
36	3	25	Total 25	O 25	0
36	5	7	Total 7	O 7	0
36	6	2	Total 2	O 2	0
36	7	25	Total 25	O 25	0
36	8	24	Total 24	O 24	0
36	L	1	Total 1	O 1	0

3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:  98% ..



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  98% .



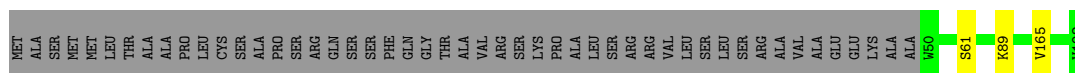
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  99% .




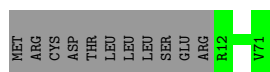
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:  73% . 26%



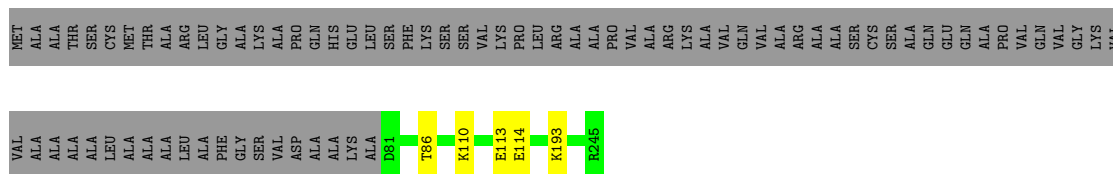
- Molecule 5: Photosystem I reaction centre subunit IV/PsaE

Chain E:  85% 15%



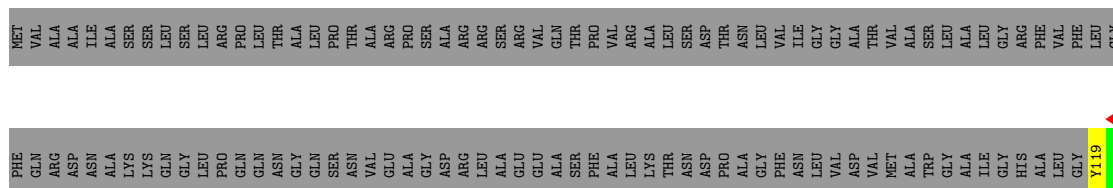
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  65% 33%




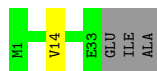
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:  14% 86% 7%



- Molecule 8: Photosystem I reaction center subunit VIII

Chain I:  89% 8%



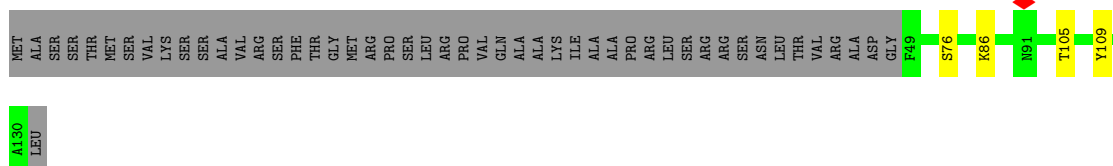
- Molecule 9: Photosystem I reaction center subunit IX

Chain J:  95% 5%



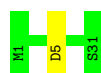
- Molecule 10: PSI-K

Chain K:  60% 37%



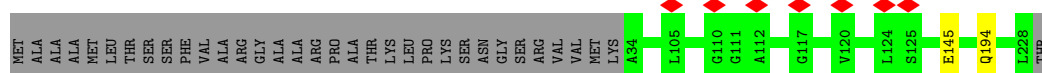
- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  97%



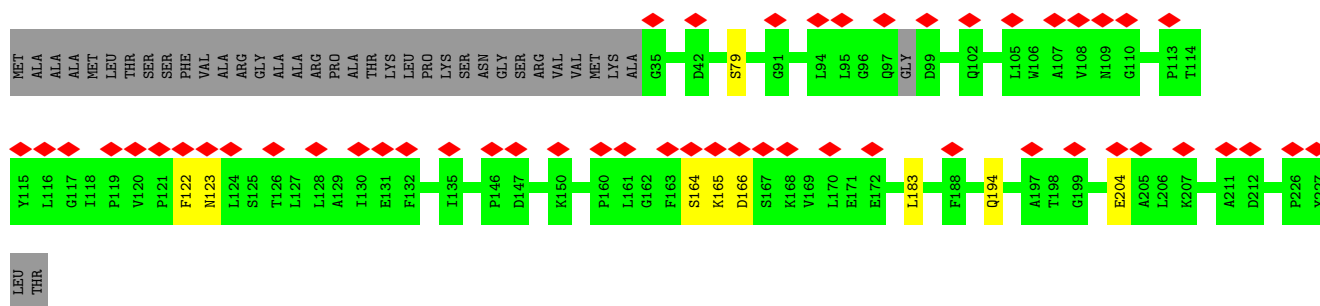
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain a: 84% 15%



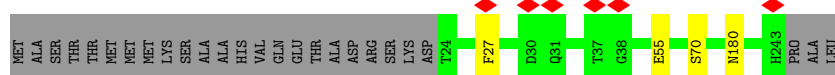
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain b: 23% 80% 16%



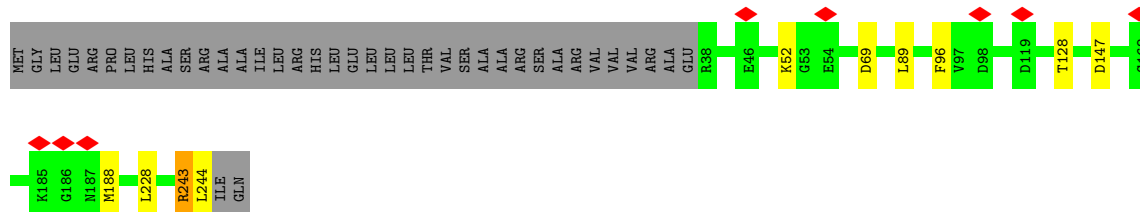
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 88% 11%



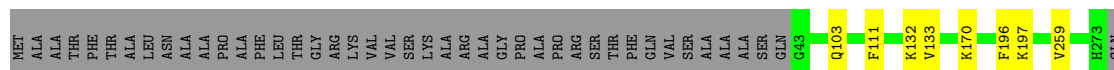
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 80% 16%




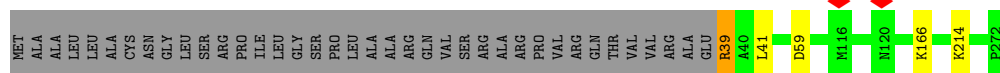
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 81% 16%




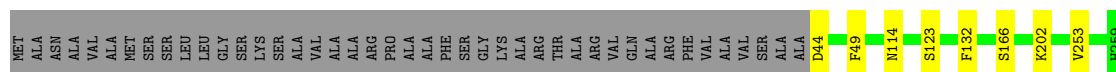
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 6:  84% 14%




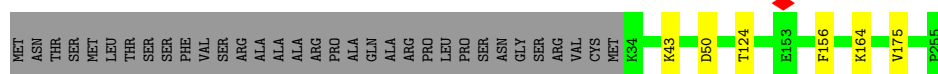
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  80% 17%



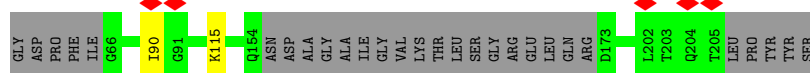
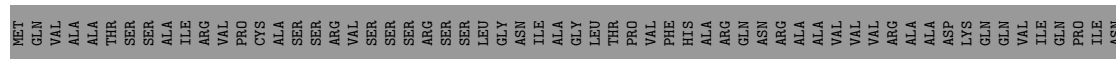
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 8:  85% 13%



- Molecule 19: PSI subunit V

Chain L:  57% 42%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.519	Depositor
Minimum map value	-0.166	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, DGD, BCR, CL0, LMG, LUT, AXT, PQN, SQD, DGA, SF4, XAT, LMT, UNL, PTY, CHL

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	A	0.31	0/6021	0.49	1/8213 (0.0%)
2	B	0.30	0/6041	0.48	0/8247
3	C	0.32	0/606	0.57	0/822
4	D	0.29	0/1136	0.53	0/1537
5	E	0.32	0/502	0.51	0/686
6	F	0.28	0/1288	0.50	0/1737
7	G	0.25	0/165	0.35	0/226
8	I	0.35	0/254	0.58	0/347
9	J	0.29	0/348	0.45	0/476
10	K	0.27	0/580	0.47	0/789
11	M	0.30	0/240	0.54	0/325
12	a	0.28	0/1501	0.47	0/2045
12	b	0.30	0/1483	0.51	1/2019 (0.0%)
13	3	0.31	0/1759	0.47	0/2394
14	4	0.30	0/1653	0.50	1/2250 (0.0%)
15	5	0.29	0/1834	0.49	0/2496
16	6	0.29	0/1832	0.48	1/2501 (0.0%)
17	7	0.29	0/1702	0.45	0/2323
18	8	0.30	0/1752	0.45	0/2379
19	L	0.27	0/912	0.45	0/1247
All	All	0.30	0/31609	0.48	4/43059 (0.0%)

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
14	4	0	1
16	6	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	147	ASP	CB-CG-OD1	6.54	124.19	118.30
16	6	59	ASP	CB-CG-OD1	6.31	123.97	118.30
1	A	157	LEU	CA-CB-CG	5.87	128.79	115.30
12	b	183	LEU	CA-CB-CG	5.33	127.57	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	4	243	ARG	Sidechain
16	6	39	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A	739/751 (98%)	720 (97%)	19 (3%)	0	100	100
2	B	732/734 (100%)	719 (98%)	13 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/192 (73%)	138 (98%)	3 (2%)	0	100	100
5	E	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
6	F	163/245 (66%)	161 (99%)	2 (1%)	0	100	100
7	G	18/138 (13%)	17 (94%)	1 (6%)	0	100	100
8	I	31/36 (86%)	31 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
10	K	80/131 (61%)	80 (100%)	0	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
12	a	193/229 (84%)	188 (97%)	5 (3%)	0	100	100
12	b	188/229 (82%)	177 (94%)	9 (5%)	2 (1%)	12	4
13	3	218/246 (89%)	214 (98%)	4 (2%)	0	100	100
14	4	205/246 (83%)	198 (97%)	7 (3%)	0	100	100
15	5	229/274 (84%)	219 (96%)	10 (4%)	0	100	100
16	6	232/272 (85%)	227 (98%)	5 (2%)	0	100	100
17	7	214/259 (83%)	209 (98%)	5 (2%)	0	100	100
18	8	220/255 (86%)	217 (99%)	3 (1%)	0	100	100
19	L	118/210 (56%)	116 (98%)	2 (2%)	0	100	100
All	All	3925/4671 (84%)	3831 (98%)	92 (2%)	2 (0%)	50	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	b	165	LYS
12	b	164	SER

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 PDB entries followed by that with respect to all EM entries.

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	A	604/613 (98%)	597 (99%)	7 (1%)	67	68
2	B	594/593 (100%)	578 (97%)	16 (3%)	40	35
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	118/156 (76%)	115 (98%)	3 (2%)	42	38
5	E	56/67 (84%)	56 (100%)	0	100	100
6	F	131/183 (72%)	126 (96%)	5 (4%)	28	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	18/106 (17%)	17 (94%)	1 (6%)	17	10
8	I	26/28 (93%)	25 (96%)	1 (4%)	28	22
9	J	37/37 (100%)	35 (95%)	2 (5%)	18	11
10	K	60/100 (60%)	56 (93%)	4 (7%)	13	7
11	M	26/26 (100%)	25 (96%)	1 (4%)	28	22
12	a	141/166 (85%)	139 (99%)	2 (1%)	62	62
12	b	140/166 (84%)	134 (96%)	6 (4%)	25	18
13	3	176/197 (89%)	172 (98%)	4 (2%)	45	41
14	4	164/195 (84%)	155 (94%)	9 (6%)	18	11
15	5	179/208 (86%)	171 (96%)	8 (4%)	23	17
16	6	183/212 (86%)	179 (98%)	4 (2%)	47	43
17	7	168/195 (86%)	160 (95%)	8 (5%)	21	15
18	8	175/202 (87%)	169 (97%)	6 (3%)	32	26
19	L	91/161 (56%)	89 (98%)	2 (2%)	47	43
All	All	3155/3680 (86%)	3066 (97%)	89 (3%)	40	34

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	60	ASP
1	A	247	ARG
1	A	278	PHE
1	A	360	PHE
1	A	372	TYR
1	A	524	MET
2	B	7	LYS
2	B	14	LYS
2	B	186	SER
2	B	257	PHE
2	B	292	ARG
2	B	294	ASN
2	B	302	GLN
2	B	309	THR
2	B	394	PHE
2	B	402	GLN
2	B	475	ASP

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Mol	Chain	Res	Type
2	B	481	SER
2	B	577	TYR
2	B	607	ASN
2	B	644	SER
2	B	692	ARG
4	D	61	SER
4	D	89	LYS
4	D	165	VAL
6	F	86	THR
6	F	110	LYS
6	F	113	GLU
6	F	114	GLU
6	F	193	LYS
7	G	119	TYR
8	I	14	VAL
9	J	1	MET
9	J	40	SER
10	K	76	SER
10	K	86	LYS
10	K	105	THR
10	K	109	TYR
11	M	5	ASP
12	a	145	GLU
12	a	194	GLN
13	3	27	PHE
13	3	55	GLU
13	3	70	SER
13	3	180	ASN
14	4	52	LYS
14	4	69	ASP
14	4	89	LEU
14	4	96	PHE
14	4	128	THR
14	4	188	MET
14	4	228	LEU
14	4	243	ARG
14	4	244	LEU
15	5	103	GLN
15	5	111	PHE
15	5	132	LYS
15	5	133	VAL
15	5	170	LYS

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Mol	Chain	Res	Type
15	5	196	PHE
15	5	197	LYS
15	5	259	VAL
16	6	39	ARG
16	6	41	LEU
16	6	166	LYS
16	6	214	LYS
17	7	44	ASP
17	7	49	PHE
17	7	114	ASN
17	7	123	SER
17	7	132	PHE
17	7	166	SER
17	7	202	LYS
17	7	253	VAL
18	8	43	LYS
18	8	50	ASP
18	8	124	THR
18	8	156	PHE
18	8	164	LYS
18	8	175	VAL
19	L	90	ILE
19	L	115	LYS
12	b	79	SER
12	b	122	PHE
12	b	123	ASN
12	b	166	ASP
12	b	194	GLN
12	b	204	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	HIS
1	A	659	GLN
2	B	34	HIS
2	B	64	ASN
2	B	98	GLN
2	B	229	ASN
2	B	504	ASN
3	C	38	GLN
6	F	111	GLN

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Mol	Chain	Res	Type
13	3	68	GLN
13	3	180	ASN
14	4	102	HIS
14	4	156	GLN
15	5	172	ASN
15	5	260	GLN
16	6	242	GLN
17	7	46	GLN
17	7	114	ASN
17	7	127	GLN
17	7	131	ASN
18	8	74	GLN
18	8	222	ASN
18	8	245	GLN
19	L	84	ASN
19	L	176	GLN
12	b	67	ASN
12	b	69	GLN
12	b	72	GLN
12	b	173	ASN
12	b	194	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 318 ligands modelled in this entry, 21 are unknown - leaving 297 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
27	CHL	5	315	15	65,73,74	2.59	19 (29%)	76,113,114	4.35	24 (31%)
29	LUT	3	304	-	42,43,43	5.53	19 (45%)	51,60,60	5.58	32 (62%)
27	CHL	4	309	-	47,55,74	2.54	15 (31%)	50,91,114	2.09	17 (34%)
27	CHL	6	310	16	55,63,74	2.85	21 (38%)	64,101,114	2.34	23 (35%)
27	CHL	7	316	36	54,62,74	2.62	18 (33%)	63,100,114	2.30	23 (36%)
27	CHL	A	851	1	46,54,74	2.78	19 (41%)	53,90,114	2.55	20 (37%)
29	LUT	7	304	-	42,43,43	5.54	21 (50%)	51,60,60	5.78	29 (56%)
29	LUT	4	302	-	42,43,43	5.62	19 (45%)	51,60,60	5.60	31 (60%)
27	CHL	B	822	2	65,73,74	2.59	18 (27%)	76,113,114	2.14	21 (27%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-
22	BCR	3	301	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
27	CHL	8	321	36	66,74,74	2.11	15 (22%)	73,114,114	2.03	21 (28%)
27	CHL	a	318	36	48,56,74	2.69	17 (35%)	51,92,114	2.24	19 (37%)
22	BCR	K	203	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	6 (10%)
27	CHL	A	841	36	56,64,74	2.07	15 (26%)	61,102,114	2.42	23 (37%)
21	SF4	A	802	1,2	0,12,12	-	-	-	-	-
27	CHL	a	307	12	60,68,74	2.76	19 (31%)	70,107,114	2.21	23 (32%)
27	CHL	6	318	-	47,55,74	2.77	14 (29%)	50,91,114	2.21	17 (34%)
27	CHL	A	834	1	65,73,74	2.35	19 (29%)	76,113,114	2.07	23 (30%)
27	CHL	B	836	2	65,73,74	2.56	18 (27%)	76,113,114	2.04	20 (26%)
27	CHL	B	850	2	50,58,74	3.05	20 (40%)	58,95,114	2.54	25 (43%)
22	BCR	A	807	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
27	CHL	5	318	15	65,73,74	2.65	18 (27%)	76,113,114	2.17	24 (31%)
27	CHL	A	838	1	60,68,74	2.74	18 (30%)	70,107,114	2.22	23 (32%)
27	CHL	5	320	15	46,54,74	2.86	20 (43%)	53,90,114	2.44	21 (39%)
27	CHL	A	846	-	50,58,74	2.22	12 (24%)	58,95,114	4.33	29 (50%)
29	LUT	8	304	-	42,43,43	5.52	19 (45%)	51,60,60	5.83	33 (64%)
27	CHL	4	307	14	60,68,74	2.50	19 (31%)	70,107,114	2.24	23 (32%)
27	CHL	A	825	1	65,73,74	2.73	19 (29%)	76,113,114	2.21	24 (31%)
27	CHL	A	823	1	65,73,74	2.27	17 (26%)	76,113,114	2.21	24 (31%)
27	CHL	A	837	1	55,63,74	2.73	19 (34%)	64,101,114	2.41	22 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LHG	b	302	27	34,34,48	0.74	1 (2%)	37,40,54	1.28	4 (10%)
27	CHL	A	839	1	65,73,74	2.46	18 (27%)	76,113,114	2.15	23 (30%)
23	LMT	7	308	-	36,36,36	1.19	6 (16%)	47,47,47	0.89	0
27	CHL	B	831	2	46,54,74	2.79	19 (41%)	53,90,114	2.43	22 (41%)
22	BCR	I	801	-	41,41,41	1.11	2 (4%)	56,56,56	1.15	4 (7%)
27	CHL	A	816	36	65,73,74	2.38	18 (27%)	76,113,114	2.21	22 (28%)
23	LMT	5	326	-	36,36,36	1.23	6 (16%)	47,47,47	0.94	2 (4%)
27	CHL	B	851	2	62,70,74	2.64	20 (32%)	72,109,114	2.17	24 (33%)
27	CHL	3	315	13	52,60,74	2.54	18 (34%)	60,97,114	2.39	22 (36%)
20	PQN	B	801	-	34,34,34	0.47	0	42,45,45	0.73	1 (2%)
27	CHL	8	323	-	50,58,74	3.27	21 (42%)	58,95,114	2.79	23 (39%)
27	CHL	B	819	2	65,73,74	2.53	19 (29%)	76,113,114	2.21	22 (28%)
22	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	5 (8%)
27	CHL	3	320	13	61,69,74	2.28	18 (29%)	71,108,114	2.25	26 (36%)
22	BCR	3	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	5 (8%)
27	CHL	B	846	36	65,73,74	2.30	18 (27%)	76,113,114	2.17	23 (30%)
32	PTY	5	305	-	30,30,49	0.56	0	33,35,54	0.55	1 (3%)
27	CHL	B	834	2	65,73,74	3.02	18 (27%)	76,113,114	2.27	25 (32%)
27	CHL	4	316	-	46,54,74	2.85	15 (32%)	49,90,114	2.16	18 (36%)
27	CHL	B	820	2	65,73,74	2.61	19 (29%)	76,113,114	2.14	23 (30%)
27	CHL	8	326	18	46,54,74	3.06	17 (36%)	53,90,114	2.60	22 (41%)
27	CHL	A	843	1	65,73,74	1.95	12 (18%)	76,113,114	4.66	36 (47%)
27	CHL	A	828	1	65,73,74	2.52	19 (29%)	76,113,114	2.14	22 (28%)
27	CHL	A	819	1	55,63,74	2.68	19 (34%)	64,101,114	2.35	20 (31%)
27	CHL	4	317	14	45,53,74	2.77	18 (40%)	52,89,114	3.00	18 (34%)
22	BCR	L	302	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	4 (7%)
24	LHG	a	305	27	48,48,48	0.28	0	51,54,54	0.30	0
24	LHG	4	303	27	48,48,48	0.27	0	51,54,54	0.37	0
27	CHL	B	848	2	65,73,74	2.69	19 (29%)	76,113,114	2.16	21 (27%)
27	CHL	8	320	18	52,60,74	2.86	19 (36%)	60,97,114	2.43	23 (38%)
24	LHG	A	811	27	41,41,48	0.69	2 (4%)	44,47,54	1.18	4 (9%)
27	CHL	B	847	36	65,73,74	2.90	19 (29%)	76,113,114	2.19	23 (30%)
27	CHL	b	307	12	55,63,74	2.57	18 (32%)	64,101,114	2.25	24 (37%)
24	LHG	7	306	27	43,43,48	0.70	1 (2%)	46,49,54	1.22	4 (8%)
30	LMG	J	104	-	29,29,55	0.99	1 (3%)	37,37,63	1.21	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	B	813	2	55,63,74	2.76	20 (36%)	64,101,114	2.43	21 (32%)
35	DGA	8	306	-	27,27,43	0.22	0	29,29,45	0.17	0
27	CHL	3	308	13	65,73,74	2.88	18 (27%)	76,113,114	2.26	25 (32%)
27	CHL	L	304	-	45,53,74	2.88	19 (42%)	52,89,114	2.47	19 (36%)
27	CHL	b	306	12	46,54,74	4.26	18 (39%)	53,90,114	2.38	22 (41%)
27	CHL	5	313	-	57,65,74	2.10	12 (21%)	66,103,114	4.36	34 (51%)
27	CHL	5	325	16	47,55,74	2.21	16 (34%)	50,91,114	2.21	20 (40%)
27	CHL	a	312	36	50,58,74	3.31	18 (36%)	58,95,114	2.43	22 (37%)
27	CHL	7	320	36,28	47,55,74	2.10	14 (29%)	50,91,114	2.41	19 (38%)
27	CHL	5	323	15	56,64,74	3.20	17 (30%)	65,102,114	2.43	23 (35%)
27	CHL	B	817	2	65,73,74	2.39	18 (27%)	76,113,114	2.29	22 (28%)
27	CHL	A	835	1	47,55,74	3.12	19 (40%)	54,91,114	2.51	21 (38%)
27	CHL	B	842	2	65,73,74	2.78	18 (27%)	76,113,114	2.24	23 (30%)
27	CHL	4	314	-	45,53,74	2.96	20 (44%)	52,89,114	2.47	21 (40%)
27	CHL	B	840	2	65,73,74	2.63	17 (26%)	76,113,114	2.18	23 (30%)
27	CHL	B	833	36	55,63,74	2.62	19 (34%)	64,101,114	2.26	22 (34%)
23	LMT	A	808	-	36,36,36	1.24	6 (16%)	47,47,47	1.05	2 (4%)
30	LMG	J	101	-	49,49,55	0.81	1 (2%)	57,57,63	1.26	3 (5%)
27	CHL	A	858	1	65,73,74	2.60	19 (29%)	76,113,114	2.23	25 (32%)
27	CHL	b	313	12	46,54,74	3.66	19 (41%)	53,90,114	2.48	20 (37%)
27	CHL	B	843	36	45,53,74	3.13	17 (37%)	52,89,114	2.52	18 (34%)
27	CHL	b	314	12	46,54,74	3.00	19 (41%)	53,90,114	2.40	21 (39%)
27	CHL	A	856	36	65,73,74	2.35	18 (27%)	76,113,114	2.22	25 (32%)
27	CHL	7	321	17	47,55,74	2.53	15 (31%)	50,91,114	2.53	18 (36%)
27	CHL	A	855	1	65,73,74	2.48	19 (29%)	76,113,114	2.18	24 (31%)
27	CHL	3	321	13	45,53,74	3.25	19 (42%)	52,89,114	2.50	18 (34%)
27	CHL	5	311	15	46,54,74	3.04	19 (41%)	53,90,114	2.59	24 (45%)
27	CHL	b	305	-	46,54,74	3.39	19 (41%)	53,90,114	2.52	20 (37%)
23	LMT	5	306	-	31,31,36	1.28	5 (16%)	42,42,47	0.96	3 (7%)
27	CHL	7	319	17	66,74,74	1.77	15 (22%)	73,114,114	2.08	23 (31%)
27	CHL	B	811	2	65,73,74	2.50	18 (27%)	76,113,114	2.26	23 (30%)
27	CHL	6	305	16	46,54,74	2.74	19 (41%)	53,90,114	2.40	19 (35%)
27	CHL	8	324	36	45,53,74	2.40	16 (35%)	46,88,114	2.36	19 (41%)
27	CHL	b	316	-	48,56,74	2.60	16 (33%)	51,92,114	2.17	19 (37%)
27	CHL	7	317	24	65,73,74	2.44	19 (29%)	76,113,114	2.18	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	8	313	18	50,58,74	3.08	19 (38%)	58,95,114	2.46	22 (37%)
27	CHL	A	857	24	46,54,74	2.89	17 (36%)	53,90,114	2.56	22 (41%)
27	CHL	A	852	1	51,59,74	3.23	17 (33%)	59,96,114	2.64	25 (42%)
27	CHL	4	320	14	50,58,74	2.89	20 (40%)	58,95,114	2.43	25 (43%)
27	CHL	A	832	1	60,68,74	2.83	19 (31%)	70,107,114	2.38	24 (34%)
22	BCR	B	805	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	4 (7%)
27	CHL	A	826	1	62,70,74	2.81	18 (29%)	72,109,114	2.21	22 (30%)
27	CHL	a	313	24	55,63,74	2.57	19 (34%)	64,101,114	2.33	24 (37%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
27	CHL	B	814	2	65,73,74	2.46	19 (29%)	76,113,114	2.18	23 (30%)
22	BCR	B	802	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	7 (12%)
27	CHL	6	313	16	47,55,74	3.65	19 (40%)	54,91,114	2.50	21 (38%)
27	CHL	b	312	-	46,54,74	3.10	18 (39%)	53,90,114	2.43	22 (41%)
27	CHL	3	313	36	65,73,74	2.50	19 (29%)	76,113,114	2.13	23 (30%)
27	CHL	5	321	15	46,54,74	3.09	18 (39%)	53,90,114	2.47	21 (39%)
27	CHL	5	314	15	45,53,74	3.29	18 (40%)	52,89,114	2.43	18 (34%)
27	CHL	3	309	13	46,54,74	3.22	19 (41%)	53,90,114	2.52	19 (35%)
22	BCR	B	804	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	3 (5%)
22	BCR	7	303	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	5 (8%)
27	CHL	A	859	36	65,73,74	2.72	17 (26%)	76,113,114	2.20	25 (32%)
27	CHL	B	832	36	65,73,74	2.36	18 (27%)	76,113,114	2.23	26 (34%)
27	CHL	a	316	36	48,56,74	2.47	15 (31%)	51,92,114	2.20	20 (39%)
27	CHL	5	319	-	47,55,74	2.83	16 (34%)	50,91,114	2.16	19 (38%)
27	CHL	8	314	18	66,74,74	1.91	14 (21%)	73,114,114	1.97	24 (32%)
33	XAT	7	305	-	39,47,47	1.64	8 (20%)	54,74,74	1.61	10 (18%)
27	CHL	4	319	14	45,53,74	3.07	19 (42%)	52,89,114	2.60	17 (32%)
27	CHL	6	316	36	46,54,74	2.91	16 (34%)	49,90,114	2.31	18 (36%)
27	CHL	B	844	2	65,73,74	2.40	18 (27%)	76,113,114	2.12	23 (30%)
29	LUT	6	303	-	42,43,43	5.58	20 (47%)	51,60,60	5.63	32 (62%)
28	DGD	7	307	27	67,67,67	0.91	2 (2%)	81,81,81	1.38	10 (12%)
29	LUT	3	305	-	42,43,43	5.47	19 (45%)	51,60,60	5.84	33 (64%)
27	CHL	A	847	1	56,64,74	2.85	18 (32%)	65,102,114	2.30	23 (35%)
23	LMT	A	809	-	36,36,36	1.21	5 (13%)	47,47,47	0.93	1 (2%)
27	CHL	4	308	14	60,68,74	2.80	19 (31%)	70,107,114	2.23	23 (32%)
27	CHL	6	307	-	65,73,74	1.99	14 (21%)	76,113,114	4.03	33 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	AXT	a	303	-	44,44,45	0.70	1 (2%)	55,62,64	0.99	1 (1%)
27	CHL	8	316	18	65,73,74	2.53	19 (29%)	76,113,114	2.13	24 (31%)
27	CHL	B	849	24	65,73,74	2.42	19 (29%)	76,113,114	2.10	21 (27%)
22	BCR	5	301	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	4 (7%)
27	CHL	3	319	13	55,63,74	2.98	18 (32%)	64,101,114	2.30	21 (32%)
27	CHL	6	314	24	46,54,74	3.24	19 (41%)	53,90,114	2.50	19 (35%)
27	CHL	3	311	13	60,68,74	2.50	17 (28%)	70,107,114	2.28	23 (32%)
27	CHL	F	309	36	50,58,74	2.78	19 (38%)	58,95,114	2.45	22 (37%)
27	CHL	7	314	17	62,70,74	3.03	18 (29%)	72,109,114	2.21	23 (31%)
27	CHL	4	315	14	47,55,74	2.79	19 (40%)	54,91,114	2.48	21 (38%)
27	CHL	A	827	1	54,62,74	2.77	19 (35%)	62,99,114	2.35	22 (35%)
27	CHL	K	204	36	50,58,74	3.77	20 (40%)	58,95,114	2.45	22 (37%)
27	CHL	8	311	18	46,54,74	2.93	19 (41%)	53,90,114	2.48	19 (35%)
27	CHL	8	322	36	50,58,74	2.63	16 (32%)	58,95,114	2.53	21 (36%)
29	LUT	b	303	-	42,43,43	1.65	8 (19%)	51,60,60	1.74	10 (19%)
22	BCR	K	202	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	6 (10%)
27	CHL	B	845	2	50,58,74	2.67	18 (36%)	58,95,114	2.55	24 (41%)
30	LMG	8	307	-	32,32,55	0.27	0	40,40,63	0.33	0
23	LMT	F	302	-	30,30,36	1.33	6 (20%)	41,41,47	1.01	3 (7%)
27	CHL	A	836	36	65,73,74	2.73	19 (29%)	76,113,114	2.14	23 (30%)
27	CHL	A	844	1	65,73,74	2.60	20 (30%)	76,113,114	2.12	21 (27%)
27	CHL	A	842	1	66,74,74	2.10	15 (22%)	73,114,114	1.89	21 (28%)
27	CHL	b	310	12	46,54,74	3.59	20 (43%)	53,90,114	2.48	22 (41%)
27	CHL	B	841	2	55,63,74	2.51	17 (30%)	64,101,114	2.35	21 (32%)
27	CHL	7	322	36	61,69,74	2.10	17 (27%)	67,108,114	2.10	23 (34%)
22	BCR	B	806	-	41,41,41	1.10	2 (4%)	56,56,56	1.36	5 (8%)
27	CHL	8	312	18	65,73,74	2.82	18 (27%)	76,113,114	2.11	23 (30%)
27	CHL	B	827	2	60,68,74	2.36	17 (28%)	70,107,114	2.22	24 (34%)
27	CHL	4	305	14	45,53,74	3.14	18 (40%)	52,89,114	2.42	21 (40%)
27	CHL	4	304	14	55,63,74	2.83	18 (32%)	64,101,114	2.32	24 (37%)
27	CHL	7	312	17	44,52,74	3.08	18 (40%)	51,88,114	2.52	21 (41%)
22	BCR	B	807	-	41,41,41	1.11	2 (4%)	56,56,56	1.09	3 (5%)
27	CHL	B	821	2	58,66,74	2.54	19 (32%)	67,104,114	2.31	23 (34%)
27	CHL	B	829	2	55,63,74	2.61	19 (34%)	64,101,114	2.36	23 (35%)
27	CHL	3	310	13	65,73,74	2.37	19 (29%)	76,113,114	2.12	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	7	311	17	60,68,74	2.43	19 (31%)	70,107,114	2.24	26 (37%)
27	CHL	a	319	36	50,58,74	2.83	19 (38%)	58,95,114	2.46	24 (41%)
27	CHL	b	309	24	46,54,74	3.72	19 (41%)	53,90,114	2.50	21 (39%)
27	CHL	8	315	18	65,73,74	2.30	19 (29%)	76,113,114	2.20	21 (27%)
27	CHL	6	309	16	47,55,74	3.14	19 (40%)	54,91,114	2.38	20 (37%)
29	LUT	6	302	-	42,43,43	5.56	19 (45%)	51,60,60	5.91	31 (60%)
27	CHL	B	839	2	60,68,74	2.59	19 (31%)	70,107,114	2.22	24 (34%)
22	BCR	8	302	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	8 (14%)
27	CHL	B	816	2	61,69,74	2.62	18 (29%)	71,108,114	2.26	25 (35%)
27	CHL	5	316	36	66,74,74	1.78	13 (19%)	73,114,114	2.57	22 (30%)
27	CHL	6	308	16	66,74,74	1.85	15 (22%)	73,114,114	2.50	22 (30%)
27	CHL	b	311	12	47,55,74	2.67	16 (34%)	50,91,114	2.20	21 (42%)
28	DGD	B	809	-	62,62,67	0.98	2 (3%)	76,76,81	1.35	10 (13%)
29	LUT	8	303	-	42,43,43	5.48	19 (45%)	51,60,60	5.73	33 (64%)
27	CHL	J	106	9	42,50,74	3.34	18 (42%)	48,85,114	2.54	18 (37%)
27	CHL	6	315	16	50,58,74	3.42	20 (40%)	58,95,114	2.46	23 (39%)
27	CHL	A	853	1	65,73,74	2.53	19 (29%)	76,113,114	2.18	23 (30%)
27	CHL	4	313	-	45,53,74	3.32	17 (37%)	52,89,114	3.09	20 (38%)
27	CHL	7	315	17	43,52,74	3.04	20 (46%)	49,88,114	2.40	19 (38%)
27	CHL	8	325	18	65,73,74	2.41	18 (27%)	76,113,114	2.10	21 (27%)
27	CHL	b	308	-	46,54,74	5.19	22 (47%)	53,90,114	5.00	23 (43%)
27	CHL	A	849	1	65,73,74	2.58	19 (29%)	76,113,114	2.19	21 (27%)
27	CHL	B	838	2	65,73,74	2.61	18 (27%)	76,113,114	2.15	23 (30%)
27	CHL	3	316	36	66,74,74	1.87	13 (19%)	73,114,114	2.09	24 (32%)
29	LUT	a	302	-	42,43,43	5.58	19 (45%)	51,60,60	5.75	34 (66%)
24	LHG	A	812	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	6 (11%)
27	CHL	K	206	10	46,54,74	3.16	19 (41%)	53,90,114	2.48	21 (39%)
27	CHL	5	308	15	46,54,74	3.03	18 (39%)	53,90,114	2.52	19 (35%)
27	CHL	B	828	36	60,68,74	2.38	18 (30%)	70,107,114	2.21	24 (34%)
27	CHL	7	323	-	52,60,74	2.95	17 (32%)	60,97,114	2.74	23 (38%)
27	CHL	8	319	36	55,63,74	2.71	19 (34%)	64,101,114	2.36	23 (35%)
27	CHL	b	315	12	65,73,74	2.94	20 (30%)	76,113,114	2.16	22 (28%)
34	SQD	8	301	-	34,35,54	1.79	7 (20%)	43,46,65	1.51	6 (13%)
22	BCR	A	805	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	5 (8%)
24	LHG	5	324	27	31,31,48	0.79	1 (3%)	34,37,54	1.27	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LUT	a	304	-	42,43,43	5.54	19 (45%)	51,60,60	6.07	32 (62%)
27	CHL	a	309	36	60,68,74	3.25	19 (31%)	70,107,114	2.31	24 (34%)
27	CHL	4	312	14	48,56,74	2.16	16 (33%)	51,92,114	2.21	20 (39%)
27	CHL	B	824	2	57,65,74	2.69	18 (31%)	66,103,114	2.33	24 (36%)
22	BCR	A	803	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	3 (5%)
27	CHL	4	311	14	47,55,74	3.73	19 (40%)	54,91,114	2.47	21 (38%)
29	LUT	F	303	-	42,43,43	5.51	19 (45%)	51,60,60	5.90	33 (64%)
27	CHL	8	318	24	46,54,74	3.48	18 (39%)	53,90,114	2.44	18 (33%)
27	CHL	a	317	12	65,73,74	2.36	19 (29%)	76,113,114	2.14	22 (28%)
27	CHL	6	306	16	57,65,74	4.24	19 (33%)	66,103,114	2.31	25 (37%)
27	CHL	A	829	1	55,63,74	2.62	18 (32%)	64,101,114	2.39	20 (31%)
27	CHL	L	303	-	60,68,74	2.03	14 (23%)	70,107,114	4.14	30 (42%)
27	CHL	a	314	12	45,53,74	2.96	19 (42%)	52,89,114	2.46	21 (40%)
27	CHL	5	309	15	60,68,74	2.49	19 (31%)	70,107,114	2.23	23 (32%)
27	CHL	6	317	-	47,55,74	2.98	16 (34%)	50,91,114	2.36	20 (40%)
29	LUT	5	303	-	42,43,43	5.51	20 (47%)	51,60,60	5.89	32 (62%)
27	CHL	B	830	2	60,68,74	2.64	20 (33%)	70,107,114	2.27	23 (32%)
27	CHL	K	207	10	47,55,74	3.21	16 (34%)	50,91,114	2.11	18 (36%)
27	CHL	6	319	16	43,51,74	2.42	16 (37%)	45,86,114	2.89	17 (37%)
27	CHL	8	317	36	65,73,74	2.37	19 (29%)	76,113,114	2.14	22 (28%)
22	BCR	B	803	-	41,41,41	1.15	2 (4%)	56,56,56	1.13	4 (7%)
27	CHL	A	817	-	65,73,74	2.58	17 (26%)	76,113,114	2.19	22 (28%)
27	CHL	7	313	17	65,73,74	2.61	19 (29%)	76,113,114	2.15	22 (28%)
27	CHL	a	315	12	61,69,74	2.36	16 (26%)	67,108,114	2.09	25 (37%)
27	CHL	A	840	36	65,73,74	2.69	19 (29%)	76,113,114	2.25	22 (28%)
27	CHL	5	310	15	65,73,74	3.39	20 (30%)	76,113,114	2.26	22 (28%)
27	CHL	A	833	1	61,69,74	2.05	15 (24%)	67,108,114	2.22	24 (35%)
27	CHL	7	318	17	55,63,74	2.78	19 (34%)	64,101,114	2.42	23 (35%)
29	LUT	J	103	-	42,43,43	5.59	20 (47%)	51,60,60	5.87	31 (60%)
27	CHL	4	310	24	46,54,74	3.83	20 (43%)	53,90,114	2.50	22 (41%)
27	CHL	A	850	1	65,73,74	2.37	18 (27%)	76,113,114	2.12	23 (30%)
30	LMG	a	301	-	44,44,55	0.87	2 (4%)	52,52,63	1.27	6 (11%)
20	PQN	A	801	-	34,34,34	0.37	0	42,45,45	0.56	0
22	BCR	F	301	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	4 (7%)
27	CHL	a	308	12	45,53,74	3.09	19 (42%)	52,89,114	2.58	20 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LUT	b	301	-	42,43,43	5.62	19 (45%)	51,60,60	5.71	34 (66%)
30	LMG	7	301	-	41,41,55	0.87	1 (2%)	49,49,63	1.21	3 (6%)
27	CHL	a	310	12	65,73,74	2.93	18 (27%)	76,113,114	2.17	22 (28%)
27	CHL	5	307	15	55,63,74	3.45	18 (32%)	64,101,114	2.30	25 (39%)
27	CHL	a	311	12	60,68,74	2.71	18 (30%)	70,107,114	2.33	24 (34%)
27	CHL	5	322	15	47,55,74	2.80	16 (34%)	50,91,114	2.23	19 (38%)
27	CHL	B	823	2	55,63,74	2.64	19 (34%)	64,101,114	2.37	23 (35%)
27	CHL	B	835	2	57,65,74	2.66	19 (33%)	66,103,114	2.36	22 (33%)
27	CHL	A	854	1	56,64,74	2.91	20 (35%)	65,102,114	2.41	23 (35%)
27	CHL	3	314	36	60,68,74	2.68	17 (28%)	70,107,114	2.29	22 (31%)
22	BCR	A	804	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	5 (8%)
24	LHG	8	305	27	48,48,48	0.64	1 (2%)	51,54,54	1.25	6 (11%)
27	CHL	B	826	2	50,58,74	3.33	19 (38%)	58,95,114	2.48	21 (36%)
27	CHL	A	821	1	65,73,74	2.51	20 (30%)	76,113,114	2.17	23 (30%)
27	CHL	A	824	1	60,68,74	2.46	17 (28%)	70,107,114	2.20	22 (31%)
27	CHL	F	308	6	46,54,74	3.17	19 (41%)	53,90,114	2.48	19 (35%)
26	CL0	A	815	1	65,73,73	1.79	11 (16%)	76,113,113	3.37	29 (38%)
24	LHG	5	304	-	34,34,48	0.36	0	37,40,54	0.44	0
27	CHL	B	818	2	55,63,74	2.59	19 (34%)	64,101,114	2.38	21 (32%)
27	CHL	A	830	1	65,73,74	2.39	18 (27%)	76,113,114	2.27	22 (28%)
22	BCR	L	301	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	4 (7%)
27	CHL	A	831	-	55,63,74	2.15	11 (20%)	64,101,114	4.15	31 (48%)
27	CHL	5	312	36	50,58,74	3.81	19 (38%)	58,95,114	2.42	22 (37%)
27	CHL	b	317	-	48,56,74	2.83	16 (33%)	51,92,114	2.20	19 (37%)
22	BCR	6	301	-	41,41,41	1.68	8 (19%)	56,56,56	1.61	11 (19%)
27	CHL	5	317	36	47,55,74	2.26	14 (29%)	50,91,114	2.29	19 (38%)
22	BCR	M	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.21	5 (8%)
22	BCR	3	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	7 (12%)
27	CHL	a	320	12	46,54,74	3.19	19 (41%)	53,90,114	2.40	21 (39%)
27	CHL	K	205	10	46,54,74	3.04	19 (41%)	53,90,114	2.40	20 (37%)
27	CHL	4	318	-	42,50,74	3.94	19 (45%)	48,85,114	2.52	20 (41%)
27	CHL	B	825	2	60,68,74	2.71	20 (33%)	70,107,114	2.30	26 (37%)
27	CHL	6	320	16	46,54,74	3.33	17 (36%)	53,90,114	2.44	21 (39%)
27	CHL	B	837	2	65,73,74	2.73	19 (29%)	76,113,114	2.12	23 (30%)
24	LHG	7	302	-	48,48,48	0.60	0	51,54,54	1.24	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CHL	A	845	1	65,73,74	2.79	19 (29%)	76,113,114	2.14	23 (30%)
27	CHL	A	818	1	65,73,74	2.32	20 (30%)	76,113,114	2.20	25 (32%)
27	CHL	7	324	17	46,54,74	2.83	19 (41%)	53,90,114	2.35	18 (33%)
27	CHL	3	318	36	51,59,74	2.76	20 (39%)	59,96,114	2.46	23 (38%)
27	CHL	3	317	36	62,70,74	2.53	19 (30%)	72,109,114	2.26	21 (29%)
27	CHL	A	820	1	65,73,74	2.40	18 (27%)	76,113,114	2.24	24 (31%)
24	LHG	A	810	-	41,41,48	0.68	1 (2%)	44,47,54	1.32	6 (13%)
24	LHG	B	808	27	31,31,48	0.78	1 (3%)	34,37,54	1.31	4 (11%)
27	CHL	A	822	1	55,63,74	2.92	20 (36%)	64,101,114	2.37	24 (37%)
27	CHL	B	812	-	65,73,74	2.47	17 (26%)	76,113,114	2.24	22 (28%)
23	LMT	B	810	-	36,36,36	1.20	5 (13%)	47,47,47	0.94	1 (2%)
27	CHL	B	815	2	65,73,74	2.45	20 (30%)	76,113,114	2.17	26 (34%)
22	BCR	A	806	-	41,41,41	1.15	2 (4%)	56,56,56	1.28	6 (10%)
27	CHL	3	312	13	65,73,74	2.80	20 (30%)	76,113,114	2.16	24 (31%)
27	CHL	4	306	14	56,64,74	2.63	18 (32%)	65,102,114	2.31	23 (35%)
27	CHL	6	312	16	46,54,74	3.25	19 (41%)	53,90,114	2.55	22 (41%)
27	CHL	6	311	16	65,73,74	2.67	19 (29%)	76,113,114	2.20	24 (31%)
27	CHL	b	304	12	46,54,74	3.62	19 (41%)	53,90,114	2.50	22 (41%)
27	CHL	A	848	1	65,73,74	2.43	18 (27%)	76,113,114	2.18	22 (28%)
29	LUT	5	302	-	42,43,43	5.57	19 (45%)	51,60,60	5.71	33 (64%)
29	LUT	4	301	-	42,43,43	5.61	20 (47%)	51,60,60	5.69	34 (66%)

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
27	CHL	5	315	15	3/3/20/26	8/37/135/137	-
29	LUT	3	304	-	-	15/29/67/67	0/2/2/2
27	CHL	4	309	-	3/3/16/26	9/17/115/137	-
27	CHL	6	310	16	3/3/18/26	10/25/123/137	-
27	CHL	7	316	36	3/3/18/26	9/23/121/137	-
27	CHL	A	851	1	3/3/16/26	4/15/113/137	-
29	LUT	7	304	-	-	17/29/67/67	0/2/2/2
29	LUT	4	302	-	-	19/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	B	822	2	2/2/20/26	14/37/135/137	-
22	BCR	3	301	-	-	8/29/63/63	0/2/2/2
21	SF4	C	102	3	-	-	0/6/5/5
27	CHL	8	321	36	3/3/20/26	17/39/137/137	-
27	CHL	a	318	36	3/3/16/26	6/18/116/137	-
22	BCR	K	203	-	-	5/29/63/63	0/2/2/2
27	CHL	A	841	36	3/3/18/26	10/27/125/137	-
27	CHL	a	307	12	3/3/19/26	4/31/129/137	-
21	SF4	A	802	1,2	-	-	0/6/5/5
27	CHL	6	318	-	3/3/16/26	9/17/115/137	-
27	CHL	A	834	1	2/2/20/26	6/37/135/137	-
27	CHL	B	836	2	2/2/20/26	5/37/135/137	-
27	CHL	B	850	2	2/2/17/26	3/19/117/137	-
22	BCR	A	807	-	-	11/29/63/63	0/2/2/2
27	CHL	5	318	15	3/3/20/26	9/37/135/137	-
27	CHL	A	838	1	1/1/19/26	8/31/129/137	-
27	CHL	5	320	15	3/3/16/26	2/15/113/137	-
27	CHL	A	846	-	2/2/17/26	3/19/117/137	-
29	LUT	8	304	-	-	14/29/67/67	0/2/2/2
27	CHL	4	307	14	2/2/19/26	7/31/129/137	-
27	CHL	A	825	1	1/1/20/26	11/37/135/137	-
27	CHL	A	823	1	3/3/20/26	13/37/135/137	-
27	CHL	A	837	1	2/2/18/26	5/25/123/137	-
27	CHL	A	839	1	2/2/20/26	13/37/135/137	-
27	CHL	B	831	2	2/2/16/26	4/15/113/137	-
27	CHL	B	851	2	2/2/19/26	7/34/132/137	-
27	CHL	5	323	15	2/2/18/26	8/27/125/137	-
27	CHL	A	816	36	3/3/20/26	6/37/135/137	-
27	CHL	b	305	-	3/3/16/26	6/15/113/137	-
27	CHL	3	315	13	2/2/17/26	8/22/120/137	-
22	BCR	I	801	-	-	11/29/63/63	0/2/2/2
23	LMT	5	326	-	-	9/21/61/61	0/2/2/2
27	CHL	8	323	-	2/2/17/26	4/19/117/137	-
20	PQN	B	801	-	-	3/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	B	819	2	3/3/20/26	11/37/135/137	-
27	CHL	3	320	13	3/3/19/26	6/33/131/137	-
22	BCR	J	102	-	-	8/29/63/63	0/2/2/2
22	BCR	3	302	-	-	11/29/63/63	0/2/2/2
27	CHL	B	846	36	3/3/20/26	13/37/135/137	-
32	PTY	5	305	-	-	17/34/34/53	-
27	CHL	B	834	2	3/3/20/26	6/37/135/137	-
27	CHL	4	316	-	3/3/16/26	8/15/113/137	-
27	CHL	B	820	2	1/1/20/26	10/37/135/137	-
27	CHL	8	326	18	3/3/16/26	3/15/113/137	-
27	CHL	A	843	1	2/2/20/26	13/37/135/137	-
27	CHL	A	828	1	2/2/20/26	12/37/135/137	-
27	CHL	A	819	1	2/2/18/26	8/25/123/137	-
27	CHL	4	317	14	2/2/16/26	6/13/111/137	-
22	BCR	L	302	-	-	8/29/63/63	0/2/2/2
27	CHL	B	848	2	1/1/20/26	7/37/135/137	-
24	LHG	a	305	27	-	24/53/53/53	-
24	LHG	4	303	27	-	30/53/53/53	-
27	CHL	8	320	18	2/2/17/26	6/22/120/137	-
24	LHG	A	811	27	-	26/46/46/53	-
27	CHL	B	847	36	2/2/20/26	8/37/135/137	-
27	CHL	b	307	12	2/2/18/26	6/25/123/137	-
24	LHG	7	306	27	-	20/48/48/53	-
30	LMG	J	104	-	-	7/24/44/70	0/1/1/1
27	CHL	B	813	2	3/3/18/26	9/25/123/137	-
35	DGA	8	306	-	-	5/29/29/45	-
27	CHL	3	308	13	3/3/20/26	6/37/135/137	-
27	CHL	L	304	-	2/2/16/26	2/13/111/137	-
27	CHL	b	306	12	2/2/16/26	5/15/113/137	-
27	CHL	5	313	-	2/2/18/26	10/28/126/137	-
27	CHL	5	325	16	2/2/16/26	8/17/115/137	-
27	CHL	a	312	36	3/3/17/26	4/19/117/137	-
27	CHL	7	320	36,28	2/2/16/26	8/17/115/137	-
27	CHL	B	817	2	3/3/20/26	9/37/135/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	A	835	1	3/3/16/26	6/16/114/137	-
27	CHL	B	842	2	2/2/20/26	5/37/135/137	-
27	CHL	4	314	-	3/3/16/26	5/13/111/137	-
27	CHL	B	840	2	3/3/20/26	10/37/135/137	-
27	CHL	B	833	36	3/3/18/26	7/25/123/137	-
23	LMT	A	808	-	-	8/21/61/61	0/2/2/2
30	LMG	J	101	-	-	26/44/64/70	0/1/1/1
27	CHL	A	858	1	2/2/20/26	14/37/135/137	-
27	CHL	b	313	12	3/3/16/26	7/15/113/137	-
27	CHL	B	843	36	3/3/16/26	2/13/111/137	-
27	CHL	b	314	12	3/3/16/26	4/15/113/137	-
27	CHL	A	856	36	2/2/20/26	4/37/135/137	-
27	CHL	7	321	17	3/3/16/26	1/17/115/137	-
27	CHL	A	855	1	1/1/20/26	10/37/135/137	-
27	CHL	3	321	13	2/2/16/26	5/13/111/137	-
27	CHL	5	311	15	3/3/16/26	5/15/113/137	-
23	LMT	5	306	-	-	6/16/56/61	0/2/2/2
27	CHL	7	319	17	3/3/20/26	19/39/137/137	-
27	CHL	B	811	2	2/2/20/26	7/37/135/137	-
27	CHL	6	305	16	3/3/16/26	7/15/113/137	-
27	CHL	8	324	36	3/3/15/26	2/13/112/137	-
27	CHL	b	316	-	3/3/16/26	6/18/116/137	-
27	CHL	7	317	24	3/3/20/26	13/37/135/137	-
27	CHL	8	313	18	3/3/17/26	4/19/117/137	-
27	CHL	A	857	24	3/3/16/26	5/15/113/137	-
27	CHL	A	852	1	3/3/17/26	4/21/119/137	-
27	CHL	4	320	14	3/3/17/26	7/19/117/137	-
27	CHL	A	832	1	2/2/19/26	13/31/129/137	-
22	BCR	B	805	-	-	8/29/63/63	0/2/2/2
27	CHL	A	826	1	1/1/19/26	11/34/132/137	-
27	CHL	a	313	24	3/3/18/26	10/25/123/137	-
27	CHL	B	814	2	3/3/20/26	15/37/135/137	-
21	SF4	C	101	3	-	-	0/6/5/5
27	CHL	b	312	-	1/1/16/26	4/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	6	313	16	2/2/16/26	6/16/114/137	-
22	BCR	B	802	-	-	9/29/63/63	0/2/2/2
27	CHL	3	313	36	3/3/20/26	7/37/135/137	-
27	CHL	5	321	15	2/2/16/26	3/15/113/137	-
27	CHL	5	314	15	2/2/16/26	4/13/111/137	-
27	CHL	3	309	13	3/3/16/26	2/15/113/137	-
22	BCR	B	804	-	-	10/29/63/63	0/2/2/2
27	CHL	5	319	-	2/2/16/26	10/17/115/137	-
27	CHL	A	859	36	3/3/20/26	7/37/135/137	-
27	CHL	B	832	36	3/3/20/26	7/37/135/137	-
27	CHL	a	316	36	3/3/16/26	8/18/116/137	-
27	CHL	8	314	18	3/3/20/26	10/39/137/137	-
22	BCR	7	303	-	-	8/29/63/63	0/2/2/2
33	XAT	7	305	-	-	7/31/93/93	0/4/4/4
27	CHL	4	319	14	2/2/16/26	5/13/111/137	-
27	CHL	6	316	36	3/3/16/26	9/15/113/137	-
27	CHL	B	844	2	3/3/20/26	11/37/135/137	-
29	LUT	6	303	-	-	18/29/67/67	0/2/2/2
28	DGD	7	307	27	-	22/55/95/95	0/2/2/2
29	LUT	3	305	-	-	12/29/67/67	0/2/2/2
27	CHL	A	847	1	2/2/18/26	6/27/125/137	-
27	CHL	4	308	14	3/3/19/26	9/31/129/137	-
27	CHL	6	307	-	2/2/20/26	14/37/135/137	-
23	LMT	A	809	-	-	6/21/61/61	0/2/2/2
31	AXT	a	303	-	-	1/29/71/75	0/2/2/2
27	CHL	8	316	18	2/2/20/26	11/37/135/137	-
27	CHL	B	849	24	3/3/20/26	6/37/135/137	-
22	BCR	5	301	-	-	13/29/63/63	0/2/2/2
27	CHL	3	319	13	2/2/18/26	9/25/123/137	-
27	CHL	6	314	24	3/3/16/26	3/15/113/137	-
27	CHL	3	311	13	3/3/19/26	15/31/129/137	-
27	CHL	F	309	36	3/3/17/26	5/19/117/137	-
27	CHL	7	314	17	3/3/19/26	9/34/132/137	-
27	CHL	4	315	14	3/3/16/26	2/16/114/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	A	827	1	2/2/17/26	7/24/122/137	-
27	CHL	K	204	36	3/3/17/26	4/19/117/137	-
27	CHL	8	311	18	3/3/16/26	2/15/113/137	-
27	CHL	8	322	36	2/2/17/26	2/19/117/137	-
29	LUT	b	303	-	-	23/29/67/67	0/2/2/2
22	BCR	K	202	-	-	9/29/63/63	0/2/2/2
27	CHL	B	845	2	2/2/17/26	2/19/117/137	-
30	LMG	8	307	-	-	13/27/47/70	0/1/1/1
23	LMT	F	302	-	-	5/15/55/61	0/2/2/2
27	CHL	A	836	36	3/3/20/26	11/37/135/137	-
27	CHL	A	844	1	1/1/20/26	6/37/135/137	-
24	LHG	b	302	27	-	17/39/39/53	-
27	CHL	A	842	1	2/2/20/26	8/39/137/137	-
27	CHL	b	310	12	2/2/16/26	4/15/113/137	-
27	CHL	B	841	2	2/2/18/26	7/25/123/137	-
27	CHL	7	322	36	2/2/19/26	10/33/131/137	-
27	CHL	8	312	18	3/3/20/26	14/37/135/137	-
22	BCR	B	806	-	-	9/29/63/63	0/2/2/2
27	CHL	B	827	2	3/3/19/26	10/31/129/137	-
27	CHL	4	305	14	3/3/16/26	4/13/111/137	-
27	CHL	4	304	14	3/3/18/26	4/25/123/137	-
27	CHL	7	312	17	3/3/16/26	4/11/109/137	-
27	CHL	B	821	2	2/2/18/26	9/29/127/137	-
27	CHL	B	829	2	2/2/18/26	7/25/123/137	-
27	CHL	3	310	13	3/3/20/26	13/37/135/137	-
22	BCR	B	807	-	-	6/29/63/63	0/2/2/2
27	CHL	7	311	17	3/3/19/26	4/31/129/137	-
27	CHL	a	319	36	2/2/17/26	6/19/117/137	-
27	CHL	b	309	24	3/3/16/26	3/15/113/137	-
27	CHL	8	315	18	2/2/20/26	14/37/135/137	-
27	CHL	6	309	16	3/3/16/26	5/16/114/137	-
29	LUT	6	302	-	-	16/29/67/67	0/2/2/2
27	CHL	B	839	2	2/2/19/26	6/31/129/137	-
22	BCR	8	302	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	B	816	2	3/3/19/26	6/33/131/137	-
27	CHL	5	316	36	3/3/20/26	25/39/137/137	-
27	CHL	6	308	16	3/3/20/26	19/39/137/137	-
27	CHL	b	311	12	3/3/16/26	8/17/115/137	-
28	DGD	B	809	-	-	22/50/90/95	0/2/2/2
29	LUT	8	303	-	-	13/29/67/67	0/2/2/2
27	CHL	J	106	9	3/3/15/26	4/10/108/137	-
27	CHL	6	315	16	2/2/17/26	2/19/117/137	-
27	CHL	A	853	1	3/3/20/26	10/37/135/137	-
27	CHL	4	313	-	1/1/16/26	6/13/111/137	-
27	CHL	7	315	17	2/2/16/26	3/11/109/137	-
27	CHL	8	325	18	2/2/20/26	10/37/135/137	-
27	CHL	b	308	-	2/2/16/26	5/15/113/137	-
27	CHL	A	849	1	2/2/20/26	7/37/135/137	-
27	CHL	B	838	2	1/1/20/26	11/37/135/137	-
27	CHL	3	316	36	2/2/20/26	8/39/137/137	-
29	LUT	a	302	-	-	15/29/67/67	0/2/2/2
24	LHG	A	812	-	-	21/53/53/53	-
27	CHL	K	206	10	2/2/16/26	2/15/113/137	-
27	CHL	5	308	15	3/3/16/26	3/15/113/137	-
27	CHL	B	828	36	3/3/19/26	2/31/129/137	-
27	CHL	7	323	-	2/2/17/26	8/22/120/137	-
27	CHL	8	319	36	3/3/18/26	6/25/123/137	-
27	CHL	b	315	12	3/3/20/26	14/37/135/137	-
34	SQD	8	301	-	-	15/30/50/69	0/1/1/1
22	BCR	A	805	-	-	4/29/63/63	0/2/2/2
24	LHG	5	324	27	-	14/36/36/53	-
29	LUT	a	304	-	-	14/29/67/67	0/2/2/2
27	CHL	a	309	36	3/3/19/26	7/31/129/137	-
27	CHL	4	312	14	2/2/16/26	9/18/116/137	-
27	CHL	B	824	2	2/2/18/26	6/28/126/137	-
22	BCR	A	803	-	-	7/29/63/63	0/2/2/2
27	CHL	4	311	14	3/3/16/26	5/16/114/137	-
29	LUT	F	303	-	-	18/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	8	318	24	3/3/16/26	6/15/113/137	-
27	CHL	a	317	12	3/3/20/26	9/37/135/137	-
27	CHL	6	306	16	3/3/18/26	10/28/126/137	-
27	CHL	A	829	1	2/2/18/26	9/25/123/137	-
27	CHL	L	303	-	2/2/19/26	10/31/129/137	-
27	CHL	a	314	12	2/2/16/26	8/13/111/137	-
27	CHL	5	309	15	2/2/19/26	15/31/129/137	-
27	CHL	6	317	-	2/2/16/26	7/17/115/137	-
29	LUT	5	303	-	-	19/29/67/67	0/2/2/2
27	CHL	B	830	2	2/2/19/26	3/31/129/137	-
27	CHL	K	207	10	3/3/16/26	6/17/115/137	-
27	CHL	6	319	16	3/3/15/26	6/12/110/137	-
27	CHL	8	317	36	3/3/20/26	12/37/135/137	-
22	BCR	B	803	-	-	9/29/63/63	0/2/2/2
27	CHL	A	817	-	1/1/20/26	3/37/135/137	-
27	CHL	7	313	17	2/2/20/26	10/37/135/137	-
27	CHL	a	315	12	2/2/19/26	12/33/131/137	-
27	CHL	A	840	36	3/3/20/26	8/37/135/137	-
27	CHL	5	310	15	3/3/20/26	5/37/135/137	-
27	CHL	A	833	1	2/2/19/26	11/33/131/137	-
27	CHL	7	318	17	2/2/18/26	7/25/123/137	-
29	LUT	J	103	-	-	18/29/67/67	0/2/2/2
27	CHL	4	310	24	3/3/16/26	6/15/113/137	-
27	CHL	A	850	1	1/1/20/26	10/37/135/137	-
30	LMG	a	301	-	-	16/39/59/70	0/1/1/1
27	CHL	a	308	12	3/3/16/26	5/13/111/137	-
20	PQN	A	801	-	-	3/23/43/43	0/2/2/2
22	BCR	F	301	-	-	10/29/63/63	0/2/2/2
29	LUT	b	301	-	-	15/29/67/67	0/2/2/2
30	LMG	7	301	-	-	18/36/56/70	0/1/1/1
27	CHL	a	310	12	2/2/20/26	12/37/135/137	-
27	CHL	5	307	15	3/3/18/26	6/25/123/137	-
27	CHL	a	311	12	2/2/19/26	7/31/129/137	-
27	CHL	5	322	15	3/3/16/26	3/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	B	823	2	3/3/18/26	8/25/123/137	-
27	CHL	B	835	2	2/2/18/26	11/28/126/137	-
24	LHG	B	808	27	-	6/36/36/53	-
27	CHL	A	854	1	1/1/18/26	3/27/125/137	-
27	CHL	3	314	36	3/3/19/26	10/31/129/137	-
27	CHL	B	826	2	1/1/17/26	7/19/117/137	-
22	BCR	A	804	-	-	6/29/63/63	0/2/2/2
24	LHG	8	305	27	-	16/53/53/53	-
27	CHL	A	821	1	3/3/20/26	11/37/135/137	-
27	CHL	A	824	1	2/2/19/26	8/31/129/137	-
27	CHL	F	308	6	3/3/16/26	6/15/113/137	-
26	CL0	A	815	1	1/1/20/25	6/37/135/135	-
27	CHL	B	818	2	2/2/18/26	6/25/123/137	-
24	LHG	5	304	-	-	21/39/39/53	-
27	CHL	A	830	1	2/2/20/26	7/37/135/137	-
27	CHL	A	831	-	2/2/18/26	12/25/123/137	-
27	CHL	5	312	36	3/3/17/26	4/19/117/137	-
27	CHL	b	317	-	2/2/16/26	5/18/116/137	-
22	BCR	L	301	-	-	10/29/63/63	0/2/2/2
22	BCR	6	301	-	-	23/29/63/63	0/2/2/2
27	CHL	5	317	36	2/2/16/26	5/17/115/137	-
22	BCR	M	102	-	-	9/29/63/63	0/2/2/2
27	CHL	4	318	-	3/3/15/26	3/10/108/137	-
27	CHL	a	320	12	3/3/16/26	5/15/113/137	-
27	CHL	K	205	10	3/3/16/26	3/15/113/137	-
22	BCR	3	303	-	-	10/29/63/63	0/2/2/2
27	CHL	B	825	2	2/2/19/26	8/31/129/137	-
27	CHL	6	320	16	3/3/16/26	4/15/113/137	-
27	CHL	B	837	2	1/1/20/26	9/37/135/137	-
24	LHG	7	302	-	-	32/53/53/53	-
27	CHL	A	845	1	1/1/20/26	10/37/135/137	-
27	CHL	A	818	1	3/3/20/26	7/37/135/137	-
27	CHL	7	324	17	2/2/16/26	6/15/113/137	-
27	CHL	3	318	36	3/3/17/26	7/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	3	317	36	2/2/19/26	9/34/132/137	-
27	CHL	A	820	1	3/3/20/26	7/37/135/137	-
24	LHG	A	810	-	-	21/46/46/53	-
27	CHL	A	822	1	1/1/18/26	5/25/123/137	-
27	CHL	B	812	-	2/2/20/26	6/37/135/137	-
27	CHL	4	306	14	3/3/18/26	7/27/125/137	-
27	CHL	B	815	2	3/3/20/26	12/37/135/137	-
27	CHL	6	312	16	3/3/16/26	7/15/113/137	-
22	BCR	A	806	-	-	9/29/63/63	0/2/2/2
27	CHL	3	312	13	2/2/20/26	7/37/135/137	-
23	LMT	B	810	-	-	7/21/61/61	0/2/2/2
23	LMT	7	308	-	-	9/21/61/61	0/2/2/2
27	CHL	6	311	16	3/3/20/26	9/37/135/137	-
27	CHL	b	304	12	2/2/16/26	4/15/113/137	-
27	CHL	A	848	1	2/2/20/26	4/37/135/137	-
29	LUT	5	302	-	-	14/29/67/67	0/2/2/2
29	LUT	4	301	-	-	15/29/67/67	0/2/2/2

All (4370) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	306	CHL	MG-NA	23.77	2.62	2.06
27	6	306	CHL	MG-NA	23.39	2.61	2.06
27	5	310	CHL	MG-NA	20.63	2.55	2.06
27	b	308	CHL	C1B-NB	20.41	1.53	1.35
27	5	312	CHL	MG-NA	19.85	2.53	2.06
27	4	311	CHL	MG-NA	18.64	2.50	2.06
27	K	204	CHL	MG-ND	-18.47	1.69	2.05
27	B	834	CHL	MG-NA	18.45	2.50	2.06
27	5	307	CHL	MG-NA	18.22	2.49	2.06
27	b	304	CHL	MG-NC	17.82	2.48	2.06
27	5	323	CHL	MG-NA	17.80	2.48	2.06
27	4	318	CHL	MG-NA	17.53	2.47	2.06
27	4	310	CHL	MG-NA	17.51	2.47	2.06
27	b	308	CHL	C4B-NB	17.37	1.50	1.35
29	a	302	LUT	C24-C25	17.19	1.54	1.33
29	6	302	LUT	C24-C25	16.96	1.54	1.33
29	b	301	LUT	C24-C25	16.91	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3	305	LUT	C24-C25	16.75	1.54	1.33
27	A	852	CHL	MG-NA	16.70	2.46	2.06
29	3	304	LUT	C24-C25	16.70	1.53	1.33
29	5	302	LUT	C24-C25	16.69	1.53	1.33
29	a	304	LUT	C24-C25	16.65	1.53	1.33
29	J	103	LUT	C24-C25	16.65	1.53	1.33
27	B	847	CHL	MG-NA	16.64	2.45	2.06
29	4	301	LUT	C24-C25	16.62	1.53	1.33
29	8	304	LUT	C24-C25	16.61	1.53	1.33
29	5	303	LUT	C24-C25	16.54	1.53	1.33
29	8	303	LUT	C24-C25	16.50	1.53	1.33
29	6	303	LUT	C24-C25	16.47	1.53	1.33
29	F	303	LUT	C24-C25	16.45	1.53	1.33
29	4	302	LUT	C24-C25	16.45	1.53	1.33
27	b	309	CHL	MG-NA	16.42	2.45	2.06
29	7	304	LUT	C24-C25	16.41	1.53	1.33
27	B	826	CHL	MG-NA	16.28	2.44	2.06
27	6	315	CHL	MG-NA	15.81	2.43	2.06
27	6	320	CHL	MG-NA	15.76	2.43	2.06
27	8	312	CHL	MG-NA	15.54	2.43	2.06
27	a	310	CHL	MG-NA	15.41	2.42	2.06
27	A	826	CHL	MG-NA	14.66	2.41	2.06
27	8	318	CHL	MG-NA	14.56	2.40	2.06
27	b	313	CHL	MG-NA	14.53	2.40	2.06
27	6	314	CHL	MG-NA	14.37	2.40	2.06
27	3	321	CHL	MG-NA	14.23	2.40	2.06
27	A	845	CHL	MG-NA	14.16	2.39	2.06
27	3	319	CHL	MG-NA	14.13	2.39	2.06
29	4	302	LUT	C30-C29	14.08	1.54	1.35
27	6	312	CHL	MG-NA	14.04	2.39	2.06
27	5	314	CHL	MG-NA	14.03	2.39	2.06
27	B	837	CHL	MG-NA	14.03	2.39	2.06
27	b	310	CHL	MG-ND	13.93	2.33	2.05
27	7	314	CHL	MG-NA	13.90	2.39	2.06
27	a	309	CHL	MG-NC	13.90	2.39	2.06
29	4	301	LUT	C30-C29	13.83	1.54	1.35
27	A	847	CHL	MG-NA	13.81	2.39	2.06
29	a	304	LUT	C30-C29	13.78	1.54	1.35
29	b	301	LUT	C14-C13	13.76	1.54	1.35
29	5	303	LUT	C10-C9	13.74	1.54	1.35
29	b	301	LUT	C30-C29	13.73	1.54	1.35
29	6	302	LUT	C30-C29	13.72	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	303	LUT	C14-C13	13.71	1.54	1.35
29	3	305	LUT	C30-C29	13.70	1.53	1.35
27	B	840	CHL	MG-NA	13.69	2.38	2.06
29	6	303	LUT	C30-C29	13.68	1.53	1.35
29	4	302	LUT	C14-C13	13.67	1.53	1.35
29	6	303	LUT	C10-C9	13.63	1.53	1.35
27	B	842	CHL	MG-NA	13.61	2.38	2.06
29	8	304	LUT	C14-C13	13.61	1.53	1.35
29	7	304	LUT	C30-C29	13.60	1.53	1.35
29	a	302	LUT	C30-C29	13.60	1.53	1.35
29	3	304	LUT	C30-C29	13.57	1.53	1.35
29	5	302	LUT	C30-C29	13.56	1.53	1.35
29	F	303	LUT	C30-C29	13.52	1.53	1.35
29	4	302	LUT	C10-C9	13.52	1.53	1.35
29	8	304	LUT	C10-C9	13.50	1.53	1.35
29	8	304	LUT	C30-C29	13.50	1.53	1.35
29	J	103	LUT	C30-C29	13.48	1.53	1.35
29	6	303	LUT	C14-C13	13.48	1.53	1.35
27	8	326	CHL	MG-NA	13.47	2.38	2.06
29	4	302	LUT	C34-C33	13.47	1.53	1.35
27	A	832	CHL	MG-NC	13.44	2.38	2.06
29	4	301	LUT	C10-C9	13.40	1.53	1.35
29	6	302	LUT	C10-C9	13.40	1.53	1.35
29	5	302	LUT	C10-C9	13.40	1.53	1.35
29	5	303	LUT	C30-C29	13.39	1.53	1.35
29	8	303	LUT	C30-C29	13.37	1.53	1.35
29	a	304	LUT	C34-C33	13.37	1.53	1.35
27	b	315	CHL	MG-ND	13.36	2.32	2.05
27	4	304	CHL	MG-NA	13.30	2.37	2.06
29	4	301	LUT	C14-C13	13.30	1.53	1.35
29	5	302	LUT	C14-C13	13.29	1.53	1.35
29	3	304	LUT	C14-C13	13.28	1.53	1.35
27	5	321	CHL	MG-NA	13.28	2.37	2.06
29	3	305	LUT	C14-C13	13.28	1.53	1.35
29	6	302	LUT	C14-C13	13.28	1.53	1.35
29	b	301	LUT	C10-C9	13.28	1.53	1.35
29	8	303	LUT	C10-C9	13.27	1.53	1.35
29	J	103	LUT	C10-C9	13.27	1.53	1.35
29	a	304	LUT	C14-C13	13.25	1.53	1.35
29	J	103	LUT	C34-C33	13.23	1.53	1.35
27	a	309	CHL	MG-ND	13.21	2.32	2.05
29	F	303	LUT	C10-C9	13.20	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	302	LUT	C14-C13	13.19	1.53	1.35
29	3	304	LUT	C10-C9	13.18	1.53	1.35
29	J	103	LUT	C14-C13	13.18	1.53	1.35
29	7	304	LUT	C10-C9	13.16	1.53	1.35
29	3	305	LUT	C10-C9	13.16	1.53	1.35
27	B	843	CHL	MG-NA	13.14	2.37	2.06
29	a	302	LUT	C10-C9	13.14	1.53	1.35
27	3	308	CHL	MG-ND	-13.10	1.79	2.05
29	8	303	LUT	C34-C33	13.09	1.53	1.35
29	5	302	LUT	C34-C33	13.08	1.53	1.35
29	4	301	LUT	C34-C33	13.08	1.53	1.35
29	7	304	LUT	C14-C13	13.07	1.53	1.35
27	b	312	CHL	MG-NA	13.05	2.37	2.06
27	a	311	CHL	MG-NA	13.04	2.37	2.06
29	F	303	LUT	C34-C33	13.03	1.53	1.35
29	a	304	LUT	C10-C9	13.02	1.53	1.35
27	6	313	CHL	MG-NC	13.02	2.37	2.06
27	4	308	CHL	MG-NA	13.02	2.37	2.06
29	b	301	LUT	C34-C33	13.01	1.53	1.35
29	F	303	LUT	C14-C13	13.01	1.53	1.35
29	6	302	LUT	C34-C33	13.00	1.53	1.35
29	5	303	LUT	C14-C13	12.99	1.53	1.35
27	A	859	CHL	MG-NA	12.99	2.37	2.06
29	6	303	LUT	C34-C33	12.98	1.53	1.35
27	a	307	CHL	MG-NA	12.97	2.37	2.06
27	B	850	CHL	MG-NC	12.96	2.37	2.06
27	8	313	CHL	MG-NA	12.88	2.36	2.06
29	7	304	LUT	C5-C6	12.87	1.56	1.34
29	a	302	LUT	C34-C33	12.85	1.52	1.35
27	K	207	CHL	MG-NC	12.84	2.36	2.06
27	3	314	CHL	MG-NA	12.77	2.36	2.06
27	B	851	CHL	MG-NA	12.70	2.36	2.06
29	5	303	LUT	C34-C33	12.70	1.52	1.35
29	3	305	LUT	C34-C33	12.64	1.52	1.35
29	8	304	LUT	C34-C33	12.63	1.52	1.35
29	3	304	LUT	C34-C33	12.60	1.52	1.35
27	A	838	CHL	MG-NA	12.60	2.36	2.06
29	7	304	LUT	C34-C33	12.56	1.52	1.35
27	3	309	CHL	MG-NA	12.56	2.36	2.06
27	7	313	CHL	MG-NA	12.53	2.36	2.06
29	J	103	LUT	C5-C6	12.52	1.56	1.34
27	6	309	CHL	MG-NA	12.51	2.36	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	323	CHL	MG-NC	12.47	2.35	2.06
27	A	836	CHL	MG-NA	12.46	2.35	2.06
27	B	816	CHL	MG-NC	12.44	2.35	2.06
27	6	317	CHL	MG-NC	12.40	2.35	2.06
29	5	302	LUT	C5-C6	12.40	1.55	1.34
29	3	304	LUT	C5-C6	12.39	1.55	1.34
27	B	825	CHL	MG-NC	12.39	2.35	2.06
29	4	301	LUT	C5-C6	12.35	1.55	1.34
29	a	302	LUT	C5-C6	12.35	1.55	1.34
29	6	303	LUT	C5-C6	12.30	1.55	1.34
27	5	319	CHL	MG-ND	12.22	2.30	2.05
27	4	305	CHL	MG-NA	12.16	2.35	2.06
29	5	303	LUT	C5-C6	12.14	1.55	1.34
27	K	206	CHL	MG-NA	12.08	2.35	2.06
29	b	301	LUT	C5-C6	12.05	1.55	1.34
27	5	311	CHL	MG-NA	11.93	2.34	2.06
27	a	312	CHL	MG-NC	11.89	2.34	2.06
27	6	306	CHL	MG-ND	11.85	2.29	2.05
29	F	303	LUT	C5-C6	11.83	1.54	1.34
27	a	312	CHL	MG-ND	11.81	2.29	2.05
27	3	312	CHL	MG-NA	11.79	2.34	2.06
27	B	813	CHL	MG-NA	11.77	2.34	2.06
27	4	316	CHL	MG-ND	11.67	2.28	2.05
27	B	822	CHL	MG-NC	11.63	2.33	2.06
27	B	812	CHL	MG-NA	11.61	2.33	2.06
27	b	313	CHL	MG-ND	-11.59	1.82	2.05
27	A	817	CHL	MG-NC	11.58	2.33	2.06
27	F	308	CHL	MG-NC	11.57	2.33	2.06
27	A	854	CHL	MG-NA	11.53	2.33	2.06
27	b	311	CHL	MG-NC	11.51	2.33	2.06
27	A	825	CHL	MG-NA	11.49	2.33	2.06
27	B	838	CHL	MG-NC	11.47	2.33	2.06
27	6	316	CHL	MG-NC	11.47	2.33	2.06
29	8	304	LUT	C5-C6	11.46	1.54	1.34
29	a	304	LUT	C5-C6	11.45	1.54	1.34
29	4	302	LUT	C5-C6	11.42	1.54	1.34
27	b	308	CHL	MG-NC	11.31	2.33	2.06
27	A	840	CHL	MG-NC	11.28	2.33	2.06
27	5	308	CHL	MG-NA	11.24	2.33	2.06
27	A	857	CHL	MG-NA	11.22	2.32	2.06
29	6	302	LUT	C5-C6	11.19	1.53	1.34
27	A	844	CHL	MG-NC	11.17	2.32	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	305	CHL	MG-ND	11.14	2.27	2.05
29	3	305	LUT	C5-C6	11.13	1.53	1.34
29	8	303	LUT	C5-C6	11.01	1.53	1.34
27	3	317	CHL	MG-NA	10.99	2.32	2.06
27	3	308	CHL	MG-NA	10.96	2.32	2.06
27	B	839	CHL	MG-NA	10.93	2.32	2.06
27	7	314	CHL	MG-ND	10.84	2.27	2.05
27	a	308	CHL	MG-NA	10.83	2.32	2.06
27	J	106	CHL	MG-ND	10.80	2.27	2.05
27	7	318	CHL	MG-NA	10.73	2.31	2.06
27	a	318	CHL	MG-ND	10.72	2.27	2.05
27	4	313	CHL	MG-NC	10.72	2.31	2.06
27	B	811	CHL	MG-NC	10.72	2.31	2.06
27	b	305	CHL	MG-NC	10.71	2.31	2.06
27	4	314	CHL	MG-NC	10.68	2.31	2.06
27	3	311	CHL	MG-NA	10.63	2.31	2.06
27	8	320	CHL	MG-NA	10.55	2.31	2.06
27	A	824	CHL	MG-NA	10.53	2.31	2.06
27	6	318	CHL	MG-ND	10.49	2.26	2.05
27	K	205	CHL	MG-NA	10.46	2.31	2.06
27	a	320	CHL	MG-NC	10.45	2.31	2.06
27	8	316	CHL	MG-NC	10.44	2.31	2.06
27	B	848	CHL	MG-NC	10.40	2.31	2.06
27	B	830	CHL	MG-NA	10.40	2.31	2.06
27	4	307	CHL	MG-NA	10.39	2.30	2.06
27	A	822	CHL	MG-NA	10.37	2.30	2.06
27	B	823	CHL	MG-NC	10.36	2.30	2.06
27	A	849	CHL	MG-NA	10.33	2.30	2.06
27	7	312	CHL	MG-NC	10.30	2.30	2.06
27	5	318	CHL	MG-NC	10.28	2.30	2.06
27	b	317	CHL	MG-ND	10.28	2.26	2.05
27	7	323	CHL	MG-NC	10.26	2.30	2.06
27	5	322	CHL	MG-ND	10.24	2.26	2.05
27	B	824	CHL	MG-NA	10.24	2.30	2.06
27	B	818	CHL	MG-NA	10.23	2.30	2.06
27	8	311	CHL	MG-NA	10.21	2.30	2.06
27	A	853	CHL	MG-NA	10.16	2.30	2.06
27	8	325	CHL	MG-NC	10.15	2.30	2.06
27	A	848	CHL	MG-NA	10.09	2.30	2.06
27	6	313	CHL	MG-ND	-10.09	1.85	2.05
27	J	106	CHL	MG-NC	10.01	2.30	2.06
27	6	311	CHL	MG-ND	-9.86	1.86	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	828	CHL	MG-NC	9.85	2.29	2.06
27	B	829	CHL	MG-NA	9.84	2.29	2.06
27	A	820	CHL	MG-NA	9.83	2.29	2.06
27	B	836	CHL	MG-NA	9.82	2.29	2.06
27	8	322	CHL	MG-NA	9.80	2.29	2.06
27	a	319	CHL	MG-NA	9.76	2.29	2.06
27	A	858	CHL	MG-NC	9.73	2.29	2.06
27	6	307	CHL	C1D-ND	9.72	1.49	1.37
27	3	312	CHL	MG-ND	-9.65	1.86	2.05
27	7	316	CHL	MG-NA	9.62	2.29	2.06
27	A	835	CHL	MG-NA	9.61	2.29	2.06
27	6	313	CHL	MG-NA	9.59	2.29	2.06
27	B	821	CHL	MG-NA	9.59	2.29	2.06
27	4	309	CHL	MG-NA	9.56	2.29	2.06
27	a	320	CHL	MG-ND	-9.55	1.86	2.05
27	5	313	CHL	C1D-ND	9.51	1.49	1.37
27	5	318	CHL	MG-ND	-9.49	1.87	2.05
27	6	311	CHL	MG-NC	9.48	2.28	2.06
27	8	318	CHL	MG-ND	-9.47	1.87	2.05
27	A	831	CHL	C1D-ND	9.45	1.49	1.37
27	A	822	CHL	MG-NC	9.43	2.28	2.06
27	4	319	CHL	MG-NC	9.41	2.28	2.06
27	B	819	CHL	MG-NC	9.37	2.28	2.06
27	b	309	CHL	MG-ND	9.35	2.24	2.05
27	A	843	CHL	C1D-ND	9.32	1.49	1.37
27	4	310	CHL	MG-ND	-9.30	1.87	2.05
27	b	316	CHL	MG-NC	9.29	2.28	2.06
27	a	315	CHL	MG-NC	9.25	2.28	2.06
27	8	321	CHL	MG-NC	9.24	2.28	2.06
27	B	844	CHL	MG-NC	9.21	2.28	2.06
27	A	819	CHL	MG-NA	9.20	2.28	2.06
27	K	207	CHL	MG-ND	9.18	2.24	2.05
27	6	306	CHL	MG-NC	-9.17	1.84	2.06
27	B	828	CHL	MG-NC	9.16	2.28	2.06
27	A	839	CHL	MG-NC	9.14	2.28	2.06
27	A	846	CHL	C1D-ND	9.12	1.49	1.37
27	A	816	CHL	MG-NA	9.08	2.27	2.06
27	7	315	CHL	MG-NC	9.05	2.27	2.06
27	4	313	CHL	MG-NA	9.02	2.27	2.06
27	A	836	CHL	MG-ND	9.01	2.23	2.05
27	F	309	CHL	MG-NA	9.00	2.27	2.06
27	4	315	CHL	MG-NA	8.97	2.27	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	820	CHL	MG-NC	8.88	2.27	2.06
27	A	821	CHL	MG-NA	8.86	2.27	2.06
27	b	317	CHL	MG-NC	8.84	2.27	2.06
27	8	315	CHL	MG-NA	8.81	2.27	2.06
27	A	855	CHL	MG-NA	8.77	2.27	2.06
27	B	835	CHL	MG-NC	8.72	2.27	2.06
27	B	848	CHL	MG-NA	8.67	2.26	2.06
27	b	315	CHL	MG-NA	8.64	2.26	2.06
27	6	310	CHL	MG-NC	8.62	2.26	2.06
27	5	315	CHL	MG-ND	8.59	2.22	2.05
27	a	317	CHL	MG-NC	8.59	2.26	2.06
27	L	303	CHL	C1D-ND	8.58	1.48	1.37
27	A	837	CHL	MG-NA	8.58	2.26	2.06
27	a	313	CHL	MG-NA	8.57	2.26	2.06
27	A	829	CHL	MG-NC	8.53	2.26	2.06
27	A	851	CHL	MG-NA	8.50	2.26	2.06
27	B	814	CHL	MG-NA	8.50	2.26	2.06
27	a	316	CHL	MG-NC	8.49	2.26	2.06
27	A	823	CHL	MG-NC	8.47	2.26	2.06
27	8	319	CHL	MG-ND	-8.45	1.89	2.05
27	B	836	CHL	MG-NC	8.44	2.26	2.06
27	3	318	CHL	MG-NC	8.43	2.26	2.06
27	B	820	CHL	MG-NA	8.42	2.26	2.06
27	5	322	CHL	MG-NC	8.40	2.26	2.06
27	6	317	CHL	MG-NA	-8.39	1.86	2.06
27	3	315	CHL	MG-NA	8.38	2.26	2.06
27	7	321	CHL	MG-NC	8.38	2.26	2.06
27	B	832	CHL	MG-NA	8.38	2.26	2.06
27	4	306	CHL	MG-NA	8.36	2.26	2.06
27	B	835	CHL	MG-NA	8.33	2.26	2.06
27	3	313	CHL	MG-NC	8.27	2.25	2.06
27	a	314	CHL	MG-NC	8.27	2.25	2.06
27	B	817	CHL	MG-NA	8.24	2.25	2.06
27	A	850	CHL	MG-NC	8.24	2.25	2.06
27	A	835	CHL	MG-ND	-8.20	1.89	2.05
27	5	320	CHL	MG-NC	8.20	2.25	2.06
27	b	314	CHL	MG-NA	8.18	2.25	2.06
27	B	845	CHL	MG-NA	8.15	2.25	2.06
27	6	310	CHL	MG-NA	8.09	2.25	2.06
27	B	833	CHL	MG-NA	8.08	2.25	2.06
27	A	818	CHL	MG-NC	8.07	2.25	2.06
27	4	313	CHL	C1D-ND	8.06	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	310	CHL	MG-ND	-8.06	1.89	2.05
27	A	854	CHL	MG-NC	8.05	2.25	2.06
27	b	310	CHL	MG-NA	8.04	2.25	2.06
27	A	825	CHL	MG-NC	8.03	2.25	2.06
27	4	320	CHL	MG-NA	8.03	2.25	2.06
27	b	308	CHL	MG-NA	8.01	2.25	2.06
27	B	817	CHL	MG-NC	7.97	2.25	2.06
27	5	309	CHL	MG-NA	7.96	2.25	2.06
27	B	841	CHL	MG-NA	7.95	2.25	2.06
27	K	204	CHL	MG-NA	7.94	2.25	2.06
27	7	315	CHL	MG-NA	7.93	2.25	2.06
27	B	842	CHL	MG-ND	7.93	2.21	2.05
27	5	312	CHL	MG-NC	-7.88	1.87	2.06
27	5	315	CHL	MG-NA	7.88	2.25	2.06
27	A	842	CHL	MG-NA	7.85	2.24	2.06
27	7	311	CHL	MG-NA	7.82	2.24	2.06
27	7	317	CHL	MG-NC	7.82	2.24	2.06
27	5	307	CHL	MG-NC	-7.81	1.87	2.06
27	A	830	CHL	MG-NA	7.80	2.24	2.06
27	b	310	CHL	MG-NC	7.78	2.24	2.06
27	8	323	CHL	MG-NA	7.77	2.24	2.06
27	B	831	CHL	MG-NA	7.75	2.24	2.06
27	6	318	CHL	MG-NC	7.75	2.24	2.06
27	6	305	CHL	MG-NC	7.68	2.24	2.06
27	7	323	CHL	MG-NA	7.67	2.24	2.06
27	8	323	CHL	C1D-ND	7.65	1.47	1.37
27	A	827	CHL	MG-NC	7.64	2.24	2.06
27	A	859	CHL	MG-ND	-7.64	1.90	2.05
27	6	315	CHL	MG-ND	7.63	2.20	2.05
27	5	310	CHL	MG-NC	-7.62	1.88	2.06
27	A	827	CHL	MG-NA	7.60	2.24	2.06
27	B	849	CHL	MG-NA	7.58	2.24	2.06
27	A	858	CHL	MG-NA	7.55	2.24	2.06
27	A	837	CHL	MG-ND	-7.49	1.90	2.05
27	8	317	CHL	MG-NA	7.47	2.24	2.06
27	b	307	CHL	MG-NC	7.46	2.24	2.06
27	B	815	CHL	MG-ND	-7.42	1.91	2.05
27	B	838	CHL	MG-NA	7.42	2.23	2.06
27	A	856	CHL	MG-NC	7.42	2.23	2.06
27	7	324	CHL	MG-NA	7.40	2.23	2.06
27	b	314	CHL	MG-NC	7.40	2.23	2.06
27	a	315	CHL	MG-ND	7.38	2.20	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	312	CHL	MG-NA	7.38	2.23	2.06
27	A	834	CHL	MG-NC	7.38	2.23	2.06
27	A	819	CHL	MG-NC	7.37	2.23	2.06
27	3	310	CHL	MG-NA	7.37	2.23	2.06
27	F	308	CHL	MG-ND	7.37	2.20	2.05
27	3	313	CHL	MG-ND	7.35	2.20	2.05
27	A	840	CHL	MG-ND	-7.30	1.91	2.05
27	K	204	CHL	MG-NC	7.30	2.23	2.06
27	4	306	CHL	MG-NC	7.30	2.23	2.06
27	B	815	CHL	MG-NA	7.30	2.23	2.06
27	A	856	CHL	MG-NA	7.30	2.23	2.06
27	B	819	CHL	MG-NA	7.25	2.23	2.06
27	A	855	CHL	MG-NC	7.25	2.23	2.06
27	B	827	CHL	MG-NA	7.24	2.23	2.06
27	7	318	CHL	MG-NC	7.22	2.23	2.06
27	4	317	CHL	C1D-ND	7.21	1.46	1.37
27	A	830	CHL	MG-NC	7.15	2.23	2.06
27	A	853	CHL	MG-NC	7.14	2.23	2.06
27	3	320	CHL	MG-NA	7.12	2.23	2.06
26	A	815	CL0	C1D-ND	7.11	1.46	1.37
27	L	304	CHL	MG-NA	7.09	2.23	2.06
27	A	834	CHL	MG-NA	7.09	2.23	2.06
27	6	310	CHL	MG-ND	-7.06	1.91	2.05
27	8	320	CHL	MG-NC	7.04	2.23	2.06
27	b	315	CHL	MG-NC	7.04	2.23	2.06
27	A	839	CHL	MG-NA	7.03	2.23	2.06
27	K	206	CHL	MG-ND	7.00	2.19	2.05
27	8	314	CHL	MG-NA	6.95	2.22	2.06
27	B	814	CHL	MG-NC	6.93	2.22	2.06
27	3	316	CHL	MG-NA	6.88	2.22	2.06
27	B	846	CHL	MG-NC	6.88	2.22	2.06
27	7	322	CHL	MG-ND	6.88	2.19	2.05
27	A	821	CHL	MG-NC	6.81	2.22	2.06
27	b	307	CHL	MG-NA	6.80	2.22	2.06
27	5	317	CHL	MG-NC	6.80	2.22	2.06
27	B	824	CHL	MG-NC	6.79	2.22	2.06
27	B	846	CHL	MG-NA	6.77	2.22	2.06
27	4	318	CHL	MG-ND	6.77	2.19	2.05
27	4	320	CHL	MG-ND	-6.75	1.92	2.05
27	4	318	CHL	MG-NC	-6.74	1.90	2.06
27	A	817	CHL	MG-NA	6.71	2.22	2.06
27	A	829	CHL	MG-NA	6.69	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	319	CHL	MG-NA	6.68	2.22	2.06
27	K	207	CHL	MG-NA	-6.68	1.90	2.06
27	A	849	CHL	MG-NC	6.65	2.22	2.06
27	L	304	CHL	MG-NC	6.65	2.22	2.06
27	a	308	CHL	MG-NC	6.62	2.22	2.06
27	a	314	CHL	MG-NA	6.60	2.21	2.06
27	A	835	CHL	MG-NC	6.59	2.21	2.06
27	7	317	CHL	MG-NA	6.59	2.21	2.06
27	5	309	CHL	MG-NC	6.57	2.21	2.06
27	A	832	CHL	MG-NA	6.54	2.21	2.06
27	4	316	CHL	MG-NC	6.49	2.21	2.06
27	4	320	CHL	MG-NC	6.49	2.21	2.06
27	A	850	CHL	MG-NA	6.46	2.21	2.06
27	F	309	CHL	MG-NC	6.46	2.21	2.06
27	B	832	CHL	MG-NC	6.41	2.21	2.06
27	B	822	CHL	MG-NA	6.40	2.21	2.06
27	7	321	CHL	MG-ND	-6.38	1.93	2.05
27	5	308	CHL	MG-NC	6.37	2.21	2.06
27	7	323	CHL	C1D-ND	6.36	1.45	1.37
27	4	319	CHL	MG-ND	-6.34	1.93	2.05
27	A	844	CHL	MG-NA	6.33	2.21	2.06
27	b	308	CHL	C3C-C2C	6.30	1.50	1.36
27	B	815	CHL	MG-NC	6.26	2.21	2.06
27	7	324	CHL	MG-NC	6.24	2.21	2.06
27	B	831	CHL	MG-NC	6.23	2.21	2.06
27	B	849	CHL	MG-ND	-6.17	1.93	2.05
27	4	317	CHL	MG-NC	6.14	2.20	2.06
27	6	316	CHL	MG-NA	-6.11	1.91	2.06
27	A	827	CHL	MG-ND	-6.10	1.93	2.05
27	5	320	CHL	MG-NA	6.09	2.20	2.06
27	3	309	CHL	MG-ND	6.09	2.17	2.05
27	8	313	CHL	MG-ND	-6.09	1.93	2.05
27	3	318	CHL	MG-NA	6.08	2.20	2.06
27	K	205	CHL	MG-ND	-6.07	1.93	2.05
27	5	315	CHL	MG-NC	6.06	2.20	2.06
27	A	828	CHL	MG-NA	6.04	2.20	2.06
27	A	821	CHL	MG-ND	-6.03	1.93	2.05
27	8	324	CHL	MG-ND	5.95	2.17	2.05
27	4	308	CHL	MG-ND	5.92	2.17	2.05
27	A	840	CHL	MG-NA	5.91	2.20	2.06
27	b	308	CHL	C4D-ND	5.90	1.45	1.37
27	B	827	CHL	MG-NC	5.87	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	841	CHL	MG-NC	5.87	2.20	2.06
27	7	316	CHL	C3C-C2C	5.87	1.48	1.36
27	B	848	CHL	MG-ND	5.86	2.17	2.05
27	A	841	CHL	MG-ND	5.86	2.17	2.05
27	B	825	CHL	MG-NA	5.85	2.20	2.06
27	A	833	CHL	MG-NC	5.84	2.20	2.06
27	4	311	CHL	MG-ND	5.84	2.17	2.05
27	7	311	CHL	MG-ND	-5.83	1.94	2.05
27	A	825	CHL	MG-ND	-5.78	1.94	2.05
27	8	317	CHL	MG-NC	5.75	2.19	2.06
27	4	319	CHL	C3C-C2C	5.74	1.48	1.36
27	5	325	CHL	MG-NC	5.74	2.19	2.06
27	B	814	CHL	C3B-C2B	5.73	1.48	1.40
27	4	305	CHL	MG-NC	5.71	2.19	2.06
27	B	830	CHL	MG-NC	5.70	2.19	2.06
27	B	845	CHL	MG-NC	5.70	2.19	2.06
27	7	312	CHL	C3C-C2C	5.69	1.47	1.36
27	4	319	CHL	C3B-C2B	5.69	1.48	1.40
27	A	833	CHL	MG-ND	5.68	2.17	2.05
27	A	842	CHL	MG-ND	5.67	2.17	2.05
27	B	811	CHL	MG-NA	5.64	2.19	2.06
27	B	845	CHL	C3B-C2B	5.63	1.48	1.40
27	A	832	CHL	C3B-C2B	5.63	1.48	1.40
27	L	304	CHL	C3B-C2B	5.63	1.48	1.40
27	B	833	CHL	MG-ND	5.62	2.16	2.05
27	B	850	CHL	C3B-C2B	5.61	1.48	1.40
27	A	845	CHL	MG-NC	5.60	2.19	2.06
27	8	326	CHL	C3B-C2B	5.60	1.48	1.40
27	A	857	CHL	C3B-C2B	5.60	1.48	1.40
27	a	319	CHL	C3C-C2C	5.60	1.48	1.36
27	B	850	CHL	MG-NA	5.59	2.19	2.06
27	b	314	CHL	MG-ND	-5.59	1.94	2.05
27	3	310	CHL	MG-NC	5.58	2.19	2.06
27	L	304	CHL	C3C-C2C	5.58	1.48	1.36
27	A	830	CHL	C3B-C2B	5.58	1.48	1.40
27	A	827	CHL	C3B-C2B	5.58	1.48	1.40
27	B	826	CHL	MG-ND	-5.57	1.94	2.05
27	b	308	CHL	CHC-C1C	5.56	1.49	1.35
27	A	840	CHL	C3B-C2B	5.56	1.48	1.40
27	5	307	CHL	C3B-C2B	5.55	1.48	1.40
27	b	306	CHL	C3B-C2B	5.55	1.48	1.40
27	A	858	CHL	MG-ND	5.55	2.16	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	843	CHL	C3B-C2B	5.54	1.48	1.40
27	A	816	CHL	C3B-C2B	5.54	1.48	1.40
27	8	319	CHL	C3B-C2B	5.54	1.48	1.40
27	8	316	CHL	MG-NA	5.54	2.19	2.06
27	A	852	CHL	C3B-C2B	5.53	1.48	1.40
27	3	320	CHL	C3B-C2B	5.53	1.48	1.40
27	B	839	CHL	C3B-C2B	5.52	1.48	1.40
27	a	307	CHL	MG-ND	5.52	2.16	2.05
27	4	310	CHL	C3C-C2C	5.51	1.48	1.36
27	b	308	CHL	C1D-ND	5.51	1.44	1.37
27	B	821	CHL	C3B-C2B	5.50	1.48	1.40
27	B	840	CHL	C3B-C2B	5.50	1.48	1.40
27	B	822	CHL	C3C-C2C	5.49	1.48	1.36
27	5	320	CHL	C3B-C2B	5.49	1.48	1.40
27	A	818	CHL	C3B-C2B	5.49	1.48	1.40
27	A	838	CHL	C3B-C2B	5.49	1.48	1.40
27	a	307	CHL	C3B-C2B	5.49	1.48	1.40
27	4	318	CHL	C3C-C2C	5.48	1.48	1.36
27	B	812	CHL	C3B-C2B	5.48	1.48	1.40
27	7	323	CHL	C3C-C2C	5.48	1.48	1.36
27	a	317	CHL	C3C-C2C	5.48	1.48	1.36
27	a	318	CHL	MG-NC	5.47	2.19	2.06
27	b	313	CHL	C3C-C2C	5.47	1.48	1.36
27	A	854	CHL	C3B-C2B	5.46	1.47	1.40
27	8	323	CHL	C3C-C2C	5.46	1.48	1.36
27	5	318	CHL	C3C-C2C	5.46	1.48	1.36
27	B	820	CHL	MG-ND	5.46	2.16	2.05
27	B	824	CHL	C3B-C2B	5.45	1.47	1.40
27	A	844	CHL	C3B-C2B	5.45	1.47	1.40
27	7	324	CHL	C3C-C2C	5.45	1.48	1.36
27	A	838	CHL	MG-NC	5.45	2.19	2.06
27	B	844	CHL	C3B-C2B	5.45	1.47	1.40
27	a	312	CHL	C3C-C2C	5.45	1.48	1.36
27	A	847	CHL	C3B-C2B	5.45	1.47	1.40
27	A	824	CHL	C3B-C2B	5.44	1.47	1.40
27	5	311	CHL	C3B-C2B	5.44	1.47	1.40
27	3	311	CHL	C3C-C2C	5.44	1.48	1.36
27	A	820	CHL	C3B-C2B	5.44	1.47	1.40
27	A	837	CHL	C3B-C2B	5.44	1.47	1.40
27	3	321	CHL	C3C-C2C	5.43	1.48	1.36
27	B	837	CHL	C3B-C2B	5.43	1.47	1.40
27	5	320	CHL	C3C-C2C	5.43	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	835	CHL	C3B-C2B	5.43	1.47	1.40
27	4	318	CHL	C3B-C2B	5.43	1.47	1.40
27	b	310	CHL	C3B-C2B	5.43	1.47	1.40
27	b	309	CHL	C3C-C2C	5.42	1.48	1.36
27	A	826	CHL	C3B-C2B	5.42	1.47	1.40
27	8	318	CHL	C3C-C2C	5.42	1.48	1.36
27	B	819	CHL	C3C-C2C	5.42	1.48	1.36
27	4	317	CHL	C3C-C2C	5.42	1.48	1.36
27	3	320	CHL	CHC-C1C	5.42	1.48	1.35
27	b	309	CHL	C3B-C2B	5.41	1.47	1.40
27	B	825	CHL	C3B-C2B	5.41	1.47	1.40
27	3	318	CHL	C3B-C2B	5.41	1.47	1.40
27	b	312	CHL	C3B-C2B	5.41	1.47	1.40
27	3	308	CHL	C3B-C2B	5.41	1.47	1.40
27	6	311	CHL	C3B-C2B	5.41	1.47	1.40
27	b	314	CHL	C3B-C2B	5.41	1.47	1.40
27	b	304	CHL	C3C-C2C	5.41	1.48	1.36
27	b	313	CHL	C3B-C2B	5.40	1.47	1.40
27	6	314	CHL	C3C-C2C	5.40	1.48	1.36
27	a	313	CHL	C3C-C2C	5.40	1.48	1.36
27	4	319	CHL	CHC-C1C	5.40	1.48	1.35
27	7	314	CHL	C3B-C2B	5.40	1.47	1.40
27	a	311	CHL	C3B-C2B	5.40	1.47	1.40
27	b	316	CHL	MG-ND	5.40	2.16	2.05
27	B	849	CHL	MG-NC	5.40	2.19	2.06
27	B	833	CHL	C3B-C2B	5.39	1.47	1.40
27	4	320	CHL	C3C-C2C	5.39	1.48	1.36
27	b	315	CHL	C3C-C2C	5.38	1.48	1.36
27	b	310	CHL	C3C-C2C	5.38	1.48	1.36
27	8	312	CHL	C3B-C2B	5.38	1.47	1.40
27	B	851	CHL	CHC-C1C	5.38	1.48	1.35
27	5	315	CHL	C3C-C2C	5.37	1.48	1.36
27	8	319	CHL	MG-NC	5.37	2.19	2.06
27	K	206	CHL	C3C-C2C	5.37	1.48	1.36
27	4	305	CHL	C3C-C2C	5.37	1.48	1.36
27	A	836	CHL	C3C-C2C	5.37	1.48	1.36
27	3	312	CHL	C3B-C2B	5.37	1.47	1.40
27	a	314	CHL	C3C-C2C	5.37	1.48	1.36
27	b	305	CHL	CHD-C1D	5.36	1.48	1.38
27	B	840	CHL	C3C-C2C	5.36	1.48	1.36
27	B	836	CHL	C3B-C2B	5.36	1.47	1.40
27	4	304	CHL	C3B-C2B	5.36	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	310	CHL	C3B-C2B	5.36	1.47	1.40
27	3	319	CHL	C3C-C2C	5.36	1.48	1.36
27	B	848	CHL	C3C-C2C	5.36	1.48	1.36
27	K	205	CHL	C3C-C2C	5.36	1.48	1.36
27	A	845	CHL	C3C-C2C	5.36	1.48	1.36
27	4	315	CHL	C3C-C2C	5.35	1.48	1.36
27	6	309	CHL	C3C-C2C	5.35	1.48	1.36
27	3	314	CHL	C3B-C2B	5.35	1.47	1.40
27	b	315	CHL	C3B-C2B	5.35	1.47	1.40
27	a	313	CHL	C3B-C2B	5.35	1.47	1.40
27	A	816	CHL	C3C-C2C	5.35	1.48	1.36
27	B	814	CHL	C3C-C2C	5.35	1.48	1.36
27	B	834	CHL	C3B-C2B	5.34	1.47	1.40
27	6	305	CHL	C3B-C2B	5.34	1.47	1.40
27	B	843	CHL	C3C-C2C	5.34	1.48	1.36
27	a	317	CHL	C3B-C2B	5.34	1.47	1.40
27	4	315	CHL	C3B-C2B	5.34	1.47	1.40
27	7	315	CHL	C3B-C2B	5.34	1.47	1.40
27	8	316	CHL	C3B-C2B	5.34	1.47	1.40
27	A	817	CHL	C3B-C2B	5.34	1.47	1.40
27	3	321	CHL	C3B-C2B	5.34	1.47	1.40
27	4	311	CHL	C3C-C2C	5.34	1.48	1.36
27	a	311	CHL	C3C-C2C	5.33	1.48	1.36
27	8	315	CHL	CHC-C1C	5.33	1.48	1.35
27	5	321	CHL	C3C-C2C	5.33	1.48	1.36
27	5	314	CHL	C3C-C2C	5.33	1.48	1.36
27	B	828	CHL	C3C-C2C	5.33	1.48	1.36
27	8	311	CHL	C3C-C2C	5.33	1.48	1.36
27	4	310	CHL	C3B-C2B	5.33	1.47	1.40
27	5	312	CHL	C3C-C2C	5.33	1.48	1.36
27	8	317	CHL	C3C-C2C	5.33	1.48	1.36
27	A	819	CHL	C3B-C2B	5.32	1.47	1.40
27	A	854	CHL	C3C-C2C	5.32	1.48	1.36
27	B	826	CHL	C3C-C2C	5.32	1.48	1.36
27	B	837	CHL	C3C-C2C	5.32	1.48	1.36
27	6	314	CHL	C3B-C2B	5.32	1.47	1.40
27	b	305	CHL	C3C-C2C	5.32	1.48	1.36
27	A	851	CHL	C3C-C2C	5.32	1.48	1.36
27	a	308	CHL	C3C-C2C	5.32	1.48	1.36
27	6	316	CHL	MG-ND	5.32	2.16	2.05
27	b	312	CHL	C3C-C2C	5.32	1.48	1.36
27	B	831	CHL	C3B-C2B	5.32	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	850	CHL	C3C-C2C	5.32	1.48	1.36
27	3	309	CHL	C3C-C2C	5.32	1.48	1.36
27	b	307	CHL	C3C-C2C	5.32	1.48	1.36
27	8	324	CHL	MG-NC	5.32	2.18	2.06
27	B	849	CHL	C3B-C2B	5.31	1.47	1.40
27	A	840	CHL	C3C-C2C	5.31	1.48	1.36
27	6	311	CHL	CHC-C1C	5.31	1.48	1.35
27	B	819	CHL	C3B-C2B	5.31	1.47	1.40
27	3	319	CHL	C3B-C2B	5.31	1.47	1.40
27	4	319	CHL	CHD-C1D	5.31	1.48	1.38
27	A	829	CHL	C3C-C2C	5.31	1.48	1.36
27	6	315	CHL	C3B-C2B	5.31	1.47	1.40
27	8	319	CHL	C3C-C2C	5.31	1.48	1.36
27	b	314	CHL	C3C-C2C	5.31	1.48	1.36
27	B	829	CHL	C3B-C2B	5.30	1.47	1.40
27	4	320	CHL	O2D-CGD	5.30	1.46	1.33
27	B	839	CHL	C3C-C2C	5.30	1.48	1.36
27	8	315	CHL	C3B-C2B	5.30	1.47	1.40
27	K	205	CHL	C3B-C2B	5.30	1.47	1.40
27	B	823	CHL	C3C-C2C	5.30	1.48	1.36
27	6	320	CHL	C3C-C2C	5.30	1.48	1.36
27	B	830	CHL	C3C-C2C	5.30	1.48	1.36
27	A	819	CHL	CHC-C1C	5.30	1.48	1.35
27	b	310	CHL	CHC-C1C	5.30	1.48	1.35
27	A	848	CHL	C3C-C2C	5.29	1.48	1.36
27	8	325	CHL	C3C-C2C	5.29	1.48	1.36
27	A	844	CHL	C3C-C2C	5.29	1.48	1.36
27	A	822	CHL	C3B-C2B	5.29	1.47	1.40
27	B	826	CHL	C3B-C2B	5.29	1.47	1.40
27	A	853	CHL	C3C-C2C	5.29	1.48	1.36
27	3	315	CHL	C3C-C2C	5.29	1.48	1.36
27	L	304	CHL	O2D-CGD	5.29	1.46	1.33
27	A	849	CHL	C3C-C2C	5.29	1.48	1.36
27	B	816	CHL	C3B-C2B	5.29	1.47	1.40
27	b	315	CHL	CHC-C1C	5.29	1.48	1.35
27	B	835	CHL	C3C-C2C	5.29	1.48	1.36
27	b	304	CHL	C3B-C2B	5.28	1.47	1.40
27	b	310	CHL	CHD-C1D	5.28	1.48	1.38
27	3	310	CHL	C3C-C2C	5.28	1.48	1.36
27	B	823	CHL	C3B-C2B	5.28	1.47	1.40
27	b	306	CHL	C3C-C2C	5.28	1.48	1.36
27	B	814	CHL	CHC-C1C	5.28	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	320	CHL	C3C-C2C	5.28	1.48	1.36
27	a	319	CHL	C3B-C2B	5.28	1.47	1.40
27	B	844	CHL	C3C-C2C	5.28	1.47	1.36
27	3	312	CHL	C3C-C2C	5.28	1.47	1.36
27	6	315	CHL	C3C-C2C	5.28	1.47	1.36
27	4	307	CHL	C3B-C2B	5.28	1.47	1.40
27	5	320	CHL	CHC-C1C	5.28	1.48	1.35
27	A	825	CHL	C3C-C2C	5.28	1.47	1.36
27	A	828	CHL	C3B-C2B	5.28	1.47	1.40
27	B	832	CHL	C3B-C2B	5.28	1.47	1.40
27	A	835	CHL	C3C-C2C	5.27	1.47	1.36
27	B	820	CHL	C3B-C2B	5.27	1.47	1.40
27	A	838	CHL	C3C-C2C	5.27	1.47	1.36
27	B	831	CHL	C3C-C2C	5.27	1.47	1.36
27	A	822	CHL	CHC-C1C	5.27	1.48	1.35
27	6	312	CHL	C3C-C2C	5.27	1.47	1.36
27	B	833	CHL	C3C-C2C	5.27	1.47	1.36
27	7	317	CHL	C3B-C2B	5.27	1.47	1.40
27	6	314	CHL	CHC-C1C	5.27	1.48	1.35
27	3	310	CHL	C3B-C2B	5.27	1.47	1.40
27	4	307	CHL	C3C-C2C	5.27	1.47	1.36
27	A	858	CHL	C3C-C2C	5.27	1.47	1.36
27	7	324	CHL	C3B-C2B	5.27	1.47	1.40
27	5	310	CHL	CHC-C1C	5.27	1.48	1.35
27	B	840	CHL	CHC-C1C	5.27	1.48	1.35
27	A	822	CHL	C3C-C2C	5.26	1.47	1.36
27	a	320	CHL	C3B-C2B	5.26	1.47	1.40
27	b	306	CHL	CHC-C1C	5.26	1.48	1.35
27	K	206	CHL	O2D-CGD	5.26	1.46	1.33
27	7	317	CHL	C3C-C2C	5.26	1.47	1.36
27	5	314	CHL	C3B-C2B	5.26	1.47	1.40
27	J	106	CHL	C3C-C2C	5.26	1.47	1.36
27	5	309	CHL	C3C-C2C	5.26	1.47	1.36
27	8	322	CHL	C3B-C2B	5.26	1.47	1.40
27	7	311	CHL	C3B-C2B	5.26	1.47	1.40
27	A	830	CHL	C3C-C2C	5.26	1.47	1.36
27	B	838	CHL	C3C-C2C	5.25	1.47	1.36
27	B	820	CHL	C3C-C2C	5.25	1.47	1.36
27	A	850	CHL	C3C-C2C	5.25	1.47	1.36
27	7	313	CHL	C3C-C2C	5.25	1.47	1.36
27	4	318	CHL	CHC-C1C	5.25	1.48	1.35
27	b	308	CHL	C3B-C2B	5.25	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	816	CHL	CHC-C1C	5.25	1.48	1.35
27	A	847	CHL	C3C-C2C	5.25	1.47	1.36
27	8	312	CHL	CHC-C1C	5.25	1.48	1.35
27	a	314	CHL	CHC-C1C	5.25	1.48	1.35
27	3	314	CHL	CHC-C1C	5.25	1.48	1.35
27	4	315	CHL	CHC-C1C	5.25	1.48	1.35
27	5	307	CHL	CHC-C1C	5.25	1.48	1.35
27	B	817	CHL	C3C-C2C	5.25	1.47	1.36
27	7	314	CHL	CHC-C1C	5.25	1.48	1.35
27	F	308	CHL	C3C-C2C	5.24	1.47	1.36
27	3	318	CHL	C3C-C2C	5.24	1.47	1.36
27	B	824	CHL	C3C-C2C	5.24	1.47	1.36
27	A	856	CHL	C3B-C2B	5.24	1.47	1.40
27	a	308	CHL	C3B-C2B	5.24	1.47	1.40
27	A	827	CHL	CHC-C1C	5.24	1.48	1.35
27	F	309	CHL	C3C-C2C	5.24	1.47	1.36
27	A	826	CHL	C3C-C2C	5.24	1.47	1.36
27	5	308	CHL	C3C-C2C	5.24	1.47	1.36
27	6	313	CHL	C3C-C2C	5.24	1.47	1.36
27	a	307	CHL	CHC-C1C	5.24	1.48	1.35
27	6	310	CHL	C3C-C2C	5.24	1.47	1.36
27	a	319	CHL	MG-ND	-5.24	1.95	2.05
27	L	304	CHL	CHD-C1D	5.24	1.48	1.38
27	6	320	CHL	C3B-C2B	5.24	1.47	1.40
27	7	315	CHL	C3C-C2C	5.24	1.47	1.36
27	3	314	CHL	C3C-C2C	5.24	1.47	1.36
27	4	310	CHL	CHC-C1C	5.24	1.48	1.35
27	B	847	CHL	C3C-C2C	5.24	1.47	1.36
27	6	315	CHL	O2D-CGD	5.24	1.46	1.33
27	5	309	CHL	C3B-C2B	5.23	1.47	1.40
27	8	311	CHL	C3B-C2B	5.23	1.47	1.40
27	A	834	CHL	C3C-C2C	5.23	1.47	1.36
27	A	820	CHL	CHC-C1C	5.23	1.48	1.35
27	7	317	CHL	MG-ND	-5.23	1.95	2.05
27	b	314	CHL	CHC-C1C	5.23	1.48	1.35
27	B	836	CHL	C3C-C2C	5.23	1.47	1.36
27	a	314	CHL	C3B-C2B	5.23	1.47	1.40
27	A	828	CHL	C3C-C2C	5.23	1.47	1.36
27	6	305	CHL	C3C-C2C	5.23	1.47	1.36
27	a	308	CHL	O2D-CGD	5.22	1.45	1.33
27	A	827	CHL	C3C-C2C	5.22	1.47	1.36
27	4	314	CHL	CHC-C1C	5.22	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	316	CHL	C3C-C2C	5.22	1.47	1.36
27	a	312	CHL	CHC-C1C	5.22	1.48	1.35
27	6	310	CHL	CHC-C1C	5.22	1.48	1.35
27	6	305	CHL	MG-NA	5.22	2.18	2.06
27	5	311	CHL	O2D-CGD	5.22	1.45	1.33
27	4	306	CHL	C3B-C2B	5.22	1.47	1.40
27	a	320	CHL	C3C-C2C	5.22	1.47	1.36
27	B	850	CHL	CHC-C1C	5.22	1.48	1.35
27	6	313	CHL	CHD-C1D	5.22	1.48	1.38
27	4	311	CHL	CHC-C1C	5.22	1.48	1.35
27	6	312	CHL	C3B-C2B	5.22	1.47	1.40
27	3	309	CHL	CHC-C1C	5.22	1.48	1.35
27	L	304	CHL	CHC-C1C	5.22	1.48	1.35
27	B	813	CHL	CHC-C1C	5.21	1.48	1.35
27	B	841	CHL	C3B-C2B	5.21	1.47	1.40
27	4	318	CHL	CHD-C1D	5.21	1.48	1.38
27	A	821	CHL	C3C-C2C	5.21	1.47	1.36
27	6	309	CHL	C3B-C2B	5.21	1.47	1.40
27	6	313	CHL	C3B-C2B	5.21	1.47	1.40
27	4	306	CHL	C3C-C2C	5.21	1.47	1.36
27	B	849	CHL	CHC-C1C	5.21	1.48	1.35
27	B	847	CHL	CHC-C1C	5.21	1.48	1.35
27	b	313	CHL	CHC-C1C	5.21	1.48	1.35
27	K	204	CHL	C3C-C2C	5.21	1.47	1.36
27	a	309	CHL	C3C-C2C	5.21	1.47	1.36
27	A	853	CHL	C3B-C2B	5.21	1.47	1.40
27	b	304	CHL	CHC-C1C	5.21	1.48	1.35
27	b	309	CHL	CHD-C1D	5.21	1.48	1.38
27	B	849	CHL	C3C-C2C	5.21	1.47	1.36
27	8	312	CHL	C3C-C2C	5.21	1.47	1.36
27	B	813	CHL	C3B-C2B	5.21	1.47	1.40
27	K	205	CHL	CHC-C1C	5.21	1.48	1.35
27	a	310	CHL	C3B-C2B	5.20	1.47	1.40
27	B	820	CHL	CHC-C1C	5.20	1.48	1.35
27	A	829	CHL	C3B-C2B	5.20	1.47	1.40
27	b	307	CHL	O2D-CGD	5.20	1.45	1.33
27	A	859	CHL	C3C-C2C	5.20	1.47	1.36
27	b	304	CHL	O2D-CGD	5.20	1.45	1.33
27	B	834	CHL	C3C-C2C	5.20	1.47	1.36
27	A	817	CHL	C3C-C2C	5.20	1.47	1.36
27	3	313	CHL	C3C-C2C	5.20	1.47	1.36
27	5	307	CHL	C3C-C2C	5.20	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	857	CHL	O2D-CGD	5.20	1.45	1.33
27	7	314	CHL	C3C-C2C	5.20	1.47	1.36
27	5	320	CHL	O2D-CGD	5.20	1.45	1.33
27	a	313	CHL	CHC-C1C	5.20	1.48	1.35
27	B	835	CHL	CHC-C1C	5.20	1.48	1.35
27	A	855	CHL	C3C-C2C	5.20	1.47	1.36
27	A	859	CHL	C3B-C2B	5.20	1.47	1.40
27	B	816	CHL	C3C-C2C	5.20	1.47	1.36
27	8	319	CHL	CHC-C1C	5.19	1.48	1.35
27	3	321	CHL	CHC-C1C	5.19	1.48	1.35
27	A	837	CHL	C3C-C2C	5.19	1.47	1.36
27	a	312	CHL	CHD-C1D	5.19	1.48	1.38
27	B	844	CHL	CHC-C1C	5.19	1.48	1.35
27	3	309	CHL	C3B-C2B	5.19	1.47	1.40
27	7	324	CHL	CHC-C1C	5.19	1.48	1.35
27	5	323	CHL	C3C-C2C	5.19	1.47	1.36
27	F	309	CHL	CHC-C1C	5.19	1.48	1.35
27	b	312	CHL	CHC-C1C	5.19	1.48	1.35
27	5	321	CHL	CHC-C1C	5.19	1.48	1.35
27	a	320	CHL	CHC-C1C	5.19	1.48	1.35
27	B	829	CHL	C3C-C2C	5.19	1.47	1.36
27	b	310	CHL	O2D-CGD	5.19	1.45	1.33
27	b	312	CHL	O2D-CGD	5.19	1.45	1.33
27	3	321	CHL	O2D-CGD	5.18	1.45	1.33
27	A	823	CHL	C3C-C2C	5.18	1.47	1.36
27	a	310	CHL	CHC-C1C	5.18	1.48	1.35
27	5	315	CHL	C3B-C2B	5.18	1.47	1.40
27	b	307	CHL	CHC-C1C	5.18	1.48	1.35
27	A	851	CHL	C3B-C2B	5.18	1.47	1.40
27	6	315	CHL	CHC-C1C	5.18	1.48	1.35
27	a	308	CHL	CHC-C1C	5.18	1.48	1.35
27	5	321	CHL	C3B-C2B	5.18	1.47	1.40
27	J	106	CHL	C3B-C2B	5.18	1.47	1.40
27	A	836	CHL	CHC-C1C	5.18	1.48	1.35
27	6	313	CHL	CHC-C1C	5.17	1.48	1.35
27	B	831	CHL	CHC-C1C	5.17	1.48	1.35
27	B	832	CHL	C3C-C2C	5.17	1.47	1.36
27	8	318	CHL	CHC-C1C	5.17	1.48	1.35
27	A	823	CHL	C3B-C2B	5.17	1.47	1.40
27	B	846	CHL	C3C-C2C	5.17	1.47	1.36
27	A	823	CHL	CHC-C1C	5.17	1.48	1.35
27	B	823	CHL	CHC-C1C	5.17	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	318	CHL	CHC-C1C	5.17	1.48	1.35
27	6	320	CHL	CHC-C1C	5.17	1.48	1.35
27	B	821	CHL	C3C-C2C	5.17	1.47	1.36
27	B	841	CHL	CHC-C1C	5.17	1.48	1.35
27	3	319	CHL	CHC-C1C	5.17	1.48	1.35
27	7	318	CHL	C3C-C2C	5.17	1.47	1.36
27	3	319	CHL	CHD-C1D	5.17	1.48	1.38
27	A	851	CHL	CHC-C1C	5.17	1.48	1.35
27	a	311	CHL	CHC-C1C	5.17	1.48	1.35
27	4	305	CHL	C3B-C2B	5.17	1.47	1.40
27	5	312	CHL	C3B-C2B	5.17	1.47	1.40
27	8	317	CHL	CHC-C1C	5.17	1.48	1.35
27	3	310	CHL	CHC-C1C	5.17	1.48	1.35
27	5	314	CHL	CHC-C1C	5.17	1.48	1.35
27	b	309	CHL	O2D-CGD	5.17	1.45	1.33
27	A	836	CHL	C3B-C2B	5.17	1.47	1.40
27	F	308	CHL	C3B-C2B	5.16	1.47	1.40
27	5	318	CHL	C3B-C2B	5.16	1.47	1.40
27	5	315	CHL	CHC-C1C	5.16	1.48	1.35
27	K	204	CHL	C3B-C2B	5.16	1.47	1.40
27	8	313	CHL	C3B-C2B	5.16	1.47	1.40
27	4	308	CHL	C3C-C2C	5.16	1.47	1.36
27	A	849	CHL	C3B-C2B	5.16	1.47	1.40
27	3	317	CHL	CHC-C1C	5.16	1.48	1.35
27	B	842	CHL	C3C-C2C	5.16	1.47	1.36
27	a	309	CHL	CHD-C1D	5.16	1.48	1.38
27	b	314	CHL	CHD-C1D	5.16	1.48	1.38
27	4	320	CHL	CHC-C1C	5.16	1.48	1.35
27	B	833	CHL	CHC-C1C	5.16	1.48	1.35
27	4	307	CHL	CHC-C1C	5.16	1.48	1.35
27	A	855	CHL	O2D-CGD	5.16	1.45	1.33
27	B	825	CHL	CHC-C1C	5.16	1.48	1.35
27	A	852	CHL	C3C-C2C	5.16	1.47	1.36
27	4	320	CHL	C3B-C2B	5.16	1.47	1.40
27	A	858	CHL	C3B-C2B	5.16	1.47	1.40
27	B	847	CHL	C3B-C2B	5.16	1.47	1.40
27	3	317	CHL	C3B-C2B	5.16	1.47	1.40
27	7	316	CHL	CHC-C1C	5.16	1.48	1.35
27	4	306	CHL	CHC-C1C	5.15	1.48	1.35
27	4	306	CHL	CHD-C1D	5.15	1.48	1.38
27	6	306	CHL	CHC-C1C	5.15	1.48	1.35
27	A	821	CHL	C3B-C2B	5.15	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	310	CHL	C3B-C2B	5.15	1.47	1.40
27	6	311	CHL	C3C-C2C	5.15	1.47	1.36
27	A	849	CHL	MG-ND	-5.15	1.95	2.05
27	7	317	CHL	O2D-CGD	5.15	1.45	1.33
27	A	847	CHL	CHC-C1C	5.15	1.48	1.35
27	4	314	CHL	C3C-C2C	5.15	1.47	1.36
27	4	308	CHL	C3B-C2B	5.15	1.47	1.40
27	A	830	CHL	CHC-C1C	5.15	1.48	1.35
27	a	317	CHL	CHC-C1C	5.15	1.48	1.35
27	3	309	CHL	MG-NC	5.15	2.18	2.06
27	5	312	CHL	CHC-C1C	5.15	1.48	1.35
27	8	319	CHL	O2D-CGD	5.15	1.45	1.33
27	b	307	CHL	C3B-C2B	5.15	1.47	1.40
27	A	826	CHL	CHC-C1C	5.15	1.48	1.35
27	A	858	CHL	CHC-C1C	5.15	1.48	1.35
27	b	309	CHL	CHC-C1C	5.15	1.48	1.35
27	3	317	CHL	C3C-C2C	5.15	1.47	1.36
27	4	311	CHL	CHD-C1D	5.15	1.48	1.38
27	a	307	CHL	C3C-C2C	5.15	1.47	1.36
27	6	306	CHL	O2D-CGD	5.15	1.45	1.33
27	7	311	CHL	CHC-C1C	5.15	1.48	1.35
27	8	313	CHL	C3C-C2C	5.15	1.47	1.36
27	A	855	CHL	CHC-C1C	5.15	1.48	1.35
27	B	822	CHL	CHC-C1C	5.14	1.48	1.35
27	A	852	CHL	O2D-CGD	5.14	1.45	1.33
27	5	308	CHL	O2D-CGD	5.14	1.45	1.33
27	A	854	CHL	CHC-C1C	5.14	1.48	1.35
27	b	313	CHL	O2D-CGD	5.14	1.45	1.33
27	K	205	CHL	CHD-C1D	5.14	1.48	1.38
27	b	312	CHL	CHD-C1D	5.14	1.48	1.38
27	b	314	CHL	O2D-CGD	5.14	1.45	1.33
27	K	206	CHL	CHD-C1D	5.14	1.48	1.38
27	A	844	CHL	CHC-C1C	5.14	1.48	1.35
27	5	323	CHL	O2D-CGD	5.14	1.45	1.33
27	4	311	CHL	O2D-CGD	5.14	1.45	1.33
27	8	317	CHL	C3B-C2B	5.14	1.47	1.40
27	a	320	CHL	O2D-CGD	5.14	1.45	1.33
27	a	319	CHL	CHD-C1D	5.14	1.48	1.38
27	8	316	CHL	O2D-CGD	5.14	1.45	1.33
27	5	314	CHL	O2D-CGD	5.14	1.45	1.33
27	B	838	CHL	C3B-C2B	5.14	1.47	1.40
27	6	315	CHL	CHD-C1D	5.14	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	839	CHL	CHD-C1D	5.13	1.48	1.38
27	A	832	CHL	CHC-C1C	5.13	1.48	1.35
27	A	849	CHL	CHC-C1C	5.13	1.48	1.35
27	5	316	CHL	C3D-C4D	-5.13	1.32	1.44
27	8	317	CHL	O2D-CGD	5.13	1.45	1.33
27	a	310	CHL	C3C-C2C	5.13	1.47	1.36
27	A	825	CHL	C3B-C2B	5.13	1.47	1.40
27	8	311	CHL	CHC-C1C	5.13	1.48	1.35
27	A	837	CHL	CHC-C1C	5.13	1.48	1.35
27	B	815	CHL	C3B-C2B	5.13	1.47	1.40
27	B	815	CHL	CHC-C1C	5.13	1.48	1.35
27	B	811	CHL	O2D-CGD	5.13	1.45	1.33
27	B	826	CHL	CHC-C1C	5.13	1.48	1.35
27	4	305	CHL	CHC-C1C	5.13	1.48	1.35
27	5	318	CHL	CHC-C1C	5.13	1.48	1.35
27	3	315	CHL	CHC-C1C	5.13	1.48	1.35
27	B	822	CHL	C3B-C2B	5.13	1.47	1.40
27	6	320	CHL	O2D-CGD	5.13	1.45	1.33
27	8	316	CHL	CHC-C1C	5.13	1.48	1.35
27	4	305	CHL	O2D-CGD	5.13	1.45	1.33
27	4	319	CHL	O2D-CGD	5.13	1.45	1.33
27	5	315	CHL	CHD-C1D	5.13	1.48	1.38
27	4	306	CHL	O2D-CGD	5.13	1.45	1.33
27	4	318	CHL	O2D-CGD	5.13	1.45	1.33
27	A	819	CHL	C3C-C2C	5.13	1.47	1.36
27	A	848	CHL	CHC-C1C	5.13	1.48	1.35
27	B	839	CHL	CHC-C1C	5.12	1.48	1.35
27	a	313	CHL	O2D-CGD	5.12	1.45	1.33
27	6	312	CHL	O2D-CGD	5.12	1.45	1.33
27	B	851	CHL	C3C-C2C	5.12	1.47	1.36
27	8	320	CHL	C3B-C2B	5.12	1.47	1.40
27	6	309	CHL	CHC-C1C	5.12	1.48	1.35
27	B	832	CHL	CHC-C1C	5.12	1.48	1.35
27	4	310	CHL	O2D-CGD	5.12	1.45	1.33
27	B	829	CHL	O2D-CGD	5.12	1.45	1.33
27	a	312	CHL	O2D-CGD	5.12	1.45	1.33
27	5	308	CHL	C3B-C2B	5.12	1.47	1.40
27	7	313	CHL	CHC-C1C	5.12	1.48	1.35
27	B	837	CHL	CHC-C1C	5.12	1.48	1.35
27	A	818	CHL	MG-NA	5.12	2.18	2.06
27	7	316	CHL	O2D-CGD	5.12	1.45	1.33
27	7	312	CHL	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	308	CHL	C3D-C4D	-5.11	1.32	1.44
27	A	859	CHL	CHC-C1C	5.11	1.48	1.35
27	3	313	CHL	CHD-C1D	5.11	1.48	1.38
27	3	314	CHL	CHD-C1D	5.11	1.48	1.38
27	B	818	CHL	C3C-C2C	5.11	1.47	1.36
27	4	308	CHL	O2D-CGD	5.11	1.45	1.33
27	B	815	CHL	C3C-C2C	5.11	1.47	1.36
27	8	311	CHL	O2D-CGD	5.11	1.45	1.33
27	A	853	CHL	CHD-C1D	5.11	1.48	1.38
27	b	313	CHL	CHD-C1D	5.11	1.48	1.38
27	A	828	CHL	CHC-C1C	5.11	1.48	1.35
27	8	326	CHL	C3C-C2C	5.11	1.47	1.36
27	8	320	CHL	CHC-C1C	5.11	1.48	1.35
27	4	320	CHL	CHD-C1D	5.11	1.48	1.38
27	b	306	CHL	O2D-CGD	5.11	1.45	1.33
27	A	825	CHL	CHC-C1C	5.11	1.48	1.35
27	3	308	CHL	CHC-C1C	5.11	1.48	1.35
27	3	311	CHL	CHC-C1C	5.11	1.48	1.35
27	6	313	CHL	O2D-CGD	5.11	1.45	1.33
27	7	312	CHL	C3B-C2B	5.11	1.47	1.40
27	B	821	CHL	O2D-CGD	5.11	1.45	1.33
27	a	317	CHL	O2D-CGD	5.11	1.45	1.33
27	A	829	CHL	CHC-C1C	5.11	1.48	1.35
27	8	325	CHL	CHC-C1C	5.11	1.48	1.35
27	A	839	CHL	C3C-C2C	5.11	1.47	1.36
27	F	309	CHL	C3B-C2B	5.11	1.47	1.40
27	A	856	CHL	C3C-C2C	5.11	1.47	1.36
27	B	812	CHL	CHC-C1C	5.11	1.48	1.35
27	6	305	CHL	CHC-C1C	5.11	1.48	1.35
27	5	312	CHL	CHD-C1D	5.11	1.48	1.38
27	A	838	CHL	CHC-C1C	5.11	1.48	1.35
27	B	845	CHL	C3C-C2C	5.11	1.47	1.36
27	8	320	CHL	CHD-C1D	5.10	1.48	1.38
27	3	309	CHL	O2D-CGD	5.10	1.45	1.33
27	A	839	CHL	O2D-CGD	5.10	1.45	1.33
27	b	305	CHL	CHC-C1C	5.10	1.48	1.35
27	a	320	CHL	CHD-C1D	5.10	1.48	1.38
27	8	313	CHL	CHC-C1C	5.10	1.48	1.35
27	5	309	CHL	CHD-C1D	5.10	1.48	1.38
27	5	310	CHL	C3C-C2C	5.10	1.47	1.36
27	a	314	CHL	CHD-C1D	5.10	1.48	1.38
27	a	312	CHL	C3B-C2B	5.10	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	834	CHL	CHC-C1C	5.10	1.48	1.35
27	3	311	CHL	C3B-C2B	5.10	1.47	1.40
27	7	316	CHL	C3B-C2B	5.10	1.47	1.40
27	6	314	CHL	O2D-CGD	5.10	1.45	1.33
27	B	843	CHL	CHC-C1C	5.10	1.48	1.35
27	J	106	CHL	O2D-CGD	5.10	1.45	1.33
27	4	314	CHL	C3B-C2B	5.10	1.47	1.40
27	B	842	CHL	C3B-C2B	5.10	1.47	1.40
27	4	310	CHL	CHD-C1D	5.09	1.48	1.38
27	8	318	CHL	C3B-C2B	5.09	1.47	1.40
27	a	319	CHL	CHC-C1C	5.09	1.48	1.35
27	4	311	CHL	C3B-C2B	5.09	1.47	1.40
27	5	320	CHL	CHD-C1D	5.09	1.48	1.38
27	7	312	CHL	CHC-C1C	5.09	1.48	1.35
27	6	306	CHL	C3C-C2C	5.09	1.47	1.36
27	A	839	CHL	CHC-C1C	5.09	1.48	1.35
27	K	205	CHL	O2D-CGD	5.09	1.45	1.33
27	B	837	CHL	CHD-C1D	5.09	1.48	1.38
27	5	308	CHL	CHC-C1C	5.09	1.48	1.35
27	6	311	CHL	O2D-CGD	5.09	1.45	1.33
27	B	824	CHL	CHC-C1C	5.09	1.48	1.35
27	A	853	CHL	CHC-C1C	5.09	1.48	1.35
27	5	309	CHL	O2D-CGD	5.09	1.45	1.33
27	B	829	CHL	CHC-C1C	5.09	1.48	1.35
27	B	838	CHL	CHC-C1C	5.08	1.48	1.35
27	5	309	CHL	CHC-C1C	5.08	1.48	1.35
27	a	311	CHL	O2D-CGD	5.08	1.45	1.33
27	A	857	CHL	C3C-C2C	5.08	1.47	1.36
27	6	312	CHL	CHC-C1C	5.08	1.48	1.35
27	B	819	CHL	O2D-CGD	5.08	1.45	1.33
27	6	310	CHL	O2D-CGD	5.08	1.45	1.33
27	8	318	CHL	O2D-CGD	5.08	1.45	1.33
27	7	313	CHL	CHD-C1D	5.08	1.48	1.38
27	3	312	CHL	CHD-C1D	5.08	1.48	1.38
27	a	314	CHL	O2D-CGD	5.08	1.45	1.33
27	6	306	CHL	C3B-C2B	5.08	1.47	1.40
27	B	825	CHL	O2D-CGD	5.08	1.45	1.33
27	7	315	CHL	CHC-C1C	5.08	1.48	1.35
27	a	319	CHL	O2D-CGD	5.07	1.45	1.33
27	7	316	CHL	CHD-C1D	5.07	1.48	1.38
27	B	836	CHL	CHC-C1C	5.07	1.48	1.35
27	A	835	CHL	C3B-C2B	5.07	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	827	CHL	C3C-C2C	5.07	1.47	1.36
27	A	837	CHL	O2D-CGD	5.07	1.45	1.33
27	b	308	CHL	O2D-CGD	5.07	1.45	1.33
27	3	318	CHL	O2D-CGD	5.07	1.45	1.33
27	B	838	CHL	CHD-C1D	5.07	1.48	1.38
27	A	835	CHL	CHD-C1D	5.07	1.48	1.38
27	4	304	CHL	O2D-CGD	5.07	1.45	1.33
27	b	305	CHL	C3B-C2B	5.07	1.47	1.40
27	b	305	CHL	O2D-CGD	5.07	1.45	1.33
27	4	314	CHL	O2D-CGD	5.07	1.45	1.33
27	F	308	CHL	O2D-CGD	5.07	1.45	1.33
27	6	309	CHL	MG-NC	5.06	2.18	2.06
27	B	824	CHL	CHD-C1D	5.06	1.48	1.38
27	4	307	CHL	O2D-CGD	5.06	1.45	1.33
27	6	310	CHL	CHD-C1D	5.06	1.48	1.38
27	B	811	CHL	CHC-C1C	5.06	1.47	1.35
27	5	311	CHL	C3C-C2C	5.06	1.47	1.36
27	B	851	CHL	C3B-C2B	5.06	1.47	1.40
27	B	839	CHL	O2D-CGD	5.06	1.45	1.33
27	K	204	CHL	CHC-C1C	5.06	1.47	1.35
27	A	858	CHL	O2D-CGD	5.06	1.45	1.33
27	4	304	CHL	CHC-C1C	5.06	1.47	1.35
27	B	830	CHL	C3B-C2B	5.06	1.47	1.40
27	B	837	CHL	MG-NC	5.06	2.18	2.06
27	A	817	CHL	CHC-C1C	5.06	1.47	1.35
27	8	311	CHL	CHD-C1D	5.06	1.48	1.38
27	5	322	CHL	O2D-CGD	5.06	1.45	1.33
27	a	317	CHL	CHD-C1D	5.06	1.48	1.38
27	5	323	CHL	CHD-C1D	5.05	1.48	1.38
27	b	304	CHL	CHD-C1D	5.05	1.48	1.38
27	A	857	CHL	CHC-C1C	5.05	1.47	1.35
27	B	843	CHL	O2D-CGD	5.05	1.45	1.33
27	B	811	CHL	C3C-C2C	5.05	1.47	1.36
27	6	320	CHL	CHD-C1D	5.05	1.48	1.38
27	A	848	CHL	MG-NC	5.05	2.18	2.06
27	5	314	CHL	CHD-C1D	5.05	1.48	1.38
27	A	854	CHL	O2D-CGD	5.05	1.45	1.33
27	3	319	CHL	O2D-CGD	5.05	1.45	1.33
27	K	206	CHL	CHC-C1C	5.05	1.47	1.35
27	7	311	CHL	C3C-C2C	5.05	1.47	1.36
27	3	314	CHL	O2D-CGD	5.05	1.45	1.33
27	A	850	CHL	C3B-C2B	5.05	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	845	CHL	CHC-C1C	5.05	1.47	1.35
27	J	106	CHL	CHC-C1C	5.05	1.47	1.35
27	B	820	CHL	CHD-C1D	5.05	1.48	1.38
27	B	822	CHL	CHD-C1D	5.05	1.48	1.38
27	B	836	CHL	O2D-CGD	5.05	1.45	1.33
27	7	324	CHL	O2D-CGD	5.05	1.45	1.33
27	A	821	CHL	CHC-C1C	5.05	1.47	1.35
27	3	320	CHL	O2D-CGD	5.04	1.45	1.33
27	8	322	CHL	C3C-C2C	5.04	1.47	1.36
27	4	304	CHL	C3C-C2C	5.04	1.47	1.36
27	B	830	CHL	CHC-C1C	5.04	1.47	1.35
27	K	204	CHL	O2D-CGD	5.04	1.45	1.33
27	B	811	CHL	C3B-C2B	5.04	1.47	1.40
27	B	831	CHL	O2D-CGD	5.04	1.45	1.33
27	B	851	CHL	O2D-CGD	5.04	1.45	1.33
27	3	313	CHL	O2D-CGD	5.04	1.45	1.33
27	8	320	CHL	O2D-CGD	5.04	1.45	1.33
27	7	324	CHL	CHD-C1D	5.04	1.48	1.38
27	A	855	CHL	C3B-C2B	5.04	1.47	1.40
27	A	825	CHL	O2D-CGD	5.04	1.45	1.33
27	B	813	CHL	C3C-C2C	5.04	1.47	1.36
27	A	844	CHL	CHD-C1D	5.04	1.48	1.38
27	B	828	CHL	CHD-C1D	5.04	1.48	1.38
27	B	824	CHL	O2D-CGD	5.04	1.45	1.33
27	8	326	CHL	O2D-CGD	5.04	1.45	1.33
27	B	828	CHL	CHC-C1C	5.04	1.47	1.35
27	A	856	CHL	CHC-C1C	5.03	1.47	1.35
27	a	309	CHL	CHC-C1C	5.03	1.47	1.35
27	B	821	CHL	CHC-C1C	5.03	1.47	1.35
27	3	317	CHL	O2D-CGD	5.03	1.45	1.33
27	A	824	CHL	C3C-C2C	5.03	1.47	1.36
27	a	309	CHL	O2D-CGD	5.03	1.45	1.33
27	A	845	CHL	CHD-C1D	5.03	1.48	1.38
27	4	313	CHL	O2D-CGD	5.03	1.45	1.33
27	B	846	CHL	CHC-C1C	5.03	1.47	1.35
27	8	325	CHL	CHD-C1D	5.03	1.48	1.38
27	A	845	CHL	C3B-C2B	5.03	1.47	1.40
27	8	322	CHL	CHC-C1C	5.03	1.47	1.35
27	a	309	CHL	C3B-C2B	5.03	1.47	1.40
27	3	313	CHL	CHC-C1C	5.03	1.47	1.35
27	F	309	CHL	O2D-CGD	5.03	1.45	1.33
27	F	308	CHL	CHC-C1C	5.03	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	848	CHL	C3B-C2B	5.03	1.47	1.40
27	5	311	CHL	CHC-C1C	5.02	1.47	1.35
27	B	816	CHL	CHC-C1C	5.02	1.47	1.35
27	B	842	CHL	CHC-C1C	5.02	1.47	1.35
27	A	839	CHL	C3B-C2B	5.02	1.47	1.40
27	B	850	CHL	O2D-CGD	5.02	1.45	1.33
27	8	322	CHL	O2D-CGD	5.02	1.45	1.33
27	A	838	CHL	CHD-C1D	5.02	1.48	1.38
27	4	305	CHL	CHD-C1D	5.02	1.48	1.38
27	B	836	CHL	CHD-C1D	5.02	1.48	1.38
27	a	313	CHL	CHD-C1D	5.02	1.48	1.38
27	5	315	CHL	O2D-CGD	5.02	1.45	1.33
27	A	824	CHL	CHC-C1C	5.02	1.47	1.35
27	5	321	CHL	CHD-C1D	5.02	1.48	1.38
27	8	325	CHL	O2D-CGD	5.02	1.45	1.33
27	B	830	CHL	O2D-CGD	5.02	1.45	1.33
27	A	829	CHL	CHD-C1D	5.02	1.48	1.38
27	A	854	CHL	CHD-C1D	5.02	1.48	1.38
27	b	305	CHL	MG-NA	5.02	2.18	2.06
27	A	834	CHL	CHC-C1C	5.02	1.47	1.35
27	8	318	CHL	CHD-C1D	5.02	1.48	1.38
27	A	844	CHL	O2D-CGD	5.01	1.45	1.33
27	B	819	CHL	CHC-C1C	5.01	1.47	1.35
27	B	812	CHL	O2D-CGD	5.01	1.45	1.33
27	8	313	CHL	O2D-CGD	5.01	1.45	1.33
27	B	823	CHL	O2D-CGD	5.01	1.45	1.33
27	A	818	CHL	CHC-C1C	5.01	1.47	1.35
27	3	318	CHL	CHD-C1D	5.01	1.48	1.38
27	8	323	CHL	CHD-C4C	5.01	1.50	1.39
27	A	826	CHL	CHD-C1D	5.01	1.48	1.38
27	B	827	CHL	CHC-C1C	5.01	1.47	1.35
27	A	818	CHL	C3C-C2C	5.01	1.47	1.36
27	A	835	CHL	CHC-C1C	5.01	1.47	1.35
27	a	307	CHL	O2D-CGD	5.01	1.45	1.33
27	6	305	CHL	O2D-CGD	5.01	1.45	1.33
27	6	309	CHL	O2D-CGD	5.01	1.45	1.33
27	A	856	CHL	O2D-CGD	5.01	1.45	1.33
27	B	815	CHL	O2D-CGD	5.01	1.45	1.33
27	6	319	CHL	O2D-CGD	5.01	1.45	1.33
27	B	825	CHL	C3C-C2C	5.00	1.47	1.36
27	7	317	CHL	CHC-C1C	5.00	1.47	1.35
27	8	326	CHL	CHC-C1C	5.00	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	311	CHL	O2D-CGD	5.00	1.45	1.33
27	3	320	CHL	C3C-C2C	5.00	1.47	1.36
27	6	311	CHL	CHD-C1D	5.00	1.48	1.38
27	b	307	CHL	CHD-C1D	5.00	1.48	1.38
27	A	847	CHL	O2D-CGD	5.00	1.45	1.33
27	A	838	CHL	O2D-CGD	5.00	1.45	1.33
27	A	848	CHL	O2D-CGD	5.00	1.45	1.33
27	3	313	CHL	C3B-C2B	5.00	1.47	1.40
27	A	849	CHL	O2D-CGD	5.00	1.45	1.33
27	B	813	CHL	O2D-CGD	5.00	1.45	1.33
27	a	308	CHL	CHD-C1D	5.00	1.48	1.38
27	A	822	CHL	CHD-C1D	4.99	1.48	1.38
27	4	315	CHL	CHD-C1D	4.99	1.48	1.38
27	A	850	CHL	CHC-C1C	4.99	1.47	1.35
27	6	309	CHL	CHD-C1D	4.99	1.48	1.38
27	B	821	CHL	CHD-C1D	4.99	1.48	1.38
27	B	848	CHL	CHD-C1D	4.99	1.48	1.38
27	5	307	CHL	O2D-CGD	4.99	1.45	1.33
27	A	859	CHL	CHD-C1D	4.99	1.48	1.38
27	3	309	CHL	CHD-C1D	4.99	1.48	1.38
27	7	313	CHL	O2D-CGD	4.99	1.45	1.33
27	B	841	CHL	C3C-C2C	4.99	1.47	1.36
27	a	310	CHL	O2D-CGD	4.99	1.45	1.33
27	A	851	CHL	CHD-C1D	4.99	1.48	1.38
27	B	849	CHL	CHD-C1D	4.99	1.48	1.38
27	F	309	CHL	CHD-C1D	4.99	1.48	1.38
27	7	318	CHL	C3B-C2B	4.99	1.47	1.40
27	5	318	CHL	CHD-C1D	4.99	1.48	1.38
27	A	825	CHL	CHD-C1D	4.99	1.48	1.38
27	3	311	CHL	CHD-C1D	4.99	1.48	1.38
27	6	314	CHL	CHD-C1D	4.99	1.48	1.38
27	a	311	CHL	CHD-C1D	4.98	1.48	1.38
27	5	312	CHL	O2D-CGD	4.98	1.45	1.33
27	4	308	CHL	CHC-C1C	4.98	1.47	1.35
27	B	832	CHL	CHD-C1D	4.98	1.48	1.38
27	6	319	CHL	CHD-C4C	4.98	1.50	1.39
27	3	315	CHL	CHD-C1D	4.98	1.48	1.38
27	B	816	CHL	O2D-CGD	4.98	1.45	1.33
27	B	828	CHL	O2D-CGD	4.98	1.45	1.33
27	B	845	CHL	O2D-CGD	4.98	1.45	1.33
27	3	310	CHL	O2D-CGD	4.98	1.45	1.33
27	3	315	CHL	C3B-C2B	4.98	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	855	CHL	CHD-C1D	4.98	1.48	1.38
27	B	846	CHL	O2D-CGD	4.98	1.45	1.33
27	B	813	CHL	CHD-C1D	4.98	1.48	1.38
27	A	823	CHL	O2D-CGD	4.98	1.45	1.33
27	A	818	CHL	CHD-C1D	4.98	1.48	1.38
27	6	306	CHL	CHD-C1D	4.98	1.48	1.38
27	3	312	CHL	O2D-CGD	4.97	1.45	1.33
27	6	305	CHL	CHD-C1D	4.97	1.48	1.38
27	A	847	CHL	CHD-C1D	4.97	1.48	1.38
27	B	846	CHL	CHD-C1D	4.97	1.48	1.38
27	7	314	CHL	O2D-CGD	4.97	1.45	1.33
27	B	833	CHL	CHD-C1D	4.97	1.48	1.38
27	3	312	CHL	CHC-C1C	4.97	1.47	1.35
27	7	318	CHL	CHC-C1C	4.97	1.47	1.35
27	A	850	CHL	CHD-C1D	4.97	1.48	1.38
27	B	820	CHL	O2D-CGD	4.97	1.45	1.33
27	B	822	CHL	O2D-CGD	4.97	1.45	1.33
27	A	828	CHL	CHD-C1D	4.97	1.48	1.38
27	B	826	CHL	O2D-CGD	4.97	1.45	1.33
27	8	324	CHL	O2D-CGD	4.97	1.45	1.33
27	4	315	CHL	O2D-CGD	4.97	1.45	1.33
27	A	840	CHL	O2D-CGD	4.96	1.45	1.33
27	3	308	CHL	O2D-CGD	4.96	1.45	1.33
27	8	317	CHL	CHD-C1D	4.96	1.48	1.38
27	8	311	CHL	MG-NC	4.96	2.18	2.06
27	A	817	CHL	O2D-CGD	4.96	1.45	1.33
27	A	840	CHL	CHC-C1C	4.96	1.47	1.35
27	A	828	CHL	O2D-CGD	4.96	1.45	1.33
27	B	818	CHL	O2D-CGD	4.96	1.45	1.33
27	B	844	CHL	O2D-CGD	4.96	1.45	1.33
27	A	826	CHL	O2D-CGD	4.96	1.45	1.33
27	A	830	CHL	O2D-CGD	4.96	1.45	1.33
27	B	835	CHL	CHD-C1D	4.96	1.48	1.38
27	B	843	CHL	CHD-C1D	4.95	1.48	1.38
27	b	316	CHL	O2D-CGD	4.95	1.45	1.33
27	5	310	CHL	O2D-CGD	4.95	1.45	1.33
27	5	318	CHL	O2D-CGD	4.95	1.45	1.33
27	A	827	CHL	CHD-C1D	4.95	1.48	1.38
27	3	315	CHL	O2D-CGD	4.95	1.45	1.33
27	8	315	CHL	O2D-CGD	4.95	1.45	1.33
27	B	838	CHL	O2D-CGD	4.95	1.45	1.33
27	A	840	CHL	CHD-C1D	4.95	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	314	CHL	CHD-C1D	4.95	1.48	1.38
27	a	318	CHL	O2D-CGD	4.95	1.45	1.33
27	3	321	CHL	CHD-C1D	4.95	1.48	1.38
27	A	848	CHL	CHD-C1D	4.95	1.48	1.38
27	A	850	CHL	O2D-CGD	4.94	1.45	1.33
27	5	308	CHL	CHD-C1D	4.94	1.48	1.38
27	B	844	CHL	CHD-C1D	4.94	1.48	1.38
27	B	830	CHL	CHD-C1D	4.94	1.48	1.38
27	A	852	CHL	CHC-C1C	4.94	1.47	1.35
27	B	840	CHL	CHD-C1D	4.94	1.48	1.38
27	8	325	CHL	C3B-C2B	4.94	1.47	1.40
27	A	834	CHL	CHD-C1D	4.94	1.48	1.38
26	A	815	CL0	C3D-C4D	-4.94	1.33	1.44
27	A	816	CHL	MG-NC	4.94	2.18	2.06
27	3	317	CHL	CHD-C1D	4.94	1.48	1.38
27	A	853	CHL	O2D-CGD	4.94	1.45	1.33
27	B	835	CHL	O2D-CGD	4.94	1.45	1.33
27	A	849	CHL	CHD-C1D	4.93	1.48	1.38
27	b	304	CHL	MG-ND	-4.93	1.96	2.05
27	B	827	CHL	O2D-CGD	4.93	1.45	1.33
27	3	310	CHL	CHD-C1D	4.93	1.48	1.38
27	B	814	CHL	CHD-C1D	4.93	1.48	1.38
27	A	845	CHL	CHC-C1C	4.93	1.47	1.35
27	B	817	CHL	O2D-CGD	4.93	1.45	1.33
27	A	835	CHL	O2D-CGD	4.93	1.45	1.33
27	7	318	CHL	O2D-CGD	4.93	1.45	1.33
27	b	306	CHL	CHD-C1D	4.93	1.48	1.38
27	6	312	CHL	CHD-C1D	4.93	1.48	1.38
27	b	315	CHL	O2D-CGD	4.92	1.45	1.33
27	A	832	CHL	C3C-C2C	4.92	1.47	1.36
27	B	839	CHL	CHD-C1D	4.92	1.47	1.38
27	B	829	CHL	CHD-C1D	4.92	1.47	1.38
27	8	316	CHL	CHD-C1D	4.92	1.47	1.38
27	B	847	CHL	CHD-C1D	4.92	1.47	1.38
27	5	321	CHL	O2D-CGD	4.92	1.45	1.33
27	A	821	CHL	O2D-CGD	4.92	1.45	1.33
27	A	846	CHL	C3D-C4D	-4.92	1.33	1.44
27	B	831	CHL	CHD-C1D	4.92	1.47	1.38
27	6	319	CHL	C2C-C3C	4.92	1.47	1.36
27	B	827	CHL	CHD-C1D	4.91	1.47	1.38
27	a	310	CHL	CHD-C1D	4.91	1.47	1.38
27	A	832	CHL	O2D-CGD	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	314	CHL	CHD-C1D	4.91	1.47	1.38
27	5	323	CHL	CHC-C1C	4.91	1.47	1.35
27	B	826	CHL	CHD-C1D	4.91	1.47	1.38
27	B	817	CHL	C3B-C2B	4.91	1.47	1.40
27	A	836	CHL	O2D-CGD	4.91	1.45	1.33
27	B	849	CHL	O2D-CGD	4.91	1.45	1.33
27	6	318	CHL	O2D-CGD	4.91	1.45	1.33
27	A	830	CHL	CHD-C1D	4.90	1.47	1.38
27	4	307	CHL	CHD-C1D	4.90	1.47	1.38
27	4	316	CHL	O2D-CGD	4.90	1.45	1.33
27	A	831	CHL	C3D-C4D	-4.90	1.33	1.44
27	B	832	CHL	O2D-CGD	4.90	1.45	1.33
27	8	315	CHL	C3C-C2C	4.90	1.47	1.36
27	A	834	CHL	C3B-C2B	4.90	1.47	1.40
27	8	313	CHL	CHD-C1D	4.90	1.47	1.38
27	5	314	CHL	MG-ND	4.90	2.15	2.05
27	8	319	CHL	CHD-C1D	4.89	1.47	1.38
27	5	310	CHL	CHD-C1D	4.89	1.47	1.38
27	A	843	CHL	C3D-C4D	-4.89	1.33	1.44
27	A	819	CHL	O2D-CGD	4.89	1.45	1.33
27	5	323	CHL	C3B-C2B	4.89	1.47	1.40
27	b	317	CHL	O2D-CGD	4.89	1.45	1.33
27	B	847	CHL	O2D-CGD	4.89	1.45	1.33
27	a	315	CHL	O2D-CGD	4.89	1.45	1.33
27	5	325	CHL	O2D-CGD	4.89	1.45	1.33
27	7	323	CHL	O2D-CGD	4.89	1.45	1.33
27	7	313	CHL	C3B-C2B	4.89	1.47	1.40
27	5	311	CHL	CHD-C1D	4.89	1.47	1.38
27	A	822	CHL	O2D-CGD	4.88	1.45	1.33
27	6	319	CHL	C3B-C2B	4.88	1.47	1.40
27	A	821	CHL	CHD-C1D	4.88	1.47	1.38
27	B	846	CHL	C3B-C2B	4.88	1.47	1.40
27	B	851	CHL	CHD-C1D	4.88	1.47	1.38
27	B	819	CHL	CHD-C1D	4.88	1.47	1.38
27	B	841	CHL	O2D-CGD	4.88	1.45	1.33
27	B	842	CHL	CHD-C1D	4.88	1.47	1.38
27	A	823	CHL	CHD-C1D	4.88	1.47	1.38
27	B	833	CHL	O2D-CGD	4.87	1.45	1.33
27	a	316	CHL	O2D-CGD	4.87	1.45	1.33
27	4	304	CHL	CHD-C1D	4.87	1.47	1.38
27	4	317	CHL	O2D-CGD	4.87	1.45	1.33
27	A	828	CHL	MG-ND	4.87	2.15	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	858	CHL	CHD-C1D	4.87	1.47	1.38
27	7	311	CHL	CHD-C1D	4.87	1.47	1.38
27	B	842	CHL	O2D-CGD	4.87	1.45	1.33
27	8	314	CHL	O2D-CGD	4.87	1.45	1.33
27	A	816	CHL	CHD-C1D	4.87	1.47	1.38
27	A	818	CHL	O2D-CGD	4.86	1.45	1.33
27	4	312	CHL	O2D-CGD	4.86	1.45	1.33
27	5	307	CHL	CHD-C1D	4.86	1.47	1.38
27	3	311	CHL	O2D-CGD	4.86	1.45	1.33
27	A	829	CHL	O2D-CGD	4.86	1.45	1.33
27	B	848	CHL	O2D-CGD	4.85	1.45	1.33
27	7	312	CHL	CHD-C1D	4.85	1.47	1.38
27	B	837	CHL	O2D-CGD	4.85	1.45	1.33
27	A	851	CHL	O2D-CGD	4.85	1.45	1.33
27	A	827	CHL	O2D-CGD	4.85	1.45	1.33
27	7	317	CHL	CHD-C1D	4.85	1.47	1.38
27	3	313	CHL	MG-NA	4.85	2.17	2.06
27	b	311	CHL	O2D-CGD	4.85	1.45	1.33
27	B	827	CHL	C3B-C2B	4.85	1.47	1.40
27	a	313	CHL	MG-NC	4.84	2.17	2.06
27	7	315	CHL	CHD-C1D	4.84	1.47	1.38
27	F	308	CHL	CHD-C1D	4.84	1.47	1.38
27	B	844	CHL	MG-NA	4.84	2.17	2.06
27	A	859	CHL	O2D-CGD	4.84	1.45	1.33
27	A	836	CHL	CHD-C1D	4.84	1.47	1.38
27	A	820	CHL	O2D-CGD	4.83	1.45	1.33
27	J	106	CHL	CHD-C1D	4.83	1.47	1.38
27	A	837	CHL	CHD-C1D	4.83	1.47	1.38
27	B	823	CHL	CHD-C1D	4.83	1.47	1.38
27	B	848	CHL	CHC-C1C	4.83	1.47	1.35
27	7	323	CHL	C3B-C2B	4.83	1.47	1.40
27	B	850	CHL	CHD-C1D	4.83	1.47	1.38
27	7	318	CHL	CHD-C1D	4.83	1.47	1.38
27	8	312	CHL	O2D-CGD	4.83	1.45	1.33
27	K	207	CHL	O2D-CGD	4.82	1.45	1.33
27	B	814	CHL	O2D-CGD	4.82	1.45	1.33
27	A	856	CHL	CHD-C1D	4.82	1.47	1.38
27	A	816	CHL	O2D-CGD	4.82	1.45	1.33
27	B	848	CHL	C3B-C2B	4.82	1.47	1.40
27	B	828	CHL	C3B-C2B	4.82	1.47	1.40
27	B	845	CHL	CHD-C1D	4.82	1.47	1.38
27	8	321	CHL	O2D-CGD	4.81	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	319	CHL	O2D-CGD	4.81	1.44	1.33
27	7	322	CHL	O2D-CGD	4.81	1.44	1.33
27	A	857	CHL	CHD-C1D	4.81	1.47	1.38
27	B	817	CHL	CHC-C1C	4.81	1.47	1.35
27	8	323	CHL	O2D-CGD	4.81	1.44	1.33
27	B	812	CHL	C3C-C2C	4.80	1.46	1.36
27	B	830	CHL	MG-ND	-4.80	1.96	2.05
27	4	308	CHL	CHD-C1D	4.80	1.47	1.38
27	A	852	CHL	CHD-C1D	4.80	1.47	1.38
27	3	308	CHL	CHD-C1D	4.80	1.47	1.38
27	4	317	CHL	C3B-C2B	4.80	1.47	1.40
27	A	824	CHL	CHD-C1D	4.79	1.47	1.38
27	4	313	CHL	CHC-C1C	4.79	1.47	1.35
27	b	308	CHL	CHD-C4C	4.79	1.50	1.39
27	B	816	CHL	CHD-C1D	4.79	1.47	1.38
27	4	309	CHL	O2D-CGD	4.78	1.44	1.33
27	A	819	CHL	CHD-C1D	4.78	1.47	1.38
27	K	204	CHL	CHD-C1D	4.78	1.47	1.38
27	6	308	CHL	C3B-C2B	4.78	1.47	1.40
27	b	315	CHL	CHD-C1D	4.77	1.47	1.38
27	5	319	CHL	MG-NA	4.77	2.17	2.06
27	A	832	CHL	CHD-C1D	4.77	1.47	1.38
27	8	312	CHL	CHD-C1D	4.76	1.47	1.38
27	a	307	CHL	CHD-C1D	4.76	1.47	1.38
27	B	811	CHL	CHD-C1D	4.76	1.47	1.38
27	B	818	CHL	C3B-C2B	4.76	1.47	1.40
27	B	818	CHL	CHC-C1C	4.76	1.47	1.35
27	8	315	CHL	CHD-C1D	4.75	1.47	1.38
27	A	845	CHL	O2D-CGD	4.75	1.44	1.33
27	A	834	CHL	O2D-CGD	4.75	1.44	1.33
27	3	316	CHL	O2D-CGD	4.75	1.44	1.33
27	B	817	CHL	CHD-C1D	4.75	1.47	1.38
27	6	319	CHL	MG-NC	4.74	2.17	2.06
27	6	308	CHL	O2D-CGD	4.74	1.44	1.33
27	A	842	CHL	O2D-CGD	4.73	1.44	1.33
27	6	307	CHL	C3D-C4D	-4.72	1.33	1.44
27	B	815	CHL	CHD-C1D	4.72	1.47	1.38
27	8	322	CHL	CHD-C1D	4.72	1.47	1.38
27	A	820	CHL	CHD-C1D	4.71	1.47	1.38
27	3	312	CHL	MG-NC	4.71	2.17	2.06
27	7	319	CHL	O2D-CGD	4.71	1.44	1.33
27	B	841	CHL	CHD-C1D	4.70	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	834	CHL	O2D-CGD	4.70	1.44	1.33
27	B	825	CHL	CHD-C1D	4.70	1.47	1.38
27	A	820	CHL	C3C-C2C	4.70	1.46	1.36
27	5	313	CHL	O2D-CGD	4.70	1.44	1.33
27	K	206	CHL	C3B-C2B	4.70	1.46	1.40
27	B	840	CHL	O2D-CGD	4.70	1.44	1.33
27	8	323	CHL	C3B-C2B	4.69	1.46	1.40
27	B	833	CHL	MG-NC	4.69	2.17	2.06
27	8	326	CHL	CHD-C1D	4.69	1.47	1.38
27	6	307	CHL	O2D-CGD	4.68	1.44	1.33
27	5	313	CHL	C3D-C4D	-4.68	1.33	1.44
27	3	320	CHL	CHD-C1D	4.68	1.47	1.38
27	6	308	CHL	CHC-C1C	4.67	1.46	1.35
27	4	317	CHL	C3D-C4D	-4.67	1.33	1.44
27	B	818	CHL	CHD-C1D	4.67	1.47	1.38
27	L	303	CHL	C3D-C4D	-4.66	1.33	1.44
27	7	323	CHL	MG-ND	4.66	2.15	2.05
27	5	316	CHL	CHC-C1C	4.66	1.46	1.35
27	A	824	CHL	O2D-CGD	4.65	1.44	1.33
27	7	323	CHL	CHC-C1C	4.63	1.46	1.35
34	8	301	SQD	O48-C23	4.63	1.46	1.33
27	B	834	CHL	CHD-C1D	4.62	1.47	1.38
27	B	812	CHL	CHD-C1D	4.62	1.47	1.38
27	7	320	CHL	O2D-CGD	4.62	1.44	1.33
27	8	324	CHL	O1A-CGA	4.61	1.46	1.19
27	A	837	CHL	MG-NC	4.60	2.17	2.06
27	F	308	CHL	MG-NA	4.60	2.17	2.06
27	4	316	CHL	O2A-CGA	4.59	1.46	1.30
27	6	309	CHL	MG-ND	-4.59	1.96	2.05
27	6	317	CHL	O2D-CGD	4.59	1.44	1.33
27	7	315	CHL	O2D-CGD	4.58	1.45	1.30
27	b	317	CHL	CHC-C1C	4.57	1.46	1.35
27	7	323	CHL	C3D-C4D	-4.57	1.33	1.44
27	6	316	CHL	O2D-CGD	4.56	1.44	1.33
27	A	817	CHL	CHD-C1D	4.56	1.47	1.38
27	4	315	CHL	MG-NC	4.55	2.17	2.06
27	6	316	CHL	O2A-CGA	4.55	1.46	1.30
27	A	833	CHL	O2D-CGD	4.54	1.44	1.33
27	6	316	CHL	CHC-C1C	4.54	1.46	1.35
27	4	317	CHL	O2A-CGA	4.54	1.46	1.30
27	4	317	CHL	CHC-C1C	4.53	1.46	1.35
27	5	317	CHL	CHC-C1C	4.53	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	317	CHL	CHD-C4C	4.53	1.49	1.39
27	A	843	CHL	O2D-CGD	4.53	1.44	1.33
27	A	851	CHL	MG-NC	4.53	2.17	2.06
27	4	313	CHL	O2A-CGA	4.52	1.45	1.30
27	A	841	CHL	CHC-C1C	4.51	1.46	1.35
27	A	833	CHL	CHC-C1C	4.50	1.46	1.35
27	a	318	CHL	CHC-C1C	4.50	1.46	1.35
27	6	319	CHL	CHD-C1D	4.50	1.47	1.38
27	a	316	CHL	CHC-C1C	4.50	1.46	1.35
27	A	846	CHL	O2D-CGD	4.50	1.44	1.33
27	b	316	CHL	CHC-C1C	4.50	1.46	1.35
27	b	311	CHL	CHC-C1C	4.49	1.46	1.35
27	L	304	CHL	O2A-CGA	4.49	1.45	1.30
27	K	207	CHL	CHC-C1C	4.49	1.46	1.35
27	4	314	CHL	MG-ND	4.48	2.14	2.05
27	A	845	CHL	MG-ND	4.48	2.14	2.05
27	8	321	CHL	CHC-C1C	4.48	1.46	1.35
27	5	314	CHL	O2A-CGA	4.48	1.45	1.30
27	3	321	CHL	O2A-CGA	4.48	1.45	1.30
27	8	321	CHL	O2A-CGA	4.47	1.46	1.33
27	8	314	CHL	CHC-C1C	4.47	1.46	1.35
27	3	308	CHL	C3C-C2C	4.47	1.46	1.36
27	B	843	CHL	O2A-CGA	4.47	1.45	1.30
27	4	319	CHL	O2A-CGA	4.46	1.45	1.30
27	4	313	CHL	CHD-C4C	4.46	1.49	1.39
27	5	317	CHL	O2D-CGD	4.46	1.44	1.33
27	4	313	CHL	C3D-C4D	-4.46	1.34	1.44
27	a	315	CHL	CHC-C1C	4.46	1.46	1.35
27	a	308	CHL	O2A-CGA	4.45	1.45	1.30
27	7	322	CHL	O2A-CGA	4.45	1.46	1.33
27	7	315	CHL	O2A-CGA	4.45	1.45	1.30
27	4	309	CHL	CHC-C1C	4.45	1.46	1.35
27	a	314	CHL	MG-ND	4.45	2.14	2.05
27	4	305	CHL	O2A-CGA	4.45	1.45	1.30
27	7	321	CHL	CHC-C1C	4.45	1.46	1.35
27	5	325	CHL	CHC-C1C	4.45	1.46	1.35
27	4	312	CHL	CHC-C1C	4.44	1.46	1.35
27	L	303	CHL	O2D-CGD	4.44	1.44	1.33
27	8	316	CHL	MG-ND	-4.44	1.97	2.05
27	A	842	CHL	CHC-C1C	4.44	1.46	1.35
27	A	841	CHL	O2D-CGD	4.43	1.44	1.33
27	a	314	CHL	O2A-CGA	4.42	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	322	CHL	CHC-C1C	4.42	1.46	1.35
27	7	322	CHL	CHC-C1C	4.42	1.46	1.35
27	6	318	CHL	CHC-C1C	4.42	1.46	1.35
27	5	319	CHL	CHC-C1C	4.42	1.46	1.35
27	4	316	CHL	CHC-C1C	4.41	1.46	1.35
27	4	314	CHL	O2A-CGA	4.41	1.45	1.30
27	3	316	CHL	CHC-C1C	4.41	1.46	1.35
29	b	303	LUT	C10-C9	4.40	1.41	1.35
27	7	319	CHL	CHC-C1C	4.40	1.46	1.35
27	b	316	CHL	O2A-CGA	4.39	1.46	1.33
27	B	819	CHL	MG-ND	-4.39	1.97	2.05
27	4	312	CHL	O2A-CGA	4.39	1.46	1.33
27	7	320	CHL	CHC-C1C	4.39	1.46	1.35
27	a	318	CHL	O2A-CGA	4.38	1.46	1.33
27	a	316	CHL	O2A-CGA	4.38	1.46	1.33
27	A	847	CHL	O2A-CGA	4.37	1.46	1.33
27	8	324	CHL	CHC-C1C	4.37	1.46	1.35
27	7	312	CHL	O2A-CGA	4.36	1.45	1.30
27	a	315	CHL	O2A-CGA	4.35	1.46	1.33
27	B	820	CHL	O2A-CGA	4.34	1.46	1.33
27	7	323	CHL	CHD-C4C	4.34	1.49	1.39
27	7	320	CHL	MG-NC	4.34	2.16	2.06
27	3	310	CHL	O2A-CGA	4.34	1.46	1.33
27	B	848	CHL	O2A-CGA	4.33	1.46	1.33
27	A	846	CHL	O2A-CGA	4.33	1.46	1.33
27	b	317	CHL	O2A-CGA	4.33	1.46	1.33
27	6	317	CHL	CHC-C1C	4.33	1.46	1.35
27	7	313	CHL	MG-NC	4.31	2.16	2.06
27	4	312	CHL	MG-NC	4.31	2.16	2.06
27	B	839	CHL	O2A-CGA	4.30	1.45	1.33
27	K	204	CHL	O2A-CGA	4.30	1.45	1.33
27	4	320	CHL	O2A-CGA	4.30	1.45	1.33
27	A	831	CHL	O2D-CGD	4.30	1.43	1.33
27	B	826	CHL	O2A-CGA	4.29	1.45	1.33
27	A	841	CHL	MG-NC	4.29	2.16	2.06
27	8	317	CHL	MG-ND	4.29	2.14	2.05
27	4	319	CHL	CHD-C4C	4.29	1.49	1.39
27	3	310	CHL	MG-ND	-4.29	1.97	2.05
27	3	317	CHL	MG-ND	4.29	2.14	2.05
27	6	312	CHL	MG-ND	4.29	2.14	2.05
26	A	815	CL0	O2D-CGD	4.29	1.43	1.33
27	4	308	CHL	O2A-CGA	4.28	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	816	CHL	O2A-CGA	4.28	1.45	1.33
27	F	309	CHL	O2A-CGA	4.28	1.45	1.33
27	5	307	CHL	O2A-CGA	4.28	1.45	1.33
27	A	842	CHL	O2A-CGA	4.28	1.45	1.33
27	A	844	CHL	MG-ND	-4.28	1.97	2.05
27	6	309	CHL	O2A-CGA	4.27	1.45	1.33
27	8	314	CHL	O2A-CGA	4.27	1.45	1.33
27	4	304	CHL	O2A-CGA	4.27	1.45	1.33
27	3	318	CHL	MG-ND	4.27	2.14	2.05
27	4	315	CHL	O2A-CGA	4.26	1.45	1.33
27	6	319	CHL	C3D-C4D	-4.26	1.34	1.44
27	b	307	CHL	O2A-CGA	4.26	1.45	1.33
27	A	837	CHL	O2A-CGA	4.26	1.45	1.33
27	6	315	CHL	O2A-CGA	4.26	1.45	1.33
27	B	823	CHL	O2A-CGA	4.26	1.45	1.33
27	B	837	CHL	O2A-CGA	4.25	1.45	1.33
27	8	312	CHL	O2A-CGA	4.25	1.45	1.33
27	6	313	CHL	O2A-CGA	4.25	1.45	1.33
27	A	833	CHL	O2A-CGA	4.25	1.45	1.33
27	a	307	CHL	O2A-CGA	4.25	1.45	1.33
27	A	826	CHL	O2A-CGA	4.25	1.45	1.33
27	3	318	CHL	O2A-CGA	4.24	1.45	1.33
27	a	313	CHL	O2A-CGA	4.24	1.45	1.33
27	8	317	CHL	O2A-CGA	4.24	1.45	1.33
27	5	312	CHL	O2A-CGA	4.24	1.45	1.33
27	a	309	CHL	O2A-CGA	4.24	1.45	1.33
27	7	319	CHL	O2A-CGA	4.24	1.45	1.33
27	b	315	CHL	O2A-CGA	4.24	1.45	1.33
27	B	841	CHL	O2A-CGA	4.23	1.45	1.33
27	A	858	CHL	O2A-CGA	4.23	1.45	1.33
27	8	313	CHL	O2A-CGA	4.23	1.45	1.33
27	A	854	CHL	O2A-CGA	4.23	1.45	1.33
27	3	320	CHL	O2A-CGA	4.23	1.45	1.33
27	5	323	CHL	O2A-CGA	4.23	1.45	1.33
27	L	303	CHL	C3C-C2C	4.22	1.45	1.36
27	a	312	CHL	O2A-CGA	4.22	1.45	1.33
27	7	316	CHL	O2A-CGA	4.22	1.45	1.33
27	A	849	CHL	O2A-CGA	4.22	1.45	1.33
27	5	318	CHL	O2A-CGA	4.22	1.45	1.33
27	4	310	CHL	MG-NC	-4.22	1.96	2.06
27	8	322	CHL	O2A-CGA	4.22	1.45	1.33
27	B	824	CHL	O2A-CGA	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	313	CHL	O2A-CGA	4.22	1.45	1.33
27	A	838	CHL	O2A-CGA	4.21	1.45	1.33
27	3	319	CHL	O2A-CGA	4.21	1.45	1.33
27	3	308	CHL	O2A-CGA	4.21	1.45	1.33
27	B	813	CHL	MG-NC	4.21	2.16	2.06
27	B	846	CHL	O2A-CGA	4.21	1.45	1.33
27	A	839	CHL	O2A-CGA	4.21	1.45	1.33
27	4	311	CHL	O2A-CGA	4.20	1.45	1.33
27	B	821	CHL	O2A-CGA	4.20	1.45	1.33
27	A	841	CHL	O2A-CGA	4.20	1.45	1.33
27	B	829	CHL	O2A-CGA	4.20	1.45	1.33
27	B	830	CHL	O2A-CGA	4.20	1.45	1.33
27	3	311	CHL	O2A-CGA	4.20	1.45	1.33
27	B	847	CHL	O2A-CGA	4.20	1.45	1.33
27	5	313	CHL	O2A-CGA	4.19	1.45	1.33
27	B	818	CHL	O2A-CGA	4.19	1.45	1.33
27	a	319	CHL	O2A-CGA	4.19	1.45	1.33
27	4	313	CHL	C3B-C2B	4.19	1.46	1.40
27	8	323	CHL	CHC-C1C	4.19	1.45	1.35
27	7	318	CHL	O2A-CGA	4.18	1.45	1.33
27	A	845	CHL	O2A-CGA	4.18	1.45	1.33
27	8	325	CHL	O2A-CGA	4.18	1.45	1.33
27	a	311	CHL	O2A-CGA	4.18	1.45	1.33
27	4	307	CHL	O2A-CGA	4.18	1.45	1.33
27	8	325	CHL	MG-NA	4.18	2.16	2.06
27	B	815	CHL	O2A-CGA	4.18	1.45	1.33
27	B	836	CHL	O2A-CGA	4.18	1.45	1.33
27	B	819	CHL	O2A-CGA	4.18	1.45	1.33
27	7	311	CHL	O2A-CGA	4.18	1.45	1.33
27	B	825	CHL	O2A-CGA	4.17	1.45	1.33
27	3	316	CHL	O2A-CGA	4.17	1.45	1.33
27	5	309	CHL	O2A-CGA	4.17	1.45	1.33
27	B	838	CHL	O2A-CGA	4.17	1.45	1.33
27	3	319	CHL	MG-ND	-4.17	1.97	2.05
27	A	818	CHL	O2A-CGA	4.17	1.45	1.33
27	B	850	CHL	O2A-CGA	4.17	1.45	1.33
27	5	315	CHL	O2A-CGA	4.17	1.45	1.33
27	5	316	CHL	O2A-CGA	4.16	1.45	1.33
27	B	833	CHL	O2A-CGA	4.16	1.45	1.33
27	7	317	CHL	O2A-CGA	4.16	1.45	1.33
27	b	310	CHL	CHD-C4C	4.16	1.48	1.39
27	a	317	CHL	O2A-CGA	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	312	CHL	MG-NC	-4.16	1.96	2.06
27	5	316	CHL	C2C-C3C	4.16	1.45	1.36
27	6	318	CHL	O2A-CGA	4.16	1.46	1.33
27	3	317	CHL	O2A-CGA	4.15	1.45	1.33
27	A	831	CHL	C3C-C2C	4.15	1.45	1.36
27	a	310	CHL	O2A-CGA	4.15	1.45	1.33
27	B	813	CHL	O2A-CGA	4.15	1.45	1.33
27	B	842	CHL	O2A-CGA	4.15	1.45	1.33
27	8	319	CHL	O2A-CGA	4.15	1.45	1.33
29	4	302	LUT	C8-C9	4.15	1.54	1.45
27	A	827	CHL	O2A-CGA	4.15	1.45	1.33
27	3	314	CHL	O2A-CGA	4.14	1.45	1.33
27	B	849	CHL	O2A-CGA	4.14	1.45	1.33
27	5	310	CHL	O2A-CGA	4.14	1.45	1.33
27	A	829	CHL	O2A-CGA	4.14	1.45	1.33
27	7	320	CHL	O2A-CGA	4.14	1.46	1.33
27	A	852	CHL	O2A-CGA	4.14	1.45	1.33
27	A	825	CHL	O2A-CGA	4.13	1.45	1.33
27	6	311	CHL	O2A-CGA	4.13	1.45	1.33
27	A	830	CHL	O2A-CGA	4.13	1.45	1.33
27	A	823	CHL	O2A-CGA	4.13	1.45	1.33
27	B	845	CHL	O2A-CGA	4.13	1.45	1.33
27	B	827	CHL	O2A-CGA	4.13	1.45	1.33
27	B	844	CHL	O2A-CGA	4.12	1.45	1.33
27	6	307	CHL	O2A-CGA	4.12	1.45	1.33
27	7	314	CHL	O2A-CGA	4.12	1.45	1.33
27	b	311	CHL	O2A-CGA	4.12	1.46	1.33
27	A	817	CHL	O2A-CGA	4.12	1.45	1.33
27	8	320	CHL	O2A-CGA	4.12	1.45	1.33
27	b	305	CHL	CHD-C4C	4.12	1.48	1.39
27	6	317	CHL	O2A-CGA	4.12	1.46	1.33
27	6	310	CHL	O2A-CGA	4.12	1.45	1.33
27	B	834	CHL	O2A-CGA	4.11	1.45	1.33
27	A	850	CHL	O2A-CGA	4.11	1.45	1.33
27	K	207	CHL	O2A-CGA	4.11	1.46	1.33
27	B	851	CHL	O2A-CGA	4.11	1.45	1.33
27	8	313	CHL	MG-NC	4.11	2.16	2.06
27	A	835	CHL	O2A-CGA	4.11	1.45	1.33
27	4	308	CHL	MG-NC	4.11	2.16	2.06
27	4	309	CHL	O2A-CGA	4.11	1.46	1.33
27	A	853	CHL	O2A-CGA	4.11	1.45	1.33
27	5	322	CHL	O2A-CGA	4.11	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	321	CHL	O2D-CGD	4.11	1.43	1.33
27	8	316	CHL	O2A-CGA	4.10	1.45	1.33
27	5	316	CHL	O2D-CGD	4.10	1.43	1.33
27	A	821	CHL	O2A-CGA	4.10	1.45	1.33
27	A	824	CHL	O2A-CGA	4.10	1.45	1.33
27	7	321	CHL	O2A-CGA	4.10	1.46	1.33
27	5	319	CHL	O2A-CGA	4.10	1.46	1.33
27	A	828	CHL	O2A-CGA	4.10	1.45	1.33
27	5	316	CHL	C3B-C2B	4.09	1.46	1.40
27	3	315	CHL	O2A-CGA	4.09	1.45	1.33
27	4	306	CHL	O2A-CGA	4.09	1.45	1.33
27	A	819	CHL	O2A-CGA	4.09	1.45	1.33
27	B	832	CHL	O2A-CGA	4.09	1.45	1.33
27	5	317	CHL	O2A-CGA	4.09	1.46	1.33
29	5	303	LUT	C8-C9	4.09	1.54	1.45
27	B	821	CHL	MG-NC	4.08	2.16	2.06
27	3	312	CHL	O2A-CGA	4.08	1.45	1.33
27	4	318	CHL	CHD-C4C	4.08	1.48	1.39
27	8	315	CHL	MG-NC	4.07	2.15	2.06
27	a	319	CHL	CHD-C4C	4.07	1.48	1.39
27	B	822	CHL	O2A-CGA	4.07	1.45	1.33
27	8	323	CHL	O2A-CGA	4.07	1.45	1.33
27	a	317	CHL	MG-NA	4.07	2.15	2.06
27	6	308	CHL	C2C-C3C	4.07	1.45	1.36
27	L	304	CHL	CHD-C4C	4.07	1.48	1.39
27	B	828	CHL	O2A-CGA	4.07	1.45	1.33
27	A	848	CHL	O2A-CGA	4.07	1.45	1.33
29	4	302	LUT	C35-C34	4.06	1.56	1.43
27	B	817	CHL	O2A-CGA	4.06	1.45	1.33
27	K	206	CHL	O2A-CGA	4.06	1.45	1.33
27	B	814	CHL	O2A-CGA	4.06	1.45	1.33
27	5	325	CHL	O2A-CGA	4.06	1.45	1.33
27	B	831	CHL	O2A-CGA	4.05	1.45	1.33
27	b	313	CHL	O2A-CGA	4.05	1.45	1.33
27	5	320	CHL	O2A-CGA	4.05	1.45	1.33
27	b	310	CHL	O2A-CGA	4.05	1.45	1.33
27	b	305	CHL	O2A-CGA	4.05	1.45	1.33
27	7	322	CHL	MG-NC	4.05	2.15	2.06
27	A	840	CHL	O2A-CGA	4.05	1.45	1.33
27	b	304	CHL	O2A-CGA	4.05	1.45	1.33
27	A	832	CHL	O2A-CGA	4.04	1.45	1.33
27	b	316	CHL	C2C-C3C	4.04	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	822	CHL	O2A-CGA	4.04	1.45	1.33
27	K	205	CHL	O2A-CGA	4.04	1.45	1.33
27	8	315	CHL	O2A-CGA	4.04	1.45	1.33
27	8	318	CHL	O2A-CGA	4.04	1.45	1.33
29	F	303	LUT	C8-C9	4.04	1.54	1.45
27	5	311	CHL	O2A-CGA	4.04	1.45	1.33
29	8	303	LUT	C35-C34	4.03	1.55	1.43
27	4	310	CHL	O2A-CGA	4.03	1.45	1.33
27	a	320	CHL	O2A-CGA	4.03	1.45	1.33
27	5	315	CHL	CHD-C4C	4.03	1.48	1.39
27	7	313	CHL	O2A-CGA	4.03	1.45	1.33
27	A	857	CHL	O2A-CGA	4.03	1.45	1.33
27	b	312	CHL	O2A-CGA	4.03	1.45	1.33
27	A	816	CHL	O2A-CGA	4.03	1.45	1.33
27	B	835	CHL	O2A-CGA	4.03	1.45	1.33
27	A	820	CHL	MG-NC	4.03	2.15	2.06
27	8	311	CHL	O2A-CGA	4.02	1.45	1.33
27	K	206	CHL	CHD-C4C	4.02	1.48	1.39
27	b	309	CHL	O2A-CGA	4.02	1.45	1.33
27	b	306	CHL	O2A-CGA	4.02	1.45	1.33
27	B	820	CHL	CHD-C4C	4.02	1.48	1.39
27	6	306	CHL	O2A-CGA	4.02	1.45	1.33
27	b	309	CHL	CHD-C4C	4.02	1.48	1.39
27	7	323	CHL	O2A-CGA	4.02	1.45	1.33
27	A	834	CHL	O2A-CGA	4.02	1.45	1.33
27	6	314	CHL	O2A-CGA	4.01	1.45	1.33
27	8	326	CHL	O2A-CGA	4.01	1.45	1.33
27	5	311	CHL	MG-NC	4.01	2.15	2.06
29	6	302	LUT	C35-C34	4.01	1.55	1.43
27	B	840	CHL	O2A-CGA	4.01	1.45	1.33
27	b	312	CHL	CHD-C4C	4.00	1.48	1.39
27	6	320	CHL	O2A-CGA	4.00	1.45	1.33
27	A	856	CHL	O2A-CGA	4.00	1.45	1.33
27	B	811	CHL	O2A-CGA	4.00	1.45	1.33
27	a	312	CHL	CHD-C4C	4.00	1.48	1.39
27	4	311	CHL	CHD-C4C	4.00	1.48	1.39
27	b	314	CHL	O2A-CGA	4.00	1.45	1.33
27	A	843	CHL	O2A-CGA	4.00	1.45	1.33
29	b	303	LUT	C14-C13	4.00	1.41	1.35
27	A	855	CHL	O2A-CGA	4.00	1.45	1.33
27	4	316	CHL	C2C-C3C	4.00	1.45	1.36
27	A	859	CHL	O2A-CGA	4.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	312	CHL	O2A-CGA	3.99	1.45	1.33
27	J	106	CHL	MG-NA	3.99	2.15	2.06
27	A	820	CHL	O2A-CGA	3.99	1.45	1.33
29	b	303	LUT	C30-C29	3.99	1.41	1.35
29	6	303	LUT	C8-C9	3.99	1.54	1.45
27	6	315	CHL	CHD-C4C	3.99	1.48	1.39
27	5	321	CHL	O2A-CGA	3.99	1.45	1.33
27	B	837	CHL	CHD-C4C	3.99	1.48	1.39
27	A	831	CHL	O2A-CGA	3.98	1.45	1.33
27	4	314	CHL	CHD-C4C	3.98	1.48	1.39
27	A	851	CHL	O2A-CGA	3.98	1.45	1.33
27	5	309	CHL	CHD-C4C	3.98	1.48	1.39
27	B	812	CHL	O2A-CGA	3.98	1.45	1.33
29	b	303	LUT	C34-C33	3.98	1.41	1.35
27	A	855	CHL	MG-ND	-3.98	1.97	2.05
27	B	844	CHL	CHD-C4C	3.98	1.48	1.39
27	7	324	CHL	O2A-CGA	3.97	1.45	1.33
27	A	853	CHL	CHD-C4C	3.97	1.48	1.39
27	6	313	CHL	CHD-C4C	3.97	1.48	1.39
27	6	305	CHL	O2A-CGA	3.97	1.45	1.33
27	a	320	CHL	CHD-C4C	3.97	1.48	1.39
27	5	320	CHL	CHD-C4C	3.97	1.48	1.39
27	b	314	CHL	CHD-C4C	3.97	1.48	1.39
27	5	312	CHL	CHD-C4C	3.97	1.48	1.39
27	F	308	CHL	O2A-CGA	3.97	1.45	1.33
27	K	205	CHL	CHD-C4C	3.97	1.48	1.39
27	5	318	CHL	CHD-C4C	3.97	1.48	1.39
27	a	314	CHL	CHD-C4C	3.96	1.48	1.39
27	3	314	CHL	CHD-C4C	3.96	1.48	1.39
27	b	313	CHL	CHD-C4C	3.96	1.48	1.39
29	J	103	LUT	C35-C34	3.96	1.55	1.43
27	4	309	CHL	CHD-C1D	3.96	1.46	1.38
27	8	320	CHL	CHD-C4C	3.95	1.48	1.39
27	3	309	CHL	O2A-CGA	3.95	1.45	1.33
27	3	313	CHL	CHD-C4C	3.94	1.48	1.39
27	B	827	CHL	CHD-C4C	3.94	1.48	1.39
27	4	309	CHL	MG-NC	-3.94	1.96	2.06
27	A	851	CHL	CHD-C4C	3.94	1.48	1.39
27	A	836	CHL	O2A-CGA	3.94	1.44	1.33
27	a	316	CHL	C2C-C3C	3.94	1.45	1.36
27	A	849	CHL	CHD-C4C	3.94	1.48	1.39
27	5	308	CHL	O2A-CGA	3.94	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	828	CHL	CHD-C4C	3.94	1.48	1.39
27	3	311	CHL	CHD-C4C	3.94	1.48	1.39
27	6	308	CHL	CHD-C1D	3.94	1.46	1.38
27	b	317	CHL	C2C-C3C	3.93	1.45	1.36
27	4	320	CHL	CHD-C4C	3.93	1.48	1.39
27	A	844	CHL	CHD-C4C	3.93	1.48	1.39
27	6	318	CHL	C2C-C3C	3.93	1.45	1.36
27	6	319	CHL	CHC-C1C	3.93	1.45	1.35
27	b	306	CHL	CHD-C4C	3.93	1.48	1.39
27	b	316	CHL	C3B-C2B	3.93	1.45	1.40
27	4	315	CHL	CHD-C4C	3.93	1.48	1.39
27	b	316	CHL	CHD-C1D	3.93	1.46	1.38
27	4	306	CHL	CHD-C4C	3.93	1.48	1.39
27	3	315	CHL	CHD-C4C	3.92	1.48	1.39
27	A	842	CHL	MG-NC	3.92	2.15	2.06
27	5	314	CHL	CHD-C4C	3.92	1.48	1.39
27	5	321	CHL	CHD-C4C	3.92	1.48	1.39
27	A	826	CHL	CHD-C4C	3.92	1.48	1.39
27	a	309	CHL	CHD-C4C	3.92	1.48	1.39
27	B	823	CHL	MG-NA	3.92	2.15	2.06
27	A	829	CHL	CHD-C4C	3.92	1.48	1.39
27	8	325	CHL	CHD-C4C	3.91	1.48	1.39
27	B	840	CHL	CHD-C4C	3.91	1.48	1.39
27	A	822	CHL	CHD-C4C	3.91	1.48	1.39
27	8	324	CHL	C2C-C3C	3.91	1.45	1.36
27	A	843	CHL	C3C-C2C	3.91	1.45	1.36
27	A	844	CHL	O2A-CGA	3.91	1.44	1.33
29	5	302	LUT	C35-C34	3.91	1.55	1.43
27	3	321	CHL	CHD-C4C	3.91	1.48	1.39
27	A	854	CHL	CHD-C4C	3.90	1.48	1.39
27	b	317	CHL	C3B-C2B	3.90	1.45	1.40
27	B	849	CHL	CHD-C4C	3.90	1.48	1.39
27	B	839	CHL	CHD-C4C	3.90	1.48	1.39
27	3	319	CHL	CHD-C4C	3.90	1.48	1.39
27	6	320	CHL	CHD-C4C	3.90	1.48	1.39
29	a	304	LUT	C35-C34	3.90	1.55	1.43
27	b	308	CHL	O2A-CGA	3.90	1.45	1.33
29	b	301	LUT	C35-C34	3.90	1.55	1.43
27	5	319	CHL	C2C-C3C	3.90	1.45	1.36
27	B	833	CHL	CHD-C4C	3.90	1.48	1.39
27	B	818	CHL	CHD-C4C	3.90	1.48	1.39
27	a	313	CHL	CHD-C4C	3.90	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	835	CHL	CHD-C4C	3.89	1.48	1.39
27	a	318	CHL	C2C-C3C	3.89	1.45	1.36
27	B	829	CHL	CHD-C4C	3.89	1.48	1.39
27	B	831	CHL	CHD-C4C	3.89	1.48	1.39
27	3	310	CHL	CHD-C4C	3.89	1.48	1.39
27	6	307	CHL	C3C-C2C	3.89	1.45	1.36
27	B	814	CHL	CHD-C4C	3.89	1.48	1.39
29	8	304	LUT	C35-C34	3.89	1.55	1.43
27	4	310	CHL	CHD-C4C	3.89	1.48	1.39
27	6	314	CHL	CHD-C4C	3.89	1.48	1.39
27	K	205	CHL	MG-NC	3.89	2.15	2.06
27	A	816	CHL	CHD-C4C	3.88	1.48	1.39
27	b	307	CHL	CHD-C4C	3.88	1.48	1.39
27	B	842	CHL	CHD-C4C	3.88	1.48	1.39
27	B	824	CHL	CHD-C4C	3.88	1.48	1.39
27	8	323	CHL	C3D-C4D	-3.88	1.35	1.44
27	a	317	CHL	CHD-C4C	3.88	1.48	1.39
27	5	311	CHL	MG-ND	-3.88	1.98	2.05
27	A	848	CHL	CHD-C4C	3.88	1.48	1.39
27	B	838	CHL	CHD-C4C	3.88	1.48	1.39
27	6	311	CHL	CHD-C4C	3.88	1.48	1.39
27	7	318	CHL	CHD-C4C	3.88	1.48	1.39
27	A	823	CHL	CHD-C4C	3.88	1.48	1.39
27	F	309	CHL	CHD-C4C	3.88	1.48	1.39
22	6	301	BCR	C21-C22	3.87	1.40	1.35
27	b	311	CHL	C2C-C3C	3.87	1.45	1.36
27	8	319	CHL	CHD-C4C	3.87	1.48	1.39
27	b	304	CHL	CHD-C4C	3.87	1.48	1.39
27	a	311	CHL	CHD-C4C	3.87	1.48	1.39
27	a	319	CHL	MG-NC	3.87	2.15	2.06
27	L	303	CHL	CHC-C1C	3.87	1.44	1.35
27	5	323	CHL	CHD-C4C	3.87	1.48	1.39
27	7	316	CHL	CHD-C4C	3.87	1.48	1.39
27	5	322	CHL	C2C-C3C	3.87	1.45	1.36
27	6	316	CHL	C2C-C3C	3.87	1.45	1.36
27	A	839	CHL	CHD-C4C	3.87	1.48	1.39
27	6	310	CHL	CHD-C4C	3.87	1.48	1.39
27	7	322	CHL	C2C-C3C	3.87	1.45	1.36
27	K	207	CHL	CHD-C1D	3.87	1.45	1.38
27	6	312	CHL	CHD-C4C	3.86	1.48	1.39
27	4	313	CHL	C3C-C2C	3.86	1.44	1.36
27	b	308	CHL	C3D-C4D	-3.86	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	306	CHL	CHD-C4C	3.86	1.48	1.39
27	8	316	CHL	CHD-C4C	3.86	1.48	1.39
27	4	316	CHL	CHD-C1D	3.86	1.45	1.38
27	6	308	CHL	O2A-CGA	3.86	1.44	1.33
27	L	303	CHL	O2A-CGA	3.86	1.44	1.33
27	6	305	CHL	CHD-C4C	3.86	1.48	1.39
29	8	304	LUT	C8-C9	3.86	1.54	1.45
27	A	830	CHL	CHD-C4C	3.86	1.48	1.39
27	A	847	CHL	CHD-C4C	3.85	1.48	1.39
27	8	311	CHL	CHD-C4C	3.85	1.48	1.39
27	8	318	CHL	CHD-C4C	3.85	1.48	1.39
27	4	305	CHL	CHD-C4C	3.85	1.48	1.39
27	A	827	CHL	CHD-C4C	3.85	1.48	1.39
29	4	301	LUT	C35-C34	3.85	1.55	1.43
27	5	307	CHL	CHD-C4C	3.85	1.48	1.39
27	A	859	CHL	CHD-C4C	3.85	1.48	1.39
27	B	813	CHL	CHD-C4C	3.85	1.48	1.39
27	7	314	CHL	CHD-C4C	3.85	1.48	1.39
27	7	324	CHL	CHD-C4C	3.85	1.48	1.39
27	B	836	CHL	CHD-C4C	3.84	1.48	1.39
27	5	317	CHL	C2C-C3C	3.84	1.45	1.36
27	A	855	CHL	CHD-C4C	3.84	1.48	1.39
27	b	317	CHL	CHD-C1D	3.84	1.45	1.38
27	7	320	CHL	C2C-C3C	3.84	1.45	1.36
27	7	313	CHL	CHD-C4C	3.84	1.48	1.39
29	a	304	LUT	C8-C9	3.84	1.54	1.45
27	6	318	CHL	C3B-C2B	3.84	1.45	1.40
27	B	845	CHL	CHD-C4C	3.84	1.48	1.39
29	b	301	LUT	C8-C9	3.84	1.54	1.45
27	4	309	CHL	C2C-C3C	3.84	1.45	1.36
27	3	309	CHL	CHD-C4C	3.83	1.48	1.39
27	A	818	CHL	CHD-C4C	3.83	1.48	1.39
27	a	308	CHL	CHD-C4C	3.83	1.48	1.39
27	3	312	CHL	CHD-C4C	3.83	1.48	1.39
27	B	821	CHL	CHD-C4C	3.83	1.48	1.39
27	B	847	CHL	CHD-C4C	3.83	1.48	1.39
27	A	857	CHL	CHD-C4C	3.83	1.48	1.39
27	5	311	CHL	CHD-C4C	3.83	1.48	1.39
27	a	316	CHL	MG-NA	-3.83	1.97	2.06
27	A	845	CHL	CHD-C4C	3.83	1.48	1.39
27	J	106	CHL	CHD-C4C	3.82	1.48	1.39
27	3	318	CHL	CHD-C4C	3.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	322	CHL	CHD-C4C	3.82	1.48	1.39
27	a	316	CHL	C3B-C2B	3.82	1.45	1.40
27	B	843	CHL	CHD-C4C	3.82	1.48	1.39
27	8	323	CHL	CHD-C1D	3.82	1.45	1.38
27	a	307	CHL	CHD-C4C	3.82	1.48	1.39
27	5	313	CHL	C3C-C2C	3.82	1.44	1.36
27	A	825	CHL	CHD-C4C	3.82	1.48	1.39
27	B	826	CHL	CHD-C4C	3.82	1.47	1.39
27	B	823	CHL	CHD-C4C	3.82	1.47	1.39
29	6	303	LUT	C35-C34	3.82	1.55	1.43
27	4	312	CHL	C2C-C3C	3.82	1.45	1.36
27	4	317	CHL	CHD-C1D	3.81	1.45	1.38
27	7	311	CHL	CHD-C4C	3.81	1.47	1.39
27	6	309	CHL	CHD-C4C	3.81	1.47	1.39
27	4	308	CHL	CHD-C4C	3.81	1.47	1.39
29	5	303	LUT	C35-C34	3.81	1.55	1.43
27	A	831	CHL	C3B-C2B	3.81	1.45	1.40
27	B	848	CHL	CHD-C4C	3.81	1.47	1.39
27	B	822	CHL	CHD-C4C	3.80	1.47	1.39
27	8	317	CHL	CHD-C4C	3.80	1.47	1.39
27	8	321	CHL	C2C-C3C	3.80	1.44	1.36
27	A	817	CHL	CHD-C4C	3.80	1.47	1.39
27	K	207	CHL	C2C-C3C	3.80	1.44	1.36
29	7	304	LUT	C35-C34	3.80	1.55	1.43
27	4	307	CHL	CHD-C4C	3.80	1.47	1.39
27	5	319	CHL	CHD-C1D	3.80	1.45	1.38
27	A	828	CHL	CHD-C4C	3.80	1.47	1.39
27	7	313	CHL	MG-ND	3.79	2.13	2.05
27	6	314	CHL	MG-ND	-3.79	1.98	2.05
27	5	322	CHL	CHD-C1D	3.79	1.45	1.38
29	3	304	LUT	C31-C30	3.79	1.55	1.43
27	A	834	CHL	CHD-C4C	3.79	1.47	1.39
27	3	317	CHL	CHD-C4C	3.79	1.47	1.39
27	A	837	CHL	CHD-C4C	3.79	1.47	1.39
29	4	302	LUT	C15-C14	3.79	1.55	1.43
27	4	319	CHL	OBD-CAD	3.79	1.29	1.22
27	B	816	CHL	CHD-C4C	3.79	1.47	1.39
27	A	856	CHL	CHD-C4C	3.79	1.47	1.39
27	B	832	CHL	CHD-C4C	3.78	1.47	1.39
27	8	314	CHL	C2C-C3C	3.78	1.44	1.36
27	B	839	CHL	MG-NC	3.78	2.15	2.06
29	3	305	LUT	C35-C34	3.78	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	302	LUT	C31-C30	3.78	1.55	1.43
29	F	303	LUT	C35-C34	3.78	1.55	1.43
27	A	854	CHL	MG-ND	3.78	2.13	2.05
29	4	301	LUT	C31-C30	3.78	1.55	1.43
27	K	207	CHL	C3B-C2B	3.78	1.45	1.40
27	7	319	CHL	C3B-C2B	3.78	1.45	1.40
29	5	302	LUT	C8-C9	3.77	1.54	1.45
27	4	318	CHL	OBD-CAD	3.77	1.29	1.22
29	b	301	LUT	C31-C30	3.77	1.55	1.43
29	8	303	LUT	C15-C14	3.77	1.55	1.43
27	4	304	CHL	CHD-C4C	3.77	1.47	1.39
27	a	318	CHL	C3B-C2B	3.77	1.45	1.40
27	A	836	CHL	CHD-C4C	3.77	1.47	1.39
27	B	851	CHL	CHD-C4C	3.77	1.47	1.39
27	5	325	CHL	C3B-C2B	3.76	1.45	1.40
26	A	815	CL0	O2A-CGA	3.76	1.44	1.33
27	a	318	CHL	CHD-C1D	3.76	1.45	1.38
27	7	321	CHL	C2C-C3C	3.76	1.44	1.36
27	A	838	CHL	CHD-C4C	3.76	1.47	1.39
27	a	316	CHL	CHD-C1D	3.76	1.45	1.38
29	a	302	LUT	C35-C34	3.76	1.55	1.43
29	J	103	LUT	C8-C9	3.76	1.54	1.45
29	J	103	LUT	C31-C30	3.76	1.55	1.43
29	a	304	LUT	C31-C30	3.76	1.55	1.43
27	7	322	CHL	C3B-C2B	3.76	1.45	1.40
29	J	103	LUT	C15-C14	3.76	1.55	1.43
33	7	305	XAT	C10-C9	3.76	1.40	1.35
27	3	308	CHL	CHD-C4C	3.76	1.47	1.39
27	A	850	CHL	CHD-C4C	3.75	1.47	1.39
27	B	835	CHL	CHD-C4C	3.75	1.47	1.39
27	7	319	CHL	C2C-C3C	3.75	1.44	1.36
27	A	840	CHL	CHD-C4C	3.75	1.47	1.39
22	6	301	BCR	C14-C13	3.75	1.40	1.35
27	6	311	CHL	MG-NA	3.75	2.15	2.06
27	A	858	CHL	CHD-C4C	3.75	1.47	1.39
27	B	846	CHL	CHD-C4C	3.75	1.47	1.39
27	a	310	CHL	CHD-C4C	3.75	1.47	1.39
27	5	308	CHL	CHD-C4C	3.75	1.47	1.39
27	A	842	CHL	C3B-C2B	3.75	1.45	1.40
29	3	304	LUT	C35-C34	3.75	1.55	1.43
27	b	311	CHL	CHD-C1D	3.75	1.45	1.38
27	4	309	CHL	C3B-C2B	3.75	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	325	CHL	C2C-C3C	3.74	1.44	1.36
27	3	320	CHL	CHD-C4C	3.74	1.47	1.39
29	6	302	LUT	C8-C9	3.74	1.54	1.45
29	6	302	LUT	C28-C29	3.74	1.54	1.45
27	A	852	CHL	CHD-C4C	3.74	1.47	1.39
27	b	315	CHL	CHD-C4C	3.74	1.47	1.39
29	4	302	LUT	C28-C29	3.73	1.54	1.45
27	5	317	CHL	C3B-C2B	3.73	1.45	1.40
27	a	315	CHL	C2C-C3C	3.73	1.44	1.36
27	B	830	CHL	CHD-C4C	3.73	1.47	1.39
27	4	312	CHL	CHD-C1D	3.73	1.45	1.38
27	A	841	CHL	C3B-C2B	3.73	1.45	1.40
27	7	321	CHL	C3B-C2B	3.73	1.45	1.40
27	A	841	CHL	C2C-C3C	3.73	1.44	1.36
27	6	317	CHL	CHD-C1D	3.73	1.45	1.38
27	B	819	CHL	CHD-C4C	3.73	1.47	1.39
29	3	305	LUT	C31-C30	3.73	1.55	1.43
27	A	820	CHL	CHD-C4C	3.73	1.47	1.39
27	7	315	CHL	CHD-C4C	3.73	1.47	1.39
27	3	321	CHL	OBD-CAD	3.73	1.28	1.22
27	5	310	CHL	CHD-C4C	3.73	1.47	1.39
27	b	311	CHL	C3B-C2B	3.73	1.45	1.40
27	6	317	CHL	C2C-C3C	3.72	1.44	1.36
27	A	821	CHL	CHD-C4C	3.72	1.47	1.39
27	B	825	CHL	CHD-C4C	3.72	1.47	1.39
27	8	312	CHL	CHD-C4C	3.72	1.47	1.39
27	5	319	CHL	MG-NC	3.72	2.15	2.06
27	7	322	CHL	MG-NA	3.72	2.15	2.06
29	a	302	LUT	C8-C9	3.72	1.53	1.45
29	4	302	LUT	C12-C13	3.71	1.53	1.45
29	3	304	LUT	C8-C9	3.71	1.53	1.45
27	A	833	CHL	C2C-C3C	3.71	1.44	1.36
27	B	850	CHL	CHD-C4C	3.71	1.47	1.39
29	a	304	LUT	C28-C29	3.71	1.53	1.45
29	6	302	LUT	C15-C14	3.71	1.54	1.43
27	6	312	CHL	MG-NC	3.71	2.15	2.06
27	6	318	CHL	CHD-C1D	3.71	1.45	1.38
29	6	303	LUT	C31-C30	3.71	1.54	1.43
27	7	317	CHL	CHD-C4C	3.70	1.47	1.39
29	J	103	LUT	C11-C10	3.70	1.54	1.43
29	4	302	LUT	C32-C33	3.70	1.53	1.45
29	b	301	LUT	C15-C14	3.70	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	305	CHL	OBD-CAD	3.70	1.28	1.22
29	4	302	LUT	C11-C10	3.70	1.54	1.43
27	A	826	CHL	MG-NC	3.70	2.15	2.06
29	6	302	LUT	C32-C33	3.70	1.53	1.45
27	A	819	CHL	CHD-C4C	3.70	1.47	1.39
27	8	313	CHL	CHD-C4C	3.70	1.47	1.39
27	a	315	CHL	CHD-C1D	3.70	1.45	1.38
27	7	320	CHL	CHD-C1D	3.70	1.45	1.38
27	8	324	CHL	CHD-C1D	3.70	1.45	1.38
29	4	301	LUT	C15-C14	3.69	1.54	1.43
29	a	302	LUT	C31-C30	3.69	1.54	1.43
27	a	315	CHL	C3B-C2B	3.69	1.45	1.40
27	5	322	CHL	C3B-C2B	3.69	1.45	1.40
27	4	313	CHL	CHD-C1D	3.68	1.45	1.38
27	5	314	CHL	OBD-CAD	3.68	1.28	1.22
27	8	326	CHL	CHD-C4C	3.68	1.47	1.39
27	a	312	CHL	OBD-CAD	3.68	1.28	1.22
27	b	306	CHL	OBD-CAD	3.68	1.28	1.22
27	B	812	CHL	CHD-C4C	3.68	1.47	1.39
27	6	317	CHL	C3B-C2B	3.68	1.45	1.40
27	A	822	CHL	MG-ND	3.68	2.13	2.05
27	8	315	CHL	CHD-C4C	3.68	1.47	1.39
27	8	314	CHL	C3B-C2B	3.68	1.45	1.40
27	5	317	CHL	CHD-C1D	3.68	1.45	1.38
27	A	831	CHL	CHC-C1C	3.67	1.44	1.35
27	b	310	CHL	OBD-CAD	3.67	1.28	1.22
22	6	301	BCR	C17-C18	3.67	1.40	1.35
29	5	302	LUT	C31-C30	3.67	1.54	1.43
29	7	304	LUT	C31-C30	3.67	1.54	1.43
27	B	841	CHL	CHD-C4C	3.67	1.47	1.39
27	8	321	CHL	C3B-C2B	3.67	1.45	1.40
29	6	302	LUT	C31-C30	3.67	1.54	1.43
27	6	316	CHL	CHD-C1D	3.67	1.45	1.38
29	5	302	LUT	C15-C14	3.67	1.54	1.43
27	A	833	CHL	CHD-C1D	3.67	1.45	1.38
29	4	301	LUT	C8-C9	3.66	1.53	1.45
27	4	310	CHL	OBD-CAD	3.66	1.28	1.22
29	J	103	LUT	C12-C13	3.66	1.53	1.45
27	A	842	CHL	C2C-C3C	3.66	1.44	1.36
27	3	315	CHL	MG-NC	3.66	2.15	2.06
27	5	320	CHL	OBD-CAD	3.66	1.28	1.22
27	A	843	CHL	CHC-C1C	3.66	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	308	CHL	CHD-C4C	3.66	1.47	1.39
27	7	322	CHL	CHD-C1D	3.66	1.45	1.38
27	8	324	CHL	C3B-C2B	3.66	1.45	1.40
33	7	305	XAT	C34-C33	3.66	1.40	1.35
27	8	314	CHL	CHD-C1D	3.66	1.45	1.38
27	B	818	CHL	MG-NC	3.66	2.15	2.06
27	F	308	CHL	OBD-CAD	3.65	1.28	1.22
27	b	308	CHL	OBD-CAD	3.65	1.28	1.22
33	7	305	XAT	C30-C29	3.65	1.40	1.35
27	b	304	CHL	OBD-CAD	3.65	1.28	1.22
27	5	323	CHL	OBD-CAD	3.65	1.28	1.22
29	8	304	LUT	C15-C14	3.65	1.54	1.43
27	B	815	CHL	CHD-C4C	3.64	1.47	1.39
29	b	301	LUT	C28-C29	3.64	1.53	1.45
27	K	204	CHL	CHD-C4C	3.64	1.47	1.39
27	a	314	CHL	OBD-CAD	3.64	1.28	1.22
29	8	303	LUT	C8-C9	3.64	1.53	1.45
29	J	103	LUT	C32-C33	3.64	1.53	1.45
33	7	305	XAT	C14-C13	3.64	1.40	1.35
27	B	830	CHL	OBD-CAD	3.64	1.28	1.22
27	b	309	CHL	OBD-CAD	3.64	1.28	1.22
27	6	316	CHL	C3B-C2B	3.64	1.45	1.40
27	B	824	CHL	OBD-CAD	3.64	1.28	1.22
27	6	309	CHL	OBD-CAD	3.64	1.28	1.22
27	A	832	CHL	CHD-C4C	3.64	1.47	1.39
29	a	304	LUT	C15-C14	3.64	1.54	1.43
27	K	206	CHL	OBD-CAD	3.64	1.28	1.22
27	3	319	CHL	OBD-CAD	3.64	1.28	1.22
27	4	306	CHL	OBD-CAD	3.63	1.28	1.22
27	b	315	CHL	OBD-CAD	3.63	1.28	1.22
26	A	815	CL0	CHC-C1C	3.63	1.44	1.35
27	A	857	CHL	OBD-CAD	3.63	1.28	1.22
27	4	320	CHL	OBD-CAD	3.63	1.28	1.22
27	5	325	CHL	CHD-C1D	3.63	1.45	1.38
29	F	303	LUT	C31-C30	3.63	1.54	1.43
27	7	312	CHL	CHD-C4C	3.63	1.47	1.39
27	A	846	CHL	C3B-C2B	3.63	1.45	1.40
27	6	319	CHL	OBD-CAD	3.63	1.28	1.22
27	A	817	CHL	C1D-ND	-3.63	1.33	1.37
29	F	303	LUT	C15-C14	3.63	1.54	1.43
29	a	304	LUT	C32-C33	3.63	1.53	1.45
27	A	824	CHL	CHD-C4C	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	815	CL0	C3C-C2C	3.62	1.44	1.36
27	7	324	CHL	MG-ND	-3.62	1.98	2.05
27	4	316	CHL	C3B-C2B	3.62	1.45	1.40
27	5	316	CHL	CHD-C1D	3.62	1.45	1.38
27	L	303	CHL	C3B-C2B	3.62	1.45	1.40
27	A	843	CHL	C3B-C2B	3.62	1.45	1.40
29	5	303	LUT	C11-C10	3.62	1.54	1.43
27	5	308	CHL	OBD-CAD	3.62	1.28	1.22
27	7	320	CHL	C3B-C2B	3.62	1.45	1.40
27	3	316	CHL	C2C-C3C	3.62	1.44	1.36
29	6	303	LUT	C15-C14	3.62	1.54	1.43
29	4	301	LUT	C28-C29	3.61	1.53	1.45
29	7	304	LUT	C7-C6	3.61	1.57	1.45
27	B	811	CHL	CHD-C4C	3.61	1.47	1.39
27	5	319	CHL	C3B-C2B	3.61	1.45	1.40
27	b	313	CHL	OBD-CAD	3.61	1.28	1.22
27	4	305	CHL	OBD-CAD	3.61	1.28	1.22
27	L	304	CHL	OBD-CAD	3.61	1.28	1.22
27	B	820	CHL	OBD-CAD	3.61	1.28	1.22
27	3	309	CHL	OBD-CAD	3.61	1.28	1.22
27	B	829	CHL	MG-NC	3.61	2.14	2.06
29	6	302	LUT	C26-C27	3.61	1.55	1.50
29	b	301	LUT	C11-C10	3.60	1.54	1.43
27	8	311	CHL	OBD-CAD	3.60	1.28	1.22
27	A	849	CHL	OBD-CAD	3.60	1.28	1.22
27	B	829	CHL	OBD-CAD	3.60	1.28	1.22
27	a	309	CHL	OBD-CAD	3.60	1.28	1.22
27	4	311	CHL	OBD-CAD	3.60	1.28	1.22
27	7	318	CHL	OBD-CAD	3.59	1.28	1.22
27	8	323	CHL	C3D-C2D	3.59	1.48	1.39
27	5	315	CHL	OBD-CAD	3.59	1.28	1.22
27	5	321	CHL	OBD-CAD	3.59	1.28	1.22
27	B	842	CHL	OBD-CAD	3.59	1.28	1.22
27	3	314	CHL	OBD-CAD	3.59	1.28	1.22
27	7	319	CHL	CHD-C1D	3.59	1.45	1.38
27	B	817	CHL	CHD-C4C	3.59	1.47	1.39
27	b	307	CHL	OBD-CAD	3.59	1.28	1.22
29	a	302	LUT	C15-C14	3.58	1.54	1.43
27	6	308	CHL	CHD-C4C	3.58	1.47	1.39
27	7	321	CHL	CHD-C1D	3.58	1.45	1.38
22	6	301	BCR	C10-C9	3.58	1.40	1.35
27	7	319	CHL	MG-NC	3.58	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	315	CHL	OBD-CAD	3.58	1.28	1.22
29	7	304	LUT	C15-C14	3.58	1.54	1.43
27	b	312	CHL	OBD-CAD	3.58	1.28	1.22
27	B	843	CHL	OBD-CAD	3.58	1.28	1.22
27	a	319	CHL	OBD-CAD	3.58	1.28	1.22
27	6	314	CHL	OBD-CAD	3.58	1.28	1.22
27	3	316	CHL	CHD-C1D	3.58	1.45	1.38
27	8	321	CHL	MG-NA	-3.58	1.97	2.06
27	J	106	CHL	OBD-CAD	3.57	1.28	1.22
27	4	313	CHL	OBD-CAD	3.57	1.28	1.22
27	8	313	CHL	OBD-CAD	3.57	1.28	1.22
27	B	813	CHL	OBD-CAD	3.57	1.28	1.22
27	6	307	CHL	CHC-C1C	3.57	1.44	1.35
29	7	304	LUT	C8-C9	3.57	1.53	1.45
29	8	303	LUT	C31-C30	3.57	1.54	1.43
27	6	312	CHL	OBD-CAD	3.57	1.28	1.22
29	6	302	LUT	C12-C13	3.57	1.53	1.45
29	b	301	LUT	C32-C33	3.57	1.53	1.45
29	F	303	LUT	C28-C29	3.56	1.53	1.45
29	3	304	LUT	C32-C33	3.56	1.53	1.45
29	6	302	LUT	C11-C10	3.56	1.54	1.43
27	A	833	CHL	C3B-C2B	3.56	1.45	1.40
27	B	851	CHL	OBD-CAD	3.56	1.28	1.22
27	3	318	CHL	OBD-CAD	3.56	1.28	1.22
29	8	303	LUT	C12-C13	3.56	1.53	1.45
27	a	308	CHL	OBD-CAD	3.56	1.28	1.22
27	a	317	CHL	OBD-CAD	3.56	1.28	1.22
26	A	815	CL0	C3B-C2B	3.56	1.45	1.40
29	F	303	LUT	C12-C13	3.56	1.53	1.45
29	J	103	LUT	C28-C29	3.55	1.53	1.45
27	4	319	CHL	MG-NA	3.55	2.14	2.06
27	B	834	CHL	CHD-C4C	3.55	1.47	1.39
27	b	310	CHL	C3D-C2D	3.55	1.48	1.39
27	A	837	CHL	OBD-CAD	3.55	1.28	1.22
27	8	317	CHL	OBD-CAD	3.55	1.28	1.22
29	3	304	LUT	C15-C14	3.55	1.54	1.43
29	3	305	LUT	C15-C14	3.54	1.54	1.43
27	7	324	CHL	OBD-CAD	3.54	1.28	1.22
27	B	821	CHL	OBD-CAD	3.54	1.28	1.22
27	4	312	CHL	C3B-C2B	3.54	1.45	1.40
27	b	317	CHL	CHD-C4C	3.54	1.47	1.39
29	5	303	LUT	C31-C30	3.54	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	307	CHL	OBD-CAD	3.54	1.28	1.22
27	4	304	CHL	OBD-CAD	3.54	1.28	1.22
27	4	319	CHL	C3D-C2D	3.53	1.48	1.39
29	5	302	LUT	C11-C10	3.53	1.54	1.43
29	5	302	LUT	C12-C13	3.53	1.53	1.45
27	a	310	CHL	OBD-CAD	3.53	1.28	1.22
29	4	301	LUT	C11-C10	3.53	1.54	1.43
27	A	829	CHL	OBD-CAD	3.53	1.28	1.22
29	6	303	LUT	C32-C33	3.53	1.53	1.45
27	6	313	CHL	OBD-CAD	3.53	1.28	1.22
27	B	826	CHL	OBD-CAD	3.52	1.28	1.22
27	7	323	CHL	OBD-CAD	3.52	1.28	1.22
29	4	301	LUT	C12-C13	3.52	1.53	1.45
27	8	321	CHL	CHD-C1D	3.52	1.45	1.38
29	6	303	LUT	C11-C10	3.52	1.54	1.43
27	8	325	CHL	OBD-CAD	3.52	1.28	1.22
29	3	305	LUT	C28-C29	3.52	1.53	1.45
29	8	304	LUT	C31-C30	3.52	1.54	1.43
27	B	817	CHL	OBD-CAD	3.52	1.28	1.22
27	3	310	CHL	OBD-CAD	3.52	1.28	1.22
27	K	204	CHL	OBD-CAD	3.52	1.28	1.22
27	3	316	CHL	C3D-C4D	-3.52	1.36	1.44
27	4	309	CHL	CHD-C4C	3.51	1.47	1.39
27	B	838	CHL	OBD-CAD	3.51	1.28	1.22
29	a	304	LUT	C11-C10	3.51	1.54	1.43
29	b	301	LUT	C26-C27	3.51	1.55	1.50
27	5	312	CHL	OBD-CAD	3.51	1.28	1.22
29	6	303	LUT	C28-C29	3.51	1.53	1.45
27	b	316	CHL	OBD-CAD	3.51	1.28	1.22
27	4	307	CHL	OBD-CAD	3.51	1.28	1.22
27	A	839	CHL	OBD-CAD	3.50	1.28	1.22
27	5	318	CHL	OBD-CAD	3.50	1.28	1.22
27	A	820	CHL	MG-ND	-3.50	1.98	2.05
27	A	827	CHL	OBD-CAD	3.50	1.28	1.22
27	a	320	CHL	OBD-CAD	3.50	1.28	1.22
27	3	313	CHL	OBD-CAD	3.50	1.28	1.22
27	A	851	CHL	OBD-CAD	3.50	1.28	1.22
27	B	812	CHL	C1D-ND	-3.50	1.33	1.37
27	A	822	CHL	OBD-CAD	3.50	1.28	1.22
29	3	305	LUT	C8-C9	3.50	1.53	1.45
29	4	301	LUT	C26-C27	3.50	1.55	1.50
27	B	822	CHL	OBD-CAD	3.50	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	848	CHL	OBD-CAD	3.49	1.28	1.22
27	6	311	CHL	OBD-CAD	3.49	1.28	1.22
27	b	316	CHL	CHD-C4C	3.49	1.47	1.39
27	4	315	CHL	OBD-CAD	3.49	1.28	1.22
29	a	302	LUT	C28-C29	3.49	1.53	1.45
27	A	817	CHL	OBD-CAD	3.49	1.28	1.22
27	A	858	CHL	OBD-CAD	3.49	1.28	1.22
29	8	303	LUT	C11-C10	3.49	1.54	1.43
27	B	819	CHL	OBD-CAD	3.49	1.28	1.22
27	A	835	CHL	OBD-CAD	3.49	1.28	1.22
27	B	827	CHL	OBD-CAD	3.49	1.28	1.22
27	B	840	CHL	OBD-CAD	3.49	1.28	1.22
27	4	316	CHL	CHD-C4C	3.49	1.47	1.39
27	A	850	CHL	OBD-CAD	3.48	1.28	1.22
27	6	317	CHL	C3D-C4D	-3.48	1.36	1.44
27	6	305	CHL	OBD-CAD	3.48	1.28	1.22
34	8	301	SQD	O5-C1	3.48	1.50	1.41
27	A	855	CHL	OBD-CAD	3.48	1.28	1.22
27	6	307	CHL	C3B-C2B	3.48	1.45	1.40
27	4	312	CHL	CHD-C4C	3.48	1.47	1.39
27	K	205	CHL	OBD-CAD	3.48	1.28	1.22
27	B	847	CHL	OBD-CAD	3.48	1.28	1.22
27	K	207	CHL	CHD-C4C	3.48	1.47	1.39
27	A	848	CHL	OBD-CAD	3.48	1.28	1.22
29	3	304	LUT	C28-C29	3.47	1.53	1.45
29	5	303	LUT	C12-C13	3.47	1.53	1.45
27	5	307	CHL	OBD-CAD	3.47	1.28	1.22
27	a	313	CHL	OBD-CAD	3.47	1.28	1.22
27	7	320	CHL	C3D-C4D	-3.47	1.36	1.44
29	a	302	LUT	C11-C10	3.47	1.54	1.43
27	6	317	CHL	CHD-C4C	3.47	1.47	1.39
27	B	837	CHL	OBD-CAD	3.47	1.28	1.22
27	A	826	CHL	OBD-CAD	3.47	1.28	1.22
27	b	314	CHL	OBD-CAD	3.47	1.28	1.22
27	5	313	CHL	CHC-C1C	3.47	1.43	1.35
27	a	318	CHL	CHD-C4C	3.47	1.47	1.39
29	b	301	LUT	C12-C13	3.46	1.53	1.45
27	7	316	CHL	OBD-CAD	3.46	1.28	1.22
27	8	320	CHL	OBD-CAD	3.46	1.28	1.22
27	b	313	CHL	C3D-C2D	3.46	1.48	1.39
27	a	316	CHL	OBD-CAD	3.46	1.28	1.22
27	B	811	CHL	OBD-CAD	3.46	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	835	CHL	OBD-CAD	3.46	1.28	1.22
29	5	303	LUT	C15-C14	3.46	1.54	1.43
29	F	303	LUT	C11-C10	3.46	1.54	1.43
27	a	311	CHL	OBD-CAD	3.46	1.28	1.22
27	7	314	CHL	OBD-CAD	3.46	1.28	1.22
29	3	305	LUT	C32-C33	3.45	1.53	1.45
29	a	304	LUT	C12-C13	3.45	1.53	1.45
27	b	311	CHL	CHD-C4C	3.45	1.47	1.39
27	B	832	CHL	OBD-CAD	3.45	1.28	1.22
27	A	856	CHL	OBD-CAD	3.45	1.28	1.22
27	5	322	CHL	OBD-CAD	3.45	1.28	1.22
27	7	313	CHL	OBD-CAD	3.45	1.28	1.22
27	B	818	CHL	OBD-CAD	3.45	1.28	1.22
27	A	830	CHL	OBD-CAD	3.45	1.28	1.22
27	5	309	CHL	OBD-CAD	3.45	1.28	1.22
29	6	303	LUT	C12-C13	3.45	1.53	1.45
34	8	301	SQD	O47-C45	-3.45	1.38	1.46
27	A	833	CHL	CHD-C4C	3.45	1.47	1.39
27	5	317	CHL	C3D-C4D	-3.45	1.36	1.44
27	a	315	CHL	CHD-C4C	3.44	1.47	1.39
27	8	322	CHL	OBD-CAD	3.44	1.28	1.22
27	7	322	CHL	C3D-C4D	-3.44	1.36	1.44
27	b	305	CHL	C3D-C2D	3.44	1.48	1.39
27	a	318	CHL	OBD-CAD	3.44	1.28	1.22
27	A	818	CHL	OBD-CAD	3.44	1.28	1.22
27	A	828	CHL	OBD-CAD	3.44	1.28	1.22
27	3	317	CHL	OBD-CAD	3.44	1.28	1.22
27	A	816	CHL	C3D-C2D	3.44	1.48	1.39
27	4	314	CHL	OBD-CAD	3.44	1.28	1.22
27	A	816	CHL	C1D-ND	-3.44	1.33	1.37
27	L	304	CHL	C3D-C2D	3.44	1.48	1.39
27	B	831	CHL	OBD-CAD	3.44	1.28	1.22
27	B	833	CHL	OBD-CAD	3.43	1.28	1.22
27	A	854	CHL	OBD-CAD	3.43	1.28	1.22
27	b	317	CHL	OBD-CAD	3.43	1.28	1.22
27	6	306	CHL	OBD-CAD	3.43	1.28	1.22
27	a	316	CHL	CHD-C4C	3.43	1.47	1.39
27	B	846	CHL	OBD-CAD	3.43	1.28	1.22
27	3	316	CHL	C3B-C2B	3.43	1.45	1.40
27	A	841	CHL	C3D-C4D	-3.43	1.36	1.44
27	5	319	CHL	C3D-C4D	-3.43	1.36	1.44
29	a	302	LUT	C12-C13	3.43	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	849	CHL	OBD-CAD	3.43	1.28	1.22
29	7	304	LUT	C12-C13	3.43	1.53	1.45
27	A	824	CHL	OBD-CAD	3.43	1.28	1.22
27	7	317	CHL	OBD-CAD	3.43	1.28	1.22
27	4	317	CHL	C3D-C2D	3.43	1.48	1.39
27	B	841	CHL	OBD-CAD	3.43	1.28	1.22
29	8	304	LUT	C11-C10	3.43	1.54	1.43
27	A	833	CHL	C3D-C4D	-3.43	1.36	1.44
27	4	312	CHL	OBD-CAD	3.43	1.28	1.22
27	A	823	CHL	OBD-CAD	3.42	1.28	1.22
27	5	325	CHL	OBD-CAD	3.42	1.28	1.22
27	A	846	CHL	C3C-C2C	3.42	1.44	1.36
27	4	310	CHL	C3D-C2D	3.42	1.48	1.39
27	K	207	CHL	OBD-CAD	3.42	1.28	1.22
27	7	316	CHL	MG-NC	3.42	2.14	2.06
27	3	311	CHL	OBD-CAD	3.42	1.28	1.22
27	B	846	CHL	C3D-C2D	3.42	1.48	1.39
27	B	814	CHL	OBD-CAD	3.42	1.28	1.22
27	A	842	CHL	CHD-C1D	3.42	1.45	1.38
29	4	301	LUT	C32-C33	3.42	1.53	1.45
27	A	846	CHL	CHC-C1C	3.42	1.43	1.35
27	A	840	CHL	OBD-CAD	3.42	1.28	1.22
27	5	322	CHL	CHD-C4C	3.42	1.47	1.39
27	b	309	CHL	MG-NC	-3.42	1.98	2.06
27	5	317	CHL	CHD-C4C	3.42	1.47	1.39
27	8	324	CHL	C3D-C4D	-3.42	1.36	1.44
27	7	322	CHL	CHD-C4C	3.41	1.47	1.39
27	K	204	CHL	C3D-C2D	3.41	1.48	1.39
27	A	847	CHL	OBD-CAD	3.41	1.28	1.22
29	3	304	LUT	C11-C10	3.41	1.54	1.43
27	6	320	CHL	OBD-CAD	3.41	1.28	1.22
27	6	314	CHL	C3D-C2D	3.41	1.48	1.39
22	3	302	BCR	C1-C6	-3.41	1.49	1.53
27	8	318	CHL	OBD-CAD	3.41	1.28	1.22
29	8	304	LUT	C12-C13	3.40	1.53	1.45
27	b	309	CHL	C3D-C2D	3.40	1.48	1.39
27	A	854	CHL	C3D-C2D	3.40	1.48	1.39
27	a	317	CHL	C3D-C2D	3.40	1.48	1.39
27	A	825	CHL	OBD-CAD	3.39	1.28	1.22
27	A	841	CHL	CHD-C1D	3.39	1.45	1.38
27	6	316	CHL	CHD-C4C	3.39	1.47	1.39
27	6	318	CHL	CHD-C4C	3.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	316	CHL	OBD-CAD	3.39	1.28	1.22
29	4	302	LUT	C7-C6	3.39	1.57	1.45
27	B	820	CHL	C3D-C2D	3.39	1.48	1.39
27	3	315	CHL	OBD-CAD	3.39	1.28	1.22
27	3	314	CHL	C3D-C2D	3.39	1.48	1.39
27	B	812	CHL	OBD-CAD	3.39	1.28	1.22
27	a	315	CHL	C3D-C4D	-3.38	1.36	1.44
27	B	812	CHL	C3D-C2D	3.38	1.48	1.39
27	A	817	CHL	C3D-C2D	3.38	1.48	1.39
27	8	315	CHL	OBD-CAD	3.38	1.28	1.22
27	8	319	CHL	OBD-CAD	3.38	1.28	1.22
27	B	828	CHL	C3D-C2D	3.38	1.48	1.39
29	8	304	LUT	C28-C29	3.38	1.53	1.45
27	8	320	CHL	C3D-C2D	3.38	1.48	1.39
27	3	321	CHL	C3D-C2D	3.38	1.48	1.39
27	6	318	CHL	OBD-CAD	3.38	1.28	1.22
27	B	829	CHL	C3D-C2D	3.38	1.48	1.39
27	A	838	CHL	OBD-CAD	3.38	1.28	1.22
27	b	304	CHL	C3D-C2D	3.38	1.48	1.39
27	B	811	CHL	MG-ND	3.38	2.12	2.05
27	8	324	CHL	CHD-C4C	3.37	1.46	1.39
27	5	325	CHL	CHD-C4C	3.37	1.46	1.39
27	8	323	CHL	OBD-CAD	3.37	1.28	1.22
27	8	312	CHL	C3D-C2D	3.37	1.48	1.39
29	a	304	LUT	C26-C27	3.37	1.55	1.50
27	K	206	CHL	C3D-C2D	3.37	1.48	1.39
27	7	321	CHL	C3D-C4D	-3.37	1.36	1.44
27	4	309	CHL	C3D-C4D	-3.37	1.36	1.44
27	A	834	CHL	OBD-CAD	3.37	1.28	1.22
27	4	309	CHL	OBD-CAD	3.37	1.28	1.22
27	7	319	CHL	C3D-C4D	-3.37	1.36	1.44
27	B	836	CHL	OBD-CAD	3.37	1.28	1.22
29	a	302	LUT	C26-C27	3.37	1.55	1.50
27	3	320	CHL	OBD-CAD	3.37	1.28	1.22
27	7	316	CHL	C3D-C2D	3.36	1.48	1.39
27	4	317	CHL	OBD-CAD	3.36	1.28	1.22
27	A	837	CHL	C3D-C2D	3.36	1.48	1.39
27	8	312	CHL	OBD-CAD	3.36	1.28	1.22
27	4	318	CHL	C3D-C2D	3.36	1.48	1.39
29	3	305	LUT	C11-C10	3.36	1.53	1.43
29	7	304	LUT	C11-C10	3.36	1.53	1.43
29	8	303	LUT	C32-C33	3.36	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	314	CHL	C3D-C2D	3.36	1.48	1.39
27	3	316	CHL	CHD-C4C	3.36	1.46	1.39
27	b	306	CHL	C3D-C2D	3.36	1.48	1.39
29	F	303	LUT	C32-C33	3.36	1.53	1.45
27	A	839	CHL	C3D-C2D	3.36	1.48	1.39
29	8	304	LUT	C32-C33	3.36	1.53	1.45
27	A	820	CHL	C1D-ND	-3.36	1.33	1.37
27	6	306	CHL	C3D-C2D	3.36	1.48	1.39
29	3	305	LUT	C12-C13	3.35	1.53	1.45
27	B	821	CHL	C3D-C2D	3.35	1.48	1.39
27	b	311	CHL	C3D-C4D	-3.35	1.36	1.44
27	B	828	CHL	OBD-CAD	3.35	1.28	1.22
27	8	312	CHL	C1D-ND	-3.35	1.33	1.37
27	7	315	CHL	OBD-CAD	3.35	1.28	1.22
27	5	325	CHL	C3D-C4D	-3.35	1.36	1.44
29	7	304	LUT	C32-C33	3.35	1.53	1.45
27	K	205	CHL	C3D-C2D	3.35	1.48	1.39
27	4	312	CHL	MG-NA	3.35	2.14	2.06
27	5	319	CHL	CHD-C4C	3.35	1.46	1.39
27	4	311	CHL	C3D-C2D	3.35	1.48	1.39
27	A	820	CHL	OBD-CAD	3.35	1.28	1.22
29	6	302	LUT	C23-C24	3.35	1.54	1.50
27	A	822	CHL	C3D-C2D	3.35	1.48	1.39
27	7	311	CHL	C3D-C2D	3.35	1.48	1.39
27	A	842	CHL	C3D-C4D	-3.35	1.36	1.44
27	8	321	CHL	C3D-C4D	-3.35	1.36	1.44
27	8	314	CHL	C3D-C4D	-3.35	1.36	1.44
27	5	307	CHL	C3D-C2D	3.35	1.48	1.39
27	a	313	CHL	C3D-C2D	3.35	1.48	1.39
27	A	850	CHL	C3D-C2D	3.34	1.48	1.39
27	A	818	CHL	C1D-ND	-3.34	1.33	1.37
27	4	320	CHL	C3D-C2D	3.34	1.48	1.39
27	A	819	CHL	OBD-CAD	3.34	1.28	1.22
27	A	832	CHL	OBD-CAD	3.34	1.28	1.22
27	B	814	CHL	MG-ND	-3.34	1.99	2.05
27	b	316	CHL	C3D-C4D	-3.34	1.36	1.44
27	A	841	CHL	CHD-C4C	3.34	1.46	1.39
27	7	321	CHL	CHD-C4C	3.34	1.46	1.39
27	6	311	CHL	C3D-C2D	3.33	1.48	1.39
27	8	317	CHL	C3D-C2D	3.33	1.48	1.39
27	8	321	CHL	OBD-CAD	3.33	1.28	1.22
27	a	316	CHL	MG-ND	-3.33	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	313	CHL	C3D-C2D	3.33	1.48	1.39
27	A	834	CHL	C3D-C2D	3.33	1.48	1.39
27	4	316	CHL	C3D-C4D	-3.33	1.36	1.44
27	3	320	CHL	C1D-ND	-3.33	1.33	1.37
27	5	319	CHL	OBD-CAD	3.33	1.28	1.22
27	6	316	CHL	OBD-CAD	3.33	1.28	1.22
27	A	855	CHL	C3D-C2D	3.33	1.48	1.39
27	a	316	CHL	C3D-C4D	-3.33	1.36	1.44
27	b	312	CHL	C3D-C2D	3.33	1.48	1.39
27	6	316	CHL	C3D-C4D	-3.32	1.36	1.44
27	A	853	CHL	C3D-C2D	3.32	1.48	1.39
27	3	315	CHL	C3D-C2D	3.32	1.48	1.39
27	6	317	CHL	OBD-CAD	3.32	1.28	1.22
27	6	313	CHL	C3D-C2D	3.32	1.48	1.39
29	5	302	LUT	C32-C33	3.32	1.53	1.45
27	3	311	CHL	C3D-C2D	3.32	1.48	1.39
27	5	315	CHL	C3D-C2D	3.32	1.48	1.39
27	7	312	CHL	OBD-CAD	3.32	1.28	1.22
27	8	325	CHL	C3D-C2D	3.32	1.48	1.39
27	A	834	CHL	C1D-ND	-3.32	1.33	1.37
27	4	315	CHL	C3D-C2D	3.32	1.48	1.39
27	A	818	CHL	C3D-C2D	3.32	1.48	1.39
27	3	318	CHL	C3D-C2D	3.32	1.48	1.39
27	A	855	CHL	C1D-ND	-3.32	1.33	1.37
27	A	845	CHL	C3D-C2D	3.32	1.48	1.39
29	3	304	LUT	C12-C13	3.32	1.53	1.45
27	B	845	CHL	C3D-C2D	3.32	1.48	1.39
27	8	311	CHL	C3D-C2D	3.32	1.48	1.39
27	B	839	CHL	OBD-CAD	3.32	1.28	1.22
27	B	824	CHL	C3D-C2D	3.32	1.48	1.39
27	3	319	CHL	C3D-C2D	3.32	1.48	1.39
27	4	307	CHL	C3D-C2D	3.32	1.48	1.39
27	a	315	CHL	OBD-CAD	3.31	1.28	1.22
27	A	851	CHL	C3D-C2D	3.31	1.48	1.39
27	B	831	CHL	C3D-C2D	3.31	1.48	1.39
27	B	839	CHL	C3D-C2D	3.31	1.48	1.39
27	8	316	CHL	OBD-CAD	3.31	1.28	1.22
27	3	317	CHL	C3D-C2D	3.31	1.48	1.39
27	A	845	CHL	OBD-CAD	3.31	1.28	1.22
27	F	308	CHL	C3D-C2D	3.31	1.48	1.39
27	8	314	CHL	CHD-C4C	3.31	1.46	1.39
27	B	816	CHL	C3D-C2D	3.31	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	310	CHL	OBD-CAD	3.31	1.28	1.22
27	6	320	CHL	C3D-C2D	3.31	1.48	1.39
27	A	844	CHL	OBD-CAD	3.31	1.28	1.22
27	b	314	CHL	C3D-C2D	3.30	1.48	1.39
29	5	302	LUT	C28-C29	3.30	1.53	1.45
27	5	312	CHL	C3D-C2D	3.30	1.48	1.39
29	5	303	LUT	C28-C29	3.30	1.53	1.45
27	b	311	CHL	OBD-CAD	3.30	1.28	1.22
27	K	207	CHL	C3D-C4D	-3.30	1.36	1.44
27	6	309	CHL	C3D-C2D	3.30	1.48	1.39
27	7	319	CHL	OBD-CAD	3.30	1.28	1.22
27	5	323	CHL	C3D-C2D	3.30	1.48	1.39
22	I	801	BCR	C1-C6	-3.30	1.49	1.53
27	3	310	CHL	C3D-C2D	3.30	1.48	1.39
27	a	320	CHL	C3D-C2D	3.30	1.48	1.39
27	5	318	CHL	C3D-C2D	3.30	1.48	1.39
27	5	320	CHL	C3D-C2D	3.29	1.48	1.39
27	7	317	CHL	C3D-C2D	3.29	1.48	1.39
27	7	320	CHL	CHD-C4C	3.29	1.46	1.39
27	8	322	CHL	C1D-ND	-3.29	1.33	1.37
27	a	319	CHL	C3D-C2D	3.29	1.48	1.39
27	A	859	CHL	C3D-C2D	3.29	1.48	1.39
27	b	317	CHL	C3D-C4D	-3.29	1.36	1.44
27	a	307	CHL	C3D-C2D	3.29	1.48	1.39
27	A	847	CHL	C3D-C2D	3.29	1.48	1.39
27	8	318	CHL	C3D-C2D	3.29	1.48	1.39
27	5	316	CHL	CHD-C4C	3.29	1.46	1.39
29	5	303	LUT	C32-C33	3.29	1.53	1.45
27	A	825	CHL	C3D-C2D	3.29	1.48	1.39
27	a	314	CHL	C3D-C2D	3.29	1.48	1.39
27	B	840	CHL	C3D-C2D	3.29	1.48	1.39
27	B	845	CHL	OBD-CAD	3.29	1.28	1.22
27	5	317	CHL	OBD-CAD	3.29	1.28	1.22
27	B	811	CHL	C1D-ND	-3.29	1.33	1.37
27	B	848	CHL	C3D-C2D	3.28	1.48	1.39
27	b	315	CHL	C3D-C2D	3.28	1.48	1.39
27	A	829	CHL	C3D-C2D	3.28	1.48	1.39
27	B	826	CHL	C3D-C2D	3.28	1.48	1.39
27	B	841	CHL	C3D-C2D	3.28	1.48	1.39
27	B	816	CHL	OBD-CAD	3.28	1.28	1.22
27	B	836	CHL	C3D-C2D	3.28	1.48	1.39
27	a	309	CHL	C3D-C2D	3.28	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	309	CHL	C3D-C2D	3.28	1.48	1.39
27	4	305	CHL	C3D-C2D	3.28	1.48	1.39
27	B	842	CHL	C1D-ND	-3.28	1.33	1.37
27	7	314	CHL	C3D-C2D	3.28	1.48	1.39
27	7	324	CHL	C3D-C2D	3.28	1.48	1.39
27	A	849	CHL	C3D-C2D	3.28	1.48	1.39
27	B	813	CHL	C3D-C2D	3.28	1.48	1.39
27	4	312	CHL	C3D-C4D	-3.28	1.36	1.44
27	6	315	CHL	C3D-C2D	3.28	1.48	1.39
27	B	849	CHL	C3D-C2D	3.28	1.48	1.39
27	F	309	CHL	OBD-CAD	3.28	1.28	1.22
27	8	319	CHL	C3D-C2D	3.28	1.48	1.39
27	A	841	CHL	C1D-ND	-3.28	1.33	1.37
27	5	322	CHL	C3D-C4D	-3.28	1.36	1.44
22	B	803	BCR	C30-C25	-3.27	1.49	1.53
22	M	102	BCR	C1-C6	-3.27	1.49	1.53
27	a	318	CHL	C3D-C4D	-3.27	1.36	1.44
27	b	307	CHL	C3D-C2D	3.27	1.48	1.39
27	A	826	CHL	C3D-C2D	3.27	1.48	1.39
27	4	313	CHL	C3D-C2D	3.27	1.48	1.39
27	A	824	CHL	C3D-C2D	3.27	1.48	1.39
27	5	313	CHL	OBD-CAD	3.27	1.28	1.22
27	A	832	CHL	C3D-C2D	3.27	1.48	1.39
27	B	851	CHL	C3D-C2D	3.27	1.48	1.39
34	8	301	SQD	O47-C7	3.27	1.43	1.34
27	8	324	CHL	OBD-CAD	3.27	1.28	1.22
22	B	802	BCR	C30-C25	-3.27	1.49	1.53
29	8	304	LUT	C26-C27	3.26	1.55	1.50
27	6	318	CHL	C3D-C4D	-3.26	1.36	1.44
29	7	304	LUT	C28-C29	3.26	1.52	1.45
27	B	841	CHL	C1D-ND	-3.26	1.33	1.37
27	4	304	CHL	C3D-C2D	3.26	1.48	1.39
27	7	319	CHL	CHD-C4C	3.26	1.46	1.39
27	8	315	CHL	C1D-ND	-3.26	1.33	1.37
27	F	309	CHL	C3D-C2D	3.25	1.48	1.39
27	8	322	CHL	C3D-C2D	3.25	1.48	1.39
27	A	844	CHL	C3D-C2D	3.25	1.48	1.39
27	A	848	CHL	C3D-C2D	3.25	1.48	1.39
27	B	811	CHL	C3D-C2D	3.25	1.48	1.39
27	7	313	CHL	C3D-C2D	3.25	1.48	1.39
27	5	311	CHL	OBD-CAD	3.25	1.28	1.22
29	a	302	LUT	C32-C33	3.25	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	321	CHL	C3D-C2D	3.25	1.48	1.39
27	B	827	CHL	C3D-C2D	3.25	1.48	1.39
27	A	833	CHL	OBD-CAD	3.25	1.28	1.22
27	B	818	CHL	C1D-ND	-3.25	1.33	1.37
27	3	320	CHL	C3D-C2D	3.25	1.48	1.39
27	8	321	CHL	CHD-C4C	3.25	1.46	1.39
27	a	308	CHL	C3D-C2D	3.25	1.48	1.39
27	A	859	CHL	C1D-ND	-3.25	1.33	1.37
27	5	308	CHL	C3D-C2D	3.25	1.48	1.39
27	8	315	CHL	C3D-C2D	3.25	1.48	1.39
27	A	857	CHL	C3D-C2D	3.25	1.48	1.39
27	B	838	CHL	C3D-C2D	3.25	1.48	1.39
27	A	827	CHL	C3D-C2D	3.24	1.48	1.39
27	6	305	CHL	C3D-C2D	3.24	1.48	1.39
27	7	311	CHL	OBD-CAD	3.24	1.28	1.22
27	A	841	CHL	OBD-CAD	3.24	1.28	1.22
22	A	806	BCR	C1-C6	-3.24	1.49	1.53
27	4	306	CHL	C3D-C2D	3.24	1.48	1.39
27	a	312	CHL	C3D-C2D	3.24	1.48	1.39
27	B	822	CHL	C3D-C2D	3.24	1.48	1.39
27	B	842	CHL	C3D-C2D	3.24	1.48	1.39
27	8	326	CHL	OBD-CAD	3.24	1.28	1.22
27	b	308	CHL	C3D-C2D	3.24	1.48	1.39
27	7	321	CHL	MG-NA	-3.24	1.98	2.06
27	A	838	CHL	C3D-C2D	3.23	1.48	1.39
27	B	847	CHL	C3D-C2D	3.23	1.48	1.39
27	8	316	CHL	C3D-C2D	3.23	1.48	1.39
27	B	818	CHL	C3D-C2D	3.23	1.47	1.39
27	B	843	CHL	C3D-C2D	3.23	1.47	1.39
27	3	312	CHL	C3D-C2D	3.23	1.47	1.39
22	B	804	BCR	C1-C6	-3.23	1.49	1.53
27	a	310	CHL	C3D-C2D	3.23	1.47	1.39
27	3	311	CHL	C1D-ND	-3.23	1.33	1.37
27	7	318	CHL	C3D-C2D	3.23	1.47	1.39
27	B	812	CHL	MG-NC	-3.23	1.98	2.06
27	A	824	CHL	C1D-ND	-3.23	1.33	1.37
27	A	820	CHL	C3D-C2D	3.23	1.47	1.39
27	A	853	CHL	OBD-CAD	3.23	1.28	1.22
27	B	844	CHL	OBD-CAD	3.23	1.28	1.22
27	A	819	CHL	C3D-C2D	3.23	1.47	1.39
27	8	313	CHL	C3D-C2D	3.23	1.47	1.39
22	5	301	BCR	C30-C25	-3.22	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	834	CHL	MG-ND	3.22	2.12	2.05
27	5	309	CHL	C3D-C2D	3.22	1.47	1.39
29	4	301	LUT	C23-C24	3.22	1.54	1.50
27	A	858	CHL	C3D-C2D	3.22	1.47	1.39
27	7	322	CHL	OBD-CAD	3.22	1.28	1.22
27	a	311	CHL	C3D-C2D	3.22	1.47	1.39
27	A	848	CHL	C1D-ND	-3.22	1.33	1.37
27	A	836	CHL	C3D-C2D	3.22	1.47	1.39
27	A	823	CHL	C1D-ND	-3.22	1.33	1.37
27	B	816	CHL	C1D-ND	-3.22	1.33	1.37
27	6	310	CHL	C3D-C2D	3.22	1.47	1.39
27	B	817	CHL	C1D-ND	-3.22	1.33	1.37
27	3	308	CHL	C3D-C2D	3.22	1.47	1.39
27	7	312	CHL	C3D-C2D	3.22	1.47	1.39
27	B	814	CHL	C3D-C2D	3.21	1.47	1.39
27	B	823	CHL	OBD-CAD	3.21	1.28	1.22
27	7	311	CHL	C1D-ND	-3.21	1.33	1.37
27	8	326	CHL	C3D-C2D	3.21	1.47	1.39
27	A	828	CHL	C3D-C2D	3.21	1.47	1.39
27	B	835	CHL	C3D-C2D	3.21	1.47	1.39
27	A	840	CHL	C4D-CHA	3.21	1.49	1.38
27	3	315	CHL	C1D-ND	-3.21	1.33	1.37
27	J	106	CHL	C1D-ND	-3.20	1.33	1.37
27	J	106	CHL	C3D-C2D	3.20	1.47	1.39
27	4	314	CHL	C3D-C2D	3.20	1.47	1.39
27	8	314	CHL	OBD-CAD	3.20	1.28	1.22
27	7	323	CHL	C3D-C2D	3.20	1.47	1.39
27	B	840	CHL	C1D-ND	-3.20	1.33	1.37
27	A	827	CHL	C1D-ND	-3.20	1.33	1.37
27	A	850	CHL	C1D-ND	-3.19	1.33	1.37
27	B	831	CHL	C1D-ND	-3.19	1.33	1.37
27	F	308	CHL	C1D-ND	-3.19	1.33	1.37
29	4	302	LUT	C26-C27	3.19	1.55	1.50
29	F	303	LUT	C23-C24	3.19	1.54	1.50
27	6	308	CHL	OBD-CAD	3.19	1.28	1.22
27	B	823	CHL	C3D-C2D	3.19	1.47	1.39
27	A	826	CHL	C1D-ND	-3.19	1.33	1.37
27	B	847	CHL	C1D-ND	-3.19	1.33	1.37
27	A	836	CHL	C1D-ND	-3.18	1.33	1.37
27	B	844	CHL	C1D-ND	-3.18	1.33	1.37
27	A	840	CHL	C3D-C2D	3.18	1.47	1.39
27	7	324	CHL	C1D-ND	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	321	CHL	OBD-CAD	3.18	1.28	1.22
27	A	849	CHL	C1D-ND	-3.18	1.33	1.37
27	A	835	CHL	C3D-C2D	3.18	1.47	1.39
27	3	313	CHL	C1D-ND	-3.18	1.33	1.37
27	B	839	CHL	C1D-ND	-3.18	1.33	1.37
27	6	310	CHL	OBD-CAD	3.18	1.28	1.22
27	5	310	CHL	C3D-C2D	3.18	1.47	1.39
27	B	844	CHL	C3D-C2D	3.18	1.47	1.39
29	3	305	LUT	C26-C27	3.18	1.55	1.50
27	5	313	CHL	C3B-C2B	3.18	1.44	1.40
27	8	326	CHL	C1D-ND	-3.17	1.33	1.37
27	A	816	CHL	OBD-CAD	3.17	1.27	1.22
29	6	303	LUT	C26-C27	3.17	1.55	1.50
27	4	308	CHL	C3D-C2D	3.17	1.47	1.39
27	L	303	CHL	OBD-CAD	3.17	1.27	1.22
27	B	815	CHL	C3D-C2D	3.17	1.47	1.39
29	8	303	LUT	C28-C29	3.17	1.52	1.45
27	A	822	CHL	C1D-ND	-3.17	1.33	1.37
22	B	802	BCR	C1-C6	-3.17	1.49	1.53
27	B	836	CHL	C1D-ND	-3.16	1.33	1.37
27	3	308	CHL	OBD-CAD	3.16	1.27	1.22
22	K	202	BCR	C1-C6	-3.16	1.49	1.53
27	B	814	CHL	C1D-ND	-3.16	1.33	1.37
27	B	819	CHL	C3D-C2D	3.16	1.47	1.39
27	B	813	CHL	C1D-ND	-3.16	1.33	1.37
27	B	833	CHL	C3D-C2D	3.16	1.47	1.39
27	B	825	CHL	C3D-C2D	3.16	1.47	1.39
27	A	859	CHL	OBD-CAD	3.16	1.27	1.22
27	A	825	CHL	C1D-ND	-3.16	1.33	1.37
27	A	830	CHL	C1D-ND	-3.15	1.33	1.37
22	F	301	BCR	C1-C6	-3.15	1.49	1.53
27	7	315	CHL	C3D-C2D	3.15	1.47	1.39
27	A	838	CHL	C1D-ND	-3.15	1.33	1.37
27	B	845	CHL	C1D-ND	-3.15	1.33	1.37
27	A	819	CHL	C1D-ND	-3.15	1.33	1.37
27	A	845	CHL	C1D-ND	-3.15	1.33	1.37
27	B	838	CHL	C1D-ND	-3.15	1.33	1.37
27	A	842	CHL	CHD-C4C	3.15	1.46	1.39
22	B	803	BCR	C1-C6	-3.15	1.49	1.53
22	3	303	BCR	C30-C25	-3.15	1.49	1.53
27	A	823	CHL	C3D-C2D	3.15	1.47	1.39
27	B	827	CHL	C1D-ND	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	303	LUT	C7-C6	3.14	1.56	1.45
27	A	837	CHL	C1D-ND	-3.14	1.33	1.37
27	6	312	CHL	C3D-C2D	3.14	1.47	1.39
29	b	301	LUT	C23-C24	3.14	1.54	1.50
27	B	821	CHL	C1D-ND	-3.13	1.33	1.37
27	A	830	CHL	C3D-C2D	3.13	1.47	1.39
27	A	847	CHL	C1D-ND	-3.13	1.33	1.37
27	4	317	CHL	MG-NA	3.13	2.13	2.06
27	B	850	CHL	C3D-C2D	3.13	1.47	1.39
27	5	311	CHL	C3D-C2D	3.13	1.47	1.39
29	J	103	LUT	C7-C6	3.12	1.56	1.45
27	4	304	CHL	MG-ND	3.12	2.12	2.05
27	A	821	CHL	OBD-CAD	3.12	1.27	1.22
29	F	303	LUT	C26-C27	3.12	1.54	1.50
27	A	821	CHL	C4D-CHA	3.12	1.49	1.38
22	8	302	BCR	C30-C25	-3.12	1.49	1.53
27	7	314	CHL	C1D-ND	-3.12	1.34	1.37
27	b	306	CHL	C1D-ND	-3.12	1.34	1.37
27	B	846	CHL	C1D-ND	-3.12	1.34	1.37
27	4	304	CHL	C1D-ND	-3.12	1.34	1.37
27	A	852	CHL	C3D-C2D	3.11	1.47	1.39
27	A	858	CHL	C1D-ND	-3.11	1.34	1.37
27	A	844	CHL	C1D-ND	-3.11	1.34	1.37
27	5	318	CHL	C1D-ND	-3.11	1.34	1.37
27	B	825	CHL	OBD-CAD	3.11	1.27	1.22
27	B	834	CHL	C3D-C2D	3.11	1.47	1.39
27	3	316	CHL	OBD-CAD	3.10	1.27	1.22
27	7	321	CHL	C1D-ND	-3.10	1.34	1.37
27	A	832	CHL	C1D-ND	-3.10	1.34	1.37
27	7	320	CHL	OBD-CAD	3.10	1.27	1.22
27	F	309	CHL	C4D-CHA	3.10	1.49	1.38
27	5	323	CHL	C4D-CHA	3.10	1.49	1.38
29	F	303	LUT	C7-C6	3.09	1.56	1.45
27	B	848	CHL	C1D-ND	-3.09	1.34	1.37
22	K	203	BCR	C30-C25	-3.09	1.49	1.53
27	5	310	CHL	C1D-ND	-3.08	1.34	1.37
27	B	851	CHL	C1D-ND	-3.08	1.34	1.37
27	A	852	CHL	C4D-CHA	3.08	1.49	1.38
27	B	834	CHL	C4D-CHA	3.08	1.49	1.38
22	B	805	BCR	C1-C6	-3.08	1.49	1.53
27	A	856	CHL	C3D-C2D	3.08	1.47	1.39
27	4	319	CHL	C1D-ND	-3.08	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	314	CHL	C4D-CHA	3.08	1.49	1.38
27	A	857	CHL	C1D-ND	-3.07	1.34	1.37
27	A	829	CHL	C1D-ND	-3.07	1.34	1.37
27	B	817	CHL	C3D-C2D	3.07	1.47	1.39
27	4	308	CHL	OBD-CAD	3.07	1.27	1.22
27	B	822	CHL	C4D-CHA	3.07	1.49	1.38
27	3	312	CHL	OBD-CAD	3.07	1.27	1.22
27	B	830	CHL	C1D-ND	-3.07	1.34	1.37
27	B	837	CHL	C1D-ND	-3.07	1.34	1.37
27	A	821	CHL	C3D-C2D	3.06	1.47	1.39
27	B	820	CHL	C1D-ND	-3.06	1.34	1.37
27	5	321	CHL	C1D-ND	-3.06	1.34	1.37
27	B	828	CHL	C1D-ND	-3.06	1.34	1.37
27	3	317	CHL	C4D-CHA	3.06	1.49	1.38
22	L	302	BCR	C1-C6	-3.06	1.49	1.53
27	B	850	CHL	C4D-CHA	3.06	1.49	1.38
27	A	856	CHL	C1D-ND	-3.06	1.34	1.37
27	B	825	CHL	C1D-ND	-3.06	1.34	1.37
27	8	319	CHL	C1D-ND	-3.06	1.34	1.37
27	B	834	CHL	OBD-CAD	3.06	1.27	1.22
27	5	312	CHL	C4D-CHA	3.06	1.49	1.38
27	B	824	CHL	C4D-CHA	3.06	1.49	1.38
27	6	313	CHL	C4D-CHA	3.06	1.49	1.38
27	A	835	CHL	C4D-CHA	3.06	1.49	1.38
27	3	309	CHL	C4D-CHA	3.06	1.49	1.38
27	a	310	CHL	C4D-CHA	3.06	1.49	1.38
27	7	315	CHL	C1D-ND	-3.05	1.34	1.37
27	a	320	CHL	MG-NA	3.05	2.13	2.06
27	5	314	CHL	C4D-CHA	3.05	1.49	1.38
27	3	308	CHL	C1D-ND	-3.05	1.34	1.37
27	3	310	CHL	C1D-ND	-3.05	1.34	1.37
27	a	314	CHL	C1D-ND	-3.05	1.34	1.37
29	6	303	LUT	C7-C6	3.05	1.55	1.45
27	3	319	CHL	C1D-ND	-3.05	1.34	1.37
27	b	310	CHL	C1D-ND	-3.05	1.34	1.37
27	A	836	CHL	OBD-CAD	3.05	1.27	1.22
27	4	314	CHL	C1D-ND	-3.05	1.34	1.37
27	A	853	CHL	C1D-ND	-3.05	1.34	1.37
27	6	320	CHL	C1D-ND	-3.05	1.34	1.37
27	3	321	CHL	C1D-ND	-3.05	1.34	1.37
27	4	305	CHL	C4D-CHA	3.04	1.49	1.38
27	b	312	CHL	C4D-CHA	3.04	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	302	LUT	C7-C6	3.04	1.55	1.45
27	B	830	CHL	C3D-C2D	3.04	1.47	1.39
27	B	833	CHL	C1D-ND	-3.04	1.34	1.37
29	3	304	LUT	C7-C6	3.04	1.55	1.45
27	K	204	CHL	C1D-ND	-3.04	1.34	1.37
27	B	832	CHL	C4D-CHA	3.04	1.49	1.38
27	6	319	CHL	C3D-C2D	3.04	1.47	1.39
27	a	309	CHL	C4D-CHA	3.04	1.49	1.38
27	A	852	CHL	OBD-CAD	3.04	1.27	1.22
27	4	308	CHL	C1D-ND	-3.03	1.34	1.37
27	5	307	CHL	C1D-ND	-3.03	1.34	1.37
27	7	317	CHL	C4D-CHA	3.03	1.49	1.38
27	A	839	CHL	C1D-ND	-3.03	1.34	1.37
27	A	829	CHL	C4D-CHA	3.03	1.49	1.38
27	a	308	CHL	C4D-CHA	3.03	1.49	1.38
27	b	305	CHL	C4D-CHA	3.03	1.49	1.38
27	6	312	CHL	C4D-CHA	3.03	1.49	1.38
27	A	854	CHL	C1D-ND	-3.03	1.34	1.37
34	8	301	SQD	C24-C23	3.03	1.59	1.50
27	a	307	CHL	C1D-ND	-3.03	1.34	1.37
27	4	310	CHL	C1D-ND	-3.03	1.34	1.37
27	4	318	CHL	C1D-ND	-3.02	1.34	1.37
27	6	311	CHL	C4D-CHA	3.02	1.49	1.38
27	A	845	CHL	C4D-CHA	3.02	1.49	1.38
27	A	828	CHL	C4D-CHA	3.02	1.49	1.38
27	B	829	CHL	C1D-ND	-3.02	1.34	1.37
27	b	315	CHL	C4D-CHA	3.02	1.49	1.38
27	B	850	CHL	MG-ND	-3.02	1.99	2.05
27	B	851	CHL	MG-ND	-3.02	1.99	2.05
27	7	318	CHL	C4D-CHA	3.02	1.49	1.38
27	6	310	CHL	C4D-CHA	3.02	1.49	1.38
27	4	308	CHL	C4D-CHA	3.02	1.49	1.38
27	7	313	CHL	C4D-CHA	3.02	1.49	1.38
29	8	304	LUT	C7-C6	3.02	1.55	1.45
27	B	849	CHL	C4D-CHA	3.01	1.49	1.38
27	B	843	CHL	C1D-ND	-3.01	1.34	1.37
27	3	320	CHL	MG-NC	3.01	2.13	2.06
27	3	312	CHL	C4D-CHA	3.01	1.49	1.38
27	8	311	CHL	C1D-ND	-3.01	1.34	1.37
27	5	308	CHL	C4D-CHA	3.01	1.49	1.38
27	6	316	CHL	C1D-ND	-3.01	1.34	1.37
27	7	312	CHL	C4D-CHA	3.01	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	313	CHL	C1D-ND	-3.01	1.34	1.37
27	a	311	CHL	C4D-CHA	3.01	1.49	1.38
27	A	833	CHL	C1D-ND	-3.01	1.34	1.37
27	a	308	CHL	MG-ND	3.01	2.11	2.05
29	a	302	LUT	C7-C6	3.01	1.55	1.45
23	A	808	LMT	O3'-C3'	-3.01	1.35	1.43
27	A	854	CHL	C4D-CHA	3.00	1.49	1.38
22	6	301	BCR	C8-C9	-3.00	1.39	1.45
27	A	819	CHL	C4D-CHA	3.00	1.49	1.38
27	7	314	CHL	C4D-CHA	3.00	1.49	1.38
27	b	304	CHL	C4D-CHA	3.00	1.49	1.38
27	a	317	CHL	MG-ND	-3.00	1.99	2.05
27	7	319	CHL	C1D-ND	-3.00	1.34	1.37
27	K	205	CHL	C4D-CHA	3.00	1.49	1.38
27	4	306	CHL	C4D-CHA	3.00	1.49	1.38
27	B	835	CHL	C4D-CHA	3.00	1.49	1.38
27	3	318	CHL	C4D-CHA	3.00	1.49	1.38
27	6	315	CHL	C1D-ND	-3.00	1.34	1.37
27	6	305	CHL	C4D-CHA	3.00	1.49	1.38
27	8	323	CHL	C1B-CHB	3.00	1.49	1.41
27	B	815	CHL	OBD-CAD	3.00	1.27	1.22
22	M	102	BCR	C30-C25	-3.00	1.49	1.53
27	A	830	CHL	C4D-CHA	3.00	1.49	1.38
27	B	835	CHL	C1D-ND	-3.00	1.34	1.37
27	B	837	CHL	C3D-C2D	3.00	1.47	1.39
27	5	317	CHL	C1D-ND	-2.99	1.34	1.37
27	4	307	CHL	C4D-CHA	2.99	1.49	1.38
27	B	832	CHL	C3D-C2D	2.99	1.47	1.39
27	6	309	CHL	C4D-CHA	2.99	1.49	1.38
27	A	857	CHL	C4D-CHA	2.99	1.49	1.38
27	B	826	CHL	C4D-CHA	2.99	1.49	1.38
27	5	310	CHL	C4D-CHA	2.99	1.49	1.38
27	8	313	CHL	C1D-ND	-2.99	1.34	1.37
27	8	316	CHL	C1D-ND	-2.99	1.34	1.37
27	4	320	CHL	C4D-CHA	2.99	1.49	1.38
27	A	832	CHL	C4D-CHA	2.99	1.49	1.38
27	B	829	CHL	C4D-CHA	2.99	1.49	1.38
27	L	304	CHL	C4D-CHA	2.99	1.49	1.38
27	A	852	CHL	C1D-ND	-2.99	1.34	1.37
27	A	837	CHL	C4D-CHA	2.99	1.49	1.38
27	a	319	CHL	C4D-CHA	2.99	1.49	1.38
27	K	206	CHL	C1D-ND	-2.99	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	325	CHL	C1D-ND	-2.98	1.34	1.37
27	8	318	CHL	C1D-ND	-2.98	1.34	1.37
27	b	307	CHL	C1D-ND	-2.98	1.34	1.37
27	b	315	CHL	C1D-ND	-2.98	1.34	1.37
27	B	823	CHL	C4D-CHA	2.98	1.49	1.38
27	4	311	CHL	C4D-CHA	2.98	1.49	1.38
27	b	313	CHL	C4D-CHA	2.98	1.49	1.38
27	8	325	CHL	C4D-CHA	2.98	1.49	1.38
27	A	839	CHL	C4D-CHA	2.98	1.49	1.38
27	3	321	CHL	C4D-CHA	2.98	1.49	1.38
27	A	838	CHL	C4D-CHA	2.98	1.49	1.38
27	3	314	CHL	C4D-CHA	2.98	1.49	1.38
27	a	317	CHL	C4D-CHA	2.98	1.49	1.38
27	K	206	CHL	C4D-CHA	2.98	1.49	1.38
27	B	819	CHL	C4D-CHA	2.98	1.49	1.38
27	4	310	CHL	C4D-CHA	2.98	1.49	1.38
27	A	851	CHL	C4D-CHA	2.97	1.49	1.38
27	6	306	CHL	C4D-CHA	2.97	1.49	1.38
27	b	309	CHL	C4D-CHA	2.97	1.49	1.38
27	B	848	CHL	C4D-CHA	2.97	1.49	1.38
27	5	320	CHL	C1D-ND	-2.97	1.34	1.37
27	b	307	CHL	C4D-CHA	2.97	1.49	1.38
27	a	312	CHL	C1D-ND	-2.97	1.34	1.37
27	B	823	CHL	C1D-ND	-2.97	1.34	1.37
27	3	318	CHL	C1D-ND	-2.97	1.34	1.37
22	A	807	BCR	C30-C25	-2.97	1.49	1.53
27	3	310	CHL	C4D-CHA	2.97	1.48	1.38
27	4	314	CHL	C4D-CHA	2.97	1.48	1.38
27	B	813	CHL	C4D-CHA	2.97	1.48	1.38
27	4	307	CHL	MG-NC	2.97	2.13	2.06
27	8	317	CHL	C1D-ND	-2.97	1.34	1.37
27	7	316	CHL	C4D-CHA	2.97	1.48	1.38
27	6	320	CHL	C4D-CHA	2.97	1.48	1.38
27	7	315	CHL	C4D-CHA	2.97	1.48	1.38
27	3	314	CHL	C1D-ND	-2.97	1.34	1.37
27	B	845	CHL	C4D-CHA	2.97	1.48	1.38
27	4	311	CHL	MG-NC	-2.96	1.99	2.06
27	B	843	CHL	C4D-CHA	2.96	1.48	1.38
27	8	325	CHL	C1D-ND	-2.96	1.34	1.37
27	a	315	CHL	C1D-ND	-2.96	1.34	1.37
27	a	307	CHL	C4D-CHA	2.96	1.48	1.38
22	B	807	BCR	C30-C25	-2.96	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	309	CHL	C1D-ND	-2.96	1.34	1.37
27	8	320	CHL	C4D-CHA	2.96	1.48	1.38
27	8	313	CHL	C4D-CHA	2.96	1.48	1.38
27	B	815	CHL	C4D-CHA	2.96	1.48	1.38
27	b	308	CHL	C4D-CHA	2.96	1.48	1.38
29	8	304	LUT	C23-C24	2.96	1.54	1.50
27	B	814	CHL	C4D-CHA	2.96	1.48	1.38
22	L	301	BCR	C1-C6	-2.96	1.49	1.53
27	6	315	CHL	C4D-CHA	2.96	1.48	1.38
27	7	318	CHL	C1D-ND	-2.96	1.34	1.37
27	4	307	CHL	C1D-ND	-2.96	1.34	1.37
27	5	311	CHL	C4D-CHA	2.95	1.48	1.38
27	8	311	CHL	C4D-CHA	2.95	1.48	1.38
27	B	838	CHL	C4D-CHA	2.95	1.48	1.38
27	B	851	CHL	C4D-CHA	2.95	1.48	1.38
27	5	320	CHL	C4D-CHA	2.95	1.48	1.38
27	8	316	CHL	C4D-CHA	2.95	1.48	1.38
27	B	826	CHL	C1D-ND	-2.95	1.34	1.37
27	6	306	CHL	C1D-ND	-2.95	1.34	1.37
29	b	301	LUT	C7-C6	2.95	1.55	1.45
27	B	850	CHL	C1D-ND	-2.95	1.34	1.37
27	a	320	CHL	C4D-CHA	2.95	1.48	1.38
27	a	310	CHL	C1D-ND	-2.95	1.34	1.37
27	5	310	CHL	MG-ND	-2.94	2.00	2.05
22	A	805	BCR	C1-C6	-2.94	1.49	1.53
27	b	308	CHL	MG-ND	2.94	2.11	2.05
27	7	317	CHL	C1D-ND	-2.94	1.34	1.37
27	A	828	CHL	C1D-ND	-2.94	1.34	1.37
27	4	318	CHL	C4D-CHA	2.94	1.48	1.38
27	A	842	CHL	C1D-ND	-2.94	1.34	1.37
27	8	317	CHL	C4D-CHA	2.94	1.48	1.38
29	J	103	LUT	C26-C27	2.94	1.54	1.50
27	A	851	CHL	C1D-ND	-2.93	1.34	1.37
27	A	855	CHL	C4D-CHA	2.93	1.48	1.38
27	a	308	CHL	C1D-ND	-2.93	1.34	1.37
22	A	804	BCR	C30-C25	-2.93	1.49	1.53
27	A	858	CHL	C4D-CHA	2.93	1.48	1.38
27	F	308	CHL	C4D-CHA	2.93	1.48	1.38
22	A	804	BCR	C1-C6	-2.93	1.49	1.53
27	3	308	CHL	C4D-CHA	2.93	1.48	1.38
27	6	314	CHL	C4D-CHA	2.93	1.48	1.38
27	A	826	CHL	C4D-CHA	2.93	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	319	CHL	C4D-CHA	2.93	1.48	1.38
27	4	304	CHL	C4D-CHA	2.93	1.48	1.38
29	3	304	LUT	C26-C27	2.93	1.54	1.50
27	A	824	CHL	C4D-CHA	2.93	1.48	1.38
27	A	853	CHL	C4D-CHA	2.93	1.48	1.38
27	A	825	CHL	C4D-CHA	2.93	1.48	1.38
27	7	312	CHL	C1D-ND	-2.92	1.34	1.37
27	B	825	CHL	C4D-CHA	2.92	1.48	1.38
27	8	320	CHL	C1D-ND	-2.92	1.34	1.37
27	L	304	CHL	C1D-ND	-2.92	1.34	1.37
27	a	314	CHL	C4D-CHA	2.92	1.48	1.38
27	3	319	CHL	C4D-CHA	2.92	1.48	1.38
27	4	315	CHL	C1D-ND	-2.92	1.34	1.37
27	a	313	CHL	C1D-ND	-2.92	1.34	1.37
27	6	309	CHL	C1D-ND	-2.92	1.34	1.37
27	a	313	CHL	C4D-CHA	2.92	1.48	1.38
27	7	316	CHL	C1D-ND	-2.92	1.34	1.37
27	3	317	CHL	C1D-ND	-2.92	1.34	1.37
27	6	311	CHL	C1D-ND	-2.92	1.34	1.37
27	6	312	CHL	C1D-ND	-2.92	1.34	1.37
27	B	820	CHL	C4D-CHA	2.92	1.48	1.38
27	A	831	CHL	OBD-CAD	2.92	1.27	1.22
27	4	320	CHL	C1D-ND	-2.92	1.34	1.37
27	B	840	CHL	C4D-CHA	2.91	1.48	1.38
27	8	321	CHL	C1D-ND	-2.91	1.34	1.37
27	8	318	CHL	C4D-CHA	2.91	1.48	1.38
27	b	306	CHL	C4D-CHA	2.91	1.48	1.38
27	K	205	CHL	C1D-ND	-2.91	1.34	1.37
27	A	856	CHL	C4D-CHA	2.91	1.48	1.38
27	5	307	CHL	C4D-CHA	2.91	1.48	1.38
27	5	323	CHL	C1D-ND	-2.91	1.34	1.37
27	K	204	CHL	C4D-CHA	2.91	1.48	1.38
27	A	835	CHL	C1D-ND	-2.91	1.34	1.37
27	A	820	CHL	C4D-CHA	2.91	1.48	1.38
27	5	315	CHL	C4D-CHA	2.91	1.48	1.38
27	5	309	CHL	C4D-CHA	2.91	1.48	1.38
27	a	317	CHL	C1D-ND	-2.91	1.34	1.37
27	A	827	CHL	C4D-CHA	2.91	1.48	1.38
27	B	846	CHL	C4D-CHA	2.91	1.48	1.38
27	B	839	CHL	C4D-CHA	2.90	1.48	1.38
22	6	301	BCR	C23-C22	-2.90	1.39	1.45
27	A	822	CHL	C4D-CHA	2.90	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	849	CHL	C4D-CHA	2.90	1.48	1.38
27	B	847	CHL	C4D-CHA	2.90	1.48	1.38
27	3	313	CHL	C4D-CHA	2.90	1.48	1.38
27	B	839	CHL	MG-ND	2.90	2.11	2.05
27	B	836	CHL	C4D-CHA	2.90	1.48	1.38
27	B	833	CHL	C4D-CHA	2.90	1.48	1.38
27	B	821	CHL	C4D-CHA	2.90	1.48	1.38
27	5	312	CHL	C1D-ND	-2.90	1.34	1.37
27	4	313	CHL	C4B-CHC	2.90	1.49	1.41
27	4	315	CHL	C4D-CHA	2.90	1.48	1.38
27	J	106	CHL	C4D-CHA	2.90	1.48	1.38
27	a	312	CHL	C4D-CHA	2.90	1.48	1.38
27	B	850	CHL	OBD-CAD	2.90	1.27	1.22
27	A	844	CHL	C4D-CHA	2.90	1.48	1.38
27	8	324	CHL	C1D-ND	-2.89	1.34	1.37
27	5	314	CHL	C1D-ND	-2.89	1.34	1.37
27	8	315	CHL	C4D-CHA	2.89	1.48	1.38
27	A	836	CHL	C4D-CHA	2.89	1.48	1.38
27	B	811	CHL	C4D-CHA	2.89	1.48	1.38
27	7	324	CHL	C4D-CHA	2.89	1.48	1.38
27	8	326	CHL	C4D-CHA	2.89	1.48	1.38
27	3	316	CHL	C1D-ND	-2.89	1.34	1.37
27	5	309	CHL	C1B-CHB	2.89	1.49	1.41
29	a	304	LUT	C23-C24	2.89	1.54	1.50
22	K	202	BCR	C30-C25	-2.89	1.49	1.53
27	5	316	CHL	OBD-CAD	2.89	1.27	1.22
27	5	321	CHL	C4D-CHA	2.89	1.48	1.38
27	b	316	CHL	MG-NA	-2.89	1.99	2.06
27	4	311	CHL	C1D-ND	-2.89	1.34	1.37
27	B	818	CHL	C4D-CHA	2.89	1.48	1.38
27	3	319	CHL	C1B-CHB	2.89	1.49	1.41
27	B	830	CHL	C4D-CHA	2.89	1.48	1.38
27	B	841	CHL	C4D-CHA	2.88	1.48	1.38
27	B	819	CHL	C1D-ND	-2.88	1.34	1.37
27	5	308	CHL	C1D-ND	-2.88	1.34	1.37
27	B	834	CHL	C1D-ND	-2.88	1.34	1.37
27	6	318	CHL	C1D-ND	-2.88	1.34	1.37
29	4	301	LUT	C7-C6	2.88	1.55	1.45
27	A	847	CHL	C4D-CHA	2.88	1.48	1.38
27	4	319	CHL	C4D-CHA	2.88	1.48	1.38
27	A	859	CHL	C4D-CHA	2.88	1.48	1.38
27	a	311	CHL	MG-ND	-2.88	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	311	CHL	C4D-CHA	2.88	1.48	1.38
27	B	851	CHL	C4B-CHC	2.88	1.49	1.41
27	A	842	CHL	OBD-CAD	2.88	1.27	1.22
27	6	305	CHL	C1D-ND	-2.88	1.34	1.37
22	B	807	BCR	C1-C6	-2.88	1.49	1.53
22	A	803	BCR	C30-C25	-2.87	1.49	1.53
27	A	818	CHL	C4D-CHA	2.87	1.48	1.38
27	a	318	CHL	C1D-ND	-2.87	1.34	1.37
27	7	322	CHL	C1D-ND	-2.87	1.34	1.37
27	B	828	CHL	C4D-CHA	2.87	1.48	1.38
27	b	311	CHL	MG-NA	-2.87	1.99	2.06
27	b	305	CHL	C1D-ND	-2.87	1.34	1.37
27	b	313	CHL	C1B-CHB	2.87	1.49	1.41
27	B	822	CHL	C1D-ND	-2.87	1.34	1.37
24	A	812	LHG	O7-C5	-2.87	1.39	1.46
27	4	309	CHL	C1D-ND	-2.87	1.34	1.37
27	3	309	CHL	C1D-ND	-2.87	1.34	1.37
27	A	816	CHL	C4D-CHA	2.87	1.48	1.38
27	B	815	CHL	C1D-ND	-2.87	1.34	1.37
27	A	832	CHL	C1B-CHB	2.87	1.49	1.41
27	8	312	CHL	C4D-CHA	2.87	1.48	1.38
27	4	305	CHL	C1D-ND	-2.87	1.34	1.37
27	b	310	CHL	C4D-CHA	2.87	1.48	1.38
27	5	318	CHL	C4D-CHA	2.86	1.48	1.38
27	3	315	CHL	C4D-CHA	2.86	1.48	1.38
22	3	301	BCR	C30-C25	-2.86	1.49	1.53
27	7	311	CHL	C4D-CHA	2.86	1.48	1.38
27	a	316	CHL	C1D-ND	-2.86	1.34	1.37
27	8	322	CHL	C4D-CHA	2.86	1.48	1.38
27	A	823	CHL	MG-NA	2.86	2.13	2.06
27	B	817	CHL	C4D-CHA	2.86	1.48	1.38
27	3	318	CHL	C1B-CHB	2.86	1.48	1.41
27	5	319	CHL	C1D-ND	-2.86	1.34	1.37
27	b	312	CHL	C1B-CHB	2.86	1.48	1.41
27	F	309	CHL	C1D-ND	-2.85	1.34	1.37
27	a	319	CHL	C1D-ND	-2.85	1.34	1.37
27	5	315	CHL	C1D-ND	-2.85	1.34	1.37
29	6	302	LUT	C7-C6	2.85	1.55	1.45
27	A	821	CHL	C1D-ND	-2.85	1.34	1.37
27	a	309	CHL	C1D-ND	-2.85	1.34	1.37
27	B	831	CHL	C4D-CHA	2.85	1.48	1.38
27	6	307	CHL	OBD-CAD	2.85	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	848	CHL	C4D-CHA	2.85	1.48	1.38
27	B	844	CHL	MG-ND	2.85	2.11	2.05
27	B	816	CHL	C4D-CHA	2.85	1.48	1.38
27	B	847	CHL	MG-NC	-2.85	1.99	2.06
27	B	837	CHL	C4D-CHA	2.85	1.48	1.38
29	a	304	LUT	C7-C6	2.85	1.55	1.45
29	8	303	LUT	C26-C27	2.85	1.54	1.50
27	5	309	CHL	C1D-ND	-2.85	1.34	1.37
29	7	304	LUT	C1-C6	2.84	1.57	1.53
27	B	849	CHL	C1D-ND	-2.84	1.34	1.37
27	5	311	CHL	C1D-ND	-2.84	1.34	1.37
27	6	313	CHL	C1D-ND	-2.84	1.34	1.37
27	A	853	CHL	C1B-CHB	2.84	1.48	1.41
27	A	850	CHL	C4D-CHA	2.84	1.48	1.38
27	B	844	CHL	C4D-CHA	2.84	1.48	1.38
27	b	317	CHL	C1D-ND	-2.84	1.34	1.37
27	a	320	CHL	C1D-ND	-2.84	1.34	1.37
27	K	206	CHL	MG-NC	2.84	2.13	2.06
27	6	314	CHL	C1D-ND	-2.83	1.34	1.37
27	6	310	CHL	C1B-CHB	2.83	1.48	1.41
27	B	832	CHL	C1D-ND	-2.83	1.34	1.37
27	8	311	CHL	MG-ND	2.83	2.11	2.05
22	5	301	BCR	C1-C6	-2.83	1.49	1.53
27	6	311	CHL	C1B-CHB	2.83	1.48	1.41
22	B	805	BCR	C30-C25	-2.82	1.49	1.53
27	4	312	CHL	C1D-ND	-2.82	1.34	1.37
27	B	842	CHL	C4D-CHA	2.82	1.48	1.38
27	A	823	CHL	C4D-CHA	2.82	1.48	1.38
27	B	830	CHL	C1B-CHB	2.82	1.48	1.41
29	8	303	LUT	C7-C6	2.82	1.55	1.45
27	B	824	CHL	C1D-ND	-2.82	1.34	1.37
27	8	313	CHL	C1B-CHB	2.82	1.48	1.41
27	b	315	CHL	C4B-CHC	2.82	1.48	1.41
27	6	319	CHL	C4C-C3C	2.82	1.49	1.45
27	5	325	CHL	MG-ND	2.82	2.11	2.05
27	B	827	CHL	C4D-CHA	2.82	1.48	1.38
27	7	313	CHL	C1B-CHB	2.82	1.48	1.41
27	K	204	CHL	C1B-CHB	2.81	1.48	1.41
27	6	311	CHL	C4B-CHC	2.81	1.48	1.41
27	5	314	CHL	C1B-CHB	2.81	1.48	1.41
27	A	819	CHL	C4B-CHC	2.81	1.48	1.41
27	6	308	CHL	C3D-C2D	2.81	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	315	CHL	C1B-CHB	2.81	1.48	1.41
27	8	317	CHL	C1B-CHB	2.81	1.48	1.41
27	3	312	CHL	C1D-ND	-2.81	1.34	1.37
27	A	834	CHL	C4D-CHA	2.81	1.48	1.38
27	7	311	CHL	MG-NC	2.81	2.12	2.06
27	A	840	CHL	C1D-ND	-2.81	1.34	1.37
29	5	302	LUT	C26-C27	2.80	1.54	1.50
27	3	320	CHL	C4D-CHA	2.80	1.48	1.38
27	7	313	CHL	C1D-ND	-2.80	1.34	1.37
27	B	811	CHL	C1B-CHB	2.80	1.48	1.41
27	5	310	CHL	C1B-CHB	2.80	1.48	1.41
27	7	318	CHL	C1B-CHB	2.80	1.48	1.41
27	L	304	CHL	C1B-CHB	2.80	1.48	1.41
27	5	320	CHL	C4B-CHC	2.80	1.48	1.41
27	7	312	CHL	C1B-CHB	2.80	1.48	1.41
27	a	311	CHL	C1D-ND	-2.80	1.34	1.37
27	6	313	CHL	C1B-CHB	2.80	1.48	1.41
27	B	826	CHL	C1B-CHB	2.79	1.48	1.41
27	F	308	CHL	C1B-CHB	2.79	1.48	1.41
27	b	312	CHL	C1D-ND	-2.79	1.34	1.37
27	F	309	CHL	C1B-CHB	2.79	1.48	1.41
27	6	309	CHL	C1B-CHB	2.79	1.48	1.41
27	7	318	CHL	MG-ND	2.79	2.11	2.05
27	5	320	CHL	C1B-CHB	2.79	1.48	1.41
27	4	311	CHL	C1B-CHB	2.79	1.48	1.41
27	B	825	CHL	C1B-CHB	2.79	1.48	1.41
27	b	304	CHL	C1D-ND	-2.79	1.34	1.37
27	6	315	CHL	C1B-CHB	2.78	1.48	1.41
27	4	306	CHL	C1D-ND	-2.78	1.34	1.37
27	5	308	CHL	C1B-CHB	2.78	1.48	1.41
22	K	203	BCR	C1-C6	-2.78	1.49	1.53
27	3	320	CHL	C4B-CHC	2.78	1.48	1.41
27	A	845	CHL	C1C-NC	-2.78	1.33	1.37
23	5	326	LMT	O3'-C3'	-2.78	1.36	1.43
27	4	315	CHL	C1B-CHB	2.78	1.48	1.41
27	7	320	CHL	C1D-ND	-2.78	1.34	1.37
27	4	320	CHL	C1B-CHB	2.78	1.48	1.41
27	4	316	CHL	C1D-ND	-2.78	1.34	1.37
27	B	816	CHL	MG-NA	2.77	2.12	2.06
27	B	829	CHL	C1B-CHB	2.77	1.48	1.41
27	5	316	CHL	C1D-ND	-2.77	1.34	1.37
27	6	314	CHL	C1B-CHB	2.77	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	315	CHL	C4B-CHC	2.77	1.48	1.41
27	b	309	CHL	C1B-CHB	2.77	1.48	1.41
27	4	306	CHL	C1B-CHB	2.77	1.48	1.41
27	B	813	CHL	C4B-CHC	2.77	1.48	1.41
27	L	304	CHL	C4B-CHC	2.77	1.48	1.41
27	8	321	CHL	MG-ND	2.76	2.11	2.05
27	5	323	CHL	C1B-CHB	2.76	1.48	1.41
27	b	307	CHL	C1B-CHB	2.76	1.48	1.41
27	B	812	CHL	C4D-CHA	2.76	1.48	1.38
27	6	314	CHL	C4B-CHC	2.76	1.48	1.41
27	b	305	CHL	C1B-CHB	2.76	1.48	1.41
27	B	848	CHL	C1B-CHB	2.76	1.48	1.41
27	4	318	CHL	C1B-CHB	2.76	1.48	1.41
27	4	319	CHL	C4C-C3C	2.76	1.49	1.45
27	a	317	CHL	C1B-CHB	2.76	1.48	1.41
27	a	309	CHL	MG-NA	2.76	2.12	2.06
27	A	840	CHL	C1B-CHB	2.76	1.48	1.41
27	A	845	CHL	C1B-CHB	2.76	1.48	1.41
27	L	304	CHL	C4C-C3C	2.76	1.49	1.45
27	3	321	CHL	C1B-CHB	2.75	1.48	1.41
27	6	317	CHL	C1D-ND	-2.75	1.34	1.37
27	b	310	CHL	C4C-C3C	2.75	1.49	1.45
27	A	857	CHL	C1B-CHB	2.75	1.48	1.41
27	b	306	CHL	C4B-CHC	2.75	1.48	1.41
27	6	315	CHL	C4B-CHC	2.75	1.48	1.41
27	8	320	CHL	C1B-CHB	2.75	1.48	1.41
23	F	302	LMT	O3'-C3'	-2.75	1.36	1.43
27	B	818	CHL	C1B-CHB	2.75	1.48	1.41
27	8	325	CHL	C1B-CHB	2.75	1.48	1.41
29	7	304	LUT	C26-C27	2.75	1.54	1.50
27	b	310	CHL	C1B-CHB	2.75	1.48	1.41
29	a	302	LUT	C23-C24	2.75	1.54	1.50
27	a	309	CHL	C1B-CHB	2.75	1.48	1.41
27	b	314	CHL	C1B-CHB	2.75	1.48	1.41
27	A	817	CHL	C4D-CHA	2.75	1.48	1.38
27	A	852	CHL	C1B-CHB	2.75	1.48	1.41
29	5	302	LUT	C23-C24	2.74	1.54	1.50
27	B	821	CHL	C1B-CHB	2.74	1.48	1.41
27	B	837	CHL	C1B-CHB	2.74	1.48	1.41
27	5	310	CHL	C4B-CHC	2.74	1.48	1.41
27	7	315	CHL	C1B-CHB	2.74	1.48	1.41
27	3	310	CHL	C1B-CHB	2.74	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	825	CHL	C4B-CHC	2.74	1.48	1.41
27	B	835	CHL	C1B-CHB	2.74	1.48	1.41
27	b	313	CHL	C4B-CHC	2.74	1.48	1.41
27	7	324	CHL	C1B-CHB	2.74	1.48	1.41
27	b	305	CHL	C4C-C3C	2.74	1.49	1.45
27	a	312	CHL	C1B-CHB	2.74	1.48	1.41
29	3	305	LUT	C7-C6	2.74	1.54	1.45
27	B	824	CHL	C1B-CHB	2.74	1.48	1.41
27	A	821	CHL	C1B-CHB	2.74	1.48	1.41
27	B	849	CHL	C1B-CHB	2.74	1.48	1.41
27	b	306	CHL	C1B-CHB	2.74	1.48	1.41
27	B	846	CHL	C1B-CHB	2.74	1.48	1.41
27	B	823	CHL	C1B-CHB	2.74	1.48	1.41
27	A	837	CHL	C1B-CHB	2.74	1.48	1.41
27	B	822	CHL	C1C-NC	-2.74	1.33	1.37
27	5	321	CHL	C1B-CHB	2.74	1.48	1.41
27	8	311	CHL	C1B-CHB	2.74	1.48	1.41
27	6	305	CHL	C1B-CHB	2.74	1.48	1.41
27	8	314	CHL	C1D-ND	-2.74	1.34	1.37
27	A	858	CHL	C1B-CHB	2.74	1.48	1.41
27	4	310	CHL	C4B-CHC	2.73	1.48	1.41
27	a	313	CHL	C4B-CHC	2.73	1.48	1.41
27	4	314	CHL	C4B-CHC	2.73	1.48	1.41
27	A	827	CHL	C1B-CHB	2.73	1.48	1.41
27	K	206	CHL	C1B-CHB	2.73	1.48	1.41
27	A	851	CHL	C1B-CHB	2.73	1.48	1.41
27	B	837	CHL	C4C-C3C	2.73	1.49	1.45
27	a	320	CHL	C1B-CHB	2.73	1.48	1.41
27	6	310	CHL	C1D-ND	-2.73	1.34	1.37
27	B	818	CHL	C4C-C3C	2.73	1.49	1.45
27	b	315	CHL	C1B-CHB	2.73	1.48	1.41
27	4	306	CHL	C4B-CHC	2.73	1.48	1.41
27	6	317	CHL	MG-ND	-2.73	2.00	2.05
27	b	314	CHL	C4C-C3C	2.73	1.49	1.45
27	3	313	CHL	C1B-CHB	2.73	1.48	1.41
27	b	304	CHL	C4B-CHC	2.73	1.48	1.41
27	b	314	CHL	C1D-ND	-2.73	1.34	1.37
27	a	307	CHL	C4B-CHC	2.73	1.48	1.41
27	6	312	CHL	C1B-CHB	2.73	1.48	1.41
27	4	319	CHL	C4B-CHC	2.73	1.48	1.41
27	F	309	CHL	C4B-CHC	2.73	1.48	1.41
27	8	315	CHL	C4B-CHC	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	320	CHL	C1B-CHB	2.73	1.48	1.41
27	J	106	CHL	C1B-CHB	2.73	1.48	1.41
27	4	305	CHL	C1B-CHB	2.72	1.48	1.41
27	4	307	CHL	C4B-CHC	2.72	1.48	1.41
27	4	310	CHL	C1B-CHB	2.72	1.48	1.41
27	A	816	CHL	C4B-CHC	2.72	1.48	1.41
27	A	827	CHL	C4B-CHC	2.72	1.48	1.41
27	6	315	CHL	MG-NC	2.72	2.12	2.06
27	b	312	CHL	C4B-CHC	2.72	1.48	1.41
27	B	850	CHL	C4B-CHC	2.72	1.48	1.41
27	B	847	CHL	C1B-CHB	2.72	1.48	1.41
27	3	319	CHL	C4B-CHC	2.72	1.48	1.41
27	7	317	CHL	C1B-CHB	2.72	1.48	1.41
27	K	207	CHL	C1D-ND	-2.72	1.34	1.37
27	A	832	CHL	C4B-CHC	2.72	1.48	1.41
27	B	816	CHL	C1B-CHB	2.72	1.48	1.41
27	5	321	CHL	C4B-CHC	2.72	1.48	1.41
27	A	818	CHL	C1B-CHB	2.72	1.48	1.41
27	A	853	CHL	C4C-C3C	2.72	1.49	1.45
27	7	312	CHL	C1C-NC	-2.71	1.33	1.37
27	5	322	CHL	C1D-ND	-2.71	1.34	1.37
29	5	303	LUT	C26-C27	2.71	1.54	1.50
27	A	828	CHL	C1C-NC	-2.71	1.33	1.37
27	4	318	CHL	C4B-CHC	2.71	1.48	1.41
27	K	205	CHL	C1B-CHB	2.71	1.48	1.41
27	a	311	CHL	C1B-CHB	2.71	1.48	1.41
27	A	816	CHL	C1B-CHB	2.71	1.48	1.41
27	7	312	CHL	C4B-CHC	2.71	1.48	1.41
23	7	308	LMT	O3'-C3'	-2.71	1.36	1.43
27	A	829	CHL	C1B-CHB	2.71	1.48	1.41
23	B	810	LMT	O3'-C3'	-2.71	1.36	1.43
27	B	826	CHL	C4B-CHC	2.71	1.48	1.41
27	3	309	CHL	C1B-CHB	2.71	1.48	1.41
27	7	323	CHL	CHD-C1D	2.71	1.43	1.38
27	A	824	CHL	C1B-CHB	2.71	1.48	1.41
27	8	318	CHL	C1B-CHB	2.71	1.48	1.41
27	8	320	CHL	MG-ND	2.71	2.11	2.05
27	5	307	CHL	C4B-CHC	2.70	1.48	1.41
27	b	304	CHL	C1B-CHB	2.70	1.48	1.41
27	a	310	CHL	C1B-CHB	2.70	1.48	1.41
27	B	840	CHL	C1B-CHB	2.70	1.48	1.41
27	b	307	CHL	C4B-CHC	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	847	CHL	MG-ND	2.70	2.11	2.05
27	B	845	CHL	C1B-CHB	2.70	1.48	1.41
29	8	303	LUT	C23-C24	2.70	1.54	1.50
27	a	310	CHL	C4B-CHC	2.70	1.48	1.41
27	b	314	CHL	C4B-CHC	2.70	1.48	1.41
27	5	312	CHL	MG-ND	2.70	2.11	2.05
27	3	321	CHL	C4B-CHC	2.70	1.48	1.41
27	4	319	CHL	C1B-CHB	2.70	1.48	1.41
27	b	309	CHL	C4B-CHC	2.70	1.48	1.41
27	A	826	CHL	C4B-CHC	2.70	1.48	1.41
28	B	809	DGD	O2G-C2G	-2.70	1.39	1.46
27	6	306	CHL	C1B-CHB	2.70	1.48	1.41
27	A	835	CHL	C1B-CHB	2.70	1.48	1.41
27	6	306	CHL	C4B-CHC	2.70	1.48	1.41
27	6	310	CHL	C4B-CHC	2.70	1.48	1.41
27	5	312	CHL	C1B-CHB	2.69	1.48	1.41
27	4	320	CHL	C4B-CHC	2.69	1.48	1.41
27	5	314	CHL	C4B-CHC	2.69	1.48	1.41
27	4	317	CHL	C1D-C2D	2.69	1.50	1.45
27	3	314	CHL	C4B-CHC	2.69	1.48	1.41
27	B	834	CHL	C4B-CHC	2.69	1.48	1.41
27	3	313	CHL	C4C-C3C	2.69	1.49	1.45
27	4	318	CHL	C4C-C3C	2.69	1.49	1.45
27	6	319	CHL	C1D-C2D	2.69	1.50	1.45
27	3	314	CHL	C1B-CHB	2.69	1.48	1.41
27	a	313	CHL	C1B-CHB	2.69	1.48	1.41
27	B	814	CHL	C4B-CHC	2.69	1.48	1.41
27	7	314	CHL	C1B-CHB	2.69	1.48	1.41
27	7	324	CHL	C4B-CHC	2.69	1.48	1.41
27	8	326	CHL	C1B-CHB	2.69	1.48	1.41
27	7	316	CHL	C1B-CHB	2.69	1.48	1.41
27	L	303	CHL	CHD-C1D	2.69	1.43	1.38
27	5	315	CHL	C4B-CHC	2.68	1.48	1.41
27	A	856	CHL	C1B-CHB	2.68	1.48	1.41
27	6	308	CHL	C1D-ND	-2.68	1.34	1.37
27	A	847	CHL	C1B-CHB	2.68	1.48	1.41
27	B	835	CHL	C4B-CHC	2.68	1.48	1.41
27	a	319	CHL	C1B-CHB	2.68	1.48	1.41
27	8	317	CHL	C4B-CHC	2.68	1.48	1.41
27	B	819	CHL	C1B-CHB	2.68	1.48	1.41
27	B	820	CHL	C1B-CHB	2.68	1.48	1.41
27	A	840	CHL	C1C-NC	-2.68	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	320	CHL	MG-NA	2.68	2.12	2.06
27	B	844	CHL	C4B-CHC	2.68	1.48	1.41
27	b	310	CHL	C4B-CHC	2.68	1.48	1.41
27	B	831	CHL	C1B-CHB	2.68	1.48	1.41
27	B	840	CHL	C4B-CHC	2.68	1.48	1.41
27	a	317	CHL	C4B-CHC	2.68	1.48	1.41
27	A	846	CHL	OBD-CAD	2.68	1.27	1.22
23	A	809	LMT	O3'-C3'	-2.68	1.36	1.43
27	B	849	CHL	C4B-CHC	2.68	1.48	1.41
27	A	816	CHL	C4C-C3C	2.68	1.49	1.45
23	A	809	LMT	O2'-C2'	-2.67	1.36	1.43
27	A	838	CHL	C1B-CHB	2.67	1.48	1.41
27	5	318	CHL	C1B-CHB	2.67	1.48	1.41
27	8	315	CHL	C1B-CHB	2.67	1.48	1.41
27	A	824	CHL	C1C-NC	-2.67	1.33	1.37
27	A	835	CHL	C4C-C3C	2.67	1.49	1.45
27	B	843	CHL	C1B-CHB	2.67	1.48	1.41
27	B	818	CHL	C1C-NC	-2.67	1.33	1.37
27	L	303	CHL	CHD-C4C	2.67	1.45	1.39
27	3	318	CHL	C4B-CHC	2.67	1.48	1.41
27	4	311	CHL	C4B-CHC	2.67	1.48	1.41
27	4	306	CHL	C4C-C3C	2.67	1.49	1.45
27	4	314	CHL	C1B-CHB	2.67	1.48	1.41
27	K	204	CHL	C4B-CHC	2.67	1.48	1.41
27	B	813	CHL	C1B-CHB	2.67	1.48	1.41
26	A	815	CL0	OBD-CAD	2.67	1.27	1.22
27	b	316	CHL	C1D-ND	-2.67	1.34	1.37
27	B	831	CHL	C4B-CHC	2.67	1.48	1.41
27	7	313	CHL	C4B-CHC	2.66	1.48	1.41
27	6	312	CHL	C4C-C3C	2.66	1.49	1.45
27	A	845	CHL	C4C-C3C	2.66	1.49	1.45
27	A	859	CHL	C1B-CHB	2.66	1.48	1.41
27	B	847	CHL	C4B-CHC	2.66	1.48	1.41
27	6	313	CHL	C4B-CHC	2.66	1.48	1.41
27	4	304	CHL	C4B-CHC	2.66	1.48	1.41
27	A	819	CHL	C1B-CHB	2.66	1.48	1.41
27	8	312	CHL	C4B-CHC	2.66	1.48	1.41
27	6	305	CHL	MG-ND	-2.66	2.00	2.05
27	A	858	CHL	C4B-CHC	2.66	1.48	1.41
27	B	817	CHL	C1B-CHB	2.66	1.48	1.41
27	A	837	CHL	C4B-CHC	2.66	1.48	1.41
27	6	313	CHL	C4C-C3C	2.66	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	806	BCR	C30-C25	-2.66	1.50	1.53
27	3	320	CHL	C1B-CHB	2.66	1.48	1.41
27	b	305	CHL	C4B-CHC	2.65	1.48	1.41
27	7	311	CHL	C1B-CHB	2.65	1.48	1.41
27	B	828	CHL	C1B-CHB	2.65	1.48	1.41
27	8	312	CHL	C1B-CHB	2.65	1.48	1.41
27	8	311	CHL	C4B-CHC	2.65	1.48	1.41
27	B	817	CHL	C1C-NC	-2.65	1.33	1.37
27	A	855	CHL	C4B-CHC	2.65	1.48	1.41
27	5	308	CHL	C4B-CHC	2.65	1.48	1.41
27	B	843	CHL	C4B-CHC	2.65	1.48	1.41
27	A	822	CHL	C4B-CHC	2.65	1.48	1.41
27	3	309	CHL	C4B-CHC	2.65	1.48	1.41
27	8	325	CHL	C4B-CHC	2.65	1.48	1.41
27	B	833	CHL	C1B-CHB	2.65	1.48	1.41
27	a	314	CHL	C1B-CHB	2.65	1.48	1.41
29	J	103	LUT	C23-C24	2.65	1.53	1.50
27	4	307	CHL	C1B-CHB	2.65	1.48	1.41
27	3	308	CHL	C1B-CHB	2.65	1.48	1.41
27	B	833	CHL	C4B-CHC	2.65	1.48	1.41
27	B	832	CHL	C1B-CHB	2.65	1.48	1.41
27	B	850	CHL	C1B-CHB	2.65	1.48	1.41
27	a	314	CHL	C4B-CHC	2.65	1.48	1.41
27	7	314	CHL	C4B-CHC	2.65	1.48	1.41
27	8	319	CHL	C1B-CHB	2.64	1.48	1.41
27	8	319	CHL	C4B-CHC	2.64	1.48	1.41
27	B	822	CHL	C4B-CHC	2.64	1.48	1.41
27	A	847	CHL	C4B-CHC	2.64	1.48	1.41
27	A	826	CHL	C1B-CHB	2.64	1.48	1.41
29	3	304	LUT	C23-C24	2.64	1.53	1.50
23	A	808	LMT	O2'-C2'	-2.64	1.36	1.43
27	B	822	CHL	C4C-C3C	2.64	1.49	1.45
29	7	304	LUT	C23-C24	2.64	1.53	1.50
23	5	306	LMT	O3'-C3'	-2.64	1.36	1.43
27	B	841	CHL	C1B-CHB	2.64	1.48	1.41
27	a	320	CHL	C4B-CHC	2.64	1.48	1.41
27	b	309	CHL	C4C-C3C	2.64	1.49	1.45
27	A	850	CHL	C1B-CHB	2.64	1.48	1.41
27	B	829	CHL	C4B-CHC	2.64	1.48	1.41
27	5	320	CHL	C4C-C3C	2.64	1.49	1.45
27	B	813	CHL	MG-ND	2.64	2.11	2.05
27	A	828	CHL	C4C-C3C	2.64	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	803	BCR	C1-C6	-2.64	1.50	1.53
27	6	320	CHL	C4B-CHC	2.64	1.48	1.41
27	a	308	CHL	C4B-CHC	2.64	1.48	1.41
27	A	825	CHL	C1B-CHB	2.64	1.48	1.41
27	7	324	CHL	C4C-C3C	2.63	1.49	1.45
27	6	305	CHL	C4B-CHC	2.63	1.48	1.41
27	A	830	CHL	C1B-CHB	2.63	1.48	1.41
27	8	318	CHL	C4B-CHC	2.63	1.48	1.41
27	a	307	CHL	C1B-CHB	2.63	1.48	1.41
27	8	320	CHL	C4B-CHC	2.63	1.48	1.41
27	B	842	CHL	C1B-CHB	2.63	1.48	1.41
27	6	309	CHL	C4B-CHC	2.63	1.48	1.41
27	B	831	CHL	C4C-C3C	2.63	1.49	1.45
27	a	312	CHL	C4B-CHC	2.63	1.48	1.41
27	8	313	CHL	C4B-CHC	2.63	1.48	1.41
27	3	312	CHL	C1B-CHB	2.63	1.48	1.41
27	B	839	CHL	C1B-CHB	2.63	1.48	1.41
27	5	309	CHL	C4B-CHC	2.63	1.48	1.41
27	A	821	CHL	C1C-NC	-2.63	1.33	1.37
27	K	205	CHL	C4C-C3C	2.63	1.49	1.45
27	3	308	CHL	C4B-CHC	2.63	1.48	1.41
27	6	312	CHL	C4B-CHC	2.63	1.48	1.41
27	A	854	CHL	C4B-CHC	2.63	1.48	1.41
27	B	822	CHL	C1B-CHB	2.63	1.48	1.41
26	A	815	CL0	CHD-C1D	2.62	1.43	1.38
27	F	308	CHL	C4B-CHC	2.62	1.48	1.41
27	3	310	CHL	C4B-CHC	2.62	1.48	1.41
27	A	852	CHL	C1C-NC	-2.62	1.33	1.37
27	B	823	CHL	MG-ND	-2.62	2.00	2.05
27	4	311	CHL	C4C-C3C	2.62	1.49	1.45
27	A	851	CHL	C4B-CHC	2.62	1.48	1.41
27	B	851	CHL	C1B-CHB	2.62	1.48	1.41
27	a	308	CHL	C1B-CHB	2.62	1.48	1.41
27	5	312	CHL	C4B-CHC	2.62	1.48	1.41
29	4	302	LUT	C23-C24	2.62	1.53	1.50
27	b	306	CHL	MG-NC	-2.62	2.00	2.06
27	b	311	CHL	C1D-ND	-2.62	1.34	1.37
27	A	848	CHL	C1B-CHB	2.62	1.48	1.41
27	A	821	CHL	C4B-CHC	2.62	1.48	1.41
27	A	840	CHL	C4B-CHC	2.62	1.48	1.41
27	B	848	CHL	C1C-NC	-2.62	1.33	1.37
27	K	205	CHL	C4B-CHC	2.62	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	303	BCR	C30-C25	-2.62	1.50	1.53
27	B	850	CHL	C1C-NC	-2.62	1.33	1.37
27	5	314	CHL	C4C-C3C	2.62	1.49	1.45
27	B	814	CHL	C1B-CHB	2.62	1.48	1.41
27	4	314	CHL	MG-NA	2.62	2.12	2.06
27	a	311	CHL	C4B-CHC	2.62	1.48	1.41
27	5	312	CHL	C4C-C3C	2.62	1.49	1.45
27	B	830	CHL	C4B-CHC	2.62	1.48	1.41
27	3	315	CHL	C1B-CHB	2.62	1.48	1.41
27	4	305	CHL	C4B-CHC	2.61	1.48	1.41
27	6	315	CHL	C4C-C3C	2.61	1.49	1.45
27	7	313	CHL	C4C-C3C	2.61	1.49	1.45
27	A	838	CHL	C4B-CHC	2.61	1.48	1.41
27	B	820	CHL	C4B-CHC	2.61	1.48	1.41
27	A	850	CHL	C1C-NC	-2.61	1.33	1.37
27	5	311	CHL	C1B-CHB	2.61	1.48	1.41
27	J	106	CHL	C4B-CHC	2.61	1.48	1.41
27	4	308	CHL	C1B-CHB	2.61	1.48	1.41
27	A	846	CHL	CHD-C1D	2.61	1.43	1.38
27	B	839	CHL	C4B-CHC	2.61	1.48	1.41
27	B	819	CHL	C4B-CHC	2.61	1.48	1.41
27	B	844	CHL	C1B-CHB	2.61	1.48	1.41
27	A	851	CHL	MG-ND	-2.61	2.00	2.05
27	A	859	CHL	C1C-NC	-2.61	1.33	1.37
27	3	311	CHL	C1B-CHB	2.60	1.48	1.41
27	3	317	CHL	C4B-CHC	2.60	1.48	1.41
27	A	854	CHL	C1B-CHB	2.60	1.48	1.41
27	A	848	CHL	C4B-CHC	2.60	1.48	1.41
27	A	817	CHL	C4C-C3C	2.60	1.49	1.45
27	A	823	CHL	C4B-CHC	2.60	1.48	1.41
27	B	815	CHL	C1B-CHB	2.60	1.48	1.41
27	A	856	CHL	C1C-NC	-2.60	1.33	1.37
27	B	837	CHL	C1C-NC	-2.60	1.33	1.37
27	B	818	CHL	MG-ND	-2.60	2.00	2.05
27	A	822	CHL	C1B-CHB	2.60	1.48	1.41
27	4	304	CHL	C1B-CHB	2.60	1.48	1.41
27	B	838	CHL	C1B-CHB	2.60	1.48	1.41
22	B	804	BCR	C30-C25	-2.60	1.50	1.53
27	8	322	CHL	C1B-CHB	2.60	1.48	1.41
27	5	311	CHL	C4B-CHC	2.59	1.48	1.41
27	A	816	CHL	C1C-NC	-2.59	1.33	1.37
27	b	304	CHL	C4C-C3C	2.59	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3	304	LUT	C18-C5	2.59	1.55	1.50
27	A	858	CHL	C1C-NC	-2.59	1.33	1.37
27	A	825	CHL	C4B-CHC	2.59	1.48	1.41
22	3	301	BCR	C1-C6	-2.59	1.50	1.53
27	5	307	CHL	C1B-CHB	2.59	1.48	1.41
27	B	821	CHL	C4B-CHC	2.59	1.48	1.41
27	B	815	CHL	C4B-CHC	2.59	1.48	1.41
27	B	837	CHL	C4B-CHC	2.59	1.48	1.41
27	B	823	CHL	C4B-CHC	2.58	1.48	1.41
27	B	834	CHL	C1B-CHB	2.58	1.48	1.41
27	5	309	CHL	C4C-C3C	2.58	1.49	1.45
27	7	315	CHL	C4B-CHC	2.58	1.48	1.41
27	7	316	CHL	C4B-CHC	2.58	1.48	1.41
27	F	308	CHL	C1C-NC	-2.58	1.34	1.37
27	B	824	CHL	C1C-NC	-2.58	1.34	1.37
27	A	828	CHL	C1B-CHB	2.58	1.48	1.41
27	3	317	CHL	C1B-CHB	2.58	1.48	1.41
27	B	838	CHL	C4B-CHC	2.58	1.48	1.41
27	7	311	CHL	C4B-CHC	2.58	1.48	1.41
27	B	816	CHL	C1C-NC	-2.58	1.34	1.37
27	A	835	CHL	C1C-NC	-2.57	1.34	1.37
27	K	206	CHL	C4C-C3C	2.57	1.49	1.45
27	A	835	CHL	C4B-CHC	2.57	1.48	1.41
27	8	316	CHL	C1B-CHB	2.57	1.48	1.41
27	B	812	CHL	C4C-C3C	2.57	1.49	1.45
27	4	313	CHL	C4D-ND	2.57	1.41	1.37
27	A	855	CHL	C1B-CHB	2.57	1.48	1.41
27	A	859	CHL	C4B-CHC	2.57	1.48	1.41
27	A	843	CHL	CHD-C1D	2.57	1.43	1.38
27	7	317	CHL	C4B-CHC	2.57	1.48	1.41
27	7	317	CHL	C1C-NC	-2.57	1.34	1.37
27	A	838	CHL	C1C-NC	-2.57	1.34	1.37
23	5	326	LMT	O2'-C2'	-2.57	1.36	1.43
27	B	815	CHL	C1C-NC	-2.57	1.34	1.37
27	A	823	CHL	C1B-CHB	2.57	1.48	1.41
27	7	323	CHL	C1B-CHB	2.57	1.48	1.41
29	J	103	LUT	C18-C5	2.57	1.55	1.50
27	A	844	CHL	C4B-CHC	2.57	1.48	1.41
23	5	326	LMT	O2B-C2B	-2.57	1.36	1.43
22	J	102	BCR	C1-C6	-2.57	1.50	1.53
27	a	314	CHL	C4C-C3C	2.57	1.49	1.45
22	7	303	BCR	C1-C6	-2.56	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	830	CHL	C4B-CHC	2.56	1.48	1.41
27	B	833	CHL	C1C-NC	-2.56	1.34	1.37
27	B	846	CHL	C1C-NC	-2.56	1.34	1.37
27	A	829	CHL	C4B-CHC	2.56	1.48	1.41
27	B	832	CHL	C4B-CHC	2.56	1.48	1.41
27	A	837	CHL	C1C-NC	-2.56	1.34	1.37
27	a	309	CHL	C4B-CHC	2.56	1.48	1.41
27	B	816	CHL	C4C-C3C	2.56	1.49	1.45
27	B	845	CHL	C4B-CHC	2.56	1.48	1.41
27	5	318	CHL	C4B-CHC	2.56	1.48	1.41
27	A	836	CHL	C4B-CHC	2.55	1.48	1.41
27	B	828	CHL	C4B-CHC	2.55	1.48	1.41
27	a	309	CHL	C4C-C3C	2.55	1.49	1.45
27	A	834	CHL	C1C-NC	-2.55	1.34	1.37
27	A	849	CHL	C1B-CHB	2.55	1.48	1.41
27	8	316	CHL	C4B-CHC	2.55	1.48	1.41
23	7	308	LMT	O2'-C2'	-2.55	1.37	1.43
29	4	301	LUT	C4-C5	2.55	1.55	1.51
27	B	811	CHL	C4B-CHC	2.55	1.48	1.41
27	5	316	CHL	C3D-C2D	2.55	1.46	1.39
22	B	806	BCR	C1-C6	-2.55	1.50	1.53
27	8	319	CHL	C4C-C3C	2.55	1.49	1.45
27	A	857	CHL	C4B-CHC	2.55	1.48	1.41
29	3	305	LUT	C23-C24	2.55	1.53	1.50
27	B	812	CHL	C1C-NC	-2.55	1.34	1.37
27	3	314	CHL	C4C-C3C	2.54	1.49	1.45
27	K	206	CHL	C4B-CHC	2.54	1.48	1.41
27	B	842	CHL	C4B-CHC	2.54	1.48	1.41
27	A	817	CHL	C1B-CHB	2.54	1.48	1.41
27	a	312	CHL	C4C-C3C	2.54	1.49	1.45
27	A	856	CHL	C4B-CHC	2.54	1.48	1.41
27	B	846	CHL	C4B-CHC	2.54	1.48	1.41
27	A	820	CHL	C4B-CHC	2.54	1.48	1.41
27	b	312	CHL	C4C-C3C	2.54	1.49	1.45
27	7	318	CHL	C4B-CHC	2.54	1.48	1.41
27	B	849	CHL	C4C-C3C	2.54	1.49	1.45
22	A	805	BCR	C30-C25	-2.54	1.50	1.53
27	A	839	CHL	C1B-CHB	2.54	1.48	1.41
26	A	815	CL0	CHD-C4C	2.54	1.45	1.39
27	B	831	CHL	C1C-NC	-2.54	1.34	1.37
27	4	308	CHL	C1C-NC	-2.54	1.34	1.37
27	b	313	CHL	C4C-C3C	2.54	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	811	CHL	C1C-NC	-2.54	1.34	1.37
27	B	835	CHL	C1C-NC	-2.54	1.34	1.37
27	J	106	CHL	C1C-NC	-2.54	1.34	1.37
27	a	320	CHL	C4C-C3C	2.54	1.49	1.45
27	B	836	CHL	C1B-CHB	2.54	1.48	1.41
27	B	827	CHL	C1B-CHB	2.54	1.48	1.41
27	4	308	CHL	C4B-CHC	2.54	1.48	1.41
27	B	844	CHL	C4C-C3C	2.54	1.49	1.45
27	b	308	CHL	C1B-CHB	2.54	1.48	1.41
27	3	318	CHL	C4C-C3C	2.53	1.49	1.45
27	6	310	CHL	C4C-C3C	2.53	1.49	1.45
27	A	850	CHL	C4B-CHC	2.53	1.48	1.41
29	b	303	LUT	C8-C9	-2.53	1.40	1.45
27	3	310	CHL	C1C-NC	-2.53	1.34	1.37
27	A	844	CHL	C1B-CHB	2.53	1.48	1.41
27	A	817	CHL	C1C-NC	-2.53	1.34	1.37
27	A	839	CHL	C4B-CHC	2.53	1.48	1.41
27	A	836	CHL	C1B-CHB	2.53	1.48	1.41
29	a	302	LUT	C18-C5	2.53	1.55	1.50
27	8	323	CHL	MG-ND	2.53	2.10	2.05
22	J	102	BCR	C30-C25	-2.53	1.50	1.53
27	B	834	CHL	C1C-NC	-2.53	1.34	1.37
31	a	303	AXT	C4-C5	-2.53	1.47	1.51
27	B	832	CHL	C1C-NC	-2.53	1.34	1.37
27	A	834	CHL	C1B-CHB	2.52	1.48	1.41
27	a	319	CHL	C4B-CHC	2.52	1.48	1.41
27	4	320	CHL	C4C-C3C	2.52	1.49	1.45
27	8	320	CHL	C4C-C3C	2.52	1.49	1.45
27	B	830	CHL	C1C-NC	-2.52	1.34	1.37
27	A	834	CHL	C4B-CHC	2.52	1.48	1.41
27	B	824	CHL	C4B-CHC	2.52	1.48	1.41
29	8	304	LUT	C38-C25	2.52	1.55	1.50
27	B	836	CHL	C4C-C3C	2.52	1.49	1.45
27	A	820	CHL	C1B-CHB	2.52	1.48	1.41
27	B	838	CHL	C4C-C3C	2.52	1.49	1.45
27	B	828	CHL	C4C-C3C	2.52	1.49	1.45
29	a	302	LUT	C38-C25	2.52	1.55	1.50
33	7	305	XAT	C28-C29	-2.52	1.40	1.45
27	4	305	CHL	C4C-C3C	2.52	1.49	1.45
27	B	838	CHL	C1C-NC	-2.52	1.34	1.37
27	3	315	CHL	C4B-CHC	2.51	1.48	1.41
22	8	302	BCR	C1-C6	-2.51	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	839	CHL	C4C-C3C	2.51	1.49	1.45
27	B	848	CHL	C4B-CHC	2.51	1.48	1.41
27	B	824	CHL	C4C-C3C	2.51	1.49	1.45
27	A	832	CHL	C1C-NC	-2.51	1.34	1.37
27	3	312	CHL	C4B-CHC	2.51	1.48	1.41
27	A	853	CHL	C4B-CHC	2.51	1.48	1.41
27	4	310	CHL	C4C-C3C	2.51	1.49	1.45
27	A	825	CHL	C1C-NC	-2.51	1.34	1.37
22	6	301	BCR	C19-C18	-2.51	1.40	1.45
27	4	315	CHL	C4C-C3C	2.51	1.49	1.45
27	A	844	CHL	C1C-NC	-2.51	1.34	1.37
27	7	316	CHL	C4C-C3C	2.51	1.49	1.44
27	b	307	CHL	C4C-C3C	2.51	1.49	1.45
27	b	308	CHL	CHD-C1D	2.50	1.43	1.38
27	6	312	CHL	C1C-NC	-2.50	1.34	1.37
27	4	306	CHL	C4D-ND	2.50	1.41	1.37
27	b	305	CHL	C4D-ND	2.50	1.41	1.37
29	b	301	LUT	C38-C25	2.50	1.55	1.50
27	5	308	CHL	C1C-NC	-2.50	1.34	1.37
27	8	325	CHL	C1C-NC	-2.50	1.34	1.37
27	3	313	CHL	C4B-CHC	2.50	1.47	1.41
27	7	315	CHL	C1C-NC	-2.50	1.34	1.37
27	5	311	CHL	C1C-NC	-2.50	1.34	1.37
27	B	839	CHL	C4C-C3C	2.50	1.49	1.45
27	8	313	CHL	C1C-NC	-2.50	1.34	1.37
27	8	323	CHL	C1C-NC	-2.50	1.34	1.37
27	A	851	CHL	C4C-C3C	2.50	1.49	1.45
27	B	843	CHL	C1C-NC	-2.50	1.34	1.37
27	B	819	CHL	C1C-NC	-2.50	1.34	1.37
27	B	847	CHL	C1C-NC	-2.50	1.34	1.37
27	8	312	CHL	C1C-NC	-2.50	1.34	1.37
27	b	308	CHL	C1C-NC	-2.50	1.34	1.37
27	5	321	CHL	C4C-C3C	2.49	1.49	1.45
27	B	830	CHL	C4C-C3C	2.49	1.49	1.45
27	A	855	CHL	C1C-NC	-2.49	1.34	1.37
27	F	309	CHL	C1C-NC	-2.49	1.34	1.37
27	3	312	CHL	C1C-NC	-2.49	1.34	1.37
27	a	319	CHL	C4C-C3C	2.49	1.49	1.45
27	A	857	CHL	C1C-NC	-2.49	1.34	1.37
27	5	323	CHL	C4C-C3C	2.49	1.49	1.45
27	3	318	CHL	C1C-NC	-2.49	1.34	1.37
29	4	301	LUT	C18-C5	2.49	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	313	CHL	C4C-C3C	2.49	1.49	1.45
27	B	814	CHL	C4C-C3C	2.49	1.49	1.45
27	8	322	CHL	C4B-CHC	2.49	1.47	1.41
27	3	312	CHL	C4C-C3C	2.49	1.49	1.45
27	4	305	CHL	C1C-NC	-2.49	1.34	1.37
27	A	852	CHL	C4C-C3C	2.49	1.49	1.45
27	3	311	CHL	C4B-CHC	2.49	1.47	1.41
27	B	823	CHL	C1C-NC	-2.49	1.34	1.37
27	7	324	CHL	C1C-NC	-2.49	1.34	1.37
27	8	326	CHL	C4B-CHC	2.48	1.47	1.41
27	a	308	CHL	C4C-C3C	2.48	1.49	1.45
27	A	823	CHL	C1C-NC	-2.48	1.34	1.37
27	A	838	CHL	C4C-C3C	2.48	1.49	1.45
27	A	817	CHL	C4B-CHC	2.48	1.47	1.41
27	a	317	CHL	C4C-C3C	2.48	1.49	1.45
27	B	841	CHL	C1C-NC	-2.48	1.34	1.37
27	A	824	CHL	C4B-CHC	2.48	1.47	1.41
22	F	301	BCR	C30-C25	-2.48	1.50	1.53
27	F	309	CHL	C4C-C3C	2.48	1.49	1.45
33	7	305	XAT	C32-C33	-2.48	1.40	1.45
23	7	308	LMT	O2B-C2B	-2.48	1.37	1.43
29	5	303	LUT	C23-C24	2.48	1.53	1.50
27	K	206	CHL	C4D-ND	2.48	1.41	1.37
27	A	822	CHL	C4C-C3C	2.48	1.49	1.45
27	6	320	CHL	C4C-C3C	2.48	1.49	1.45
27	B	827	CHL	C4B-CHC	2.48	1.47	1.41
27	A	857	CHL	C4C-C3C	2.48	1.49	1.45
27	4	309	CHL	C3D-C2D	2.48	1.45	1.39
27	K	205	CHL	C1C-NC	-2.48	1.34	1.37
27	5	315	CHL	C4C-C3C	2.48	1.49	1.45
27	6	310	CHL	C4D-ND	2.47	1.41	1.37
27	B	836	CHL	C1C-NC	-2.47	1.34	1.37
27	3	313	CHL	C1C-NC	-2.47	1.34	1.37
27	8	326	CHL	C1C-NC	-2.47	1.34	1.37
27	7	319	CHL	MG-NA	2.47	2.12	2.06
27	4	317	CHL	C1B-CHB	2.47	1.47	1.41
27	F	309	CHL	C4D-ND	2.47	1.41	1.37
27	b	306	CHL	C4C-C3C	2.47	1.49	1.45
27	5	308	CHL	C4D-ND	2.47	1.41	1.37
27	B	816	CHL	C4B-CHC	2.47	1.47	1.41
22	6	301	BCR	C12-C13	-2.47	1.40	1.45
27	7	313	CHL	C1C-NC	-2.47	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	841	CHL	C4B-CHC	2.47	1.47	1.41
24	7	306	LHG	O7-C5	-2.47	1.40	1.46
29	F	303	LUT	C18-C5	2.47	1.55	1.50
27	A	839	CHL	C1C-NC	-2.47	1.34	1.37
27	4	307	CHL	C1C-NC	-2.47	1.34	1.37
27	3	309	CHL	C1C-NC	-2.46	1.34	1.37
27	A	828	CHL	C4B-CHC	2.46	1.47	1.41
27	A	846	CHL	CHD-C4C	2.46	1.44	1.39
29	6	303	LUT	C23-C24	2.46	1.53	1.50
27	B	812	CHL	C4B-CHC	2.46	1.47	1.41
27	A	850	CHL	C4C-C3C	2.46	1.49	1.45
27	5	323	CHL	C4B-CHC	2.46	1.47	1.41
27	A	858	CHL	C4C-C3C	2.46	1.49	1.45
27	B	814	CHL	C1C-NC	-2.46	1.34	1.37
27	a	317	CHL	C1C-NC	-2.46	1.34	1.37
27	b	314	CHL	C4D-ND	2.46	1.41	1.37
27	A	852	CHL	C4B-CHC	2.46	1.47	1.41
27	6	306	CHL	C4C-C3C	2.46	1.49	1.45
27	3	309	CHL	C4C-C3C	2.46	1.49	1.45
27	8	312	CHL	C4C-C3C	2.46	1.49	1.45
27	A	836	CHL	C1C-NC	-2.46	1.34	1.37
27	5	323	CHL	C1C-NC	-2.46	1.34	1.37
27	B	820	CHL	C4C-C3C	2.46	1.49	1.45
27	A	818	CHL	C1C-NC	-2.46	1.34	1.37
27	B	829	CHL	C1C-NC	-2.46	1.34	1.37
23	B	810	LMT	O2'-C2'	-2.46	1.37	1.43
27	A	849	CHL	C4C-C3C	2.46	1.49	1.45
27	8	317	CHL	C4C-C3C	2.46	1.49	1.45
27	A	853	CHL	C1C-NC	-2.46	1.34	1.37
27	A	840	CHL	C4C-C3C	2.46	1.49	1.45
27	6	305	CHL	C4C-C3C	2.45	1.49	1.45
27	A	818	CHL	C4B-CHC	2.45	1.47	1.41
27	7	318	CHL	C1C-NC	-2.45	1.34	1.37
27	A	844	CHL	C4C-C3C	2.45	1.49	1.45
27	A	829	CHL	C1C-NC	-2.45	1.34	1.37
27	A	856	CHL	C4C-C3C	2.45	1.49	1.45
27	A	849	CHL	C4B-CHC	2.45	1.47	1.41
27	B	828	CHL	C1C-NC	-2.45	1.34	1.37
27	b	316	CHL	C3D-C2D	2.45	1.45	1.39
27	3	319	CHL	C4C-C3C	2.45	1.49	1.45
29	7	304	LUT	C18-C5	2.45	1.54	1.50
22	L	302	BCR	C30-C25	-2.44	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	847	CHL	C4C-C3C	2.44	1.49	1.45
27	4	306	CHL	C1C-NC	-2.44	1.34	1.37
27	8	316	CHL	C1C-NC	-2.44	1.34	1.37
22	A	807	BCR	C1-C6	-2.44	1.50	1.53
27	b	317	CHL	C3D-C2D	2.44	1.45	1.39
27	4	309	CHL	C4C-C3C	2.44	1.49	1.45
33	7	305	XAT	C8-C9	-2.44	1.40	1.45
27	A	823	CHL	C4C-C3C	2.44	1.49	1.45
27	4	305	CHL	C4D-ND	2.44	1.41	1.37
27	3	317	CHL	C1C-NC	-2.44	1.34	1.37
27	B	848	CHL	C4C-C3C	2.43	1.49	1.45
27	a	307	CHL	C1C-NC	-2.43	1.34	1.37
29	5	302	LUT	C18-C5	2.43	1.54	1.50
27	3	310	CHL	C4C-C3C	2.43	1.49	1.45
27	3	319	CHL	C1C-NC	-2.43	1.34	1.37
27	A	825	CHL	C4C-C3C	2.43	1.49	1.45
27	6	311	CHL	C4C-C3C	2.43	1.49	1.45
27	A	826	CHL	C1C-NC	-2.43	1.34	1.37
27	A	845	CHL	C4B-CHC	2.43	1.47	1.41
27	B	832	CHL	C4C-C3C	2.43	1.49	1.45
27	a	316	CHL	C3D-C2D	2.43	1.45	1.39
27	A	818	CHL	C4C-C3C	2.43	1.49	1.45
27	A	830	CHL	C1C-NC	-2.43	1.34	1.37
29	6	302	LUT	C38-C25	2.43	1.55	1.50
27	A	840	CHL	C4D-ND	2.43	1.41	1.37
27	4	320	CHL	C1C-NC	-2.43	1.34	1.37
27	8	325	CHL	C4C-C3C	2.43	1.49	1.45
27	6	309	CHL	C1C-NC	-2.43	1.34	1.37
27	7	311	CHL	C1C-NC	-2.43	1.34	1.37
27	B	833	CHL	C4C-C3C	2.43	1.49	1.45
23	B	810	LMT	O2B-C2B	-2.43	1.37	1.43
23	F	302	LMT	O2'-C2'	-2.43	1.37	1.43
27	B	843	CHL	C4C-C3C	2.43	1.49	1.45
27	5	309	CHL	C1C-NC	-2.43	1.34	1.37
27	6	313	CHL	C4D-ND	2.42	1.41	1.37
27	B	835	CHL	C4C-C3C	2.42	1.49	1.45
27	8	319	CHL	C1C-NC	-2.42	1.34	1.37
27	B	826	CHL	C1C-NC	-2.42	1.34	1.37
27	K	204	CHL	C1C-NC	-2.42	1.34	1.37
27	J	106	CHL	C4C-C3C	2.42	1.49	1.45
27	8	323	CHL	CMB-C2B	-2.42	1.46	1.51
27	B	844	CHL	C1C-NC	-2.42	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	312	CHL	C4D-ND	2.42	1.41	1.37
27	5	323	CHL	C4D-ND	2.42	1.41	1.37
27	8	318	CHL	C4C-C3C	2.42	1.49	1.45
27	B	845	CHL	C1C-NC	-2.42	1.34	1.37
22	I	801	BCR	C30-C25	-2.42	1.50	1.53
27	a	308	CHL	C4D-ND	2.42	1.41	1.37
27	5	318	CHL	C4C-C3C	2.42	1.49	1.45
27	A	827	CHL	C1C-NC	-2.42	1.34	1.37
27	4	315	CHL	C1C-NC	-2.42	1.34	1.37
27	6	314	CHL	C4C-C3C	2.42	1.49	1.45
27	A	848	CHL	C1C-NC	-2.42	1.34	1.37
27	B	827	CHL	C1C-NC	-2.42	1.34	1.37
27	8	311	CHL	C1C-NC	-2.42	1.34	1.37
27	A	854	CHL	C4C-C3C	2.42	1.49	1.45
27	8	318	CHL	C1C-NC	-2.42	1.34	1.37
27	4	313	CHL	C1B-CHB	2.42	1.47	1.41
27	6	307	CHL	CHD-C1D	2.42	1.43	1.38
27	A	826	CHL	C4C-C3C	2.41	1.49	1.45
23	A	808	LMT	O3B-C3B	-2.41	1.37	1.43
27	5	307	CHL	C1C-NC	-2.41	1.34	1.37
23	A	808	LMT	O2B-C2B	-2.41	1.37	1.43
27	F	309	CHL	MG-ND	2.41	2.10	2.05
27	A	855	CHL	C4C-C3C	2.41	1.49	1.45
27	A	843	CHL	OBD-CAD	2.41	1.26	1.22
27	B	825	CHL	C1C-NC	-2.41	1.34	1.37
27	8	315	CHL	C1C-NC	-2.41	1.34	1.37
27	6	311	CHL	C4D-ND	2.41	1.41	1.37
27	3	319	CHL	C4D-ND	2.41	1.41	1.37
27	A	820	CHL	C1C-NC	-2.41	1.34	1.37
27	A	849	CHL	C1C-NC	-2.41	1.34	1.37
27	4	316	CHL	C3D-C2D	2.41	1.45	1.39
27	7	317	CHL	C4C-C3C	2.41	1.49	1.45
27	B	821	CHL	C1C-NC	-2.41	1.34	1.37
27	7	318	CHL	C4C-C3C	2.41	1.49	1.45
27	3	321	CHL	C4D-ND	2.41	1.41	1.37
33	7	305	XAT	C12-C13	-2.40	1.40	1.45
27	A	830	CHL	C4C-C3C	2.40	1.49	1.45
22	3	303	BCR	C1-C6	-2.40	1.50	1.53
27	B	819	CHL	C4C-C3C	2.40	1.49	1.45
27	7	313	CHL	C4D-ND	2.40	1.40	1.37
27	a	309	CHL	C1C-NC	-2.40	1.34	1.37
29	b	301	LUT	C18-C5	2.40	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	309	CHL	C4C-C3C	2.40	1.49	1.45
27	B	836	CHL	C4B-CHC	2.40	1.47	1.41
27	6	316	CHL	C3D-C2D	2.40	1.45	1.39
27	B	839	CHL	C1C-NC	-2.40	1.34	1.37
27	3	311	CHL	C1C-NC	-2.40	1.34	1.37
27	B	812	CHL	C1B-CHB	2.40	1.47	1.41
27	A	847	CHL	C1C-NC	-2.40	1.34	1.37
27	B	851	CHL	C1C-NC	-2.40	1.34	1.37
27	B	846	CHL	C4C-C3C	2.40	1.49	1.45
27	6	314	CHL	C1C-NC	-2.40	1.34	1.37
27	A	822	CHL	C1C-NC	-2.39	1.34	1.37
27	6	318	CHL	C3D-C2D	2.39	1.45	1.39
27	A	854	CHL	C1C-NC	-2.39	1.34	1.37
27	a	307	CHL	C4C-C3C	2.39	1.49	1.45
27	a	313	CHL	C1C-NC	-2.39	1.34	1.37
22	3	302	BCR	C30-C25	-2.39	1.50	1.53
27	5	319	CHL	C3D-C2D	2.39	1.45	1.39
29	6	303	LUT	C18-C5	2.39	1.54	1.50
27	5	308	CHL	C4C-C3C	2.39	1.49	1.45
27	3	311	CHL	C4C-C3C	2.39	1.49	1.45
23	5	306	LMT	O2B-C2B	-2.39	1.37	1.43
27	A	837	CHL	C4C-C3C	2.39	1.49	1.45
27	F	308	CHL	C4C-C3C	2.39	1.49	1.45
29	4	301	LUT	C38-C25	2.39	1.55	1.50
27	a	318	CHL	C3D-C2D	2.39	1.45	1.39
27	5	321	CHL	C1C-NC	-2.39	1.34	1.37
27	L	304	CHL	C1C-NC	-2.39	1.34	1.37
27	A	833	CHL	C4C-C3C	2.38	1.49	1.45
27	A	843	CHL	MG-NC	2.38	2.11	2.06
27	7	314	CHL	C4C-C3C	2.38	1.49	1.45
27	7	323	CHL	C4B-CHC	2.38	1.47	1.41
27	8	320	CHL	C1C-NC	-2.38	1.34	1.37
27	a	310	CHL	C1C-NC	-2.38	1.34	1.37
23	A	809	LMT	O2B-C2B	-2.38	1.37	1.43
27	4	307	CHL	C4C-C3C	2.38	1.49	1.45
27	B	817	CHL	C4B-CHC	2.38	1.47	1.41
27	5	318	CHL	C1C-NC	-2.38	1.34	1.37
27	A	831	CHL	MG-NC	2.38	2.11	2.06
23	F	302	LMT	O2B-C2B	-2.38	1.37	1.43
27	b	309	CHL	C4D-ND	2.38	1.40	1.37
27	6	310	CHL	C1C-NC	-2.37	1.34	1.37
27	3	315	CHL	C4C-C3C	2.37	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	312	CHL	C4D-ND	2.37	1.40	1.37
27	4	317	CHL	C4D-ND	2.37	1.40	1.37
27	A	835	CHL	C4D-ND	2.37	1.40	1.37
27	A	829	CHL	C4C-C3C	2.37	1.49	1.45
27	4	310	CHL	C1C-NC	-2.37	1.34	1.37
27	5	320	CHL	C1C-NC	-2.37	1.34	1.37
28	B	809	DGD	O1G-C1G	-2.37	1.39	1.45
23	5	306	LMT	O3B-C3B	-2.37	1.37	1.43
27	5	325	CHL	C3D-C2D	2.37	1.45	1.39
27	B	821	CHL	C4C-C3C	2.37	1.49	1.45
27	a	311	CHL	C4C-C3C	2.37	1.49	1.45
27	7	316	CHL	C1C-NC	-2.37	1.34	1.37
27	B	823	CHL	C4C-C3C	2.37	1.49	1.45
27	3	321	CHL	C4C-C3C	2.37	1.49	1.45
27	8	311	CHL	C4C-C3C	2.37	1.49	1.45
27	5	310	CHL	C1C-NC	-2.37	1.34	1.37
27	b	315	CHL	C1C-NC	-2.37	1.34	1.37
27	K	207	CHL	C3D-C2D	2.37	1.45	1.39
27	5	313	CHL	CHD-C4C	2.37	1.44	1.39
27	K	207	CHL	C4C-C3C	2.37	1.49	1.45
27	4	314	CHL	C4C-C3C	2.36	1.49	1.45
22	B	806	BCR	C30-C25	-2.36	1.50	1.53
27	7	314	CHL	C1C-NC	-2.36	1.34	1.37
27	6	312	CHL	C4D-ND	2.36	1.40	1.37
27	a	310	CHL	C4C-C3C	2.36	1.49	1.45
27	K	206	CHL	C1C-NC	-2.36	1.34	1.37
23	5	326	LMT	O3B-C3B	-2.36	1.37	1.43
27	7	323	CHL	C1C-NC	-2.36	1.34	1.37
27	b	312	CHL	C1C-NC	-2.36	1.34	1.37
27	B	832	CHL	C4D-ND	2.36	1.40	1.37
27	4	311	CHL	C4D-ND	2.36	1.40	1.37
27	4	317	CHL	C4B-CHC	2.36	1.47	1.41
27	3	308	CHL	C1C-NC	-2.36	1.34	1.37
27	7	317	CHL	C4D-ND	2.36	1.40	1.37
27	5	322	CHL	C3D-C2D	2.36	1.45	1.39
27	A	819	CHL	C1C-NC	-2.36	1.34	1.37
27	3	315	CHL	C1C-NC	-2.36	1.34	1.37
27	a	313	CHL	C4D-ND	2.36	1.40	1.37
27	7	312	CHL	C4C-C3C	2.36	1.49	1.44
27	B	851	CHL	C4C-C3C	2.36	1.49	1.45
27	5	311	CHL	C4C-C3C	2.36	1.49	1.45
29	J	103	LUT	C4-C5	2.36	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	309	CHL	C4D-ND	2.35	1.40	1.37
24	B	808	LHG	O7-C5	-2.35	1.40	1.46
27	A	820	CHL	C4C-C3C	2.35	1.49	1.45
27	7	321	CHL	C3A-C2A	-2.35	1.47	1.54
27	A	859	CHL	C4C-C3C	2.35	1.49	1.45
27	5	317	CHL	C3D-C2D	2.35	1.45	1.39
29	a	304	LUT	C18-C5	2.35	1.54	1.50
27	6	315	CHL	C1C-NC	-2.35	1.34	1.37
27	A	848	CHL	C4C-C3C	2.35	1.49	1.45
23	B	810	LMT	O3B-C3B	-2.35	1.37	1.43
27	b	312	CHL	C4D-ND	2.35	1.40	1.37
27	a	314	CHL	C1C-NC	-2.35	1.34	1.37
27	A	836	CHL	C4C-C3C	2.34	1.49	1.45
27	b	309	CHL	C1C-NC	-2.34	1.34	1.37
27	B	820	CHL	C1C-NC	-2.34	1.34	1.37
27	B	849	CHL	C1C-NC	-2.34	1.34	1.37
27	8	317	CHL	C1C-NC	-2.34	1.34	1.37
27	8	316	CHL	C4C-C3C	2.34	1.49	1.45
27	b	306	CHL	C1C-NC	-2.34	1.34	1.37
27	6	315	CHL	C4D-ND	2.34	1.40	1.37
27	6	307	CHL	CHD-C4C	2.34	1.44	1.39
27	b	304	CHL	C1C-NC	-2.34	1.34	1.37
27	6	308	CHL	C1D-C2D	2.34	1.49	1.45
27	5	307	CHL	C4C-C3C	2.34	1.49	1.45
27	A	821	CHL	C4C-C3C	2.34	1.49	1.45
27	5	313	CHL	CHD-C1D	2.34	1.42	1.38
27	6	307	CHL	MG-NC	2.34	2.11	2.06
23	7	308	LMT	O3B-C3B	-2.33	1.37	1.43
27	A	842	CHL	C3D-C2D	2.33	1.45	1.39
27	b	313	CHL	C1C-NC	-2.33	1.34	1.37
27	6	309	CHL	C4D-ND	2.33	1.40	1.37
27	b	307	CHL	C1C-NC	-2.33	1.34	1.37
27	6	314	CHL	C4D-ND	2.33	1.40	1.37
27	8	324	CHL	C3D-C2D	2.33	1.45	1.39
27	6	306	CHL	C1C-NC	-2.33	1.34	1.37
27	5	309	CHL	MG-ND	2.33	2.10	2.05
27	B	829	CHL	MG-ND	-2.33	2.01	2.05
27	a	315	CHL	C3D-C2D	2.33	1.45	1.39
27	B	843	CHL	C4D-ND	2.33	1.40	1.37
27	A	832	CHL	C4C-C3C	2.32	1.49	1.45
27	A	834	CHL	C4C-C3C	2.32	1.49	1.45
27	b	311	CHL	C4C-C3C	2.32	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	315	CHL	MG-ND	-2.32	2.01	2.05
27	B	847	CHL	C4C-C3C	2.32	1.49	1.45
27	A	851	CHL	C4D-ND	2.32	1.40	1.37
27	K	204	CHL	C4D-ND	2.32	1.40	1.37
27	3	309	CHL	C4D-ND	2.32	1.40	1.37
27	A	850	CHL	C4D-ND	2.32	1.40	1.37
27	4	317	CHL	C1C-NC	-2.32	1.34	1.37
29	5	302	LUT	C38-C25	2.32	1.54	1.50
27	5	314	CHL	C4D-ND	2.32	1.40	1.37
27	4	310	CHL	C4D-ND	2.32	1.40	1.37
27	A	841	CHL	C3A-C2A	-2.32	1.48	1.54
23	A	809	LMT	O3B-C3B	-2.32	1.37	1.43
27	7	311	CHL	C4C-C3C	2.32	1.49	1.45
26	A	815	CL0	C3D-C2D	2.32	1.45	1.39
27	5	309	CHL	C4D-ND	2.32	1.40	1.37
27	K	205	CHL	C4D-ND	2.31	1.40	1.37
27	b	304	CHL	C4D-ND	2.31	1.40	1.37
23	5	306	LMT	O4'-C4B	-2.31	1.37	1.43
27	a	308	CHL	C1C-NC	-2.31	1.34	1.37
27	K	204	CHL	C4C-C3C	2.31	1.49	1.45
27	A	827	CHL	C4C-C3C	2.31	1.49	1.45
27	7	312	CHL	C4D-ND	2.31	1.40	1.37
27	6	317	CHL	C3D-C2D	2.31	1.45	1.39
27	b	311	CHL	C3D-C2D	2.31	1.45	1.39
27	B	829	CHL	C4C-C3C	2.31	1.49	1.45
27	3	317	CHL	C4C-C3C	2.31	1.49	1.45
27	A	831	CHL	CHD-C4C	2.31	1.44	1.39
27	4	304	CHL	C1C-NC	-2.31	1.34	1.37
27	6	305	CHL	C1C-NC	-2.31	1.34	1.37
27	B	826	CHL	C4D-ND	2.31	1.40	1.37
27	a	317	CHL	C4D-ND	2.31	1.40	1.37
27	B	813	CHL	C4C-C3C	2.30	1.49	1.45
24	8	305	LHG	O7-C5	-2.30	1.40	1.46
27	B	826	CHL	C4C-C3C	2.30	1.49	1.45
27	4	312	CHL	C3D-C2D	2.30	1.45	1.39
27	6	319	CHL	C1B-CHB	2.30	1.47	1.41
27	B	845	CHL	C4C-C3C	2.30	1.49	1.45
27	8	322	CHL	C1C-NC	-2.30	1.34	1.37
27	B	842	CHL	C1C-NC	-2.30	1.34	1.37
27	a	311	CHL	C1C-NC	-2.30	1.34	1.37
27	A	821	CHL	C4D-ND	2.30	1.40	1.37
27	a	310	CHL	C4D-ND	2.30	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	833	CHL	C3D-C2D	2.30	1.45	1.39
27	6	311	CHL	C1C-NC	-2.30	1.34	1.37
29	5	303	LUT	C18-C5	2.30	1.54	1.50
27	a	320	CHL	C4D-ND	2.30	1.40	1.37
27	5	311	CHL	C4D-ND	2.30	1.40	1.37
27	8	311	CHL	C4D-ND	2.30	1.40	1.37
27	8	317	CHL	C4D-ND	2.30	1.40	1.37
27	A	851	CHL	C1C-NC	-2.30	1.34	1.37
29	5	303	LUT	C38-C25	2.30	1.54	1.50
27	7	315	CHL	C4C-C3C	2.30	1.49	1.45
27	5	320	CHL	C4D-ND	2.29	1.40	1.37
27	7	321	CHL	C3D-C2D	2.29	1.45	1.39
27	B	840	CHL	C1C-NC	-2.29	1.34	1.37
27	L	303	CHL	MG-NC	2.29	2.11	2.06
27	a	312	CHL	C4D-ND	2.29	1.40	1.37
27	8	323	CHL	C4B-CHC	2.29	1.47	1.41
27	4	315	CHL	C4D-ND	2.29	1.40	1.37
27	B	818	CHL	C4B-CHC	2.29	1.47	1.41
27	b	314	CHL	C1C-NC	-2.29	1.34	1.37
27	a	312	CHL	C1C-NC	-2.29	1.34	1.37
24	b	302	LHG	O7-C5	-2.29	1.40	1.46
27	7	315	CHL	C4D-ND	2.29	1.40	1.37
27	7	316	CHL	C4D-ND	2.29	1.40	1.37
27	8	313	CHL	C4D-ND	2.29	1.40	1.37
29	6	302	LUT	C18-C5	2.28	1.54	1.50
23	5	306	LMT	O2'-C2'	-2.28	1.37	1.43
27	B	850	CHL	C4C-C3C	2.28	1.49	1.45
29	4	302	LUT	C38-C25	2.28	1.54	1.50
27	B	840	CHL	C4C-C3C	2.28	1.49	1.45
27	A	844	CHL	C4D-ND	2.28	1.40	1.37
27	4	320	CHL	C4D-ND	2.28	1.40	1.37
29	8	303	LUT	C38-C25	2.28	1.54	1.50
23	5	326	LMT	O4'-C4B	-2.28	1.37	1.43
27	5	317	CHL	C3A-C2A	-2.28	1.48	1.54
27	B	841	CHL	C4C-C3C	2.28	1.49	1.45
27	B	838	CHL	C4D-ND	2.28	1.40	1.37
27	8	320	CHL	C4D-ND	2.28	1.40	1.37
27	a	315	CHL	MG-NA	-2.28	2.00	2.06
27	6	313	CHL	C1C-NC	-2.28	1.34	1.37
27	8	318	CHL	C4D-ND	2.28	1.40	1.37
27	A	831	CHL	CHD-C1D	2.28	1.42	1.38
27	4	318	CHL	C4D-ND	2.28	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	310	CHL	C4D-ND	2.28	1.40	1.37
27	8	313	CHL	C4C-C3C	2.28	1.49	1.45
27	5	315	CHL	C1C-NC	-2.27	1.34	1.37
27	5	314	CHL	C1C-NC	-2.27	1.34	1.37
27	3	317	CHL	MG-NC	2.27	2.11	2.06
27	A	843	CHL	C3D-C2D	2.27	1.45	1.39
29	6	303	LUT	C4-C5	2.27	1.54	1.51
29	J	103	LUT	C38-C25	2.27	1.54	1.50
27	4	311	CHL	C1C-NC	-2.27	1.34	1.37
27	b	305	CHL	C1C-NC	-2.27	1.34	1.37
29	6	303	LUT	C38-C25	2.27	1.54	1.50
27	5	317	CHL	MG-ND	-2.26	2.01	2.05
27	A	824	CHL	C4C-C3C	2.26	1.48	1.45
27	8	321	CHL	C3D-C2D	2.26	1.45	1.39
27	B	813	CHL	C1C-NC	-2.26	1.34	1.37
27	5	310	CHL	C4C-C3C	2.26	1.48	1.45
27	a	319	CHL	C4D-ND	2.26	1.40	1.37
27	b	313	CHL	C4D-ND	2.26	1.40	1.37
27	B	830	CHL	C4D-ND	2.26	1.40	1.37
27	a	318	CHL	MG-NA	2.26	2.11	2.06
27	7	322	CHL	C3D-C2D	2.26	1.45	1.39
27	5	315	CHL	C4D-ND	2.26	1.40	1.37
27	6	320	CHL	C4D-ND	2.26	1.40	1.37
29	3	305	LUT	C18-C5	2.26	1.54	1.50
27	3	314	CHL	C4D-ND	2.26	1.40	1.37
30	a	301	LMG	C4-C5	2.26	1.57	1.53
27	4	307	CHL	C4D-ND	2.26	1.40	1.37
27	3	320	CHL	C1C-NC	-2.25	1.34	1.37
27	A	832	CHL	C4D-ND	2.25	1.40	1.37
27	B	835	CHL	C4D-ND	2.25	1.40	1.37
27	L	304	CHL	C4D-ND	2.25	1.40	1.37
27	3	321	CHL	MG-NC	2.25	2.11	2.06
27	8	325	CHL	C4D-ND	2.25	1.40	1.37
29	8	304	LUT	C18-C5	2.25	1.54	1.50
27	5	316	CHL	MG-NA	-2.25	2.00	2.06
27	3	321	CHL	C1C-NC	-2.25	1.34	1.37
27	5	321	CHL	MG-ND	2.25	2.10	2.05
27	7	320	CHL	C3D-C2D	2.25	1.45	1.39
29	8	303	LUT	C18-C5	2.25	1.54	1.50
27	6	320	CHL	C1C-NC	-2.25	1.34	1.37
27	B	821	CHL	MG-ND	2.25	2.10	2.05
29	a	304	LUT	C38-C25	2.25	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	842	CHL	C3A-C2A	-2.25	1.48	1.54
27	B	822	CHL	C4D-ND	2.25	1.40	1.37
27	4	316	CHL	C4C-C3C	2.24	1.48	1.45
22	L	301	BCR	C30-C25	-2.24	1.50	1.53
27	4	304	CHL	C4C-C3C	2.24	1.48	1.45
27	B	842	CHL	C4C-C3C	2.24	1.48	1.45
27	a	320	CHL	C1C-NC	-2.24	1.34	1.37
27	7	319	CHL	C3D-C2D	2.24	1.45	1.39
27	b	316	CHL	C4C-C3C	2.24	1.48	1.45
27	6	316	CHL	C3A-C2A	-2.24	1.48	1.54
27	3	317	CHL	C4D-ND	2.24	1.40	1.37
27	3	308	CHL	C4C-C3C	2.24	1.48	1.45
27	B	829	CHL	C4D-ND	2.24	1.40	1.37
27	a	319	CHL	C1C-NC	-2.24	1.34	1.37
27	B	819	CHL	C4D-ND	2.24	1.40	1.37
27	8	314	CHL	C3D-C2D	2.24	1.45	1.39
27	5	312	CHL	C1C-NC	-2.24	1.34	1.37
27	3	313	CHL	C4D-ND	2.23	1.40	1.37
27	3	316	CHL	C3A-C2A	-2.23	1.48	1.54
27	b	315	CHL	C4C-C3C	2.23	1.48	1.45
27	B	837	CHL	C4D-ND	2.23	1.40	1.37
27	5	321	CHL	C4D-ND	2.23	1.40	1.37
27	B	824	CHL	C4D-ND	2.23	1.40	1.37
27	6	306	CHL	C4D-ND	2.23	1.40	1.37
23	A	808	LMT	O4'-C4B	-2.23	1.37	1.43
27	B	827	CHL	C4C-C3C	2.23	1.48	1.45
28	7	307	DGD	O5D-C6D	-2.23	1.39	1.43
27	4	308	CHL	C4C-C3C	2.23	1.48	1.45
27	4	313	CHL	C1C-NC	-2.23	1.34	1.37
23	F	302	LMT	O3B-C3B	-2.23	1.37	1.43
27	3	318	CHL	C4D-ND	2.22	1.40	1.37
27	L	303	CHL	C3D-C2D	2.22	1.45	1.39
29	F	303	LUT	C38-C25	2.22	1.54	1.50
27	b	308	CHL	C1C-C2C	2.22	1.48	1.44
27	F	308	CHL	C4D-ND	2.22	1.40	1.37
29	b	303	LUT	C32-C33	-2.22	1.41	1.45
27	3	314	CHL	C1C-NC	-2.22	1.34	1.37
27	6	305	CHL	C4D-ND	2.22	1.40	1.37
27	7	319	CHL	C3A-C2A	-2.22	1.48	1.54
28	7	307	DGD	O2G-C2G	-2.22	1.41	1.46
27	J	106	CHL	C4D-ND	2.22	1.40	1.37
27	7	324	CHL	C4D-ND	2.22	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3	304	LUT	C38-C25	2.21	1.54	1.50
27	b	307	CHL	C4D-ND	2.21	1.40	1.37
27	4	319	CHL	C4D-ND	2.21	1.40	1.37
27	A	827	CHL	C4D-ND	2.21	1.40	1.37
27	7	318	CHL	C4D-ND	2.21	1.40	1.37
29	7	304	LUT	C38-C25	2.21	1.54	1.50
27	a	311	CHL	C4D-ND	2.20	1.40	1.37
27	A	853	CHL	C4D-ND	2.20	1.40	1.37
27	b	310	CHL	C4D-ND	2.20	1.40	1.37
27	b	306	CHL	C4D-ND	2.20	1.40	1.37
27	4	318	CHL	C1C-NC	-2.20	1.34	1.37
27	A	830	CHL	C4D-ND	2.20	1.40	1.37
27	a	307	CHL	C4D-ND	2.20	1.40	1.37
27	B	849	CHL	C4D-ND	2.20	1.40	1.37
27	B	825	CHL	C4C-C3C	2.19	1.48	1.45
27	A	858	CHL	C4D-ND	2.19	1.40	1.37
27	L	303	CHL	C1D-C2D	2.19	1.49	1.45
27	A	857	CHL	C4D-ND	2.19	1.40	1.37
27	A	846	CHL	MG-NC	2.19	2.11	2.06
27	a	315	CHL	C3A-C2A	-2.19	1.48	1.54
27	b	310	CHL	C1C-NC	-2.19	1.34	1.37
27	B	820	CHL	C4D-ND	2.19	1.40	1.37
27	4	308	CHL	C4D-ND	2.18	1.40	1.37
27	A	834	CHL	MG-ND	2.18	2.10	2.05
27	6	317	CHL	C3A-C2A	-2.18	1.48	1.54
29	3	305	LUT	C38-C25	2.18	1.54	1.50
27	B	848	CHL	C4D-ND	2.18	1.40	1.37
27	A	847	CHL	C4D-ND	2.18	1.40	1.37
34	8	301	SQD	O9-S	2.18	1.51	1.45
27	B	836	CHL	C4D-ND	2.18	1.40	1.37
27	8	323	CHL	C4D-ND	2.18	1.40	1.37
27	B	813	CHL	C1C-C2C	2.18	1.48	1.44
27	b	312	CHL	MG-ND	-2.18	2.01	2.05
27	6	308	CHL	MG-NA	-2.18	2.01	2.06
27	B	813	CHL	C4D-ND	2.18	1.40	1.37
23	F	302	LMT	O1'-C1'	-2.17	1.36	1.40
23	B	810	LMT	O4'-C4B	-2.17	1.37	1.43
27	A	839	CHL	C4D-ND	2.17	1.40	1.37
23	A	808	LMT	O1'-C1'	-2.17	1.36	1.40
27	5	307	CHL	C4D-ND	2.17	1.40	1.37
27	4	314	CHL	C1C-NC	-2.17	1.34	1.37
27	A	845	CHL	C4D-ND	2.17	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	3	308	CHL	C4D-ND	2.17	1.40	1.37
27	B	811	CHL	C4C-C3C	2.17	1.48	1.45
27	B	821	CHL	C4D-ND	2.17	1.40	1.37
27	B	815	CHL	C4C-C3C	2.16	1.48	1.45
30	J	104	LMG	C1-C2	2.16	1.58	1.52
24	5	324	LHG	O7-C5	-2.16	1.41	1.46
27	b	315	CHL	C1C-C2C	2.16	1.48	1.44
27	b	315	CHL	C4D-ND	2.16	1.40	1.37
27	4	312	CHL	C4C-C3C	2.16	1.48	1.45
27	4	304	CHL	C4D-ND	2.16	1.40	1.37
27	A	846	CHL	C3D-C2D	2.15	1.45	1.39
27	3	310	CHL	C4D-ND	2.15	1.40	1.37
27	B	851	CHL	C4D-ND	2.15	1.40	1.37
27	B	825	CHL	C4D-ND	2.15	1.40	1.37
27	8	314	CHL	C4C-C3C	2.15	1.48	1.45
27	7	320	CHL	C3A-C2A	-2.15	1.48	1.54
27	B	847	CHL	C4D-ND	2.14	1.40	1.37
27	6	317	CHL	C4C-C3C	2.14	1.48	1.45
27	A	838	CHL	C4D-ND	2.14	1.40	1.37
27	7	314	CHL	C4D-ND	2.14	1.40	1.37
27	8	323	CHL	C1C-C2C	2.14	1.48	1.44
27	B	834	CHL	C4C-C3C	2.14	1.48	1.45
27	5	325	CHL	C3A-C2A	-2.14	1.48	1.54
27	a	315	CHL	C4C-C3C	2.14	1.48	1.45
27	A	856	CHL	C4D-ND	2.14	1.40	1.37
27	3	316	CHL	C3D-C2D	2.14	1.44	1.39
27	5	319	CHL	C4C-C3C	2.14	1.48	1.45
27	8	326	CHL	C4C-C3C	2.14	1.48	1.45
27	3	320	CHL	C4C-C3C	2.13	1.48	1.45
27	A	825	CHL	C4D-ND	2.13	1.40	1.37
27	K	207	CHL	C3A-C2A	-2.13	1.48	1.54
23	5	326	LMT	O1'-C1'	-2.13	1.36	1.40
27	7	322	CHL	C4C-C3C	2.13	1.48	1.45
27	b	311	CHL	MG-ND	2.13	2.10	2.05
27	a	316	CHL	C4C-C3C	2.13	1.48	1.45
27	A	841	CHL	C3D-C2D	2.13	1.44	1.39
27	A	828	CHL	C4D-ND	2.12	1.40	1.37
23	F	302	LMT	O4'-C4B	-2.12	1.38	1.43
27	7	322	CHL	C3A-C2A	-2.12	1.48	1.54
27	B	840	CHL	MG-NC	2.12	2.11	2.06
27	A	852	CHL	C4D-ND	2.12	1.40	1.37
27	6	316	CHL	C4C-C3C	2.12	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	811	LHG	P-O6	2.12	1.67	1.59
27	8	323	CHL	C4C-C3C	2.12	1.48	1.45
27	B	833	CHL	C4D-ND	2.12	1.40	1.37
27	3	311	CHL	MG-ND	2.12	2.10	2.05
27	B	814	CHL	C4D-ND	2.12	1.40	1.37
27	A	837	CHL	C4D-ND	2.12	1.40	1.37
27	6	307	CHL	C3D-C2D	2.11	1.44	1.39
27	5	320	CHL	C1C-C2C	2.11	1.48	1.44
27	A	829	CHL	C4D-ND	2.11	1.40	1.37
27	6	307	CHL	C4D-ND	2.11	1.40	1.37
27	A	833	CHL	C3A-C2A	-2.11	1.48	1.54
27	A	819	CHL	C1C-C2C	2.11	1.48	1.44
27	8	324	CHL	C3A-C2A	-2.11	1.48	1.54
27	A	853	CHL	MG-ND	2.11	2.10	2.05
27	a	314	CHL	C4D-ND	2.11	1.40	1.37
27	A	819	CHL	C4C-C3C	2.11	1.48	1.45
27	a	318	CHL	C4C-C3C	2.11	1.48	1.45
27	4	316	CHL	C3A-C2A	-2.10	1.48	1.54
27	A	843	CHL	C1C-C2C	2.10	1.48	1.44
27	B	851	CHL	MG-NC	2.10	2.11	2.06
27	8	315	CHL	C4D-ND	2.10	1.40	1.37
27	8	315	CHL	C4C-C3C	2.10	1.48	1.45
29	4	302	LUT	C18-C5	2.10	1.54	1.50
27	5	319	CHL	C3A-C2A	-2.10	1.48	1.54
27	5	310	CHL	C1C-C2C	2.10	1.48	1.44
27	5	322	CHL	C4C-C3C	2.10	1.48	1.45
23	7	308	LMT	O1'-C1'	-2.10	1.36	1.40
27	b	317	CHL	C4C-C3C	2.10	1.48	1.45
27	5	316	CHL	C1D-C2D	2.10	1.49	1.45
27	b	308	CHL	CMA-C3A	-2.10	1.48	1.53
27	5	318	CHL	C4D-ND	2.10	1.40	1.37
27	8	326	CHL	C4D-ND	2.09	1.40	1.37
27	A	848	CHL	C4D-ND	2.09	1.40	1.37
30	a	301	LMG	O7-C8	-2.09	1.41	1.46
27	4	320	CHL	C1C-C2C	2.09	1.48	1.44
27	A	854	CHL	C4D-ND	2.09	1.40	1.37
27	B	815	CHL	C4D-ND	2.09	1.40	1.37
27	8	321	CHL	C3A-C2A	-2.09	1.48	1.54
27	B	837	CHL	C3D-C4D	-2.09	1.39	1.44
27	4	309	CHL	C3A-C2A	-2.09	1.48	1.54
27	6	314	CHL	C1C-C2C	2.09	1.48	1.44
27	8	315	CHL	C1C-C2C	2.09	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	303	LUT	C28-C29	-2.09	1.41	1.45
27	3	315	CHL	C4D-ND	2.09	1.40	1.37
23	A	809	LMT	O4'-C4B	-2.09	1.38	1.43
27	3	312	CHL	C3D-C4D	-2.09	1.39	1.44
27	6	318	CHL	C3A-C2A	-2.09	1.48	1.54
27	A	824	CHL	C4D-ND	2.08	1.40	1.37
27	A	841	CHL	C4C-C3C	2.08	1.48	1.45
27	6	319	CHL	C4B-CHC	2.08	1.46	1.41
27	A	822	CHL	C4D-ND	2.08	1.40	1.37
27	8	319	CHL	C4D-ND	2.08	1.40	1.37
27	6	310	CHL	C1C-C2C	2.08	1.48	1.44
27	b	313	CHL	C1C-C2C	2.08	1.48	1.44
27	a	318	CHL	C3A-C2A	-2.08	1.48	1.54
27	B	850	CHL	C4D-ND	2.08	1.40	1.37
27	5	313	CHL	C3D-C2D	2.08	1.44	1.39
27	5	325	CHL	C4C-C3C	2.08	1.48	1.45
27	A	849	CHL	C4D-ND	2.08	1.40	1.37
27	b	317	CHL	C1B-CHB	2.08	1.46	1.41
27	A	834	CHL	C4D-ND	2.08	1.40	1.37
23	7	308	LMT	O4'-C4B	-2.08	1.38	1.43
27	b	311	CHL	C3A-C2A	-2.07	1.48	1.54
27	A	855	CHL	C4D-ND	2.07	1.40	1.37
29	b	303	LUT	C12-C13	-2.07	1.41	1.45
27	5	313	CHL	C4D-ND	2.07	1.40	1.37
27	B	817	CHL	C4D-ND	2.07	1.40	1.37
27	B	818	CHL	C4D-ND	2.07	1.40	1.37
27	8	316	CHL	C4D-ND	2.07	1.40	1.37
27	A	818	CHL	MG-ND	2.07	2.09	2.05
27	3	320	CHL	C1C-C2C	2.07	1.48	1.44
27	B	846	CHL	C4D-ND	2.07	1.40	1.37
27	a	318	CHL	C1B-CHB	2.07	1.46	1.41
27	4	312	CHL	C3A-C2A	-2.06	1.48	1.54
27	A	832	CHL	MG-ND	2.06	2.09	2.05
27	A	826	CHL	C4D-ND	2.06	1.40	1.37
27	a	307	CHL	C1C-C2C	2.06	1.48	1.44
27	4	315	CHL	C1C-C2C	2.06	1.48	1.44
27	8	314	CHL	C3A-C2A	-2.06	1.48	1.54
27	6	310	CHL	C3D-C4D	-2.06	1.39	1.44
27	B	839	CHL	C4D-ND	2.06	1.40	1.37
27	B	826	CHL	C1C-C2C	2.06	1.48	1.44
27	B	851	CHL	C1C-C2C	2.06	1.48	1.44
27	A	836	CHL	C3D-C4D	-2.06	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	8	312	CHL	C4D-ND	2.06	1.40	1.37
27	B	823	CHL	C4D-ND	2.06	1.40	1.37
34	8	301	SQD	O7-S	2.06	1.51	1.45
27	4	314	CHL	C1C-C2C	2.06	1.48	1.44
27	L	304	CHL	C1C-C2C	2.05	1.48	1.44
27	8	324	CHL	C4C-C3C	2.05	1.48	1.45
29	7	304	LUT	C4-C5	2.05	1.54	1.51
27	5	322	CHL	C3A-C2A	-2.05	1.48	1.54
27	4	314	CHL	C4D-ND	2.05	1.40	1.37
24	A	810	LHG	O7-C5	-2.05	1.41	1.46
27	3	321	CHL	C1C-C2C	2.05	1.48	1.44
27	B	831	CHL	C4D-ND	2.05	1.40	1.37
27	A	822	CHL	C1C-C2C	2.04	1.48	1.44
27	B	834	CHL	C4D-ND	2.04	1.40	1.37
27	A	844	CHL	C3D-C4D	-2.04	1.39	1.44
27	6	315	CHL	C1C-C2C	2.04	1.48	1.44
27	L	303	CHL	C1C-C2C	2.04	1.48	1.44
27	B	828	CHL	C3D-C4D	-2.04	1.39	1.44
27	A	818	CHL	C4D-ND	2.04	1.40	1.37
27	6	307	CHL	C1D-C2D	2.04	1.49	1.45
27	6	308	CHL	C4C-C3C	2.04	1.48	1.45
27	K	204	CHL	C1C-C2C	2.04	1.48	1.44
27	6	319	CHL	MG-ND	-2.03	2.01	2.05
27	b	316	CHL	C1B-CHB	2.03	1.46	1.41
30	7	301	LMG	O8-C9	-2.03	1.40	1.45
24	A	811	LHG	O7-C5	-2.03	1.41	1.46
27	A	816	CHL	C1C-C2C	2.03	1.48	1.44
27	b	304	CHL	C1C-C2C	2.03	1.48	1.44
27	5	322	CHL	C1B-CHB	2.03	1.46	1.41
27	B	845	CHL	C4D-ND	2.03	1.40	1.37
27	B	817	CHL	C4C-C3C	2.03	1.48	1.45
27	b	310	CHL	C1C-C2C	2.03	1.48	1.44
27	B	815	CHL	C3D-C4D	-2.03	1.39	1.44
27	B	842	CHL	C4D-ND	2.03	1.40	1.37
27	b	317	CHL	C3A-C2A	-2.02	1.48	1.54
27	4	307	CHL	C1C-C2C	2.02	1.48	1.44
27	4	312	CHL	C1B-CHB	2.02	1.46	1.41
27	4	319	CHL	C3D-C4D	-2.02	1.39	1.44
27	7	315	CHL	C3D-C4D	-2.02	1.39	1.44
27	7	322	CHL	C1B-CHB	2.02	1.46	1.41
27	6	319	CHL	MG-NA	2.02	2.11	2.06
27	4	310	CHL	C1C-C2C	2.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	311	CHL	C4D-ND	2.02	1.40	1.37
27	8	322	CHL	C4C-C3C	2.02	1.48	1.45
27	3	318	CHL	C1C-C2C	2.02	1.48	1.44
27	6	308	CHL	C4B-CHC	2.02	1.46	1.41
30	J	101	LMG	O8-C9	-2.02	1.40	1.45
27	B	816	CHL	MG-ND	-2.01	2.01	2.05
27	A	819	CHL	C4D-ND	2.01	1.40	1.37
27	B	825	CHL	C1C-C2C	2.01	1.48	1.44
27	a	313	CHL	C1C-C2C	2.01	1.48	1.44
27	B	825	CHL	C3D-C4D	-2.01	1.39	1.44
27	A	821	CHL	C3D-C4D	-2.01	1.39	1.44
27	A	854	CHL	C1C-C2C	2.01	1.48	1.44
27	B	850	CHL	C1C-C2C	2.01	1.48	1.44
27	B	835	CHL	C1C-C2C	2.01	1.48	1.44
27	A	836	CHL	C4D-ND	2.01	1.40	1.37
27	4	318	CHL	C1C-C2C	2.01	1.48	1.44
29	5	303	LUT	C4-C5	2.01	1.54	1.51
27	A	847	CHL	C3D-C4D	-2.01	1.39	1.44
27	B	831	CHL	C3D-C4D	-2.01	1.39	1.44
27	B	830	CHL	C3D-C4D	-2.01	1.39	1.44
22	K	202	BCR	C38-C26	-2.01	1.47	1.50
27	5	325	CHL	C1B-CHB	2.01	1.46	1.41
27	8	324	CHL	C1B-CHB	2.00	1.46	1.41
27	5	320	CHL	MG-ND	2.00	2.09	2.05
27	B	828	CHL	C4D-ND	2.00	1.40	1.37
27	A	818	CHL	C3D-C4D	-2.00	1.39	1.44
27	7	319	CHL	C1B-CHB	2.00	1.46	1.41

All (5620) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	308	CHL	CMB-C2B-C1B	-25.31	89.57	128.46
27	5	315	CHL	C4-C3-C5	-19.98	81.67	115.27
27	5	315	CHL	C5-C3-C2	19.36	160.28	121.12
27	5	313	CHL	C1D-ND-C4D	-17.88	93.63	106.33
27	A	843	CHL	O2A-CGA-O1A	-17.87	78.49	123.59
27	6	307	CHL	C1D-ND-C4D	-17.85	93.65	106.33
27	L	303	CHL	C1D-ND-C4D	-17.80	93.69	106.33
27	A	831	CHL	C1D-ND-C4D	-17.51	93.90	106.33
27	5	315	CHL	C4-C3-C2	-17.47	78.86	123.68
29	7	304	LUT	C15-C14-C13	-16.81	103.31	127.31
27	A	846	CHL	C1D-ND-C4D	-16.75	94.43	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	308	CHL	CMB-C2B-C3B	15.51	153.69	124.68
27	A	843	CHL	C1D-ND-C4D	-15.01	95.67	106.33
29	J	103	LUT	C15-C35-C34	15.01	154.22	123.47
29	8	304	LUT	C18-C5-C6	-14.54	108.19	124.53
27	A	843	CHL	O2A-CGA-CBA	14.54	157.54	111.91
29	3	305	LUT	C15-C14-C13	-14.53	106.57	127.31
29	8	304	LUT	C15-C14-C13	-14.45	106.69	127.31
29	5	303	LUT	C15-C35-C34	14.30	152.76	123.47
29	a	304	LUT	C15-C35-C34	14.09	152.33	123.47
29	a	304	LUT	C18-C5-C6	-14.05	108.75	124.53
26	A	815	CL0	C1D-ND-C4D	-13.10	97.03	106.33
29	6	303	LUT	C15-C35-C34	12.99	150.08	123.47
29	F	303	LUT	C15-C35-C34	12.94	149.98	123.47
29	F	303	LUT	C18-C5-C6	-12.79	110.17	124.53
29	3	305	LUT	C11-C10-C9	-12.65	109.25	127.31
29	5	302	LUT	C15-C35-C34	12.58	149.24	123.47
29	6	302	LUT	C15-C14-C13	-12.55	109.40	127.31
29	4	301	LUT	C15-C35-C34	12.55	149.17	123.47
29	3	304	LUT	C15-C14-C13	-12.55	109.41	127.31
29	6	302	LUT	C18-C5-C6	-12.45	110.55	124.53
29	b	301	LUT	C15-C35-C34	12.41	148.90	123.47
29	3	305	LUT	C18-C5-C6	-12.40	110.60	124.53
29	a	302	LUT	C15-C14-C13	-12.37	109.65	127.31
29	8	303	LUT	C18-C5-C6	-12.36	110.65	124.53
29	4	302	LUT	C15-C35-C34	12.22	148.51	123.47
29	4	302	LUT	C18-C5-C6	-12.17	110.86	124.53
29	6	302	LUT	C15-C35-C34	12.12	148.29	123.47
27	8	323	CHL	CHD-C1D-ND	-12.11	113.33	124.45
29	4	301	LUT	C15-C14-C13	-11.98	110.21	127.31
29	8	303	LUT	C15-C14-C13	-11.96	110.24	127.31
29	a	302	LUT	C15-C35-C34	11.95	147.96	123.47
29	3	304	LUT	C11-C10-C9	-11.80	110.47	127.31
29	8	303	LUT	C15-C35-C34	11.78	147.61	123.47
27	4	317	CHL	CHD-C1D-ND	-11.72	113.68	124.45
29	5	302	LUT	C15-C14-C13	-11.70	110.62	127.31
27	4	313	CHL	CHD-C1D-ND	-11.60	113.79	124.45
29	a	302	LUT	C11-C10-C9	-11.58	110.78	127.31
29	6	303	LUT	C18-C5-C6	-11.57	111.53	124.53
29	5	303	LUT	C31-C30-C29	-11.48	110.92	127.31
29	b	301	LUT	C11-C10-C9	-11.48	110.93	127.31
29	a	304	LUT	C11-C10-C9	-11.46	110.96	127.31
27	A	843	CHL	O1A-CGA-CBA	-11.40	79.27	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	301	LUT	C18-C5-C6	-11.35	111.78	124.53
29	3	304	LUT	C15-C35-C34	11.30	146.62	123.47
29	F	303	LUT	C11-C10-C9	-11.24	111.26	127.31
29	8	304	LUT	C31-C30-C29	-11.21	111.31	127.31
29	8	304	LUT	C15-C35-C34	11.12	146.25	123.47
29	6	302	LUT	C31-C30-C29	-11.10	111.47	127.31
27	A	846	CHL	C2C-C1C-NC	11.06	120.33	109.97
29	5	302	LUT	C18-C5-C6	-11.02	112.15	124.53
29	5	303	LUT	C18-C5-C6	-10.97	112.21	124.53
29	6	302	LUT	C31-C32-C33	10.97	157.23	126.42
29	J	103	LUT	C15-C14-C13	-10.96	111.67	127.31
27	5	313	CHL	C4A-NA-C1A	-10.93	101.79	106.71
27	5	313	CHL	C2C-C1C-NC	10.92	120.21	109.97
29	5	302	LUT	C11-C10-C9	-10.88	111.78	127.31
29	J	103	LUT	C31-C30-C29	-10.87	111.80	127.31
29	J	103	LUT	C11-C10-C9	-10.84	111.84	127.31
29	J	103	LUT	C18-C5-C6	-10.80	112.39	124.53
27	6	307	CHL	C4A-NA-C1A	-10.78	101.86	106.71
29	4	301	LUT	C18-C5-C6	-10.77	112.43	124.53
29	7	304	LUT	C15-C35-C34	10.75	145.49	123.47
29	b	301	LUT	C15-C14-C13	-10.74	111.98	127.31
29	b	301	LUT	C31-C30-C29	-10.74	111.98	127.31
29	4	301	LUT	C11-C10-C9	-10.70	112.03	127.31
29	5	303	LUT	C11-C10-C9	-10.70	112.04	127.31
27	6	307	CHL	C2C-C1C-NC	10.70	119.99	109.97
29	6	302	LUT	C11-C10-C9	-10.65	112.11	127.31
27	A	831	CHL	C2C-C1C-NC	10.63	119.93	109.97
29	3	305	LUT	C15-C35-C34	10.60	145.18	123.47
29	7	304	LUT	C31-C30-C29	-10.59	112.19	127.31
27	7	323	CHL	CHD-C1D-ND	-10.58	114.73	124.45
29	6	303	LUT	C15-C14-C13	-10.56	112.23	127.31
29	a	304	LUT	C31-C30-C29	-10.46	112.38	127.31
29	5	303	LUT	C11-C12-C13	10.44	155.75	126.42
29	3	304	LUT	C18-C5-C6	-10.43	112.82	124.53
29	4	302	LUT	C11-C10-C9	-10.41	112.46	127.31
29	a	302	LUT	C18-C5-C6	-10.40	112.84	124.53
29	3	305	LUT	C31-C30-C29	-10.39	112.48	127.31
29	F	303	LUT	C11-C12-C13	10.35	155.49	126.42
29	8	303	LUT	C31-C30-C29	-10.30	112.60	127.31
29	F	303	LUT	C31-C30-C29	-10.30	112.61	127.31
26	A	815	CL0	C2C-C1C-NC	10.30	119.62	109.97
29	4	302	LUT	C15-C14-C13	-10.29	112.62	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	304	LUT	C35-C34-C33	-10.27	112.65	127.31
29	6	303	LUT	C31-C30-C29	-10.27	112.66	127.31
29	5	302	LUT	C31-C30-C29	-10.25	112.68	127.31
29	F	303	LUT	C19-C9-C10	-10.12	108.74	122.92
27	4	313	CHL	C4A-NA-C1A	10.07	111.23	106.71
29	J	103	LUT	C39-C29-C30	-10.05	108.85	122.92
27	A	840	CHL	C4A-NA-C1A	10.00	111.20	106.71
29	a	302	LUT	C31-C30-C29	-9.99	113.05	127.31
27	A	843	CHL	C2C-C1C-NC	9.98	119.32	109.97
29	5	303	LUT	C35-C34-C33	-9.94	113.12	127.31
29	8	303	LUT	C11-C10-C9	-9.94	113.12	127.31
29	4	301	LUT	C31-C30-C29	-9.85	113.25	127.31
29	a	304	LUT	C31-C32-C33	9.83	154.04	126.42
29	7	304	LUT	C11-C10-C9	-9.83	113.28	127.31
29	a	304	LUT	C19-C9-C10	-9.80	109.19	122.92
29	4	302	LUT	C11-C12-C13	9.75	153.82	126.42
29	J	103	LUT	C11-C12-C13	9.74	153.77	126.42
29	a	304	LUT	C39-C29-C30	-9.71	109.32	122.92
29	a	304	LUT	C40-C33-C34	-9.70	109.34	122.92
27	L	303	CHL	C2C-C1C-NC	9.68	119.04	109.97
29	3	304	LUT	C31-C30-C29	-9.66	113.52	127.31
29	3	304	LUT	C31-C32-C33	9.65	153.54	126.42
29	3	305	LUT	C31-C32-C33	9.65	153.52	126.42
29	5	303	LUT	C20-C13-C14	-9.64	109.41	122.92
29	4	301	LUT	C31-C32-C33	9.62	153.45	126.42
29	4	302	LUT	C19-C9-C10	-9.59	109.48	122.92
27	B	832	CHL	C4A-NA-C1A	9.56	111.01	106.71
29	J	103	LUT	C20-C13-C14	-9.52	109.58	122.92
27	5	323	CHL	C4A-NA-C1A	9.52	110.99	106.71
29	6	302	LUT	C39-C29-C30	-9.51	109.60	122.92
29	5	302	LUT	C40-C33-C34	-9.50	109.61	122.92
29	J	103	LUT	C19-C9-C10	-9.49	109.63	122.92
29	5	303	LUT	C15-C14-C13	-9.49	113.77	127.31
29	a	302	LUT	C31-C32-C33	9.49	153.07	126.42
29	7	304	LUT	C18-C5-C6	-9.48	113.88	124.53
29	6	303	LUT	C11-C12-C13	9.48	153.03	126.42
29	b	301	LUT	C19-C9-C10	-9.46	109.68	122.92
29	8	304	LUT	C11-C10-C9	-9.42	113.87	127.31
27	A	843	CHL	C3C-C4C-NC	9.40	121.11	110.57
29	6	303	LUT	C31-C32-C33	9.40	152.82	126.42
27	A	835	CHL	C4A-NA-C1A	9.36	110.91	106.71
29	5	302	LUT	C35-C34-C33	-9.34	113.98	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	302	LUT	C20-C13-C14	-9.30	109.90	122.92
29	J	103	LUT	C40-C33-C34	-9.28	109.93	122.92
27	A	832	CHL	C4A-NA-C1A	9.27	110.88	106.71
27	B	835	CHL	C4A-NA-C1A	9.26	110.87	106.71
29	b	301	LUT	C40-C33-C34	-9.25	109.97	122.92
27	7	313	CHL	C4A-NA-C1A	9.21	110.85	106.71
29	a	302	LUT	C19-C9-C10	-9.21	110.02	122.92
29	4	302	LUT	C31-C30-C29	-9.20	114.17	127.31
27	A	829	CHL	C4A-NA-C1A	9.19	110.84	106.71
29	7	304	LUT	C11-C12-C13	9.18	152.20	126.42
29	5	303	LUT	C40-C33-C34	-9.16	110.10	122.92
27	A	816	CHL	C4A-NA-C1A	9.15	110.82	106.71
27	3	318	CHL	C4A-NA-C1A	9.12	110.81	106.71
27	b	305	CHL	C4A-NA-C1A	9.12	110.81	106.71
29	a	304	LUT	C15-C14-C13	-9.11	114.31	127.31
27	L	303	CHL	C2D-C1D-ND	9.10	116.81	110.10
27	7	318	CHL	C4A-NA-C1A	9.09	110.79	106.71
27	L	303	CHL	C4A-NA-C1A	-9.08	102.62	106.71
29	7	304	LUT	C31-C32-C33	9.08	151.91	126.42
29	b	301	LUT	C31-C32-C33	9.07	151.89	126.42
29	F	303	LUT	C35-C34-C33	-9.06	114.39	127.31
29	a	304	LUT	C11-C12-C13	9.05	151.84	126.42
29	8	303	LUT	C40-C33-C34	-9.04	110.26	122.92
29	F	303	LUT	C20-C13-C14	-9.03	110.27	122.92
29	F	303	LUT	C40-C33-C34	-9.01	110.30	122.92
29	5	302	LUT	C31-C32-C33	9.00	151.69	126.42
27	b	308	CHL	CHD-C1D-ND	-8.99	116.19	124.45
29	b	301	LUT	C39-C29-C30	-8.99	110.33	122.92
29	J	103	LUT	C31-C32-C33	8.98	151.65	126.42
29	6	303	LUT	C11-C10-C9	-8.98	114.49	127.31
29	4	301	LUT	C35-C34-C33	-8.98	114.50	127.31
27	B	830	CHL	C4A-NA-C1A	8.96	110.73	106.71
29	7	304	LUT	C40-C33-C34	-8.95	110.38	122.92
27	5	316	CHL	C2C-C3C-C4C	-8.92	100.13	106.49
27	b	309	CHL	C4A-NA-C1A	8.92	110.72	106.71
29	4	301	LUT	C40-C33-C34	-8.92	110.43	122.92
29	5	302	LUT	C20-C13-C14	-8.90	110.46	122.92
27	3	309	CHL	C4A-NA-C1A	8.89	110.70	106.71
29	5	303	LUT	C19-C9-C10	-8.89	110.47	122.92
29	5	303	LUT	C31-C32-C33	8.87	151.33	126.42
27	5	313	CHL	C2D-C1D-ND	8.87	116.64	110.10
29	b	301	LUT	C11-C12-C13	8.86	151.31	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	302	LUT	C40-C33-C34	-8.86	110.51	122.92
27	F	309	CHL	C4A-NA-C1A	8.85	110.68	106.71
27	b	304	CHL	C4A-NA-C1A	8.83	110.67	106.71
27	B	823	CHL	C4A-NA-C1A	8.81	110.67	106.71
29	6	302	LUT	C19-C9-C10	-8.81	110.58	122.92
27	a	309	CHL	C4A-NA-C1A	8.80	110.66	106.71
29	6	303	LUT	C19-C9-C10	-8.79	110.60	122.92
27	5	308	CHL	C4A-NA-C1A	8.76	110.64	106.71
29	F	303	LUT	C31-C32-C33	8.75	150.98	126.42
27	B	824	CHL	C4A-NA-C1A	8.74	110.64	106.71
29	4	301	LUT	C39-C29-C30	-8.74	110.69	122.92
27	4	306	CHL	C4A-NA-C1A	8.73	110.63	106.71
27	A	831	CHL	C2D-C1D-ND	8.73	116.54	110.10
27	5	309	CHL	C4A-NA-C1A	8.72	110.63	106.71
29	6	302	LUT	C40-C33-C34	-8.72	110.71	122.92
27	a	308	CHL	C4A-NA-C1A	8.71	110.62	106.71
27	3	317	CHL	C4A-NA-C1A	8.70	110.62	106.71
27	6	313	CHL	C4A-NA-C1A	8.70	110.62	106.71
27	A	846	CHL	C2D-C1D-ND	8.68	116.50	110.10
27	A	852	CHL	C4A-NA-C1A	8.67	110.60	106.71
27	A	856	CHL	C4A-NA-C1A	8.67	110.60	106.71
27	A	854	CHL	C4A-NA-C1A	8.66	110.60	106.71
29	8	304	LUT	C31-C32-C33	8.66	150.75	126.42
27	6	310	CHL	C4A-NA-C1A	8.65	110.59	106.71
27	6	315	CHL	C4A-NA-C1A	8.63	110.59	106.71
29	6	303	LUT	C40-C33-C34	-8.63	110.83	122.92
29	5	303	LUT	C39-C29-C30	-8.62	110.85	122.92
27	6	312	CHL	C4A-NA-C1A	8.61	110.58	106.71
27	B	840	CHL	C4A-NA-C1A	8.60	110.57	106.71
27	b	313	CHL	C4A-NA-C1A	8.60	110.57	106.71
29	F	303	LUT	C15-C14-C13	-8.59	115.05	127.31
27	6	314	CHL	C4A-NA-C1A	8.59	110.57	106.71
29	a	302	LUT	C39-C29-C30	-8.59	110.89	122.92
27	A	830	CHL	C4A-NA-C1A	8.58	110.56	106.71
27	B	813	CHL	C4A-NA-C1A	8.58	110.56	106.71
27	4	310	CHL	C4A-NA-C1A	8.58	110.56	106.71
27	3	314	CHL	C4A-NA-C1A	8.57	110.56	106.71
27	3	319	CHL	C4A-NA-C1A	8.57	110.56	106.71
27	B	847	CHL	C4A-NA-C1A	8.57	110.56	106.71
29	4	302	LUT	C20-C13-C14	-8.56	110.93	122.92
27	b	312	CHL	C4A-NA-C1A	8.55	110.55	106.71
29	3	305	LUT	C19-C9-C10	-8.55	110.95	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	851	CHL	C4A-NA-C1A	8.55	110.55	106.71
27	A	837	CHL	C4A-NA-C1A	8.54	110.55	106.71
27	8	313	CHL	C4A-NA-C1A	8.53	110.54	106.71
27	8	317	CHL	C4A-NA-C1A	8.53	110.54	106.71
27	B	826	CHL	C4A-NA-C1A	8.52	110.54	106.71
29	3	305	LUT	C39-C29-C30	-8.52	110.99	122.92
29	a	304	LUT	C20-C13-C14	-8.49	111.03	122.92
27	B	848	CHL	C4A-NA-C1A	8.49	110.52	106.71
27	B	845	CHL	C4A-NA-C1A	8.48	110.52	106.71
29	6	303	LUT	C39-C29-C30	-8.48	111.05	122.92
29	3	304	LUT	C19-C9-C10	-8.46	111.08	122.92
29	a	302	LUT	C32-C33-C34	-8.45	105.98	118.94
29	6	302	LUT	C11-C12-C13	8.45	150.14	126.42
29	4	302	LUT	C1-C6-C5	-8.44	110.72	122.61
29	8	303	LUT	C31-C32-C33	8.44	150.12	126.42
27	F	308	CHL	C4A-NA-C1A	8.43	110.49	106.71
29	5	302	LUT	C11-C12-C13	8.43	150.09	126.42
29	4	301	LUT	C19-C9-C10	-8.42	111.12	122.92
27	B	818	CHL	C4A-NA-C1A	8.42	110.49	106.71
27	A	858	CHL	C4A-NA-C1A	8.42	110.49	106.71
29	3	304	LUT	C40-C33-C34	-8.41	111.14	122.92
27	5	320	CHL	C4A-NA-C1A	8.41	110.49	106.71
27	b	314	CHL	C4A-NA-C1A	8.41	110.48	106.71
27	A	857	CHL	C4A-NA-C1A	8.39	110.48	106.71
27	6	307	CHL	C2D-C1D-ND	8.36	116.27	110.10
27	A	855	CHL	C4A-NA-C1A	8.35	110.46	106.71
29	4	302	LUT	C31-C32-C33	8.34	149.83	126.42
29	7	304	LUT	C39-C29-C30	-8.33	111.25	122.92
27	B	829	CHL	C4A-NA-C1A	8.33	110.45	106.71
29	6	303	LUT	C35-C34-C33	-8.32	115.43	127.31
29	8	303	LUT	C11-C12-C13	8.31	149.75	126.42
27	J	106	CHL	C4A-NA-C1A	8.31	110.44	106.71
27	a	317	CHL	C4A-NA-C1A	8.30	110.44	106.71
29	4	301	LUT	C20-C13-C14	-8.30	111.30	122.92
29	a	302	LUT	C11-C12-C13	8.29	149.72	126.42
29	3	304	LUT	C39-C29-C30	-8.29	111.31	122.92
29	8	304	LUT	C39-C29-C30	-8.28	111.32	122.92
27	A	853	CHL	C4A-NA-C1A	8.28	110.43	106.71
27	B	850	CHL	C4A-NA-C1A	8.28	110.43	106.71
29	8	304	LUT	C40-C33-C34	-8.28	111.33	122.92
27	8	311	CHL	C4A-NA-C1A	8.27	110.42	106.71
29	3	305	LUT	C32-C33-C34	-8.27	106.25	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	843	CHL	C4A-NA-C1A	8.27	110.42	106.71
27	6	305	CHL	C4A-NA-C1A	8.26	110.42	106.71
27	6	308	CHL	C2C-C3C-C4C	-8.26	100.60	106.49
29	5	302	LUT	C39-C29-C30	-8.26	111.35	122.92
29	3	305	LUT	C20-C13-C14	-8.26	111.36	122.92
29	8	304	LUT	C20-C13-C14	-8.26	111.36	122.92
27	A	859	CHL	C4A-NA-C1A	8.25	110.41	106.71
27	A	845	CHL	C4A-NA-C1A	8.24	110.41	106.71
27	4	311	CHL	C4A-NA-C1A	8.24	110.41	106.71
29	5	302	LUT	C19-C9-C10	-8.24	111.38	122.92
29	7	304	LUT	C20-C13-C14	-8.24	111.38	122.92
27	B	834	CHL	C4A-NA-C1A	8.24	110.41	106.71
29	F	303	LUT	C39-C29-C30	-8.23	111.39	122.92
27	A	827	CHL	C4A-NA-C1A	8.23	110.41	106.71
29	a	302	LUT	C20-C13-C14	-8.23	111.39	122.92
29	3	304	LUT	C35-C34-C33	-8.22	115.58	127.31
27	A	822	CHL	C4A-NA-C1A	8.22	110.40	106.71
29	8	304	LUT	C38-C25-C24	-8.21	105.99	123.56
29	8	303	LUT	C20-C13-C14	-8.21	111.42	122.92
27	5	321	CHL	C4A-NA-C1A	8.20	110.39	106.71
27	8	326	CHL	C4A-NA-C1A	8.20	110.39	106.71
29	8	303	LUT	C39-C29-C30	-8.19	111.45	122.92
27	a	310	CHL	C4A-NA-C1A	8.19	110.39	106.71
27	6	319	CHL	C4A-NA-C1A	8.18	110.38	106.71
27	6	307	CHL	CMD-C2D-C1D	8.18	139.13	124.71
27	7	312	CHL	C4A-NA-C1A	8.17	110.38	106.71
27	A	825	CHL	C4A-NA-C1A	8.16	110.38	106.71
27	B	814	CHL	C4A-NA-C1A	8.15	110.37	106.71
27	A	831	CHL	CMD-C2D-C1D	8.14	139.06	124.71
29	4	301	LUT	C11-C12-C13	8.14	149.28	126.42
29	4	302	LUT	C40-C33-C34	-8.14	111.53	122.92
29	7	304	LUT	C35-C34-C33	-8.13	115.71	127.31
29	6	303	LUT	C20-C13-C14	-8.13	111.54	122.92
29	8	303	LUT	C19-C9-C10	-8.12	111.54	122.92
27	7	317	CHL	C4A-NA-C1A	8.12	110.36	106.71
27	A	831	CHL	C3C-C4C-NC	8.12	119.68	110.57
27	B	822	CHL	C4A-NA-C1A	8.11	110.35	106.71
27	5	313	CHL	CMD-C2D-C1D	8.11	139.01	124.71
29	8	304	LUT	C19-C9-C10	-8.11	111.56	122.92
27	5	312	CHL	C4A-NA-C1A	8.10	110.35	106.71
29	b	301	LUT	C35-C34-C33	-8.08	115.78	127.31
27	K	206	CHL	C4A-NA-C1A	8.07	110.34	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	838	CHL	C4A-NA-C1A	8.06	110.33	106.71
27	B	838	CHL	C4A-NA-C1A	8.06	110.33	106.71
29	3	305	LUT	C38-C25-C24	-8.04	106.37	123.56
29	F	303	LUT	C12-C13-C14	-8.02	106.64	118.94
29	3	305	LUT	C40-C33-C34	-8.01	111.70	122.92
27	L	303	CHL	C3C-C4C-NC	8.01	119.55	110.57
29	3	304	LUT	C11-C12-C13	7.99	148.87	126.42
27	A	819	CHL	C4A-NA-C1A	7.98	110.30	106.71
29	8	303	LUT	C1-C6-C5	-7.98	111.38	122.61
29	3	304	LUT	C38-C25-C24	-7.97	106.51	123.56
29	4	302	LUT	C39-C29-C30	-7.97	111.76	122.92
27	5	314	CHL	C4A-NA-C1A	7.96	110.28	106.71
29	8	304	LUT	C35-C34-C33	-7.96	115.95	127.31
29	a	302	LUT	C38-C25-C24	-7.96	106.54	123.56
27	8	322	CHL	C4A-NA-C1A	7.95	110.28	106.71
27	A	826	CHL	C4A-NA-C1A	7.93	110.27	106.71
27	A	846	CHL	CMD-C2D-C1D	7.93	138.68	124.71
27	A	849	CHL	C4A-NA-C1A	7.92	110.27	106.71
27	4	315	CHL	C4A-NA-C1A	7.91	110.26	106.71
27	B	811	CHL	C4A-NA-C1A	7.91	110.26	106.71
27	B	849	CHL	C4A-NA-C1A	7.91	110.26	106.71
27	B	839	CHL	C4A-NA-C1A	7.90	110.26	106.71
29	5	302	LUT	C38-C25-C24	-7.90	106.67	123.56
27	A	828	CHL	C4A-NA-C1A	7.90	110.26	106.71
29	a	302	LUT	C35-C34-C33	-7.89	116.04	127.31
29	8	303	LUT	C38-C25-C24	-7.88	106.70	123.56
27	B	846	CHL	C4A-NA-C1A	7.87	110.25	106.71
27	5	315	CHL	C4A-NA-C1A	7.87	110.25	106.71
27	A	824	CHL	C4A-NA-C1A	7.87	110.24	106.71
27	4	319	CHL	C4A-NA-C1A	7.86	110.24	106.71
29	J	103	LUT	C35-C34-C33	-7.86	116.09	127.31
27	6	320	CHL	C4A-NA-C1A	7.86	110.24	106.71
27	7	316	CHL	C4A-NA-C1A	7.85	110.23	106.71
27	L	303	CHL	CMD-C2D-C1D	7.84	138.53	124.71
27	5	310	CHL	C4A-NA-C1A	7.83	110.23	106.71
29	6	302	LUT	C32-C33-C34	-7.83	106.92	118.94
27	6	319	CHL	CMD-C2D-C1D	7.83	138.52	124.71
27	B	821	CHL	C4A-NA-C1A	7.83	110.23	106.71
27	4	317	CHL	C4A-NA-C1A	7.82	110.22	106.71
29	7	304	LUT	C8-C9-C10	-7.82	106.94	118.94
29	b	301	LUT	C20-C13-C14	-7.81	111.98	122.92
27	8	320	CHL	C4A-NA-C1A	7.81	110.22	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	819	CHL	C4A-NA-C1A	7.80	110.21	106.71
27	B	816	CHL	C4A-NA-C1A	7.80	110.21	106.71
27	7	315	CHL	C4A-NA-C1A	7.79	110.21	106.71
27	6	308	CHL	CMD-C2D-C1D	7.78	138.43	124.71
27	3	313	CHL	C4A-NA-C1A	7.77	110.20	106.71
29	6	302	LUT	C1-C6-C5	-7.76	111.68	122.61
27	a	312	CHL	C4A-NA-C1A	7.76	110.19	106.71
29	6	303	LUT	C38-C25-C24	-7.75	106.99	123.56
27	B	817	CHL	C4A-NA-C1A	7.74	110.19	106.71
27	a	311	CHL	C4A-NA-C1A	7.74	110.19	106.71
27	6	307	CHL	C3C-C4C-NC	7.74	119.25	110.57
29	b	301	LUT	C38-C25-C24	-7.73	107.02	123.56
27	A	843	CHL	CHD-C4C-C3C	-7.72	113.49	124.84
29	3	304	LUT	C32-C33-C34	-7.72	107.10	118.94
29	5	303	LUT	C38-C25-C24	-7.71	107.06	123.56
27	5	316	CHL	CMD-C2D-C1D	7.71	138.30	124.71
27	K	204	CHL	C4A-NA-C1A	7.71	110.17	106.71
27	A	844	CHL	C4A-NA-C1A	7.70	110.17	106.71
27	A	820	CHL	C4A-NA-C1A	7.68	110.16	106.71
27	a	319	CHL	C4A-NA-C1A	7.68	110.16	106.71
27	4	318	CHL	C4A-NA-C1A	7.67	110.16	106.71
29	3	305	LUT	C1-C6-C5	-7.67	111.81	122.61
27	8	318	CHL	C4A-NA-C1A	7.67	110.15	106.71
27	3	321	CHL	C4A-NA-C1A	7.66	110.15	106.71
27	4	305	CHL	C4A-NA-C1A	7.65	110.15	106.71
27	A	841	CHL	O2D-CGD-O1D	-7.65	108.88	123.84
27	A	839	CHL	C4A-NA-C1A	7.64	110.14	106.71
27	7	314	CHL	C4A-NA-C1A	7.64	110.14	106.71
29	7	304	LUT	C38-C25-C24	-7.64	107.22	123.56
27	a	313	CHL	C4A-NA-C1A	7.62	110.13	106.71
29	4	302	LUT	C35-C34-C33	-7.62	116.44	127.31
29	6	302	LUT	C38-C25-C24	-7.62	107.27	123.56
29	3	304	LUT	C20-C13-C14	-7.61	112.26	122.92
27	B	825	CHL	C4A-NA-C1A	7.59	110.12	106.71
27	A	818	CHL	C4A-NA-C1A	7.59	110.12	106.71
27	5	311	CHL	C4A-NA-C1A	7.58	110.11	106.71
27	B	851	CHL	C4A-NA-C1A	7.57	110.11	106.71
27	5	313	CHL	C3C-C4C-NC	7.57	119.06	110.57
27	L	304	CHL	C4A-NA-C1A	7.54	110.10	106.71
29	7	304	LUT	C32-C33-C34	-7.54	107.38	118.94
27	B	837	CHL	C4A-NA-C1A	7.52	110.09	106.71
27	3	310	CHL	C4A-NA-C1A	7.51	110.08	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	8	303	LUT	C35-C34-C33	-7.49	116.62	127.31
27	B	842	CHL	C4A-NA-C1A	7.48	110.07	106.71
27	6	311	CHL	C4A-NA-C1A	7.46	110.06	106.71
27	7	323	CHL	C4A-NA-C1A	7.46	110.06	106.71
27	8	315	CHL	C4A-NA-C1A	7.45	110.06	106.71
27	a	320	CHL	C4A-NA-C1A	7.45	110.06	106.71
29	F	303	LUT	C32-C33-C34	-7.45	107.51	118.94
27	A	821	CHL	C4A-NA-C1A	7.44	110.05	106.71
27	4	320	CHL	C4A-NA-C1A	7.44	110.05	106.71
27	K	205	CHL	C4A-NA-C1A	7.43	110.05	106.71
27	b	315	CHL	C4A-NA-C1A	7.42	110.04	106.71
27	b	307	CHL	C4A-NA-C1A	7.42	110.04	106.71
27	A	846	CHL	C3C-C4C-NC	7.41	118.88	110.57
27	B	820	CHL	C4A-NA-C1A	7.40	110.03	106.71
27	B	812	CHL	C4A-NA-C1A	7.38	110.03	106.71
29	4	302	LUT	C38-C25-C24	-7.37	107.80	123.56
27	L	303	CHL	C3D-C4D-ND	7.34	122.11	110.24
27	A	823	CHL	C4A-NA-C1A	7.33	110.00	106.71
29	6	302	LUT	C35-C34-C33	-7.33	116.84	127.31
29	3	305	LUT	C11-C12-C13	7.33	146.99	126.42
27	B	841	CHL	C4A-NA-C1A	7.31	109.99	106.71
27	6	309	CHL	C4A-NA-C1A	7.31	109.99	106.71
27	8	319	CHL	C4A-NA-C1A	7.28	109.98	106.71
27	b	310	CHL	C4A-NA-C1A	7.26	109.97	106.71
29	4	301	LUT	C38-C25-C24	-7.26	108.04	123.56
29	8	303	LUT	C20-C13-C12	-7.24	106.66	118.08
27	3	311	CHL	C4A-NA-C1A	7.23	109.96	106.71
27	4	307	CHL	C4A-NA-C1A	7.23	109.96	106.71
27	6	306	CHL	C4A-NA-C1A	7.22	109.95	106.71
26	A	815	CL0	C3C-C4C-NC	7.22	118.67	110.57
29	7	304	LUT	C19-C9-C10	-7.21	112.82	122.92
27	A	843	CHL	CMD-C2D-C1D	7.20	137.41	124.71
29	8	304	LUT	C20-C13-C12	-7.19	106.74	118.08
29	a	304	LUT	C38-C25-C24	-7.18	108.19	123.56
27	A	847	CHL	C4A-NA-C1A	7.17	109.93	106.71
29	J	103	LUT	C38-C25-C24	-7.14	108.28	123.56
27	A	833	CHL	O2D-CGD-O1D	-7.14	109.88	123.84
26	A	815	CL0	CMD-C2D-C1D	7.14	137.29	124.71
29	5	302	LUT	C32-C33-C34	-7.13	108.00	118.94
27	7	321	CHL	O2D-CGD-CBD	7.13	123.94	111.27
27	A	848	CHL	C4A-NA-C1A	7.12	109.91	106.71
27	8	316	CHL	C4A-NA-C1A	7.12	109.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	8	304	LUT	C11-C12-C13	7.11	146.38	126.42
29	7	304	LUT	C39-C29-C28	-7.10	106.89	118.08
29	b	301	LUT	C20-C13-C12	-7.09	106.91	118.08
27	4	317	CHL	CMD-C2D-C1D	7.07	137.17	124.71
27	7	324	CHL	C4A-NA-C1A	7.06	109.88	106.71
29	8	303	LUT	C39-C29-C28	-7.04	106.99	118.08
27	7	320	CHL	C4A-NA-C1A	7.02	109.86	106.71
27	3	312	CHL	C4A-NA-C1A	7.01	109.86	106.71
27	6	319	CHL	C2C-C3C-C4C	-6.99	101.50	106.49
27	4	314	CHL	C4A-NA-C1A	6.99	109.85	106.71
27	4	308	CHL	C4A-NA-C1A	6.97	109.84	106.71
27	a	314	CHL	C4A-NA-C1A	6.96	109.84	106.71
27	7	320	CHL	O2D-CGD-CBD	6.95	123.62	111.27
27	7	322	CHL	O2D-CGD-CBD	6.94	123.60	111.27
27	B	815	CHL	C4A-NA-C1A	6.93	109.82	106.71
27	A	831	CHL	CHD-C4C-C3C	-6.92	114.67	124.84
29	3	304	LUT	C20-C13-C12	-6.91	107.19	118.08
27	B	844	CHL	C4A-NA-C1A	6.88	109.80	106.71
29	4	301	LUT	C32-C33-C34	-6.86	108.41	118.94
29	J	103	LUT	C32-C33-C34	-6.86	108.41	118.94
27	6	317	CHL	O2D-CGD-CBD	6.84	123.42	111.27
27	5	310	CHL	O2D-CGD-CBD	6.83	123.41	111.27
27	5	313	CHL	C3B-C4B-NB	6.82	118.03	109.21
29	3	305	LUT	C8-C9-C10	-6.80	108.50	118.94
29	F	303	LUT	C35-C15-C14	-6.80	109.54	123.47
27	8	325	CHL	C4A-NA-C1A	6.77	109.75	106.71
27	5	313	CHL	C4D-CHA-C1A	-6.73	113.06	121.25
29	5	303	LUT	C12-C13-C14	-6.70	108.67	118.94
29	8	303	LUT	C8-C9-C10	-6.69	108.67	118.94
27	L	303	CHL	CHD-C1D-ND	-6.69	118.31	124.45
27	B	833	CHL	C4A-NA-C1A	6.69	109.71	106.71
29	3	304	LUT	C39-C29-C28	-6.66	107.58	118.08
29	J	103	LUT	C19-C9-C8	-6.66	107.58	118.08
27	6	307	CHL	C3D-C4D-ND	6.66	121.01	110.24
27	7	319	CHL	C4A-NA-C1A	6.66	109.70	106.71
27	b	306	CHL	C4A-NA-C1A	6.65	109.70	106.71
29	3	304	LUT	C8-C9-C10	-6.65	108.74	118.94
27	A	850	CHL	C4A-NA-C1A	6.62	109.68	106.71
27	B	836	CHL	C4A-NA-C1A	6.62	109.68	106.71
27	A	831	CHL	C3D-C4D-ND	6.61	120.94	110.24
27	B	828	CHL	C4A-NA-C1A	6.60	109.67	106.71
29	b	301	LUT	C8-C9-C10	-6.59	108.82	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	4	301	LUT	C8-C9-C10	-6.59	108.83	118.94
29	6	302	LUT	C8-C9-C10	-6.59	108.83	118.94
27	4	304	CHL	C4A-NA-C1A	6.58	109.67	106.71
27	6	307	CHL	C4D-CHA-C1A	-6.57	113.26	121.25
27	5	313	CHL	C3D-C4D-ND	6.56	120.84	110.24
29	J	103	LUT	C39-C29-C28	-6.55	107.75	118.08
27	8	312	CHL	C4A-NA-C1A	6.53	109.64	106.71
29	a	302	LUT	C39-C29-C28	-6.53	107.79	118.08
29	a	302	LUT	C8-C9-C10	-6.52	108.93	118.94
27	8	323	CHL	C4A-NA-C1A	6.52	109.64	106.71
29	F	303	LUT	C38-C25-C24	-6.50	109.65	123.56
29	5	302	LUT	C20-C13-C12	-6.50	107.83	118.08
27	A	846	CHL	C3B-C4B-NB	6.50	117.61	109.21
29	3	305	LUT	C35-C34-C33	-6.50	118.04	127.31
27	7	323	CHL	CMD-C2D-C1D	6.48	136.13	124.71
29	6	303	LUT	C32-C33-C34	-6.48	109.00	118.94
26	A	815	CL0	C2D-C1D-ND	6.47	114.87	110.10
29	a	304	LUT	C28-C29-C30	-6.47	109.02	118.94
29	a	304	LUT	C32-C33-C34	-6.47	109.02	118.94
27	A	817	CHL	C4A-NA-C1A	6.45	109.61	106.71
27	5	318	CHL	C4A-NA-C1A	6.44	109.60	106.71
29	a	304	LUT	C8-C9-C10	-6.44	109.06	118.94
27	A	846	CHL	C3D-C4D-ND	6.44	120.65	110.24
27	3	315	CHL	C4A-NA-C1A	6.42	109.59	106.71
27	6	316	CHL	O2D-CGD-CBD	6.40	122.65	111.27
27	5	316	CHL	O2D-CGD-CBD	6.39	122.63	111.27
29	5	302	LUT	C39-C29-C28	-6.38	108.03	118.08
27	8	314	CHL	C4A-NA-C1A	6.37	109.57	106.71
29	7	304	LUT	C20-C13-C12	-6.36	108.05	118.08
27	B	811	CHL	O2D-CGD-CBD	6.35	122.55	111.27
27	b	308	CHL	CMD-C2D-C1D	6.34	135.88	124.71
27	a	307	CHL	C4A-NA-C1A	6.33	109.55	106.71
27	B	831	CHL	C4A-NA-C1A	6.33	109.55	106.71
29	8	304	LUT	C28-C29-C30	-6.32	109.24	118.94
29	5	303	LUT	C39-C29-C28	-6.32	108.12	118.08
29	8	304	LUT	C40-C33-C32	-6.32	108.12	118.08
27	A	836	CHL	C4A-NA-C1A	6.31	109.55	106.71
27	4	307	CHL	O2D-CGD-CBD	6.31	122.49	111.27
29	a	302	LUT	C20-C13-C12	-6.31	108.14	118.08
27	A	858	CHL	O2D-CGD-CBD	6.30	122.46	111.27
27	a	313	CHL	O2D-CGD-CBD	6.30	122.45	111.27
29	6	303	LUT	C20-C13-C12	-6.29	108.17	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	3	305	LUT	C20-C13-C12	-6.28	108.18	118.08
27	L	303	CHL	CHD-C4C-C3C	-6.28	115.61	124.84
29	4	301	LUT	C20-C13-C12	-6.28	108.19	118.08
27	A	830	CHL	O2D-CGD-CBD	6.27	122.42	111.27
27	L	303	CHL	C4D-CHA-C1A	-6.25	113.64	121.25
27	A	831	CHL	C4A-NA-C1A	-6.24	103.90	106.71
27	A	846	CHL	CHD-C4C-C3C	-6.24	115.67	124.84
29	6	302	LUT	C20-C13-C12	-6.23	108.27	118.08
26	A	815	CL0	CHD-C4C-C3C	-6.22	115.69	124.84
27	4	319	CHL	C4D-CHA-C1A	-6.21	113.69	121.25
27	L	303	CHL	C1B-CHB-C4A	-6.20	117.85	130.12
27	4	313	CHL	C2D-C1D-ND	-6.19	105.54	110.10
27	5	313	CHL	CHD-C4C-C3C	-6.18	115.76	124.84
27	6	311	CHL	O2D-CGD-CBD	6.17	122.23	111.27
29	7	304	LUT	C17-C1-C6	6.16	120.29	110.30
29	5	302	LUT	C8-C9-C10	-6.15	109.50	118.94
27	A	834	CHL	C4A-NA-C1A	6.13	109.46	106.71
29	5	303	LUT	C40-C33-C32	-6.13	108.42	118.08
29	a	304	LUT	C12-C13-C14	-6.11	109.56	118.94
27	6	307	CHL	O2D-CGD-CBD	6.11	122.12	111.27
27	B	827	CHL	C4A-NA-C1A	6.11	109.45	106.71
27	8	323	CHL	CMD-C2D-C1D	6.11	135.47	124.71
29	6	303	LUT	C12-C13-C14	-6.10	109.58	118.94
29	4	302	LUT	C40-C33-C32	-6.09	108.48	118.08
29	8	303	LUT	C32-C33-C34	-6.09	109.60	118.94
29	8	303	LUT	C40-C33-C32	-6.08	108.49	118.08
27	8	324	CHL	C4A-NA-C1A	6.08	109.44	106.71
29	b	301	LUT	C32-C33-C34	-6.07	109.63	118.94
27	A	843	CHL	C4A-NA-C1A	-6.06	103.98	106.71
27	6	307	CHL	CHD-C4C-C3C	-6.04	115.96	124.84
29	4	302	LUT	C39-C29-C28	-6.04	108.56	118.08
27	7	321	CHL	O2D-CGD-O1D	-6.02	112.06	123.84
29	4	301	LUT	C28-C29-C30	-6.02	109.70	118.94
29	a	304	LUT	C35-C15-C14	-6.02	111.14	123.47
27	3	308	CHL	C4A-NA-C1A	6.02	109.41	106.71
27	7	322	CHL	C4A-NA-C1A	6.01	109.41	106.71
27	6	315	CHL	O2D-CGD-CBD	6.01	121.94	111.27
27	6	308	CHL	CHD-C1D-ND	-6.01	118.94	124.45
26	A	815	CL0	O2D-CGD-CBD	6.00	121.93	111.27
27	6	307	CHL	C3B-C4B-NB	5.99	116.96	109.21
29	b	301	LUT	C40-C33-C32	-5.99	108.64	118.08
27	b	311	CHL	C4A-NA-C1A	5.99	109.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	310	CHL	O2D-CGD-CBD	5.99	121.91	111.27
27	3	314	CHL	O2D-CGD-CBD	5.97	121.88	111.27
29	3	305	LUT	C39-C29-C28	-5.96	108.68	118.08
27	b	308	CHL	C4A-NA-C1A	5.96	109.39	106.71
29	a	304	LUT	C7-C6-C5	-5.95	107.05	121.46
27	a	318	CHL	C4A-NA-C1A	5.95	109.38	106.71
27	a	311	CHL	O2D-CGD-CBD	5.94	121.83	111.27
29	F	303	LUT	C39-C29-C28	-5.94	108.72	118.08
29	4	301	LUT	C39-C29-C28	-5.92	108.74	118.08
27	4	319	CHL	O2D-CGD-CBD	5.91	121.78	111.27
27	7	311	CHL	C4A-NA-C1A	5.91	109.36	106.71
27	B	812	CHL	O2D-CGD-CBD	5.91	121.77	111.27
29	8	303	LUT	C28-C29-C30	-5.90	109.89	118.94
27	L	303	CHL	O2D-CGD-CBD	5.88	121.72	111.27
27	A	837	CHL	O2D-CGD-CBD	5.88	121.72	111.27
29	6	303	LUT	C39-C29-C28	-5.88	108.81	118.08
27	5	322	CHL	C4A-NA-C1A	5.87	109.35	106.71
29	8	304	LUT	C8-C9-C10	-5.87	109.94	118.94
29	5	303	LUT	C35-C15-C14	-5.86	111.47	123.47
29	5	303	LUT	C28-C29-C30	-5.85	109.96	118.94
29	8	304	LUT	C19-C9-C8	-5.85	108.86	118.08
29	J	103	LUT	C40-C33-C32	-5.84	108.87	118.08
27	a	309	CHL	O2D-CGD-CBD	5.83	121.63	111.27
29	F	303	LUT	C28-C29-C30	-5.83	109.99	118.94
27	5	316	CHL	C3C-C4C-NC	5.83	117.11	110.57
29	a	302	LUT	C28-C29-C30	-5.83	110.00	118.94
26	A	815	CL0	C1C-C2C-C3C	-5.83	100.83	106.96
27	A	841	CHL	O1D-CGD-CBD	-5.82	112.57	124.48
27	B	836	CHL	O2D-CGD-CBD	5.80	121.57	111.27
27	B	835	CHL	O2D-CGD-CBD	5.78	121.54	111.27
27	5	317	CHL	O2D-CGD-O1D	-5.78	112.53	123.84
29	6	303	LUT	C8-C9-C10	-5.78	110.07	118.94
27	3	308	CHL	O2D-CGD-CBD	5.78	121.54	111.27
27	b	308	CHL	CAC-C3C-C2C	5.77	137.41	127.53
27	5	322	CHL	O2D-CGD-CBD	5.77	121.53	111.27
27	A	817	CHL	C4D-CHA-C1A	-5.77	114.22	121.25
27	4	317	CHL	C2D-C1D-ND	-5.76	105.86	110.10
27	4	319	CHL	CHD-C1D-ND	-5.76	119.16	124.45
27	A	844	CHL	O2D-CGD-CBD	5.76	121.50	111.27
27	5	316	CHL	CHD-C1D-ND	-5.76	119.16	124.45
29	4	302	LUT	C20-C13-C12	-5.75	109.02	118.08
27	A	846	CHL	O2D-CGD-CBD	5.75	121.48	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	856	CHL	O2D-CGD-CBD	5.75	121.48	111.27
27	a	316	CHL	C4A-NA-C1A	5.74	109.29	106.71
27	4	311	CHL	O2D-CGD-CBD	5.73	121.44	111.27
27	B	831	CHL	O2D-CGD-CBD	5.73	121.44	111.27
27	B	821	CHL	O2D-CGD-CBD	5.71	121.41	111.27
29	5	302	LUT	C28-C29-C30	-5.69	110.21	118.94
27	4	306	CHL	O2D-CGD-CBD	5.69	121.38	111.27
29	5	302	LUT	C40-C33-C32	-5.68	109.13	118.08
26	A	815	CL0	C3D-C4D-ND	5.66	119.39	110.24
29	a	304	LUT	C1-C6-C5	-5.65	114.65	122.61
27	A	843	CHL	C2D-C1D-ND	5.65	114.27	110.10
27	A	843	CHL	C4D-CHA-C1A	-5.65	114.37	121.25
27	5	307	CHL	O2D-CGD-CBD	5.65	121.30	111.27
26	A	815	CL0	C3B-C4B-NB	5.64	116.51	109.21
29	b	301	LUT	C39-C29-C28	-5.64	109.19	118.08
27	b	305	CHL	O2D-CGD-CBD	5.63	121.27	111.27
27	7	319	CHL	C1-C2-C3	-5.62	116.32	126.04
29	8	304	LUT	C1-C6-C5	-5.62	114.70	122.61
27	6	317	CHL	C4A-NA-C1A	5.61	109.23	106.71
27	8	321	CHL	C4A-NA-C1A	5.61	109.23	106.71
27	8	326	CHL	O2D-CGD-CBD	5.60	121.23	111.27
29	a	304	LUT	C20-C13-C12	-5.60	109.26	118.08
29	J	103	LUT	C20-C13-C12	-5.59	109.27	118.08
29	8	304	LUT	C7-C8-C9	-5.58	117.80	126.23
27	4	312	CHL	C4A-NA-C1A	5.58	109.22	106.71
27	b	317	CHL	C4A-NA-C1A	5.58	109.22	106.71
27	7	324	CHL	O2D-CGD-CBD	5.58	121.19	111.27
29	a	304	LUT	C19-C9-C8	-5.57	109.30	118.08
29	6	302	LUT	C39-C29-C28	-5.57	109.30	118.08
29	7	304	LUT	C40-C33-C32	-5.57	109.31	118.08
27	7	317	CHL	O2D-CGD-CBD	5.56	121.15	111.27
27	A	847	CHL	O2D-CGD-CBD	5.56	121.15	111.27
27	a	320	CHL	O2D-CGD-CBD	5.56	121.15	111.27
27	4	310	CHL	O2D-CGD-CBD	5.55	121.14	111.27
27	A	846	CHL	C1C-C2C-C3C	-5.55	101.12	106.96
27	A	853	CHL	O2D-CGD-CBD	5.55	121.13	111.27
27	5	315	CHL	O2D-CGD-CBD	5.55	121.12	111.27
27	a	318	CHL	O2D-CGD-CBD	5.54	121.11	111.27
27	A	846	CHL	C3D-C2D-C1D	-5.53	98.29	105.83
27	A	831	CHL	C3D-C2D-C1D	-5.53	98.29	105.83
29	4	302	LUT	C32-C33-C34	-5.52	110.47	118.94
27	6	308	CHL	O2D-CGD-CBD	5.52	121.08	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	313	CHL	O2D-CGD-CBD	5.52	121.08	111.27
27	5	313	CHL	C1C-C2C-C3C	-5.51	101.16	106.96
29	6	303	LUT	C28-C29-C30	-5.51	110.49	118.94
27	B	818	CHL	C2C-C1C-NC	5.50	115.13	109.97
27	b	316	CHL	C4A-NA-C1A	5.50	109.18	106.71
27	3	316	CHL	O2D-CGD-CBD	5.50	121.04	111.27
27	B	814	CHL	O2D-CGD-CBD	5.49	121.03	111.27
29	8	304	LUT	C39-C29-C28	-5.49	109.42	118.08
27	6	319	CHL	CHD-C1D-ND	-5.48	119.42	124.45
29	8	304	LUT	C32-C33-C34	-5.48	110.53	118.94
27	a	307	CHL	O2D-CGD-CBD	5.48	121.00	111.27
27	b	310	CHL	O2D-CGD-CBD	5.48	121.00	111.27
27	b	306	CHL	CHD-C1D-ND	-5.47	119.43	124.45
27	B	848	CHL	C2C-C1C-NC	5.47	115.09	109.97
29	F	303	LUT	C40-C33-C32	-5.47	109.47	118.08
27	B	839	CHL	O2D-CGD-CBD	5.46	120.97	111.27
27	A	843	CHL	C3B-C4B-NB	5.45	116.26	109.21
29	F	303	LUT	C8-C9-C10	-5.45	110.58	118.94
27	A	817	CHL	O2D-CGD-CBD	5.45	120.94	111.27
27	a	314	CHL	O2D-CGD-CBD	5.44	120.94	111.27
29	b	301	LUT	C28-C29-C30	-5.43	110.61	118.94
27	b	311	CHL	O2D-CGD-CBD	5.42	120.90	111.27
29	F	303	LUT	C1-C6-C5	-5.42	114.98	122.61
27	6	306	CHL	O2D-CGD-CBD	5.42	120.89	111.27
29	5	303	LUT	C20-C13-C12	-5.41	109.55	118.08
27	A	849	CHL	CHD-C1D-ND	-5.41	119.48	124.45
27	8	323	CHL	O2D-CGD-CBD	5.41	120.88	111.27
27	8	322	CHL	CHD-C1D-ND	-5.40	119.49	124.45
27	B	848	CHL	O2D-CGD-CBD	5.40	120.87	111.27
27	A	833	CHL	C4A-NA-C1A	5.40	109.13	106.71
27	7	312	CHL	O2D-CGD-CBD	5.40	120.86	111.27
27	4	304	CHL	O2D-CGD-CBD	5.40	120.86	111.27
27	B	843	CHL	O2D-CGD-CBD	5.39	120.85	111.27
29	a	302	LUT	C40-C33-C32	-5.39	109.59	118.08
27	4	316	CHL	C4A-NA-C1A	5.39	109.13	106.71
27	A	825	CHL	O2D-CGD-CBD	5.39	120.84	111.27
27	A	821	CHL	O2D-CGD-CBD	5.38	120.84	111.27
29	4	302	LUT	C28-C29-C30	-5.38	110.68	118.94
27	5	313	CHL	CHD-C1D-ND	-5.38	119.51	124.45
27	A	831	CHL	C4D-CHA-C1A	-5.38	114.71	121.25
29	5	303	LUT	C32-C33-C34	-5.37	110.69	118.94
27	A	839	CHL	O2D-CGD-CBD	5.37	120.81	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	307	CHL	CHD-C1D-ND	-5.37	119.52	124.45
27	B	818	CHL	O2D-CGD-CBD	5.37	120.80	111.27
29	3	305	LUT	C28-C29-C30	-5.36	110.71	118.94
27	8	312	CHL	O2D-CGD-CBD	5.36	120.79	111.27
27	5	325	CHL	C4A-NA-C1A	5.36	109.11	106.71
27	B	845	CHL	O2D-CGD-CBD	5.35	120.78	111.27
27	A	854	CHL	O2D-CGD-CBD	5.35	120.78	111.27
27	A	831	CHL	C3B-C4B-NB	5.35	116.13	109.21
29	7	304	LUT	C28-C29-C30	-5.33	110.76	118.94
27	5	318	CHL	CHD-C1D-ND	-5.33	119.55	124.45
27	B	811	CHL	C4D-CHA-C1A	-5.33	114.76	121.25
27	A	850	CHL	O2D-CGD-CBD	5.33	120.74	111.27
27	B	838	CHL	O2D-CGD-CBD	5.33	120.74	111.27
27	B	825	CHL	O2D-CGD-CBD	5.33	120.73	111.27
27	b	309	CHL	O2D-CGD-CBD	5.32	120.72	111.27
27	6	318	CHL	C4A-NA-C1A	5.32	109.10	106.71
27	b	313	CHL	O2D-CGD-CBD	5.30	120.68	111.27
27	A	852	CHL	O2D-CGD-CBD	5.30	120.68	111.27
27	a	319	CHL	O2D-CGD-CBD	5.29	120.67	111.27
27	a	317	CHL	O2D-CGD-CBD	5.29	120.67	111.27
27	5	313	CHL	C3D-C2D-C1D	-5.29	98.62	105.83
27	3	321	CHL	O2D-CGD-CBD	5.29	120.66	111.27
27	B	834	CHL	C2D-C1D-ND	5.28	114.00	110.10
27	6	314	CHL	O2D-CGD-CBD	5.28	120.64	111.27
27	8	322	CHL	O2D-CGD-CBD	5.27	120.64	111.27
29	4	301	LUT	C19-C9-C8	-5.27	109.77	118.08
27	J	106	CHL	O2D-CGD-CBD	5.27	120.63	111.27
27	6	318	CHL	O2D-CGD-CBD	5.27	120.62	111.27
27	A	838	CHL	O2D-CGD-CBD	5.26	120.61	111.27
27	3	311	CHL	CHD-C1D-ND	-5.26	119.62	124.45
27	4	313	CHL	CMD-C2D-C1D	5.25	133.97	124.71
27	A	849	CHL	O2D-CGD-CBD	5.25	120.60	111.27
27	B	834	CHL	O2D-CGD-O1D	-5.25	113.57	123.84
27	B	850	CHL	O2D-CGD-CBD	5.25	120.59	111.27
27	3	319	CHL	O2D-CGD-CBD	5.25	120.59	111.27
27	3	312	CHL	O2D-CGD-CBD	5.25	120.59	111.27
27	5	313	CHL	O2D-CGD-CBD	5.25	120.59	111.27
27	4	314	CHL	CHD-C1D-ND	-5.24	119.63	124.45
27	A	846	CHL	C4D-CHA-C1A	-5.23	114.89	121.25
27	4	305	CHL	O2D-CGD-CBD	5.23	120.56	111.27
27	7	316	CHL	C1C-C2C-C3C	-5.22	102.28	107.07
29	J	103	LUT	C35-C15-C14	-5.22	112.78	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	849	CHL	O2D-CGD-CBD	5.22	120.54	111.27
27	B	817	CHL	C2C-C1C-NC	5.22	114.86	109.97
27	8	311	CHL	O2D-CGD-CBD	5.21	120.53	111.27
27	5	323	CHL	O2D-CGD-CBD	5.21	120.52	111.27
27	A	817	CHL	C2D-C1D-ND	5.19	113.93	110.10
27	B	828	CHL	O2D-CGD-CBD	5.19	120.49	111.27
27	L	303	CHL	C3D-C2D-C1D	-5.19	98.75	105.83
27	B	815	CHL	O2D-CGD-CBD	5.18	120.48	111.27
29	6	303	LUT	C40-C33-C32	-5.18	109.91	118.08
27	A	857	CHL	O2D-CGD-CBD	5.18	120.48	111.27
27	4	312	CHL	O2D-CGD-CBD	5.18	120.48	111.27
27	L	303	CHL	C3B-C4B-NB	5.17	115.90	109.21
27	6	308	CHL	C3C-C4C-NC	5.17	116.37	110.57
27	6	307	CHL	C3D-C2D-C1D	-5.17	98.77	105.83
27	5	309	CHL	O2D-CGD-CBD	5.17	120.45	111.27
27	5	321	CHL	C4D-CHA-C1A	-5.17	114.96	121.25
27	K	207	CHL	C4A-NA-C1A	5.16	109.03	106.71
27	B	827	CHL	CHD-C1D-ND	-5.16	119.71	124.45
27	5	311	CHL	O2D-CGD-CBD	5.16	120.44	111.27
27	b	312	CHL	O2D-CGD-CBD	5.16	120.43	111.27
27	A	826	CHL	O2D-CGD-CBD	5.15	120.42	111.27
27	B	842	CHL	CHD-C1D-ND	-5.15	119.72	124.45
27	B	817	CHL	O2D-CGD-CBD	5.15	120.41	111.27
27	3	316	CHL	C4A-NA-C1A	5.14	109.02	106.71
27	7	313	CHL	O2D-CGD-CBD	5.14	120.40	111.27
29	6	302	LUT	C19-C9-C8	-5.14	109.98	118.08
27	5	319	CHL	C4A-NA-C1A	5.13	109.01	106.71
29	6	302	LUT	C28-C29-C30	-5.13	111.07	118.94
27	a	316	CHL	O2D-CGD-CBD	5.13	120.38	111.27
27	b	310	CHL	CHD-C1D-ND	-5.12	119.75	124.45
27	b	304	CHL	O2D-CGD-CBD	5.12	120.36	111.27
27	7	321	CHL	O1D-CGD-CBD	-5.12	114.01	124.48
27	3	311	CHL	O2D-CGD-CBD	5.11	120.35	111.27
27	5	323	CHL	C2C-C1C-NC	5.11	114.76	109.97
27	A	818	CHL	O2D-CGD-CBD	5.11	120.35	111.27
27	K	205	CHL	CHD-C1D-ND	-5.11	119.76	124.45
27	7	317	CHL	C2C-C1C-NC	5.10	114.75	109.97
27	B	825	CHL	C2D-C1D-ND	5.10	113.86	110.10
27	A	846	CHL	CHD-C1D-ND	-5.10	119.77	124.45
27	A	833	CHL	O1D-CGD-CBD	-5.10	114.06	124.48
27	A	851	CHL	O2D-CGD-CBD	5.10	120.32	111.27
27	B	812	CHL	C2D-C1D-ND	5.09	113.86	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	314	CHL	O2D-CGD-CBD	5.08	120.30	111.27
27	6	307	CHL	C1C-C2C-C3C	-5.08	101.62	106.96
27	A	859	CHL	CHD-C1D-ND	-5.08	119.79	124.45
27	A	833	CHL	O2D-CGD-CBD	5.07	120.28	111.27
27	A	816	CHL	O2D-CGD-CBD	5.07	120.28	111.27
27	7	316	CHL	O2D-CGD-CBD	5.07	120.28	111.27
27	B	830	CHL	O2D-CGD-CBD	5.07	120.27	111.27
29	4	301	LUT	C40-C33-C32	-5.06	110.10	118.08
27	4	318	CHL	O2D-CGD-CBD	5.06	120.27	111.27
27	a	314	CHL	CHD-C1D-ND	-5.05	119.81	124.45
27	F	308	CHL	O2D-CGD-CBD	5.05	120.24	111.27
27	8	326	CHL	C2D-C1D-ND	5.05	113.82	110.10
29	5	303	LUT	C19-C9-C8	-5.04	110.13	118.08
29	4	302	LUT	C8-C9-C10	-5.04	111.21	118.94
27	4	318	CHL	CHD-C1D-ND	-5.04	119.82	124.45
27	3	313	CHL	C2C-C1C-NC	5.04	114.69	109.97
27	3	320	CHL	CHD-C1D-ND	-5.02	119.84	124.45
27	a	315	CHL	O2D-CGD-CBD	5.02	120.18	111.27
27	8	324	CHL	O2D-CGD-CBD	5.02	120.18	111.27
27	A	852	CHL	C2C-C1C-NC	5.02	114.67	109.97
27	A	831	CHL	O2D-CGD-CBD	5.02	120.18	111.27
27	A	820	CHL	O2D-CGD-O1D	-5.02	114.03	123.84
27	4	308	CHL	O2D-CGD-CBD	5.01	120.18	111.27
26	A	815	CL0	C3D-C2D-C1D	-5.01	98.99	105.83
27	3	311	CHL	C2C-C1C-NC	5.01	114.67	109.97
27	A	816	CHL	C4D-CHA-C1A	-5.01	115.15	121.25
27	b	306	CHL	O2D-CGD-CBD	5.01	120.17	111.27
27	7	318	CHL	C2C-C1C-NC	5.01	114.66	109.97
27	5	319	CHL	O2D-CGD-CBD	5.00	120.15	111.27
27	6	310	CHL	O2D-CGD-CBD	5.00	120.15	111.27
27	a	315	CHL	C4A-NA-C1A	5.00	108.95	106.71
27	B	851	CHL	O2D-CGD-CBD	5.00	120.14	111.27
29	a	304	LUT	C40-C33-C32	-4.99	110.21	118.08
27	B	812	CHL	CHD-C1D-ND	-4.99	119.87	124.45
27	A	846	CHL	C1-C2-C3	-4.99	118.68	126.75
27	A	845	CHL	C2C-C1C-NC	4.99	114.64	109.97
27	B	842	CHL	C2C-C1C-NC	4.98	114.64	109.97
27	8	316	CHL	O2D-CGD-CBD	4.98	120.11	111.27
27	A	843	CHL	C1-C2-C3	-4.97	117.44	126.04
27	L	304	CHL	CHD-C1D-ND	-4.97	119.88	124.45
27	A	819	CHL	O2D-CGD-CBD	4.97	120.10	111.27
27	8	326	CHL	C2C-C1C-NC	4.97	114.63	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	812	CHL	C4D-CHA-C1A	-4.97	115.20	121.25
27	A	852	CHL	O2D-CGD-O1D	-4.97	114.13	123.84
27	B	818	CHL	C2D-C1D-ND	4.96	113.76	110.10
27	B	848	CHL	C1C-C2C-C3C	-4.96	101.74	106.96
27	3	318	CHL	O2D-CGD-CBD	4.96	120.08	111.27
27	B	817	CHL	C4D-CHA-C1A	-4.96	115.21	121.25
29	5	303	LUT	C8-C9-C10	-4.96	111.33	118.94
29	b	301	LUT	C12-C13-C14	-4.96	111.33	118.94
29	3	304	LUT	C28-C29-C30	-4.96	111.34	118.94
27	3	312	CHL	C2C-C1C-NC	4.95	114.61	109.97
27	a	319	CHL	C2C-C1C-NC	4.95	114.61	109.97
27	7	318	CHL	O2D-CGD-CBD	4.95	120.06	111.27
27	B	829	CHL	O2D-CGD-CBD	4.95	120.06	111.27
27	K	206	CHL	C2C-C1C-NC	4.95	114.61	109.97
27	5	314	CHL	O2D-CGD-CBD	4.94	120.05	111.27
27	3	320	CHL	CHD-C4C-C3C	-4.94	117.59	124.84
26	A	815	CL0	C4D-CHA-C1A	-4.93	115.25	121.25
27	4	308	CHL	C2C-C1C-NC	4.93	114.59	109.97
27	A	831	CHL	C1C-C2C-C3C	-4.92	101.78	106.96
27	A	843	CHL	C3D-C2D-C1D	-4.92	99.11	105.83
27	A	852	CHL	C4-C3-C5	4.92	121.61	115.98
27	8	323	CHL	C1-C2-C3	-4.92	118.80	126.75
27	A	846	CHL	C4A-NA-C1A	-4.92	104.50	106.71
29	4	302	LUT	C4-C5-C6	-4.91	109.90	120.85
27	A	837	CHL	C2D-C1D-ND	4.91	113.72	110.10
27	5	322	CHL	C1C-C2C-C3C	-4.91	103.22	107.11
29	8	303	LUT	C19-C9-C8	-4.91	110.35	118.08
27	B	841	CHL	C2D-C1D-ND	4.91	113.72	110.10
27	B	816	CHL	C2D-C1D-ND	4.90	113.72	110.10
27	b	308	CHL	C2C-C1C-NC	4.90	114.57	109.97
29	a	302	LUT	C19-C9-C8	-4.90	110.35	118.08
27	a	319	CHL	C1C-C2C-C3C	-4.89	101.81	106.96
27	7	312	CHL	C1C-C2C-C3C	-4.89	102.58	107.07
27	B	844	CHL	CHD-C1D-ND	-4.89	119.96	124.45
27	6	320	CHL	O2D-CGD-CBD	4.89	119.96	111.27
27	5	316	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
27	A	829	CHL	O2D-CGD-CBD	4.89	119.95	111.27
27	K	204	CHL	C2D-C1D-ND	4.88	113.70	110.10
29	F	303	LUT	C19-C9-C8	-4.88	110.39	118.08
27	8	322	CHL	C2D-C1D-ND	4.88	113.70	110.10
27	5	311	CHL	C2C-C1C-NC	4.88	114.54	109.97
27	3	315	CHL	CHD-C1D-ND	-4.87	119.97	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	308	CHL	C2D-C1D-ND	4.87	113.69	110.10
27	L	304	CHL	O2D-CGD-CBD	4.87	119.92	111.27
29	a	304	LUT	C7-C8-C9	-4.87	118.88	126.23
27	3	320	CHL	C2D-C1D-ND	4.87	113.69	110.10
27	8	313	CHL	O2D-CGD-CBD	4.86	119.91	111.27
27	8	312	CHL	C2D-C1D-ND	4.86	113.69	110.10
29	5	303	LUT	C7-C6-C5	-4.86	109.68	121.46
27	B	827	CHL	C1C-C2C-C3C	-4.86	101.84	106.96
27	B	840	CHL	CHD-C1D-ND	-4.86	119.98	124.45
27	a	319	CHL	CHD-C1D-ND	-4.86	119.99	124.45
27	3	315	CHL	O2D-CGD-O1D	-4.86	114.34	123.84
27	B	842	CHL	O2D-CGD-CBD	4.86	119.90	111.27
29	b	301	LUT	C7-C6-C5	-4.86	109.70	121.46
27	F	309	CHL	O2D-CGD-CBD	4.86	119.90	111.27
27	4	309	CHL	O2D-CGD-CBD	4.85	119.89	111.27
27	7	311	CHL	CHD-C1D-ND	-4.85	120.00	124.45
27	B	818	CHL	C1C-C2C-C3C	-4.85	101.86	106.96
27	B	842	CHL	C1C-C2C-C3C	-4.85	101.86	106.96
27	5	311	CHL	C1C-C2C-C3C	-4.84	101.87	106.96
27	B	819	CHL	C2C-C1C-NC	4.84	114.51	109.97
27	A	832	CHL	C2D-C1D-ND	4.84	113.67	110.10
27	A	841	CHL	C4A-NA-C1A	4.84	108.88	106.71
27	4	320	CHL	O2D-CGD-CBD	4.83	119.86	111.27
29	F	303	LUT	C7-C8-C9	-4.83	118.93	126.23
27	3	313	CHL	O2D-CGD-CBD	4.83	119.86	111.27
27	8	322	CHL	C2C-C1C-NC	4.83	114.50	109.97
27	B	841	CHL	CHD-C1D-ND	-4.83	120.01	124.45
27	B	834	CHL	CHD-C4C-C3C	-4.83	117.74	124.84
27	4	316	CHL	O2D-CGD-CBD	4.83	119.85	111.27
27	A	850	CHL	C2C-C1C-NC	4.83	114.50	109.97
27	K	204	CHL	C2C-C1C-NC	4.83	114.49	109.97
27	5	321	CHL	O2D-CGD-CBD	4.82	119.83	111.27
29	4	302	LUT	C19-C9-C8	-4.82	110.48	118.08
27	5	308	CHL	O2D-CGD-CBD	4.82	119.83	111.27
27	A	853	CHL	C2C-C1C-NC	4.82	114.48	109.97
27	B	827	CHL	C2C-C1C-NC	4.82	114.48	109.97
27	3	311	CHL	C1C-C2C-C3C	-4.82	101.89	106.96
27	8	320	CHL	O2D-CGD-CBD	4.81	119.82	111.27
27	3	316	CHL	C1C-C2C-C3C	-4.81	103.29	107.11
29	a	302	LUT	C12-C13-C14	-4.81	111.56	118.94
27	A	829	CHL	C2C-C1C-NC	4.81	114.48	109.97
27	A	831	CHL	C1D-CHD-C4C	-4.81	115.68	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	324	CHL	C1C-C2C-C3C	-4.81	103.30	107.11
27	8	315	CHL	C2D-C1D-ND	4.81	113.65	110.10
27	6	316	CHL	C4A-NA-C1A	4.81	108.87	106.71
27	B	843	CHL	C2C-C1C-NC	4.81	114.48	109.97
27	7	323	CHL	O2D-CGD-CBD	4.81	119.81	111.27
27	A	826	CHL	CHD-C1D-ND	-4.81	120.04	124.45
27	8	315	CHL	CHD-C4C-C3C	-4.81	117.78	124.84
29	3	305	LUT	C4-C5-C6	-4.80	110.14	120.85
27	J	106	CHL	C2C-C1C-NC	4.80	114.47	109.97
27	5	323	CHL	C1C-C2C-C3C	-4.80	101.91	106.96
27	7	321	CHL	C4A-NA-C1A	4.80	108.86	106.71
27	4	315	CHL	CHD-C1D-ND	-4.80	120.04	124.45
27	5	307	CHL	CHD-C1D-ND	-4.80	120.04	124.45
27	B	844	CHL	O2D-CGD-CBD	4.80	119.80	111.27
27	5	307	CHL	C4A-NA-C1A	4.80	108.86	106.71
27	A	857	CHL	C2D-C1D-ND	4.80	113.64	110.10
27	b	315	CHL	O2D-CGD-CBD	4.80	119.79	111.27
29	J	103	LUT	C12-C13-C14	-4.80	111.58	118.94
27	b	316	CHL	O2D-CGD-CBD	4.79	119.79	111.27
27	5	319	CHL	C1C-C2C-C3C	-4.79	103.31	107.11
27	4	308	CHL	C2D-C1D-ND	4.79	113.64	110.10
27	A	843	CHL	C3D-C4D-ND	4.79	117.99	110.24
27	7	323	CHL	C2C-C1C-NC	4.79	114.46	109.97
27	6	313	CHL	O2D-CGD-CBD	4.79	119.78	111.27
27	4	316	CHL	C1C-C2C-C3C	-4.79	103.31	107.11
27	b	305	CHL	C4D-CHA-C1A	-4.79	115.42	121.25
27	7	318	CHL	C1C-C2C-C3C	-4.78	101.93	106.96
27	4	304	CHL	C2D-C1D-ND	4.78	113.63	110.10
27	4	314	CHL	C2D-C1D-ND	4.78	113.63	110.10
27	5	320	CHL	O2D-CGD-CBD	4.78	119.77	111.27
27	5	312	CHL	O2D-CGD-O1D	-4.78	114.49	123.84
27	B	815	CHL	C2D-C1D-ND	4.78	113.63	110.10
27	B	850	CHL	C2D-C1D-ND	4.78	113.63	110.10
27	8	318	CHL	O2D-CGD-O1D	-4.78	114.50	123.84
27	a	309	CHL	C2C-C1C-NC	4.78	114.45	109.97
27	B	845	CHL	C2C-C1C-NC	4.77	114.44	109.97
27	B	817	CHL	C1C-C2C-C3C	-4.77	101.94	106.96
27	4	313	CHL	CMD-C2D-C3D	-4.77	116.64	127.61
27	b	308	CHL	C1C-C2C-C3C	-4.77	101.94	106.96
27	4	308	CHL	C1C-C2C-C3C	-4.77	101.94	106.96
27	F	308	CHL	C2C-C1C-NC	4.77	114.44	109.97
27	8	320	CHL	O2D-CGD-O1D	-4.77	114.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	823	CHL	O2D-CGD-CBD	4.77	119.74	111.27
27	B	845	CHL	C1C-C2C-C3C	-4.76	101.95	106.96
27	B	822	CHL	O2D-CGD-O1D	-4.76	114.52	123.84
27	A	834	CHL	C2C-C1C-NC	4.76	114.43	109.97
27	A	820	CHL	CHD-C1D-ND	-4.76	120.08	124.45
27	A	835	CHL	C2C-C1C-NC	4.76	114.43	109.97
27	b	315	CHL	C2D-C1D-ND	4.76	113.61	110.10
29	F	303	LUT	C20-C13-C12	-4.76	110.58	118.08
27	7	317	CHL	C1C-C2C-C3C	-4.76	101.96	106.96
27	B	820	CHL	CHD-C1D-ND	-4.76	120.08	124.45
27	B	850	CHL	O2D-CGD-O1D	-4.75	114.54	123.84
27	A	818	CHL	CHD-C1D-ND	-4.75	120.09	124.45
27	A	825	CHL	C2C-C1C-NC	4.75	114.42	109.97
27	B	827	CHL	O2D-CGD-CBD	4.75	119.71	111.27
27	8	317	CHL	O2D-CGD-CBD	4.75	119.71	111.27
27	6	312	CHL	C2C-C1C-NC	4.75	114.42	109.97
27	6	319	CHL	O2D-CGD-CBD	4.75	119.71	111.27
27	A	824	CHL	C2D-C1D-ND	4.75	113.60	110.10
27	A	840	CHL	C2C-C1C-NC	4.74	114.42	109.97
27	B	816	CHL	C2C-C1C-NC	4.74	114.42	109.97
27	B	826	CHL	O2D-CGD-CBD	4.74	119.69	111.27
27	K	204	CHL	C1C-C2C-C3C	-4.74	101.97	106.96
27	3	320	CHL	O2D-CGD-O1D	-4.74	114.57	123.84
29	F	303	LUT	C18-C5-C4	-4.73	105.59	114.36
27	5	318	CHL	C2C-C1C-NC	4.73	114.41	109.97
27	B	821	CHL	C2C-C1C-NC	4.73	114.41	109.97
27	5	325	CHL	O2D-CGD-CBD	4.73	119.68	111.27
27	A	821	CHL	C2C-C1C-NC	4.73	114.40	109.97
27	B	828	CHL	C2C-C1C-NC	4.73	114.40	109.97
27	7	311	CHL	C2D-C1D-ND	4.72	113.59	110.10
27	5	313	CHL	C1B-CHB-C4A	-4.72	120.76	130.12
27	4	305	CHL	C2C-C1C-NC	4.72	114.40	109.97
27	4	314	CHL	C1C-C2C-C3C	-4.72	101.99	106.96
27	B	817	CHL	CHD-C4C-C3C	-4.72	117.91	124.84
27	4	307	CHL	C2D-C1D-ND	4.72	113.58	110.10
27	5	316	CHL	CHD-C4C-C3C	-4.72	117.91	124.84
27	B	830	CHL	C2C-C1C-NC	4.71	114.39	109.97
27	A	820	CHL	C2D-C1D-ND	4.71	113.58	110.10
27	5	315	CHL	C1C-C2C-C3C	-4.71	102.00	106.96
27	8	326	CHL	CHD-C4C-C3C	-4.71	117.92	124.84
27	B	846	CHL	C2C-C1C-NC	4.71	114.38	109.97
27	A	835	CHL	O2D-CGD-O1D	-4.71	114.64	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	318	CHL	C1C-C2C-C3C	-4.71	103.38	107.11
29	b	301	LUT	C19-C9-C8	-4.70	110.67	118.08
27	8	322	CHL	CHD-C4C-C3C	-4.70	117.93	124.84
27	a	311	CHL	C4D-CHA-C1A	-4.70	115.53	121.25
27	8	319	CHL	C2D-C1D-ND	4.70	113.56	110.10
27	A	845	CHL	O2D-CGD-CBD	4.69	119.61	111.27
27	5	317	CHL	C4A-NA-C1A	4.69	108.81	106.71
27	b	305	CHL	C2C-C1C-NC	4.69	114.36	109.97
27	B	845	CHL	CHD-C1D-ND	-4.69	120.14	124.45
27	K	206	CHL	O2D-CGD-CBD	4.69	119.59	111.27
27	7	323	CHL	C1C-C2C-C3C	-4.68	102.03	106.96
27	B	819	CHL	O2D-CGD-O1D	-4.68	114.68	123.84
27	3	318	CHL	C2C-C1C-NC	4.68	114.36	109.97
27	7	315	CHL	C2C-C1C-NC	4.68	114.36	109.97
27	3	312	CHL	C1C-C2C-C3C	-4.68	102.04	106.96
29	3	305	LUT	C19-C9-C8	-4.68	110.70	118.08
27	8	321	CHL	O2D-CGD-O1D	-4.68	114.69	123.84
27	B	829	CHL	C2C-C1C-NC	4.68	114.36	109.97
27	b	315	CHL	CHD-C4C-C3C	-4.68	117.97	124.84
27	a	307	CHL	C2D-C1D-ND	4.67	113.55	110.10
27	5	314	CHL	C2C-C1C-NC	4.67	114.35	109.97
27	B	811	CHL	C2D-C1D-ND	4.67	113.55	110.10
27	B	817	CHL	O2D-CGD-O1D	-4.67	114.70	123.84
27	7	314	CHL	O2D-CGD-CBD	4.67	119.57	111.27
27	5	307	CHL	C2D-C1D-ND	4.67	113.55	110.10
27	A	824	CHL	CHD-C1D-ND	-4.67	120.16	124.45
27	3	315	CHL	C2C-C1C-NC	4.67	114.34	109.97
27	b	309	CHL	C2C-C1C-NC	4.67	114.34	109.97
29	8	304	LUT	C18-C5-C4	-4.67	105.71	114.36
27	A	852	CHL	C2D-C1D-ND	4.67	113.54	110.10
27	3	320	CHL	C4A-NA-C1A	4.66	108.80	106.71
27	B	843	CHL	C1C-C2C-C3C	-4.66	102.05	106.96
27	B	824	CHL	C2C-C1C-NC	4.66	114.34	109.97
27	B	846	CHL	O2D-CGD-CBD	4.66	119.55	111.27
27	B	820	CHL	C2C-C1C-NC	4.66	114.34	109.97
27	7	318	CHL	C2D-C1D-ND	4.66	113.54	110.10
27	B	819	CHL	C1C-C2C-C3C	-4.65	102.06	106.96
27	B	841	CHL	O2D-CGD-CBD	4.65	119.53	111.27
27	a	317	CHL	C2C-C1C-NC	4.65	114.33	109.97
27	A	848	CHL	O2D-CGD-CBD	4.65	119.53	111.27
29	8	303	LUT	C4-C5-C6	-4.65	110.49	120.85
27	A	848	CHL	C2C-C1C-NC	4.65	114.33	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	829	CHL	C1C-C2C-C3C	-4.65	102.07	106.96
27	B	838	CHL	C2C-C1C-NC	4.65	114.33	109.97
27	6	305	CHL	C2C-C1C-NC	4.65	114.33	109.97
27	B	841	CHL	O2D-CGD-O1D	-4.64	114.76	123.84
27	A	822	CHL	CHD-C1D-ND	-4.64	120.19	124.45
27	b	310	CHL	C4D-CHA-C1A	-4.64	115.60	121.25
27	5	310	CHL	CHD-C4C-C3C	-4.64	118.02	124.84
27	B	828	CHL	CHD-C1D-ND	-4.64	120.19	124.45
27	5	317	CHL	C1C-C2C-C3C	-4.64	103.43	107.11
27	6	308	CHL	C3D-C2D-C1D	-4.64	99.50	105.83
27	B	837	CHL	C2C-C1C-NC	4.64	114.32	109.97
27	a	318	CHL	C1C-C2C-C3C	-4.64	103.43	107.11
27	8	326	CHL	C1C-C2C-C3C	-4.63	102.09	106.96
27	A	819	CHL	C2D-C1D-ND	4.63	113.52	110.10
27	4	310	CHL	C2C-C1C-NC	4.63	114.31	109.97
27	B	813	CHL	O2D-CGD-CBD	4.63	119.49	111.27
27	4	307	CHL	C2C-C1C-NC	4.63	114.31	109.97
27	A	841	CHL	O2D-CGD-CBD	4.63	119.49	111.27
27	6	317	CHL	C1C-C2C-C3C	-4.63	103.44	107.11
27	a	309	CHL	C4D-CHA-C1A	-4.62	115.62	121.25
27	8	320	CHL	C2C-C1C-NC	4.62	114.30	109.97
27	b	316	CHL	C1C-C2C-C3C	-4.62	103.44	107.11
27	A	821	CHL	C1C-C2C-C3C	-4.62	102.10	106.96
27	A	840	CHL	C1C-C2C-C3C	-4.62	102.10	106.96
27	K	204	CHL	O2D-CGD-CBD	4.62	119.48	111.27
27	8	315	CHL	O2D-CGD-CBD	4.62	119.48	111.27
27	3	313	CHL	C1C-C2C-C3C	-4.62	102.10	106.96
27	A	852	CHL	C1C-C2C-C3C	-4.62	102.10	106.96
27	A	819	CHL	CHD-C4C-C3C	-4.62	118.05	124.84
27	K	205	CHL	C2C-C1C-NC	4.62	114.30	109.97
27	B	845	CHL	C2D-C1D-ND	4.62	113.50	110.10
27	8	316	CHL	CHD-C1D-ND	-4.61	120.21	124.45
27	a	309	CHL	C1C-C2C-C3C	-4.61	102.11	106.96
27	B	832	CHL	C2C-C1C-NC	4.61	114.29	109.97
27	A	857	CHL	C2C-C1C-NC	4.61	114.29	109.97
27	8	311	CHL	C2C-C1C-NC	4.61	114.29	109.97
27	B	813	CHL	CHD-C1D-ND	-4.61	120.22	124.45
27	3	308	CHL	CMC-C2C-C1C	4.61	132.06	125.04
27	6	309	CHL	C2C-C1C-NC	4.61	114.29	109.97
27	b	307	CHL	O2D-CGD-CBD	4.61	119.46	111.27
27	8	316	CHL	C2C-C1C-NC	4.61	114.29	109.97
29	a	304	LUT	C39-C29-C28	-4.61	110.82	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	312	CHL	C2D-C1D-ND	4.60	113.50	110.10
27	A	851	CHL	C2C-C1C-NC	4.60	114.28	109.97
27	B	826	CHL	C1C-C2C-C3C	-4.60	102.12	106.96
27	A	818	CHL	C2C-C1C-NC	4.60	114.28	109.97
27	a	312	CHL	C2C-C1C-NC	4.60	114.28	109.97
27	K	205	CHL	O2D-CGD-CBD	4.60	119.44	111.27
27	B	816	CHL	O2D-CGD-CBD	4.60	119.44	111.27
27	b	305	CHL	C1C-C2C-C3C	-4.60	102.12	106.96
27	B	833	CHL	O2D-CGD-O1D	-4.60	114.85	123.84
27	8	320	CHL	C1C-C2C-C3C	-4.60	102.12	106.96
27	b	317	CHL	O2D-CGD-CBD	4.59	119.43	111.27
27	a	312	CHL	O2D-CGD-O1D	-4.59	114.86	123.84
27	A	832	CHL	O2D-CGD-O1D	-4.59	114.86	123.84
27	A	816	CHL	C2D-C1D-ND	4.59	113.49	110.10
27	8	321	CHL	O1D-CGD-CBD	-4.59	115.09	124.48
27	A	839	CHL	CHD-C1D-ND	-4.59	120.23	124.45
27	B	836	CHL	C2C-C1C-NC	4.59	114.27	109.97
27	B	827	CHL	C2D-C1D-ND	4.59	113.49	110.10
27	A	839	CHL	C2C-C1C-NC	4.59	114.27	109.97
27	A	849	CHL	C2C-C1C-NC	4.59	114.27	109.97
27	8	325	CHL	O2D-CGD-CBD	4.59	119.42	111.27
27	A	856	CHL	C2C-C1C-NC	4.59	114.27	109.97
27	5	318	CHL	C1C-C2C-C3C	-4.59	102.13	106.96
27	A	834	CHL	C1C-C2C-C3C	-4.59	102.13	106.96
27	5	311	CHL	C2D-C1D-ND	4.59	113.48	110.10
27	B	820	CHL	C1C-C2C-C3C	-4.59	102.14	106.96
27	B	832	CHL	O2D-CGD-CBD	4.59	119.42	111.27
27	A	838	CHL	C2C-C1C-NC	4.59	114.27	109.97
27	b	309	CHL	C4D-CHA-C1A	-4.59	115.67	121.25
27	A	837	CHL	C2C-C1C-NC	4.58	114.27	109.97
27	A	843	CHL	C1C-C2C-C3C	-4.58	102.14	106.96
27	B	837	CHL	O2D-CGD-CBD	4.58	119.41	111.27
27	8	322	CHL	C1C-C2C-C3C	-4.58	102.14	106.96
27	3	316	CHL	O2D-CGD-O1D	-4.58	114.88	123.84
27	b	313	CHL	CHD-C1D-ND	-4.58	120.25	124.45
27	5	310	CHL	C2D-C1D-ND	4.58	113.48	110.10
27	A	845	CHL	O2D-CGD-O1D	-4.58	114.89	123.84
27	B	823	CHL	C2C-C1C-NC	4.58	114.26	109.97
27	B	826	CHL	C2C-C1C-NC	4.58	114.26	109.97
27	5	308	CHL	C2C-C1C-NC	4.58	114.26	109.97
27	A	850	CHL	C1C-C2C-C3C	-4.57	102.15	106.96
27	A	825	CHL	C1C-C2C-C3C	-4.57	102.15	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	834	CHL	O2D-CGD-O1D	-4.57	114.90	123.84
27	3	317	CHL	C2D-C1D-ND	4.57	113.47	110.10
27	A	823	CHL	C4D-CHA-C1A	-4.57	115.69	121.25
27	5	313	CHL	C1D-CHD-C4C	-4.57	116.20	126.06
27	B	817	CHL	C2D-C1D-ND	4.57	113.47	110.10
27	B	816	CHL	O2D-CGD-O1D	-4.57	114.91	123.84
27	A	848	CHL	C1C-C2C-C3C	-4.57	102.16	106.96
27	A	836	CHL	CHD-C1D-ND	-4.56	120.26	124.45
27	5	312	CHL	C2C-C1C-NC	4.56	114.25	109.97
29	J	103	LUT	C8-C9-C10	-4.56	111.94	118.94
27	B	823	CHL	O2D-CGD-CBD	4.56	119.38	111.27
27	7	312	CHL	C2D-C1D-ND	4.56	113.47	110.10
27	B	811	CHL	CHD-C4C-C3C	-4.56	118.14	124.84
27	4	320	CHL	CHD-C1D-ND	-4.56	120.26	124.45
27	5	315	CHL	C2C-C1C-NC	4.56	114.24	109.97
27	7	316	CHL	C2C-C1C-NC	4.56	114.24	109.97
27	3	321	CHL	C2C-C1C-NC	4.56	114.24	109.97
27	7	315	CHL	C1C-C2C-C3C	-4.56	102.17	106.96
27	3	310	CHL	C2C-C1C-NC	4.56	114.24	109.97
27	8	313	CHL	C2D-C1D-ND	4.56	113.46	110.10
27	a	308	CHL	C2C-C1C-NC	4.55	114.24	109.97
27	5	309	CHL	C2C-C1C-NC	4.55	114.24	109.97
27	B	829	CHL	C1C-C2C-C3C	-4.55	102.17	106.96
27	b	309	CHL	C1C-C2C-C3C	-4.55	102.17	106.96
27	8	318	CHL	C2C-C1C-NC	4.55	114.24	109.97
27	K	206	CHL	C1C-C2C-C3C	-4.55	102.17	106.96
27	3	321	CHL	C1C-C2C-C3C	-4.55	102.17	106.96
27	a	310	CHL	C2D-C1D-ND	4.55	113.46	110.10
27	3	318	CHL	C1C-C2C-C3C	-4.55	102.17	106.96
27	L	303	CHL	C1C-C2C-C3C	-4.55	102.17	106.96
27	A	858	CHL	C2C-C1C-NC	4.55	114.23	109.97
27	A	859	CHL	C2D-C1D-ND	4.55	113.46	110.10
27	B	824	CHL	O2D-CGD-O1D	-4.55	114.94	123.84
27	B	821	CHL	C2D-C1D-ND	4.55	113.46	110.10
27	7	313	CHL	C2C-C1C-NC	4.55	114.23	109.97
27	A	836	CHL	O2D-CGD-CBD	4.54	119.34	111.27
27	J	106	CHL	C1C-C2C-C3C	-4.54	102.18	106.96
27	A	855	CHL	C2C-C1C-NC	4.54	114.23	109.97
27	7	317	CHL	C2D-C1D-ND	4.54	113.45	110.10
27	3	309	CHL	O2D-CGD-CBD	4.54	119.34	111.27
27	B	818	CHL	C4D-CHA-C1A	-4.54	115.72	121.25
27	7	322	CHL	C1C-C2C-C3C	-4.54	103.51	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	314	CHL	C4D-CHA-C1A	-4.54	115.72	121.25
29	6	302	LUT	C4-C5-C6	-4.54	110.73	120.85
27	b	308	CHL	O2D-CGD-CBD	4.54	119.33	111.27
27	5	317	CHL	O2D-CGD-CBD	4.54	119.33	111.27
27	7	312	CHL	C2C-C1C-NC	4.54	114.22	109.97
27	a	308	CHL	O2D-CGD-O1D	-4.54	114.97	123.84
27	4	307	CHL	C1C-C2C-C3C	-4.53	102.19	106.96
27	4	314	CHL	O2D-CGD-CBD	4.53	119.32	111.27
27	6	305	CHL	C1C-C2C-C3C	-4.53	102.19	106.96
27	7	324	CHL	C2C-C1C-NC	4.53	114.22	109.97
27	B	833	CHL	O2D-CGD-CBD	4.53	119.32	111.27
27	B	831	CHL	C2C-C1C-NC	4.53	114.22	109.97
27	a	312	CHL	C1C-C2C-C3C	-4.53	102.19	106.96
27	5	321	CHL	C2C-C1C-NC	4.53	114.21	109.97
27	b	309	CHL	CHD-C1D-ND	-4.53	120.29	124.45
27	B	831	CHL	CHD-C1D-ND	-4.53	120.30	124.45
27	B	842	CHL	C2D-C1D-ND	4.53	113.44	110.10
29	5	302	LUT	C12-C13-C14	-4.53	112.00	118.94
27	B	839	CHL	C2C-C1C-NC	4.52	114.21	109.97
27	B	821	CHL	C1C-C2C-C3C	-4.52	102.20	106.96
27	6	312	CHL	O2D-CGD-CBD	4.52	119.31	111.27
27	4	320	CHL	C2C-C1C-NC	4.52	114.21	109.97
27	8	319	CHL	O2D-CGD-O1D	-4.52	114.99	123.84
27	8	311	CHL	C1C-C2C-C3C	-4.52	102.20	106.96
27	6	313	CHL	C2C-C1C-NC	4.52	114.21	109.97
27	4	313	CHL	CMC-C2C-C1C	4.52	131.93	125.04
27	7	319	CHL	O2D-CGD-CBD	4.52	119.30	111.27
27	4	306	CHL	C2C-C1C-NC	4.52	114.21	109.97
26	A	815	CL0	CHD-C1D-ND	-4.52	120.30	124.45
27	A	854	CHL	C2C-C1C-NC	4.52	114.20	109.97
27	4	320	CHL	C1C-C2C-C3C	-4.52	102.21	106.96
27	6	309	CHL	C2D-C1D-ND	4.52	113.43	110.10
27	6	306	CHL	CHD-C1D-ND	-4.52	120.30	124.45
27	4	318	CHL	C2C-C1C-NC	4.52	114.20	109.97
27	8	313	CHL	C2C-C1C-NC	4.52	114.20	109.97
27	A	822	CHL	O2D-CGD-O1D	-4.52	115.01	123.84
27	a	308	CHL	O2D-CGD-CBD	4.52	119.29	111.27
27	B	813	CHL	C2D-C1D-ND	4.52	113.43	110.10
27	b	313	CHL	C2C-C1C-NC	4.52	114.20	109.97
29	3	305	LUT	C40-C33-C32	-4.51	110.96	118.08
27	8	319	CHL	O2D-CGD-CBD	4.51	119.29	111.27
27	3	319	CHL	C1C-C2C-C3C	-4.51	102.21	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	813	CHL	O2D-CGD-O1D	-4.51	115.02	123.84
27	5	315	CHL	CHD-C1D-ND	-4.51	120.31	124.45
27	B	826	CHL	O2D-CGD-O1D	-4.51	115.02	123.84
27	4	311	CHL	C2C-C1C-NC	4.51	114.20	109.97
27	A	840	CHL	O2D-CGD-CBD	4.51	119.28	111.27
27	B	819	CHL	C2D-C1D-ND	4.51	113.43	110.10
27	6	320	CHL	CHD-C1D-ND	-4.51	120.31	124.45
27	5	325	CHL	C1C-C2C-C3C	-4.51	103.54	107.11
27	6	312	CHL	C1C-C2C-C3C	-4.51	102.22	106.96
27	a	317	CHL	C1C-C2C-C3C	-4.51	102.22	106.96
27	A	847	CHL	C2C-C1C-NC	4.51	114.19	109.97
27	b	304	CHL	C4D-CHA-C1A	-4.51	115.77	121.25
27	a	313	CHL	C2C-C1C-NC	4.50	114.19	109.97
27	3	317	CHL	CHD-C1D-ND	-4.50	120.32	124.45
27	A	818	CHL	O2D-CGD-O1D	-4.50	115.04	123.84
27	6	306	CHL	C2C-C1C-NC	4.50	114.19	109.97
27	B	846	CHL	C1C-C2C-C3C	-4.50	102.23	106.96
27	A	824	CHL	C2C-C1C-NC	4.50	114.19	109.97
27	B	831	CHL	C2D-C1D-ND	4.50	113.42	110.10
27	A	851	CHL	C1C-C2C-C3C	-4.50	102.23	106.96
27	4	310	CHL	C1C-C2C-C3C	-4.50	102.23	106.96
27	a	315	CHL	C1C-C2C-C3C	-4.50	103.55	107.11
27	6	319	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
27	8	325	CHL	C2C-C1C-NC	4.49	114.18	109.97
27	4	308	CHL	CHD-C1D-ND	-4.49	120.33	124.45
27	B	820	CHL	O2D-CGD-CBD	4.49	119.24	111.27
27	A	854	CHL	C1C-C2C-C3C	-4.49	102.24	106.96
27	5	314	CHL	C1C-C2C-C3C	-4.49	102.24	106.96
27	F	308	CHL	C1C-C2C-C3C	-4.49	102.24	106.96
27	a	310	CHL	O2D-CGD-CBD	4.49	119.24	111.27
29	3	304	LUT	C12-C13-C14	-4.48	112.06	118.94
27	A	836	CHL	C2D-C1D-ND	4.48	113.41	110.10
27	8	317	CHL	C2C-C1C-NC	4.48	114.17	109.97
27	4	312	CHL	C1C-C2C-C3C	-4.48	103.56	107.11
27	B	823	CHL	C2D-C1D-ND	4.48	113.40	110.10
29	6	302	LUT	C7-C6-C5	-4.48	110.62	121.46
27	3	318	CHL	C2D-C1D-ND	4.48	113.40	110.10
27	A	835	CHL	C1C-C2C-C3C	-4.48	102.25	106.96
27	B	814	CHL	C2D-C1D-ND	4.48	113.40	110.10
27	b	304	CHL	C2C-C1C-NC	4.47	114.16	109.97
27	8	321	CHL	CHD-C4C-C3C	-4.47	118.26	124.84
29	b	303	LUT	C39-C29-C30	-4.47	116.66	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	304	CHL	CHD-C1D-ND	-4.47	120.34	124.45
27	6	305	CHL	CHD-C1D-ND	-4.47	120.34	124.45
27	B	837	CHL	C1C-C2C-C3C	-4.47	102.25	106.96
27	K	206	CHL	O2D-CGD-O1D	-4.47	115.09	123.84
27	F	308	CHL	C2D-C1D-ND	4.47	113.40	110.10
27	3	315	CHL	C2D-C1D-ND	4.47	113.40	110.10
27	b	311	CHL	C1C-C2C-C3C	-4.47	103.56	107.11
27	6	320	CHL	C2C-C1C-NC	4.47	114.16	109.97
27	A	828	CHL	O2D-CGD-CBD	4.47	119.21	111.27
27	3	319	CHL	C2C-C1C-NC	4.47	114.16	109.97
27	B	816	CHL	C1C-C2C-C3C	-4.47	102.26	106.96
27	B	828	CHL	C1C-C2C-C3C	-4.47	102.26	106.96
27	3	309	CHL	C2C-C1C-NC	4.47	114.16	109.97
27	7	314	CHL	O2D-CGD-O1D	-4.47	115.11	123.84
27	A	821	CHL	C2D-C1D-ND	4.47	113.39	110.10
27	b	314	CHL	C2C-C1C-NC	4.47	114.16	109.97
27	b	308	CHL	CAC-C3C-C4C	-4.46	119.02	124.81
27	6	313	CHL	O2D-CGD-O1D	-4.46	115.11	123.84
27	A	836	CHL	C2C-C1C-NC	4.46	114.15	109.97
27	8	319	CHL	C2C-C1C-NC	4.46	114.15	109.97
27	F	309	CHL	C2C-C1C-NC	4.46	114.15	109.97
27	4	304	CHL	C2C-C1C-NC	4.46	114.15	109.97
27	B	829	CHL	C2D-C1D-ND	4.46	113.39	110.10
27	8	316	CHL	C1C-C2C-C3C	-4.46	102.27	106.96
27	7	320	CHL	C1C-C2C-C3C	-4.46	103.57	107.11
27	6	307	CHL	C1D-CHD-C4C	-4.46	116.44	126.06
27	A	855	CHL	C1C-C2C-C3C	-4.46	102.27	106.96
27	3	308	CHL	CAC-C3C-C4C	4.46	130.59	124.81
27	b	304	CHL	C1C-C2C-C3C	-4.46	102.27	106.96
27	A	847	CHL	C1C-C2C-C3C	-4.46	102.27	106.96
27	a	314	CHL	C2C-C1C-NC	4.46	114.15	109.97
29	5	302	LUT	C19-C9-C8	-4.45	111.06	118.08
27	4	304	CHL	C1C-C2C-C3C	-4.45	102.27	106.96
27	7	324	CHL	C4D-CHA-C1A	-4.45	115.83	121.25
27	4	309	CHL	C1C-C2C-C3C	-4.45	103.58	107.11
27	b	312	CHL	C2C-C1C-NC	4.45	114.14	109.97
27	4	318	CHL	C1C-C2C-C3C	-4.45	102.28	106.96
27	A	853	CHL	C1C-C2C-C3C	-4.45	102.28	106.96
27	7	318	CHL	CHD-C1D-ND	-4.45	120.36	124.45
27	B	847	CHL	C2C-C1C-NC	4.45	114.14	109.97
27	3	310	CHL	CHD-C1D-ND	-4.45	120.36	124.45
27	A	823	CHL	C2C-C1C-NC	4.45	114.14	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	311	CHL	CHD-C1D-ND	-4.45	120.37	124.45
27	L	304	CHL	C2C-C1C-NC	4.45	114.14	109.97
27	B	829	CHL	CHD-C1D-ND	-4.45	120.37	124.45
27	5	308	CHL	C2D-C1D-ND	4.45	113.38	110.10
27	6	309	CHL	O2D-CGD-CBD	4.45	119.17	111.27
27	A	828	CHL	O2D-CGD-O1D	-4.44	115.15	123.84
27	a	308	CHL	C1C-C2C-C3C	-4.44	102.28	106.96
27	5	321	CHL	C1C-C2C-C3C	-4.44	102.28	106.96
27	6	314	CHL	C1C-C2C-C3C	-4.44	102.28	106.96
27	4	315	CHL	O2D-CGD-O1D	-4.44	115.15	123.84
27	A	823	CHL	CHD-C1D-ND	-4.44	120.37	124.45
27	A	828	CHL	C2C-C1C-NC	4.44	114.13	109.97
27	A	830	CHL	C2C-C1C-NC	4.44	114.13	109.97
27	3	320	CHL	O2D-CGD-CBD	4.44	119.16	111.27
27	7	314	CHL	CHD-C4C-C3C	-4.44	118.32	124.84
27	a	311	CHL	C1C-C2C-C3C	-4.44	102.29	106.96
27	7	314	CHL	C2D-C1D-ND	4.44	113.37	110.10
27	4	311	CHL	CHD-C1D-ND	-4.44	120.38	124.45
27	B	851	CHL	C2D-C1D-ND	4.44	113.37	110.10
27	A	835	CHL	O2D-CGD-CBD	4.44	119.15	111.27
27	b	307	CHL	C2C-C1C-NC	4.44	114.13	109.97
29	4	302	LUT	C12-C13-C14	-4.43	112.14	118.94
27	b	313	CHL	C1C-C2C-C3C	-4.43	102.30	106.96
27	K	207	CHL	C1C-C2C-C3C	-4.43	103.60	107.11
27	B	838	CHL	C1C-C2C-C3C	-4.43	102.30	106.96
27	A	851	CHL	O2D-CGD-O1D	-4.43	115.18	123.84
27	5	312	CHL	C1C-C2C-C3C	-4.43	102.30	106.96
27	B	837	CHL	O2D-CGD-O1D	-4.43	115.18	123.84
27	a	312	CHL	O2D-CGD-CBD	4.43	119.13	111.27
27	A	845	CHL	C1C-C2C-C3C	-4.43	102.30	106.96
27	6	314	CHL	C2C-C1C-NC	4.42	114.12	109.97
27	A	823	CHL	C1C-C2C-C3C	-4.42	102.31	106.96
27	F	309	CHL	C1C-C2C-C3C	-4.42	102.31	106.96
27	5	310	CHL	C4D-CHA-C1A	-4.42	115.87	121.25
27	b	312	CHL	CHD-C1D-ND	-4.42	120.39	124.45
27	B	823	CHL	C1C-C2C-C3C	-4.42	102.31	106.96
27	B	846	CHL	C2D-C1D-ND	4.42	113.36	110.10
27	A	820	CHL	O2D-CGD-CBD	4.42	119.12	111.27
29	5	303	LUT	C21-C26-C27	-4.42	107.12	112.70
27	5	323	CHL	O2D-CGD-O1D	-4.42	115.20	123.84
27	3	317	CHL	C2C-C1C-NC	4.41	114.11	109.97
29	7	304	LUT	C19-C9-C8	-4.41	111.12	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	832	CHL	C1C-C2C-C3C	-4.41	102.32	106.96
27	B	840	CHL	C1C-C2C-C3C	-4.41	102.32	106.96
27	7	313	CHL	C1C-C2C-C3C	-4.41	102.32	106.96
27	3	321	CHL	CHD-C4C-C3C	-4.41	118.35	124.84
27	B	815	CHL	C2C-C1C-NC	4.41	114.11	109.97
27	A	849	CHL	C2D-C1D-ND	4.41	113.36	110.10
27	B	826	CHL	C2D-C1D-ND	4.41	113.36	110.10
27	6	306	CHL	C2D-C1D-ND	4.41	113.36	110.10
27	A	836	CHL	CHD-C4C-C3C	-4.41	118.36	124.84
27	5	308	CHL	CHD-C4C-C3C	-4.41	118.36	124.84
27	7	315	CHL	C2D-C1D-ND	4.41	113.35	110.10
27	B	830	CHL	C1C-C2C-C3C	-4.41	102.32	106.96
27	A	827	CHL	C2D-C1D-ND	4.41	113.35	110.10
27	8	318	CHL	C1C-C2C-C3C	-4.41	102.32	106.96
29	6	303	LUT	C19-C9-C8	-4.41	111.13	118.08
27	6	315	CHL	C2C-C1C-NC	4.41	114.10	109.97
27	B	849	CHL	C2D-C1D-ND	4.41	113.35	110.10
27	8	311	CHL	C2D-C1D-ND	4.41	113.35	110.10
27	4	310	CHL	CHD-C1D-ND	-4.41	120.41	124.45
27	b	312	CHL	C1C-C2C-C3C	-4.41	102.33	106.96
27	8	313	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
27	A	848	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
27	B	841	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
27	7	311	CHL	O2D-CGD-CBD	4.40	119.09	111.27
27	3	308	CHL	CHD-C1D-ND	-4.40	120.41	124.45
27	8	311	CHL	CHD-C1D-ND	-4.40	120.41	124.45
27	4	309	CHL	C4A-NA-C1A	4.40	108.68	106.71
27	B	842	CHL	CHD-C4C-C3C	-4.40	118.37	124.84
27	6	315	CHL	C1C-C2C-C3C	-4.40	102.33	106.96
27	a	313	CHL	C1C-C2C-C3C	-4.40	102.33	106.96
27	8	326	CHL	CHD-C1D-ND	-4.40	120.41	124.45
27	A	844	CHL	C2C-C1C-NC	4.40	114.09	109.97
27	7	311	CHL	O1D-CGD-CBD	-4.40	115.49	124.48
27	B	811	CHL	C2C-C1C-NC	4.40	114.09	109.97
27	A	842	CHL	C4A-NA-C1A	4.40	108.68	106.71
27	B	839	CHL	C2D-C1D-ND	4.40	113.34	110.10
27	A	830	CHL	CHD-C1D-ND	-4.40	120.42	124.45
27	6	313	CHL	C1C-C2C-C3C	-4.39	102.34	106.96
27	B	823	CHL	CHD-C1D-ND	-4.39	120.42	124.45
27	4	311	CHL	C1C-C2C-C3C	-4.39	102.34	106.96
27	B	825	CHL	CHD-C4C-C3C	-4.39	118.38	124.84
27	a	311	CHL	C2D-C1D-ND	4.39	113.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	310	CHL	C4D-CHA-C1A	-4.39	115.90	121.25
27	A	832	CHL	C4D-CHA-C1A	-4.39	115.91	121.25
27	B	812	CHL	CAC-C3C-C4C	4.39	130.50	124.81
27	8	325	CHL	C1C-C2C-C3C	-4.39	102.34	106.96
27	A	858	CHL	C2D-C1D-ND	4.39	113.34	110.10
27	a	320	CHL	C2C-C1C-NC	4.39	114.08	109.97
27	A	822	CHL	O2D-CGD-CBD	4.39	119.06	111.27
29	3	304	LUT	C19-C9-C8	-4.38	111.17	118.08
27	B	814	CHL	CHD-C1D-ND	-4.38	120.42	124.45
27	a	311	CHL	C2C-C1C-NC	4.38	114.08	109.97
27	A	826	CHL	C2C-C1C-NC	4.38	114.08	109.97
27	4	314	CHL	C2C-C1C-NC	4.38	114.08	109.97
27	A	824	CHL	O2D-CGD-CBD	4.38	119.06	111.27
27	A	817	CHL	C2C-C1C-NC	4.38	114.08	109.97
27	B	826	CHL	CHD-C4C-C3C	-4.38	118.40	124.84
27	A	848	CHL	C2D-C1D-ND	4.38	113.33	110.10
27	B	848	CHL	C2D-C1D-ND	4.38	113.33	110.10
27	6	314	CHL	C4D-CHA-C1A	-4.38	115.92	121.25
27	5	318	CHL	O2D-CGD-CBD	4.38	119.05	111.27
27	A	830	CHL	C2D-C1D-ND	4.38	113.33	110.10
34	8	301	SQD	O9-S-C6	4.38	112.14	106.94
27	5	309	CHL	C1C-C2C-C3C	-4.38	102.36	106.96
27	6	306	CHL	C1C-C2C-C3C	-4.38	102.36	106.96
27	b	307	CHL	CHD-C1D-ND	-4.38	120.43	124.45
27	B	825	CHL	C2C-C1C-NC	4.38	114.07	109.97
27	A	837	CHL	C1C-C2C-C3C	-4.37	102.36	106.96
29	3	304	LUT	C40-C33-C32	-4.37	111.18	118.08
27	6	309	CHL	C1C-C2C-C3C	-4.37	102.36	106.96
27	6	320	CHL	C2D-C1D-ND	4.37	113.33	110.10
27	b	310	CHL	C2C-C1C-NC	4.37	114.07	109.97
27	6	305	CHL	C2D-C1D-ND	4.37	113.33	110.10
27	5	308	CHL	C4D-CHA-C1A	-4.37	115.93	121.25
27	J	106	CHL	C2D-C1D-ND	4.37	113.32	110.10
27	4	305	CHL	C1C-C2C-C3C	-4.37	102.36	106.96
27	B	822	CHL	C2C-C1C-NC	4.37	114.06	109.97
27	A	844	CHL	C4D-CHA-C1A	-4.37	115.93	121.25
27	A	848	CHL	C4D-CHA-C1A	-4.37	115.93	121.25
27	A	846	CHL	C1D-CHD-C4C	-4.37	116.64	126.06
27	7	321	CHL	C1C-C2C-C3C	-4.37	103.65	107.11
27	L	304	CHL	C1C-C2C-C3C	-4.37	102.37	106.96
27	A	852	CHL	O1D-CGD-CBD	-4.36	115.55	124.48
27	7	321	CHL	CGD-CBD-CAD	4.36	124.87	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	823	CHL	C2D-C1D-ND	4.36	113.32	110.10
27	8	314	CHL	C1C-C2C-C3C	-4.36	103.65	107.11
27	b	315	CHL	C2C-C1C-NC	4.36	114.06	109.97
27	B	850	CHL	O1D-CGD-CBD	-4.36	115.56	124.48
29	8	303	LUT	C7-C6-C5	-4.36	110.90	121.46
27	A	832	CHL	O2D-CGD-CBD	4.36	119.02	111.27
27	a	313	CHL	C4D-CHA-C1A	-4.36	115.94	121.25
27	A	826	CHL	C1C-C2C-C3C	-4.36	102.37	106.96
27	3	309	CHL	C1C-C2C-C3C	-4.36	102.37	106.96
27	A	847	CHL	C2D-C1D-ND	4.36	113.31	110.10
27	B	824	CHL	O2D-CGD-CBD	4.36	119.01	111.27
27	8	316	CHL	C2D-C1D-ND	4.36	113.31	110.10
27	4	306	CHL	C1C-C2C-C3C	-4.35	102.38	106.96
27	A	843	CHL	C1D-CHD-C4C	-4.35	116.67	126.06
27	A	839	CHL	O2D-CGD-O1D	-4.35	115.33	123.84
27	6	320	CHL	C1C-C2C-C3C	-4.35	102.38	106.96
27	3	315	CHL	C1C-C2C-C3C	-4.35	102.38	106.96
27	B	844	CHL	C2C-C1C-NC	4.35	114.05	109.97
27	A	854	CHL	C2D-C1D-ND	4.35	113.31	110.10
27	B	840	CHL	CHD-C4C-C3C	-4.35	118.45	124.84
27	3	314	CHL	C2C-C1C-NC	4.35	114.05	109.97
27	B	831	CHL	C1C-C2C-C3C	-4.35	102.38	106.96
27	A	823	CHL	O2D-CGD-O1D	-4.35	115.34	123.84
27	a	320	CHL	C1C-C2C-C3C	-4.35	102.39	106.96
27	A	847	CHL	CHD-C1D-ND	-4.35	120.46	124.45
27	B	837	CHL	C4D-CHA-C1A	-4.35	115.96	121.25
27	b	317	CHL	C1C-C2C-C3C	-4.35	103.67	107.11
27	J	106	CHL	CHD-C4C-C3C	-4.34	118.45	124.84
27	5	320	CHL	C1C-C2C-C3C	-4.34	102.39	106.96
27	a	314	CHL	C1C-C2C-C3C	-4.34	102.39	106.96
27	A	859	CHL	C2C-C1C-NC	4.34	114.04	109.97
27	8	312	CHL	C2C-C1C-NC	4.34	114.04	109.97
29	6	303	LUT	C35-C15-C14	-4.34	114.58	123.47
27	A	839	CHL	C1C-C2C-C3C	-4.34	102.39	106.96
27	4	319	CHL	C1C-C2C-C3C	-4.34	102.39	106.96
27	5	307	CHL	C2C-C1C-NC	4.34	114.04	109.97
27	b	307	CHL	C2D-C1D-ND	4.34	113.30	110.10
27	B	815	CHL	CHD-C4C-C3C	-4.34	118.46	124.84
27	3	310	CHL	C1C-C2C-C3C	-4.34	102.39	106.96
27	3	317	CHL	O2D-CGD-CBD	4.34	118.98	111.27
27	7	319	CHL	C1C-C2C-C3C	-4.34	103.67	107.11
27	B	813	CHL	C1C-C2C-C3C	-4.34	102.39	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	318	CHL	C2D-C1D-ND	4.34	113.30	110.10
27	6	305	CHL	O2D-CGD-CBD	4.34	118.98	111.27
27	A	844	CHL	C1C-C2C-C3C	-4.34	102.40	106.96
27	3	314	CHL	C1C-C2C-C3C	-4.34	102.40	106.96
27	B	819	CHL	O2D-CGD-CBD	4.34	118.98	111.27
27	A	825	CHL	CHD-C1D-ND	-4.33	120.47	124.45
27	8	319	CHL	CHD-C1D-ND	-4.33	120.47	124.45
27	A	855	CHL	C2D-C1D-ND	4.33	113.30	110.10
27	8	317	CHL	C2D-C1D-ND	4.33	113.30	110.10
27	B	825	CHL	C1C-C2C-C3C	-4.33	102.40	106.96
27	b	317	CHL	CHD-C1D-ND	-4.33	120.47	124.45
27	A	850	CHL	C2D-C1D-ND	4.33	113.30	110.10
27	3	310	CHL	C2D-C1D-ND	4.33	113.30	110.10
27	4	315	CHL	O1D-CGD-CBD	-4.33	115.62	124.48
27	5	320	CHL	CHD-C1D-ND	-4.33	120.47	124.45
27	A	857	CHL	C4D-CHA-C1A	-4.33	115.98	121.25
27	B	833	CHL	C4D-CHA-C1A	-4.33	115.98	121.25
27	B	835	CHL	C2C-C1C-NC	4.33	114.03	109.97
27	A	827	CHL	O2D-CGD-O1D	-4.33	115.38	123.84
29	b	303	LUT	C19-C9-C10	-4.33	116.86	122.92
27	8	319	CHL	C1C-C2C-C3C	-4.32	102.41	106.96
27	b	310	CHL	C1C-C2C-C3C	-4.32	102.41	106.96
27	A	851	CHL	CHD-C1D-ND	-4.32	120.48	124.45
27	A	834	CHL	C2D-C1D-ND	4.32	113.29	110.10
27	6	310	CHL	C2C-C1C-NC	4.32	114.02	109.97
27	K	205	CHL	C1C-C2C-C3C	-4.32	102.42	106.96
29	3	305	LUT	C7-C6-C5	-4.32	111.01	121.46
27	B	847	CHL	C1C-C2C-C3C	-4.31	102.42	106.96
27	5	318	CHL	O2D-CGD-O1D	-4.31	115.40	123.84
27	B	847	CHL	CHD-C1D-ND	-4.31	120.49	124.45
27	4	308	CHL	CHD-C4C-C3C	-4.31	118.50	124.84
27	6	315	CHL	C4D-CHA-C1A	-4.31	116.00	121.25
29	4	301	LUT	C12-C13-C14	-4.31	112.32	118.94
27	4	320	CHL	O2D-CGD-O1D	-4.31	115.41	123.84
27	A	822	CHL	C1C-C2C-C3C	-4.31	102.43	106.96
27	6	314	CHL	C2D-C1D-ND	4.31	113.28	110.10
27	A	858	CHL	C1C-C2C-C3C	-4.31	102.43	106.96
27	8	321	CHL	O2D-CGD-CBD	4.31	118.92	111.27
27	A	856	CHL	C1C-C2C-C3C	-4.31	102.43	106.96
27	B	833	CHL	C2C-C1C-NC	4.30	114.00	109.97
27	B	835	CHL	C1C-C2C-C3C	-4.30	102.43	106.96
27	b	313	CHL	C2D-C1D-ND	4.30	113.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	302	LUT	C40-C33-C32	-4.30	111.30	118.08
27	4	315	CHL	C2C-C1C-NC	4.30	114.00	109.97
27	7	314	CHL	CHD-C1D-ND	-4.30	120.50	124.45
27	b	315	CHL	C1C-C2C-C3C	-4.30	102.43	106.96
27	B	815	CHL	C1C-C2C-C3C	-4.30	102.44	106.96
27	B	845	CHL	CHD-C4C-C3C	-4.30	118.52	124.84
27	3	312	CHL	C4D-CHA-C1A	-4.30	116.02	121.25
27	A	843	CHL	O2D-CGD-CBD	4.30	118.91	111.27
27	A	819	CHL	O2D-CGD-O1D	-4.30	115.44	123.84
27	6	309	CHL	CHD-C1D-ND	-4.30	120.50	124.45
27	A	840	CHL	C2D-C1D-ND	4.30	113.27	110.10
27	A	854	CHL	CHD-C1D-ND	-4.29	120.51	124.45
27	6	317	CHL	O2D-CGD-O1D	-4.29	115.44	123.84
27	7	311	CHL	CHD-C4C-C3C	-4.29	118.53	124.84
27	B	839	CHL	C1C-C2C-C3C	-4.29	102.44	106.96
27	8	313	CHL	C1C-C2C-C3C	-4.29	102.44	106.96
27	K	207	CHL	O2D-CGD-CBD	4.29	118.90	111.27
27	a	308	CHL	C4D-CHA-C1A	-4.29	116.03	121.25
27	4	318	CHL	C4D-CHA-C1A	-4.29	116.03	121.25
27	A	838	CHL	CHD-C1D-ND	-4.29	120.51	124.45
27	8	326	CHL	C4D-CHA-C1A	-4.29	116.03	121.25
27	3	311	CHL	C4D-CHA-C1A	-4.29	116.03	121.25
27	6	310	CHL	C1C-C2C-C3C	-4.29	102.45	106.96
27	B	840	CHL	C2D-C1D-ND	4.29	113.26	110.10
27	5	311	CHL	C4D-CHA-C1A	-4.28	116.04	121.25
27	6	312	CHL	O2D-CGD-O1D	-4.28	115.47	123.84
27	b	314	CHL	C1C-C2C-C3C	-4.28	102.46	106.96
27	a	311	CHL	CHD-C4C-C3C	-4.28	118.55	124.84
27	A	827	CHL	C2C-C1C-NC	4.28	113.98	109.97
27	a	307	CHL	C2C-C1C-NC	4.28	113.98	109.97
27	a	310	CHL	C2C-C1C-NC	4.28	113.98	109.97
27	A	834	CHL	CHD-C1D-ND	-4.28	120.52	124.45
27	A	849	CHL	O2D-CGD-O1D	-4.28	115.47	123.84
27	5	307	CHL	C4D-CHA-C1A	-4.28	116.04	121.25
27	a	308	CHL	CHD-C4C-C3C	-4.28	118.56	124.84
27	3	308	CHL	O1D-CGD-CBD	-4.27	115.74	124.48
27	B	816	CHL	CHD-C1D-ND	-4.27	120.53	124.45
27	a	310	CHL	O2D-CGD-O1D	-4.27	115.48	123.84
27	A	821	CHL	C4D-CHA-C1A	-4.27	116.05	121.25
27	4	315	CHL	C2D-C1D-ND	4.27	113.25	110.10
27	4	317	CHL	O2D-CGD-CBD	4.27	118.86	111.27
27	3	312	CHL	O2D-CGD-O1D	-4.27	115.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	316	CHL	C1C-C2C-C3C	-4.27	103.72	107.11
27	A	853	CHL	CHD-C1D-ND	-4.27	120.53	124.45
27	B	843	CHL	C2D-C1D-ND	4.27	113.25	110.10
27	3	321	CHL	C2D-C1D-ND	4.27	113.25	110.10
27	B	835	CHL	C4D-CHA-C1A	-4.27	116.05	121.25
27	B	847	CHL	O2D-CGD-CBD	4.27	118.85	111.27
27	A	855	CHL	CHD-C1D-ND	-4.27	120.53	124.45
27	B	842	CHL	C4D-CHA-C1A	-4.27	116.05	121.25
27	F	309	CHL	C2D-C1D-ND	4.27	113.25	110.10
27	B	844	CHL	C1C-C2C-C3C	-4.27	102.47	106.96
27	3	315	CHL	CHD-C4C-C3C	-4.27	118.57	124.84
27	A	829	CHL	CHD-C1D-ND	-4.27	120.53	124.45
27	B	840	CHL	O2D-CGD-CBD	4.27	118.85	111.27
27	5	314	CHL	C2D-C1D-ND	4.26	113.25	110.10
27	4	315	CHL	C1C-C2C-C3C	-4.26	102.47	106.96
27	7	324	CHL	C1C-C2C-C3C	-4.26	102.47	106.96
27	6	314	CHL	CHD-C1D-ND	-4.26	120.54	124.45
27	A	829	CHL	C2D-C1D-ND	4.26	113.25	110.10
27	a	312	CHL	C4D-CHA-C1A	-4.26	116.06	121.25
27	5	320	CHL	C2D-C1D-ND	4.26	113.24	110.10
27	a	312	CHL	CHD-C1D-ND	-4.26	120.54	124.45
27	4	310	CHL	C4D-CHA-C1A	-4.26	116.06	121.25
27	6	311	CHL	C2D-C1D-ND	4.26	113.24	110.10
27	B	851	CHL	CHD-C4C-C3C	-4.26	118.58	124.84
27	B	839	CHL	CHD-C1D-ND	-4.26	120.54	124.45
27	A	843	CHL	C4C-C3C-C2C	-4.26	100.69	106.90
27	8	314	CHL	O2D-CGD-CBD	4.26	118.83	111.27
27	B	847	CHL	O2D-CGD-O1D	-4.26	115.52	123.84
27	A	838	CHL	C1C-C2C-C3C	-4.26	102.48	106.96
27	A	849	CHL	C1C-C2C-C3C	-4.26	102.48	106.96
29	4	302	LUT	C18-C5-C4	-4.26	106.47	114.36
27	A	827	CHL	CHD-C4C-C3C	-4.26	118.58	124.84
27	B	813	CHL	CHD-C4C-C3C	-4.26	118.58	124.84
27	5	308	CHL	C1C-C2C-C3C	-4.26	102.48	106.96
27	B	816	CHL	C4D-CHA-C1A	-4.25	116.07	121.25
27	5	311	CHL	CHD-C1D-ND	-4.25	120.55	124.45
24	B	808	LHG	O4-P-O5	4.25	133.27	112.24
27	a	314	CHL	C2D-C1D-ND	4.25	113.24	110.10
27	A	827	CHL	C1C-C2C-C3C	-4.25	102.49	106.96
27	a	307	CHL	CHD-C1D-ND	-4.25	120.55	124.45
27	b	307	CHL	C1C-C2C-C3C	-4.25	102.49	106.96
27	4	319	CHL	C2C-C1C-NC	4.25	113.95	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	319	CHL	C1B-CHB-C4A	-4.25	121.70	130.12
27	A	856	CHL	C2D-C1D-ND	4.25	113.23	110.10
27	A	819	CHL	C1C-C2C-C3C	-4.24	102.50	106.96
27	A	859	CHL	C1C-C2C-C3C	-4.24	102.50	106.96
27	3	314	CHL	CHD-C1D-ND	-4.24	120.56	124.45
27	A	817	CHL	C1C-C2C-C3C	-4.24	102.50	106.96
27	B	813	CHL	C4D-CHA-C1A	-4.24	116.09	121.25
27	A	828	CHL	C2D-C1D-ND	4.24	113.23	110.10
27	4	317	CHL	C1B-CHB-C4A	-4.24	121.73	130.12
27	B	840	CHL	C2C-C1C-NC	4.24	113.94	109.97
27	6	311	CHL	O2D-CGD-O1D	-4.23	115.56	123.84
27	8	324	CHL	O2D-CGD-O1D	-4.23	115.56	123.84
27	A	818	CHL	C2D-C1D-ND	4.23	113.22	110.10
27	a	307	CHL	C1C-C2C-C3C	-4.23	102.51	106.96
27	4	310	CHL	C2D-C1D-ND	4.23	113.22	110.10
27	A	820	CHL	CAC-C3C-C4C	4.23	130.30	124.81
27	A	840	CHL	O2D-CGD-O1D	-4.23	115.57	123.84
27	4	305	CHL	C2D-C1D-ND	4.23	113.22	110.10
27	a	307	CHL	CHD-C4C-C3C	-4.23	118.62	124.84
27	B	821	CHL	CHD-C4C-C3C	-4.23	118.63	124.84
27	b	308	CHL	CMD-C2D-C3D	-4.23	117.89	127.61
27	3	309	CHL	O2D-CGD-O1D	-4.23	115.58	123.84
24	A	810	LHG	O4-P-O5	4.22	133.13	112.24
27	A	848	CHL	CHD-C1D-ND	-4.22	120.57	124.45
27	A	832	CHL	C2C-C1C-NC	4.22	113.93	109.97
27	4	320	CHL	C2D-C1D-ND	4.22	113.22	110.10
27	A	822	CHL	C2C-C1C-NC	4.22	113.93	109.97
27	A	829	CHL	CHD-C4C-C3C	-4.22	118.63	124.84
27	5	307	CHL	CHD-C4C-C3C	-4.22	118.63	124.84
27	5	318	CHL	C2D-C1D-ND	4.22	113.21	110.10
27	A	851	CHL	CHD-C4C-C3C	-4.22	118.64	124.84
27	7	311	CHL	C2C-C1C-NC	4.22	113.92	109.97
24	7	306	LHG	O4-P-O5	4.22	133.10	112.24
27	3	309	CHL	C2D-C1D-ND	4.22	113.21	110.10
27	b	306	CHL	C2D-C1D-ND	4.22	113.21	110.10
24	7	302	LHG	O4-P-O5	4.22	133.09	112.24
27	5	323	CHL	C2D-C1D-ND	4.22	113.21	110.10
27	5	320	CHL	C2C-C1C-NC	4.22	113.92	109.97
27	F	308	CHL	CHD-C4C-C3C	-4.21	118.64	124.84
27	8	317	CHL	C1C-C2C-C3C	-4.21	102.53	106.96
27	B	824	CHL	C1C-C2C-C3C	-4.21	102.53	106.96
27	A	841	CHL	CHD-C1D-ND	-4.21	120.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	833	CHL	CHD-C1D-ND	-4.21	120.59	124.45
27	3	311	CHL	CHD-C4C-C3C	-4.21	118.65	124.84
27	A	838	CHL	C2D-C1D-ND	4.21	113.20	110.10
27	5	309	CHL	CHD-C1D-ND	-4.21	120.59	124.45
27	B	833	CHL	C1C-C2C-C3C	-4.21	102.53	106.96
27	7	321	CHL	CHD-C1D-ND	-4.21	120.59	124.45
27	b	304	CHL	C2D-C1D-ND	4.20	113.20	110.10
27	5	307	CHL	C1C-C2C-C3C	-4.20	102.54	106.96
27	8	317	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
27	b	315	CHL	CHD-C1D-ND	-4.20	120.59	124.45
27	8	315	CHL	O2D-CGD-O1D	-4.20	115.62	123.84
27	4	305	CHL	CHD-C1D-ND	-4.20	120.59	124.45
27	a	310	CHL	C1C-C2C-C3C	-4.20	102.54	106.96
27	6	316	CHL	C1C-C2C-C3C	-4.20	103.78	107.11
27	A	818	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
27	B	835	CHL	C2D-C1D-ND	4.20	113.20	110.10
27	3	311	CHL	C2D-C1D-ND	4.20	113.20	110.10
24	8	305	LHG	O4-P-O5	4.20	132.99	112.24
27	A	851	CHL	C2D-C1D-ND	4.20	113.20	110.10
24	A	812	LHG	O4-P-O5	4.20	132.98	112.24
27	6	314	CHL	CHD-C4C-C3C	-4.19	118.67	124.84
24	5	324	LHG	O4-P-O5	4.19	132.98	112.24
27	3	308	CHL	C2C-C1C-NC	4.19	113.90	109.97
27	B	849	CHL	CHD-C1D-ND	-4.19	120.60	124.45
27	B	832	CHL	O2D-CGD-O1D	-4.19	115.64	123.84
27	b	308	CHL	CHD-C4C-C3C	-4.19	118.68	124.84
27	a	320	CHL	CHD-C1D-ND	-4.19	120.60	124.45
24	b	302	LHG	O4-P-O5	4.19	132.95	112.24
27	6	307	CHL	C2A-C1A-CHA	-4.19	116.54	123.86
27	7	319	CHL	CHD-C4C-C3C	-4.19	118.69	124.84
29	J	103	LUT	C28-C29-C30	-4.19	112.52	118.94
27	A	819	CHL	CHD-C1D-ND	-4.19	120.61	124.45
27	4	315	CHL	O2D-CGD-CBD	4.18	118.70	111.27
27	3	318	CHL	CHD-C1D-ND	-4.18	120.61	124.45
27	4	307	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
27	B	849	CHL	C2C-C1C-NC	4.18	113.89	109.97
27	A	859	CHL	O2D-CGD-CBD	4.18	118.70	111.27
27	L	304	CHL	O2D-CGD-O1D	-4.18	115.66	123.84
22	6	301	BCR	C34-C9-C10	-4.18	117.06	122.92
27	A	831	CHL	CHD-C1D-ND	-4.18	120.61	124.45
27	3	309	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
27	L	303	CHL	C1D-CHD-C4C	-4.18	117.04	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	8	303	LUT	C21-C26-C27	-4.18	107.42	112.70
27	5	312	CHL	C4D-CHA-C1A	-4.18	116.16	121.25
27	5	312	CHL	CHD-C1D-ND	-4.18	120.61	124.45
27	a	308	CHL	O1D-CGD-CBD	-4.18	115.94	124.48
27	B	842	CHL	O2D-CGD-O1D	-4.18	115.67	123.84
27	A	835	CHL	C2D-C1D-ND	4.18	113.18	110.10
27	B	836	CHL	C1C-C2C-C3C	-4.17	102.57	106.96
27	a	312	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
27	A	818	CHL	C1C-C2C-C3C	-4.17	102.57	106.96
29	7	304	LUT	C1-C6-C5	-4.17	116.75	122.61
27	3	308	CHL	C1C-C2C-C3C	-4.17	102.58	106.96
27	A	832	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
27	B	841	CHL	C2C-C1C-NC	4.16	113.87	109.97
27	B	850	CHL	C2C-C1C-NC	4.16	113.87	109.97
27	a	317	CHL	C2D-C1D-ND	4.16	113.17	110.10
27	7	320	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
27	5	315	CHL	C4D-CHA-C1A	-4.16	116.18	121.25
27	B	834	CHL	C2C-C1C-NC	4.16	113.87	109.97
27	a	308	CHL	C2D-C1D-ND	4.16	113.17	110.10
27	3	317	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
27	4	304	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
27	A	855	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
27	B	846	CHL	O2D-CGD-O1D	-4.16	115.71	123.84
27	A	825	CHL	C2D-C1D-ND	4.16	113.17	110.10
27	B	828	CHL	C2D-C1D-ND	4.16	113.17	110.10
27	8	319	CHL	O1D-CGD-CBD	-4.16	115.97	124.48
27	5	310	CHL	C1C-C2C-C3C	-4.16	102.58	106.96
27	B	822	CHL	O2D-CGD-CBD	4.16	118.66	111.27
29	6	303	LUT	C7-C8-C9	-4.16	119.96	126.23
27	B	847	CHL	CHD-C4C-C3C	-4.16	118.73	124.84
27	8	321	CHL	C1C-C2C-C3C	-4.15	103.82	107.11
27	3	313	CHL	CHD-C1D-ND	-4.15	120.64	124.45
27	A	832	CHL	C1C-C2C-C3C	-4.15	102.59	106.96
27	B	847	CHL	C2D-C1D-ND	4.15	113.16	110.10
27	B	822	CHL	C2D-C1D-ND	4.15	113.16	110.10
27	A	859	CHL	C4D-CHA-C1A	-4.15	116.20	121.25
27	A	820	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
27	a	318	CHL	CHD-C4C-C3C	-4.14	118.75	124.84
27	A	830	CHL	C1C-C2C-C3C	-4.14	102.60	106.96
27	5	310	CHL	C2C-C1C-NC	4.14	113.85	109.97
27	6	311	CHL	CHD-C4C-C3C	-4.14	118.75	124.84
27	a	313	CHL	C2D-C1D-ND	4.14	113.16	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	824	CHL	C2D-C1D-ND	4.14	113.15	110.10
27	B	850	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
27	b	312	CHL	C2D-C1D-ND	4.14	113.15	110.10
27	A	857	CHL	C1C-C2C-C3C	-4.14	102.61	106.96
24	A	811	LHG	O4-P-O5	4.13	132.68	112.24
27	B	838	CHL	C4D-CHA-C1A	-4.13	116.22	121.25
27	A	848	CHL	O2D-CGD-O1D	-4.13	115.76	123.84
33	7	305	XAT	C19-C9-C10	-4.13	117.14	122.92
27	5	320	CHL	C4D-CHA-C1A	-4.13	116.23	121.25
27	B	811	CHL	C1C-C2C-C3C	-4.13	102.62	106.96
27	8	312	CHL	CHD-C4C-C3C	-4.12	118.78	124.84
27	B	825	CHL	CHD-C1D-ND	-4.12	120.67	124.45
27	B	814	CHL	C2C-C1C-NC	4.12	113.83	109.97
27	A	847	CHL	CHD-C4C-C3C	-4.12	118.78	124.84
27	B	830	CHL	C2D-C1D-ND	4.12	113.14	110.10
27	8	325	CHL	CHD-C1D-ND	-4.12	120.67	124.45
27	K	206	CHL	C2D-C1D-ND	4.12	113.14	110.10
27	A	854	CHL	CHD-C4C-C3C	-4.12	118.79	124.84
27	6	310	CHL	C2D-C1D-ND	4.11	113.14	110.10
27	6	312	CHL	C4D-CHA-C1A	-4.11	116.24	121.25
27	B	819	CHL	CHD-C4C-C3C	-4.11	118.80	124.84
27	7	324	CHL	C2D-C1D-ND	4.11	113.13	110.10
27	7	324	CHL	CHD-C1D-ND	-4.11	120.68	124.45
27	8	312	CHL	CHD-C1D-ND	-4.11	120.68	124.45
27	A	830	CHL	CHD-C4C-C3C	-4.11	118.80	124.84
29	4	301	LUT	C7-C6-C5	-4.11	111.51	121.46
27	A	826	CHL	C2D-C1D-ND	4.11	113.13	110.10
27	7	314	CHL	C2C-C1C-NC	4.11	113.82	109.97
27	b	307	CHL	CHD-C4C-C3C	-4.11	118.80	124.84
27	A	842	CHL	O2D-CGD-CBD	4.10	118.56	111.27
27	3	321	CHL	O2D-CGD-O1D	-4.10	115.82	123.84
27	5	321	CHL	C2D-C1D-ND	4.10	113.13	110.10
27	3	321	CHL	C4D-CHA-C1A	-4.10	116.26	121.25
27	B	843	CHL	CHD-C4C-C3C	-4.10	118.81	124.84
27	a	314	CHL	CHD-C4C-C3C	-4.10	118.81	124.84
27	A	822	CHL	C2D-C1D-ND	4.10	113.12	110.10
27	A	837	CHL	C4D-CHA-C1A	-4.10	116.26	121.25
27	B	827	CHL	CHD-C4C-C3C	-4.10	118.82	124.84
27	B	850	CHL	C1C-C2C-C3C	-4.10	102.65	106.96
27	B	826	CHL	C4D-CHA-C1A	-4.10	116.27	121.25
27	A	825	CHL	C4D-CHA-C1A	-4.09	116.27	121.25
27	6	318	CHL	CHD-C4C-C3C	-4.09	118.82	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	315	CHL	C2D-C1D-ND	4.09	113.12	110.10
27	A	850	CHL	C4D-CHA-C1A	-4.09	116.27	121.25
27	B	824	CHL	CHD-C1D-ND	-4.09	120.69	124.45
27	8	316	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
27	A	854	CHL	O2D-CGD-O1D	-4.09	115.84	123.84
27	A	816	CHL	C2C-C1C-NC	4.09	113.80	109.97
27	A	829	CHL	O2D-CGD-O1D	-4.09	115.84	123.84
27	B	823	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
27	3	317	CHL	C1C-C2C-C3C	-4.09	102.66	106.96
27	a	313	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
27	8	318	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
29	5	303	LUT	C7-C8-C9	-4.09	120.06	126.23
27	B	813	CHL	C2C-C1C-NC	4.09	113.80	109.97
27	6	308	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
27	3	318	CHL	C4-C3-C5	4.09	120.65	115.98
27	A	841	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
27	B	849	CHL	C1C-C2C-C3C	-4.08	102.66	106.96
27	6	313	CHL	C4D-CHA-C1A	-4.08	116.28	121.25
27	A	853	CHL	O2D-CGD-O1D	-4.08	115.86	123.84
27	A	857	CHL	CHD-C4C-C3C	-4.08	118.84	124.84
27	6	313	CHL	CHD-C1D-ND	-4.08	120.70	124.45
27	6	320	CHL	CHD-C4C-C3C	-4.08	118.84	124.84
29	6	303	LUT	C7-C6-C5	-4.07	111.59	121.46
27	4	306	CHL	CHD-C1D-ND	-4.07	120.71	124.45
27	A	816	CHL	C1C-C2C-C3C	-4.07	102.68	106.96
29	6	302	LUT	C12-C13-C14	-4.07	112.69	118.94
27	B	840	CHL	O2D-CGD-O1D	-4.07	115.88	123.84
27	b	304	CHL	CHD-C1D-ND	-4.07	120.72	124.45
27	b	314	CHL	C2D-C1D-ND	4.07	113.10	110.10
27	5	316	CHL	C2D-C1D-ND	4.07	113.10	110.10
27	7	315	CHL	CHD-C1D-ND	-4.07	120.72	124.45
29	7	304	LUT	C10-C11-C12	-4.06	110.53	123.22
27	6	311	CHL	C4D-CHA-C1A	-4.06	116.30	121.25
27	a	310	CHL	CHD-C4C-C3C	-4.06	118.87	124.84
27	B	850	CHL	CHD-C1D-ND	-4.06	120.72	124.45
27	A	851	CHL	C4D-CHA-C1A	-4.06	116.31	121.25
27	A	839	CHL	C2D-C1D-ND	4.06	113.09	110.10
27	A	836	CHL	O2D-CGD-O1D	-4.06	115.90	123.84
27	A	824	CHL	C1C-C2C-C3C	-4.06	102.69	106.96
27	B	820	CHL	C2D-C1D-ND	4.06	113.09	110.10
27	8	320	CHL	C2D-C1D-ND	4.06	113.09	110.10
27	A	836	CHL	C1C-C2C-C3C	-4.05	102.69	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	314	CHL	C2D-C1D-ND	4.05	113.09	110.10
27	b	306	CHL	C2C-C1C-NC	4.05	113.77	109.97
27	A	823	CHL	CHD-C4C-C3C	-4.05	118.88	124.84
27	A	856	CHL	C4D-CHA-C1A	-4.05	116.32	121.25
27	K	206	CHL	CHD-C1D-ND	-4.05	120.73	124.45
27	B	815	CHL	CHD-C1D-ND	-4.05	120.73	124.45
27	8	318	CHL	C4D-CHA-C1A	-4.05	116.32	121.25
27	6	311	CHL	C1C-C2C-C3C	-4.05	102.70	106.96
22	6	301	BCR	C37-C22-C21	-4.05	117.25	122.92
27	B	819	CHL	CHD-C1D-ND	-4.05	120.73	124.45
27	5	316	CHL	O2D-CGD-O1D	-4.05	115.93	123.84
27	6	308	CHL	CMB-C2B-C3B	4.04	132.24	124.68
27	7	313	CHL	C2D-C1D-ND	4.04	113.08	110.10
27	B	821	CHL	CHD-C1D-ND	-4.04	120.74	124.45
27	B	814	CHL	C1C-C2C-C3C	-4.04	102.71	106.96
27	L	304	CHL	C4D-CHA-C1A	-4.04	116.33	121.25
27	4	311	CHL	C2D-C1D-ND	4.04	113.08	110.10
27	5	321	CHL	CHD-C4C-C3C	-4.04	118.90	124.84
27	6	309	CHL	CHD-C4C-C3C	-4.04	118.90	124.84
27	8	311	CHL	CHD-C4C-C3C	-4.04	118.90	124.84
29	6	303	LUT	C1-C6-C5	-4.04	116.92	122.61
27	8	312	CHL	C1C-C2C-C3C	-4.04	102.71	106.96
27	B	825	CHL	C4D-CHA-C1A	-4.04	116.33	121.25
27	7	315	CHL	CHD-C4C-C3C	-4.04	118.91	124.84
27	a	317	CHL	CHD-C1D-ND	-4.03	120.75	124.45
27	B	830	CHL	C4D-CHA-C1A	-4.03	116.34	121.25
27	B	829	CHL	O2D-CGD-O1D	-4.03	115.95	123.84
33	7	305	XAT	C39-C29-C30	-4.03	117.27	122.92
27	a	320	CHL	C2D-C1D-ND	4.03	113.08	110.10
27	B	829	CHL	CHD-C4C-C3C	-4.03	118.92	124.84
27	5	325	CHL	CHD-C4C-C3C	-4.03	118.92	124.84
27	B	844	CHL	C2D-C1D-ND	4.03	113.07	110.10
27	5	314	CHL	CHD-C4C-C3C	-4.03	118.92	124.84
27	A	842	CHL	C1C-C2C-C3C	-4.03	103.92	107.11
27	8	315	CHL	C1C-C2C-C3C	-4.03	102.72	106.96
27	8	314	CHL	C1-C2-C3	-4.03	119.08	126.04
27	K	204	CHL	C4D-CHA-C1A	-4.03	116.35	121.25
27	B	846	CHL	C4D-CHA-C1A	-4.03	116.35	121.25
27	A	837	CHL	CHD-C4C-C3C	-4.02	118.92	124.84
27	B	832	CHL	C4D-CHA-C1A	-4.02	116.35	121.25
27	3	316	CHL	C1-C2-C3	-4.02	119.08	126.04
27	7	322	CHL	CGD-CBD-CAD	4.02	123.77	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	313	CHL	CHD-C1D-ND	-4.02	120.76	124.45
27	B	820	CHL	CHD-C4C-C3C	-4.02	118.93	124.84
27	B	830	CHL	CHD-C4C-C3C	-4.02	118.93	124.84
27	5	312	CHL	C2D-C1D-ND	4.02	113.06	110.10
27	A	835	CHL	C4D-CHA-C1A	-4.01	116.36	121.25
27	4	304	CHL	C4D-CHA-C1A	-4.01	116.36	121.25
27	A	834	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
27	8	325	CHL	C2D-C1D-ND	4.01	113.06	110.10
27	5	314	CHL	CHD-C1D-ND	-4.01	120.77	124.45
27	4	307	CHL	CHD-C1D-ND	-4.01	120.77	124.45
27	4	314	CHL	CHD-C4C-C3C	-4.01	118.95	124.84
27	K	204	CHL	CHD-C4C-C3C	-4.01	118.95	124.84
27	3	310	CHL	CHD-C4C-C3C	-4.01	118.95	124.84
27	4	310	CHL	CHD-C4C-C3C	-4.00	118.95	124.84
27	6	306	CHL	CHD-C4C-C3C	-4.00	118.95	124.84
27	B	822	CHL	O1D-CGD-CBD	-4.00	116.29	124.48
27	B	836	CHL	C2D-C1D-ND	4.00	113.05	110.10
27	8	323	CHL	C2C-C1C-NC	4.00	113.72	109.97
27	B	832	CHL	C2D-C1D-ND	4.00	113.05	110.10
27	8	315	CHL	CHD-C1D-ND	-4.00	120.78	124.45
27	6	311	CHL	C2C-C1C-NC	4.00	113.72	109.97
27	6	316	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
27	4	315	CHL	C4D-CHA-C1A	-4.00	116.38	121.25
27	6	308	CHL	CAC-C3C-C4C	3.99	129.99	124.81
27	8	318	CHL	CHD-C1D-ND	-3.99	120.78	124.45
27	7	311	CHL	C1C-C2C-C3C	-3.99	102.76	106.96
27	a	319	CHL	C2D-C1D-ND	3.99	113.05	110.10
27	8	320	CHL	CHD-C1D-ND	-3.99	120.78	124.45
27	3	318	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
27	5	315	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
27	8	325	CHL	C4D-CHA-C1A	-3.99	116.39	121.25
27	3	315	CHL	O1D-CGD-CBD	-3.99	116.31	124.48
27	5	317	CHL	CGD-CBD-CAD	3.99	123.67	110.73
27	B	836	CHL	CHD-C1D-ND	-3.99	120.79	124.45
27	K	204	CHL	O2D-CGD-O1D	-3.99	116.04	123.84
27	3	308	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
27	4	306	CHL	C2D-C1D-ND	3.99	113.04	110.10
27	7	321	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
27	5	308	CHL	O2D-CGD-O1D	-3.99	116.04	123.84
27	3	320	CHL	C4D-CHA-C1A	-3.99	116.40	121.25
27	7	317	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
27	a	309	CHL	C2D-C1D-ND	3.98	113.04	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	302	LUT	C7-C6-C5	-3.98	111.81	121.46
27	A	858	CHL	CHD-C4C-C3C	-3.98	118.99	124.84
27	A	855	CHL	C4D-CHA-C1A	-3.98	116.41	121.25
27	A	833	CHL	C1C-C2C-C3C	-3.98	103.96	107.11
29	5	302	LUT	C1-C6-C5	-3.98	117.01	122.61
27	F	309	CHL	O2D-CGD-O1D	-3.98	116.06	123.84
27	A	843	CHL	CHD-C1D-ND	-3.98	120.80	124.45
27	B	841	CHL	O1D-CGD-CBD	-3.97	116.35	124.48
27	A	824	CHL	CHD-C4C-C3C	-3.97	119.00	124.84
27	b	313	CHL	CHD-C4C-C3C	-3.97	119.00	124.84
27	A	818	CHL	C4D-CHA-C1A	-3.97	116.41	121.25
27	6	315	CHL	CHD-C1D-ND	-3.97	120.80	124.45
27	b	305	CHL	CHD-C1D-ND	-3.97	120.80	124.45
27	6	308	CHL	C3B-C4B-NB	3.97	114.35	109.21
29	4	301	LUT	C7-C8-C9	-3.97	120.23	126.23
27	3	312	CHL	C2D-C1D-ND	3.97	113.03	110.10
27	B	848	CHL	CHD-C4C-C3C	-3.97	119.00	124.84
27	B	817	CHL	CHD-C1D-ND	-3.97	120.81	124.45
27	A	816	CHL	CHD-C1D-ND	-3.97	120.81	124.45
27	B	824	CHL	O1D-CGD-CBD	-3.97	116.36	124.48
27	B	843	CHL	C4D-CHA-C1A	-3.97	116.42	121.25
27	a	312	CHL	C2D-C1D-ND	3.96	113.03	110.10
27	5	318	CHL	O1D-CGD-CBD	-3.96	116.38	124.48
27	A	857	CHL	O2D-CGD-O1D	-3.96	116.09	123.84
27	B	814	CHL	O2D-CGD-O1D	-3.96	116.10	123.84
27	B	849	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
27	B	848	CHL	CHD-C1D-ND	-3.96	120.82	124.45
27	5	309	CHL	C2D-C1D-ND	3.96	113.02	110.10
27	7	314	CHL	C1C-C2C-C3C	-3.95	102.80	106.96
27	4	317	CHL	C2C-C1C-NC	3.95	113.68	109.97
27	6	316	CHL	CGD-CBD-CAD	3.95	123.54	110.73
27	A	853	CHL	C2D-C1D-ND	3.95	113.02	110.10
27	3	316	CHL	CHD-C4C-C3C	-3.95	119.03	124.84
29	4	301	LUT	C1-C6-C5	-3.95	117.05	122.61
27	A	859	CHL	O2D-CGD-O1D	-3.95	116.11	123.84
27	K	205	CHL	C2D-C1D-ND	3.95	113.02	110.10
27	6	313	CHL	C2D-C1D-ND	3.95	113.01	110.10
27	B	834	CHL	CHD-C1D-ND	-3.95	120.83	124.45
27	B	821	CHL	C4D-CHA-C1A	-3.95	116.44	121.25
27	A	827	CHL	O2D-CGD-CBD	3.95	118.28	111.27
27	B	838	CHL	C2D-C1D-ND	3.95	113.01	110.10
27	7	323	CHL	CHD-C4C-C3C	-3.95	119.04	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	306	CHL	C1C-C2C-C3C	-3.94	102.81	106.96
27	6	316	CHL	O2D-CGD-O1D	-3.94	116.13	123.84
27	8	315	CHL	C2C-C1C-NC	3.94	113.67	109.97
27	A	841	CHL	C1C-C2C-C3C	-3.94	103.99	107.11
27	8	318	CHL	O1D-CGD-CBD	-3.94	116.42	124.48
27	8	319	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
29	J	103	LUT	C7-C6-C5	-3.94	111.92	121.46
27	B	814	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
27	8	320	CHL	C4D-CHA-C1A	-3.94	116.46	121.25
27	5	317	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
27	3	313	CHL	C4D-CHA-C1A	-3.93	116.47	121.25
27	b	308	CHL	CMC-C2C-C3C	3.93	136.79	126.12
27	b	313	CHL	C4D-CHA-C1A	-3.93	116.47	121.25
27	7	320	CHL	O2D-CGD-O1D	-3.93	116.16	123.84
27	3	313	CHL	C2D-C1D-ND	3.93	113.00	110.10
27	B	820	CHL	O2D-CGD-O1D	-3.93	116.16	123.84
27	5	311	CHL	O2D-CGD-O1D	-3.93	116.16	123.84
27	4	317	CHL	C1C-C2C-C3C	-3.93	102.83	106.96
27	3	315	CHL	O2D-CGD-CBD	3.93	118.25	111.27
27	B	846	CHL	CHD-C4C-C3C	-3.93	119.07	124.84
27	b	317	CHL	CHD-C4C-C3C	-3.92	119.07	124.84
27	B	851	CHL	C4D-CHA-C1A	-3.92	116.47	121.25
27	A	821	CHL	CHD-C4C-C3C	-3.92	119.07	124.84
27	7	316	CHL	C2D-C1D-ND	3.92	112.99	110.10
29	3	304	LUT	C7-C6-C5	-3.92	111.97	121.46
34	8	301	SQD	O47-C7-C8	3.92	119.95	111.50
27	b	309	CHL	C2D-C1D-ND	3.92	112.99	110.10
27	A	827	CHL	CHD-C1D-ND	-3.92	120.86	124.45
27	a	320	CHL	C4D-CHA-C1A	-3.92	116.48	121.25
27	A	842	CHL	CHD-C4C-C3C	-3.92	119.08	124.84
27	3	320	CHL	O1D-CGD-CBD	-3.91	116.47	124.48
29	4	302	LUT	C7-C8-C9	-3.91	120.32	126.23
27	5	323	CHL	CHD-C4C-C3C	-3.91	119.09	124.84
27	5	318	CHL	CHD-C4C-C3C	-3.91	119.09	124.84
27	A	850	CHL	CHD-C4C-C3C	-3.91	119.09	124.84
27	a	315	CHL	CHD-C1D-ND	-3.91	120.86	124.45
27	A	844	CHL	CHD-C4C-C3C	-3.91	119.09	124.84
27	A	833	CHL	CGD-CBD-CAD	3.91	123.38	110.73
27	B	811	CHL	CHD-C1D-ND	-3.90	120.87	124.45
27	A	819	CHL	C2C-C1C-NC	3.90	113.63	109.97
27	8	313	CHL	C4D-CHA-C1A	-3.90	116.50	121.25
27	5	310	CHL	O2D-CGD-O1D	-3.90	116.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	8	303	LUT	C7-C8-C9	-3.90	120.35	126.23
27	A	857	CHL	CHD-C1D-ND	-3.90	120.87	124.45
27	K	206	CHL	CHD-C4C-C3C	-3.90	119.11	124.84
27	5	321	CHL	CHD-C1D-ND	-3.89	120.88	124.45
27	A	825	CHL	CHD-C4C-C3C	-3.89	119.12	124.84
27	6	317	CHL	C4D-CHA-C1A	-3.89	116.51	121.25
27	B	833	CHL	C2D-C1D-ND	3.89	112.97	110.10
27	A	859	CHL	CHD-C4C-C3C	-3.89	119.12	124.84
27	B	834	CHL	C1C-C2C-C3C	-3.89	102.87	106.96
27	3	308	CHL	C4D-CHA-C1A	-3.89	116.52	121.25
27	J	106	CHL	CHD-C1D-ND	-3.89	120.88	124.45
27	4	318	CHL	CHD-C4C-C3C	-3.89	119.13	124.84
27	A	831	CHL	C4C-C3C-C2C	-3.89	101.23	106.90
27	B	827	CHL	O2D-CGD-O1D	-3.88	116.25	123.84
27	A	822	CHL	C4D-CHA-C1A	-3.88	116.52	121.25
29	5	302	LUT	C21-C26-C27	-3.88	107.79	112.70
27	B	822	CHL	C1C-C2C-C3C	-3.88	102.88	106.96
27	A	837	CHL	CHD-C1D-ND	-3.88	120.89	124.45
27	A	828	CHL	O1D-CGD-CBD	-3.88	116.55	124.48
27	B	851	CHL	CHD-C1D-ND	-3.88	120.89	124.45
27	8	320	CHL	CHD-C4C-C3C	-3.87	119.14	124.84
27	8	319	CHL	C4D-CHA-C1A	-3.87	116.54	121.25
27	8	323	CHL	C1C-C2C-C3C	-3.87	102.89	106.96
27	7	323	CHL	CHC-C1C-NC	-3.87	118.33	124.20
27	a	316	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
27	5	309	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
27	7	314	CHL	O1D-CGD-CBD	-3.87	116.56	124.48
27	A	856	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
27	A	845	CHL	CHD-C1D-ND	-3.87	120.90	124.45
27	7	316	CHL	CHD-C1D-ND	-3.87	120.90	124.45
27	b	314	CHL	CHD-C1D-ND	-3.87	120.90	124.45
27	A	822	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
27	3	319	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
27	4	318	CHL	C2D-C1D-ND	3.87	112.96	110.10
27	L	304	CHL	C2D-C1D-ND	3.87	112.96	110.10
29	6	303	LUT	C21-C26-C27	-3.87	107.81	112.70
27	5	309	CHL	C4D-CHA-C1A	-3.87	116.54	121.25
27	8	312	CHL	C4D-CHA-C1A	-3.87	116.54	121.25
27	A	832	CHL	C4-C3-C5	3.87	121.78	115.27
29	5	303	LUT	C1-C6-C5	-3.87	117.17	122.61
27	A	836	CHL	O1D-CGD-CBD	-3.87	116.57	124.48
27	6	305	CHL	CHD-C4C-C3C	-3.87	119.16	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	317	CHL	O2D-CGD-O1D	-3.86	116.28	123.84
27	3	319	CHL	C2D-C1D-ND	3.86	112.95	110.10
22	B	806	BCR	C15-C16-C17	-3.86	115.57	123.47
27	5	325	CHL	CGD-CBD-CAD	3.86	123.23	110.73
27	K	206	CHL	O1D-CGD-CBD	-3.86	116.59	124.48
27	B	834	CHL	CHA-C4D-ND	3.86	140.57	132.50
27	A	839	CHL	CHD-C4C-C3C	-3.86	119.17	124.84
27	A	828	CHL	C1C-C2C-C3C	-3.86	102.90	106.96
27	a	319	CHL	CHD-C4C-C3C	-3.86	119.17	124.84
27	B	837	CHL	CHD-C1D-ND	-3.86	120.91	124.45
27	5	311	CHL	CHD-C4C-C3C	-3.85	119.17	124.84
27	3	321	CHL	CHD-C1D-ND	-3.85	120.91	124.45
27	B	839	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
27	A	816	CHL	O2D-CGD-O1D	-3.85	116.31	123.84
27	A	826	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
29	3	304	LUT	C21-C26-C27	-3.85	107.83	112.70
29	7	304	LUT	C21-C26-C27	-3.85	107.83	112.70
27	7	324	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
29	5	302	LUT	C35-C15-C14	-3.85	115.59	123.47
27	7	312	CHL	CHD-C1D-ND	-3.85	120.92	124.45
27	B	812	CHL	C2C-C1C-NC	3.85	113.58	109.97
27	4	311	CHL	CHD-C4C-C3C	-3.85	119.19	124.84
27	A	847	CHL	C4D-CHA-C1A	-3.85	116.57	121.25
27	6	310	CHL	CHD-C4C-C3C	-3.85	119.19	124.84
27	7	318	CHL	CHD-C4C-C3C	-3.85	119.19	124.84
22	A	803	BCR	C2-C1-C6	3.84	116.40	110.48
27	7	316	CHL	C4D-CHA-C1A	-3.84	116.57	121.25
27	A	852	CHL	CHD-C1D-ND	-3.84	120.92	124.45
27	A	850	CHL	O2D-CGD-O1D	-3.84	116.33	123.84
27	a	310	CHL	CHD-C1D-ND	-3.84	120.93	124.45
27	A	845	CHL	C2D-C1D-ND	3.84	112.93	110.10
27	a	310	CHL	O1D-CGD-CBD	-3.84	116.63	124.48
27	B	838	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
27	8	325	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
27	5	312	CHL	O2D-CGD-CBD	3.84	118.08	111.27
27	5	312	CHL	CHD-C4C-C3C	-3.83	119.21	124.84
27	B	838	CHL	O2D-CGD-O1D	-3.83	116.35	123.84
27	5	317	CHL	CHD-C1D-ND	-3.83	120.93	124.45
27	6	312	CHL	CHD-C1D-ND	-3.83	120.93	124.45
27	A	858	CHL	C4-C3-C5	3.83	121.71	115.27
27	6	312	CHL	O1D-CGD-CBD	-3.83	116.65	124.48
27	B	833	CHL	CHD-C4C-C3C	-3.83	119.21	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	303	LUT	C15-C35-C34	3.83	131.31	123.47
27	a	309	CHL	CHD-C4C-C3C	-3.82	119.22	124.84
27	4	306	CHL	C4D-CHA-C1A	-3.82	116.60	121.25
27	A	852	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
27	A	826	CHL	C4D-CHA-C1A	-3.82	116.60	121.25
27	F	309	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
27	A	853	CHL	C4D-CHA-C1A	-3.82	116.61	121.25
27	a	319	CHL	C1-C2-C3	-3.81	120.58	126.75
27	B	819	CHL	C4D-CHA-C1A	-3.81	116.61	121.25
27	7	316	CHL	CHD-C4C-C3C	-3.81	119.02	124.98
27	3	314	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
27	A	821	CHL	CHA-C4D-ND	3.81	140.47	132.50
27	b	306	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
27	3	309	CHL	C4D-CHA-C1A	-3.81	116.61	121.25
27	a	317	CHL	C4D-CHA-C1A	-3.81	116.62	121.25
27	A	837	CHL	O2D-CGD-O1D	-3.81	116.40	123.84
27	F	308	CHL	C4D-CHA-C1A	-3.80	116.62	121.25
27	6	315	CHL	CHD-C4C-C3C	-3.80	119.25	124.84
29	b	303	LUT	C35-C15-C14	3.80	131.27	123.47
27	6	315	CHL	C2D-C1D-ND	3.80	112.91	110.10
27	A	828	CHL	CHD-C4C-C3C	-3.80	119.25	124.84
27	A	844	CHL	C2D-C1D-ND	3.80	112.91	110.10
27	7	311	CHL	O2D-CGD-O1D	-3.80	116.41	123.84
27	B	843	CHL	CHD-C1D-ND	-3.80	120.96	124.45
27	B	823	CHL	O2D-CGD-O1D	-3.80	116.41	123.84
34	8	301	SQD	O9-S-O7	-3.80	100.81	113.95
27	A	820	CHL	C4D-CHA-C1A	-3.80	116.63	121.25
27	B	815	CHL	C4D-CHA-C1A	-3.80	116.63	121.25
27	6	308	CHL	C2D-C1D-ND	3.80	112.90	110.10
27	8	317	CHL	CHD-C1D-ND	-3.79	120.97	124.45
27	A	838	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
27	a	312	CHL	O1D-CGD-CBD	-3.79	116.72	124.48
27	8	315	CHL	O1D-CGD-CBD	-3.79	116.72	124.48
27	B	825	CHL	CHA-C4D-ND	3.79	140.43	132.50
27	4	319	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
27	b	316	CHL	CGD-CBD-CAD	3.79	123.01	110.73
27	A	817	CHL	O2D-CGD-O1D	-3.79	116.43	123.84
27	L	303	CHL	C4C-C3C-C2C	-3.79	101.38	106.90
29	a	302	LUT	C7-C8-C9	-3.79	120.51	126.23
27	4	305	CHL	CHA-C4D-ND	3.79	140.42	132.50
27	A	843	CHL	CMB-C2B-C3B	3.79	131.76	124.68
28	7	307	DGD	O3G-C3G-C2G	-3.79	101.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	828	CHL	CHD-C4C-C3C	-3.78	119.28	124.84
27	8	325	CHL	O2D-CGD-O1D	-3.78	116.44	123.84
27	L	304	CHL	O1D-CGD-CBD	-3.78	116.75	124.48
27	B	827	CHL	C4D-CHA-C1A	-3.78	116.65	121.25
27	B	844	CHL	O2D-CGD-O1D	-3.78	116.45	123.84
27	B	822	CHL	CHD-C4C-C3C	-3.78	119.28	124.84
27	B	835	CHL	CHD-C4C-C3C	-3.77	119.29	124.84
27	b	308	CHL	C1D-ND-C4D	-3.77	103.65	106.33
29	7	304	LUT	C2-C3-C4	3.77	115.47	110.30
27	4	305	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
27	A	831	CHL	CMB-C2B-C3B	3.77	131.73	124.68
27	6	310	CHL	CHA-C4D-ND	3.77	140.39	132.50
27	6	310	CHL	O2D-CGD-O1D	-3.77	116.47	123.84
27	5	322	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
27	K	206	CHL	C4D-CHA-C1A	-3.77	116.67	121.25
27	5	312	CHL	O1D-CGD-CBD	-3.77	116.78	124.48
27	b	310	CHL	C2D-C1D-ND	3.77	112.88	110.10
27	A	836	CHL	C4D-CHA-C1A	-3.77	116.67	121.25
27	a	315	CHL	CGD-CBD-CAD	3.76	122.93	110.73
27	A	858	CHL	CHD-C1D-ND	-3.76	121.00	124.45
22	K	203	BCR	C2-C1-C6	3.76	116.27	110.48
27	a	320	CHL	CHD-C4C-C3C	-3.76	119.31	124.84
27	3	316	CHL	CGD-CBD-CAD	3.76	122.91	110.73
27	8	315	CHL	C4D-CHA-C1A	-3.76	116.67	121.25
27	8	316	CHL	C4D-CHA-C1A	-3.76	116.67	121.25
27	5	321	CHL	O2D-CGD-O1D	-3.76	116.50	123.84
27	A	824	CHL	O2D-CGD-O1D	-3.75	116.50	123.84
27	B	831	CHL	C4D-CHA-C1A	-3.75	116.68	121.25
27	B	823	CHL	C4D-CHA-C1A	-3.75	116.68	121.25
27	6	318	CHL	CGD-CBD-CAD	3.75	122.88	110.73
27	8	324	CHL	O1D-CGD-CBD	-3.75	116.81	124.48
27	K	204	CHL	O1D-CGD-CBD	-3.75	116.82	124.48
27	B	844	CHL	CHD-C4C-C3C	-3.75	119.33	124.84
27	A	852	CHL	C4D-CHA-C1A	-3.75	116.69	121.25
27	8	317	CHL	C4D-CHA-C1A	-3.75	116.69	121.25
27	5	323	CHL	O1D-CGD-CBD	-3.74	116.82	124.48
27	A	854	CHL	C4D-CHA-C1A	-3.74	116.69	121.25
27	B	832	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
27	6	320	CHL	C4D-CHA-C1A	-3.74	116.70	121.25
27	B	813	CHL	O1D-CGD-CBD	-3.74	116.83	124.48
27	A	820	CHL	C2C-C1C-NC	3.74	113.47	109.97
27	4	309	CHL	CGD-CBD-CAD	3.73	122.83	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	835	CHL	O1D-CGD-CBD	-3.73	116.84	124.48
27	6	311	CHL	CHD-C1D-ND	-3.73	121.02	124.45
27	a	316	CHL	CGD-CBD-CAD	3.73	122.82	110.73
27	6	309	CHL	C4D-CHA-C1A	-3.73	116.71	121.25
27	B	839	CHL	C4D-CHA-C1A	-3.73	116.71	121.25
27	F	309	CHL	CHA-C4D-ND	3.73	140.29	132.50
27	b	311	CHL	CGD-CBD-CAD	3.72	122.80	110.73
27	3	313	CHL	O2D-CGD-O1D	-3.72	116.56	123.84
27	b	309	CHL	CHD-C4C-C3C	-3.72	119.37	124.84
27	4	314	CHL	CHA-C4D-ND	3.72	140.28	132.50
27	b	317	CHL	CGD-CBD-CAD	3.72	122.77	110.73
27	a	307	CHL	O1D-CGD-CBD	-3.72	116.88	124.48
27	6	316	CHL	CHD-C1D-ND	-3.71	121.04	124.45
27	B	817	CHL	O1D-CGD-CBD	-3.71	116.88	124.48
27	5	322	CHL	CGD-CBD-CAD	3.71	122.76	110.73
27	3	309	CHL	CHD-C1D-ND	-3.71	121.04	124.45
27	8	324	CHL	CHD-C4C-C3C	-3.71	119.39	124.84
27	7	323	CHL	CMD-C2D-C3D	-3.71	119.08	127.61
27	a	315	CHL	C1-C2-C3	-3.71	119.63	126.04
27	A	852	CHL	CHA-C4D-ND	3.71	140.26	132.50
27	a	307	CHL	C4D-CHA-C1A	-3.71	116.74	121.25
27	3	311	CHL	O2D-CGD-O1D	-3.71	116.59	123.84
27	B	822	CHL	C4D-CHA-C1A	-3.71	116.74	121.25
27	b	315	CHL	CHA-C4D-ND	3.71	140.25	132.50
27	3	309	CHL	O1D-CGD-CBD	-3.70	116.90	124.48
27	A	840	CHL	C4D-CHA-C1A	-3.70	116.74	121.25
27	B	831	CHL	O2D-CGD-O1D	-3.70	116.60	123.84
27	8	319	CHL	C4-C3-C5	3.70	121.49	115.27
27	4	312	CHL	CGD-CBD-CAD	3.70	122.72	110.73
27	8	318	CHL	O2D-CGD-CBD	3.70	117.84	111.27
27	A	845	CHL	C4D-CHA-C1A	-3.70	116.75	121.25
27	A	828	CHL	CHD-C1D-ND	-3.70	121.06	124.45
27	A	840	CHL	O1D-CGD-CBD	-3.70	116.92	124.48
27	3	320	CHL	C1C-C2C-C3C	-3.70	103.07	106.96
29	F	303	LUT	C7-C6-C5	-3.70	112.51	121.46
29	6	303	LUT	C18-C5-C4	-3.69	107.51	114.36
27	8	315	CHL	CMC-C2C-C1C	3.69	130.66	125.04
29	a	302	LUT	C1-C6-C5	-3.69	117.41	122.61
27	8	322	CHL	C4D-CHA-C1A	-3.69	116.76	121.25
27	a	317	CHL	CHD-C4C-C3C	-3.69	119.42	124.84
27	A	858	CHL	C4D-CHA-C1A	-3.69	116.76	121.25
27	B	851	CHL	C1C-C2C-C3C	-3.69	103.08	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	317	CHL	CHA-C4D-ND	3.69	140.22	132.50
27	B	828	CHL	O1D-CGD-CBD	-3.69	116.94	124.48
27	3	320	CHL	CHD-C4C-NC	3.69	130.01	124.20
27	3	312	CHL	CHA-C4D-ND	3.69	140.21	132.50
27	3	319	CHL	C4D-CHA-C1A	-3.69	116.76	121.25
27	A	841	CHL	CGD-CBD-CAD	3.69	122.67	110.73
27	6	309	CHL	CHA-C4D-ND	3.68	140.21	132.50
27	A	840	CHL	CHA-C4D-ND	3.68	140.21	132.50
27	4	311	CHL	C4D-CHA-C1A	-3.68	116.77	121.25
27	5	319	CHL	CGD-CBD-CAD	3.68	122.66	110.73
27	A	817	CHL	CHD-C4C-C3C	-3.68	119.43	124.84
27	B	851	CHL	C2C-C1C-NC	3.68	113.42	109.97
29	4	301	LUT	C35-C15-C14	-3.68	115.94	123.47
27	B	844	CHL	C4D-CHA-C1A	-3.68	116.77	121.25
27	7	313	CHL	CHA-C4D-ND	3.68	140.19	132.50
27	8	313	CHL	CHD-C1D-ND	-3.68	121.08	124.45
27	B	850	CHL	CHA-C4D-ND	3.67	140.19	132.50
27	6	307	CHL	C1B-CHB-C4A	-3.67	122.84	130.12
27	4	319	CHL	O2D-CGD-O1D	-3.67	116.66	123.84
27	B	845	CHL	C4D-CHA-C1A	-3.67	116.78	121.25
27	7	312	CHL	CHA-C4D-ND	3.67	140.18	132.50
27	a	315	CHL	CHD-C4C-C3C	-3.67	119.44	124.84
27	4	306	CHL	CHD-C4C-C3C	-3.67	119.44	124.84
27	B	834	CHL	C4D-CHA-C1A	-3.67	116.78	121.25
29	b	303	LUT	C20-C13-C14	-3.67	117.79	122.92
27	8	324	CHL	CGD-CBD-CAD	3.67	122.61	110.73
27	3	316	CHL	CHD-C1D-ND	-3.66	121.09	124.45
29	8	303	LUT	C18-C5-C4	-3.66	107.57	114.36
27	3	313	CHL	CHD-C4C-C3C	-3.66	119.46	124.84
27	7	313	CHL	CHD-C4C-C3C	-3.66	119.46	124.84
29	a	304	LUT	C10-C11-C12	-3.66	111.79	123.22
29	3	305	LUT	C7-C8-C9	-3.66	120.70	126.23
27	A	856	CHL	CHD-C1D-ND	-3.66	121.09	124.45
27	B	814	CHL	C4D-CHA-C1A	-3.66	116.79	121.25
27	7	311	CHL	C4D-CHA-C1A	-3.66	116.79	121.25
27	B	822	CHL	CHD-C1D-ND	-3.66	121.09	124.45
29	a	302	LUT	C35-C15-C14	-3.66	115.98	123.47
27	4	317	CHL	CMD-C2D-C3D	-3.66	119.20	127.61
27	a	316	CHL	CHD-C1D-ND	-3.66	121.09	124.45
22	6	301	BCR	C15-C16-C17	3.65	130.96	123.47
27	b	304	CHL	CHD-C4C-C3C	-3.65	119.47	124.84
27	b	314	CHL	CHA-C4D-ND	3.65	140.14	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	312	CHL	CHD-C4C-C3C	-3.65	119.28	124.98
27	B	815	CHL	CHA-C4D-ND	3.65	140.14	132.50
29	3	304	LUT	C1-C6-C5	-3.65	117.47	122.61
27	A	820	CHL	O1D-CGD-CBD	-3.65	117.02	124.48
27	a	311	CHL	CHA-C4D-ND	3.65	140.13	132.50
27	B	834	CHL	O1D-CGD-CBD	-3.65	117.02	124.48
27	6	319	CHL	C3C-C4C-NC	3.65	114.66	110.57
27	A	827	CHL	C4D-CHA-C1A	-3.65	116.81	121.25
27	F	309	CHL	C4D-CHA-C1A	-3.65	116.81	121.25
27	B	837	CHL	CHA-C4D-ND	3.64	140.12	132.50
27	b	310	CHL	CHD-C4C-C3C	-3.64	119.48	124.84
27	5	307	CHL	O1D-CGD-CBD	-3.64	117.03	124.48
27	B	830	CHL	CHD-C1D-ND	-3.64	121.11	124.45
27	B	838	CHL	CHD-C1D-ND	-3.64	121.11	124.45
27	B	845	CHL	O2D-CGD-O1D	-3.64	116.72	123.84
27	B	819	CHL	O1D-CGD-CBD	-3.64	117.03	124.48
27	4	311	CHL	CHA-C4D-ND	3.64	140.12	132.50
29	5	302	LUT	C7-C6-C5	-3.64	112.64	121.46
27	B	843	CHL	CMB-C2B-C3B	3.64	131.49	124.68
27	4	308	CHL	CHA-C4D-ND	3.64	140.11	132.50
27	b	305	CHL	O2D-CGD-O1D	-3.64	116.72	123.84
27	a	309	CHL	O2D-CGD-O1D	-3.64	116.73	123.84
27	B	836	CHL	CHD-C4C-C3C	-3.64	119.50	124.84
27	B	832	CHL	CHA-C4D-ND	3.64	140.10	132.50
27	B	847	CHL	C4D-CHA-C1A	-3.64	116.83	121.25
27	7	312	CHL	C4C-C3C-C2C	-3.63	103.74	107.07
27	7	315	CHL	CHA-C4D-ND	3.63	140.10	132.50
27	8	311	CHL	C4D-CHA-C1A	-3.63	116.83	121.25
27	K	205	CHL	CHA-C4D-ND	3.63	140.09	132.50
27	7	317	CHL	CHA-C4D-ND	3.63	140.09	132.50
27	A	854	CHL	CHA-C4D-ND	3.63	140.09	132.50
27	4	312	CHL	CHD-C4C-C3C	-3.63	119.51	124.84
27	K	207	CHL	CGD-CBD-CAD	3.63	122.48	110.73
27	8	322	CHL	CHD-C4C-NC	3.62	129.91	124.20
27	B	847	CHL	O1D-CGD-CBD	-3.62	117.07	124.48
27	b	312	CHL	CHA-C4D-ND	3.62	140.08	132.50
27	7	317	CHL	CHD-C1D-ND	-3.62	121.12	124.45
27	A	849	CHL	CHD-C4C-C3C	-3.62	119.52	124.84
27	a	310	CHL	CHA-C4D-ND	3.62	140.07	132.50
27	4	306	CHL	CHA-C4D-ND	3.62	140.07	132.50
29	b	301	LUT	C1-C6-C5	-3.62	117.52	122.61
27	5	312	CHL	CHA-C4D-ND	3.62	140.06	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	319	CHL	CHA-C4D-ND	3.62	140.06	132.50
27	B	851	CHL	CHA-C4D-ND	3.62	140.06	132.50
27	B	828	CHL	O2D-CGD-O1D	-3.61	116.77	123.84
27	B	822	CHL	CHA-C4D-ND	3.61	140.06	132.50
27	3	312	CHL	CHD-C4C-C3C	-3.61	119.53	124.84
27	B	834	CHL	O2D-CGD-CBD	3.61	117.68	111.27
27	3	319	CHL	CHD-C1D-ND	-3.61	121.14	124.45
27	3	320	CHL	C2C-C1C-NC	3.61	113.35	109.97
27	A	840	CHL	CHD-C4C-C3C	-3.61	119.54	124.84
27	7	314	CHL	C4D-CHA-C1A	-3.61	116.86	121.25
27	B	851	CHL	O2D-CGD-O1D	-3.61	116.79	123.84
26	A	815	CL0	C2A-C1A-CHA	-3.61	117.56	123.86
27	B	828	CHL	C4D-CHA-C1A	-3.60	116.86	121.25
27	B	836	CHL	C4D-CHA-C1A	-3.60	116.86	121.25
27	8	315	CHL	CHD-C4C-NC	3.60	129.88	124.20
27	6	312	CHL	CHA-C4D-ND	3.60	140.03	132.50
27	A	835	CHL	CHA-C4D-ND	3.60	140.03	132.50
27	A	853	CHL	CHA-C4D-ND	3.59	140.02	132.50
27	b	305	CHL	C2D-C1D-ND	3.59	112.75	110.10
27	B	835	CHL	CHA-C4D-ND	3.59	140.01	132.50
27	B	819	CHL	CHA-C4D-ND	3.59	140.01	132.50
27	B	847	CHL	CHA-C4D-ND	3.59	140.01	132.50
27	5	310	CHL	CHD-C1D-ND	-3.59	121.16	124.45
27	B	833	CHL	O1D-CGD-CBD	-3.59	117.14	124.48
27	5	311	CHL	O1D-CGD-CBD	-3.59	117.14	124.48
27	b	307	CHL	C4D-CHA-C1A	-3.59	116.88	121.25
27	A	834	CHL	C4D-CHA-C1A	-3.59	116.88	121.25
27	4	320	CHL	CHD-C4C-C3C	-3.59	119.57	124.84
27	3	315	CHL	C4-C3-C5	3.59	121.30	115.27
27	5	323	CHL	CHA-C4D-ND	3.59	140.00	132.50
27	B	832	CHL	O1D-CGD-CBD	-3.59	117.15	124.48
27	5	311	CHL	CHA-C4D-ND	3.58	140.00	132.50
27	7	315	CHL	C4D-CHA-C1A	-3.58	116.89	121.25
27	A	839	CHL	CHA-C4D-ND	3.58	140.00	132.50
31	a	303	AXT	C3-C4-C5	3.58	118.99	111.85
26	A	815	CL0	CBC-CAC-C3C	-3.58	102.56	112.43
27	B	824	CHL	CHA-C4D-ND	3.58	139.99	132.50
27	A	838	CHL	CHA-C4D-ND	3.58	139.99	132.50
27	8	323	CHL	C3D-C2D-C1D	-3.58	100.95	105.83
27	A	834	CHL	O1D-CGD-CBD	-3.58	117.17	124.48
27	7	322	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
29	3	305	LUT	C21-C26-C27	-3.57	108.18	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	814	CHL	O1D-CGD-CBD	-3.57	117.18	124.48
27	K	205	CHL	O2D-CGD-O1D	-3.57	116.86	123.84
27	A	825	CHL	C1-C2-C3	-3.57	119.87	126.04
27	6	306	CHL	C4-C3-C5	3.57	121.28	115.27
27	6	313	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
27	b	315	CHL	C1-C2-C3	-3.57	119.87	126.04
26	A	815	CL0	C1D-CHD-C4C	-3.57	118.36	126.06
27	J	106	CHL	C4D-CHA-C1A	-3.57	116.91	121.25
27	B	846	CHL	CHD-C1D-ND	-3.56	121.18	124.45
27	A	843	CHL	C16-C15-C13	-3.56	104.41	115.92
27	B	844	CHL	CHA-C4D-ND	3.56	139.95	132.50
27	8	311	CHL	CHA-C4D-ND	3.56	139.95	132.50
27	B	824	CHL	C4D-CHA-C1A	-3.56	116.92	121.25
27	A	821	CHL	O2D-CGD-O1D	-3.56	116.88	123.84
27	A	828	CHL	C4D-CHA-C1A	-3.56	116.92	121.25
27	B	820	CHL	CHA-C4D-ND	3.56	139.94	132.50
27	6	311	CHL	O1D-CGD-CBD	-3.56	117.21	124.48
27	4	315	CHL	CHD-C4C-C3C	-3.56	119.61	124.84
27	b	310	CHL	O2D-CGD-O1D	-3.55	116.89	123.84
27	B	816	CHL	CHD-C4C-C3C	-3.55	119.62	124.84
27	A	828	CHL	CHA-C4D-ND	3.55	139.93	132.50
33	7	305	XAT	C35-C15-C14	3.55	130.75	123.47
27	A	850	CHL	CHD-C1D-ND	-3.55	121.19	124.45
27	6	306	CHL	CHA-C4D-ND	3.55	139.93	132.50
27	7	318	CHL	CHA-C4D-ND	3.55	139.93	132.50
27	3	308	CHL	CHA-C4D-ND	3.55	139.92	132.50
27	B	850	CHL	C4D-CHA-C1A	-3.55	116.93	121.25
27	A	819	CHL	CHD-C4C-NC	3.55	129.79	124.20
27	5	320	CHL	CHD-C4C-C3C	-3.55	119.63	124.84
27	B	831	CHL	CHD-C4C-C3C	-3.55	119.63	124.84
27	4	316	CHL	CGD-CBD-CAD	3.54	122.21	110.73
27	4	320	CHL	CHA-C4D-ND	3.54	139.91	132.50
27	8	326	CHL	CHD-C4C-NC	3.54	129.78	124.20
22	J	102	BCR	C2-C1-C6	3.54	115.93	110.48
27	A	847	CHL	CHA-C4D-ND	3.54	139.90	132.50
27	A	841	CHL	C4D-C3D-CAD	3.54	112.27	108.10
27	a	320	CHL	CHA-C4D-ND	3.53	139.89	132.50
27	6	313	CHL	CHA-C4D-ND	3.53	139.89	132.50
27	8	320	CHL	CHA-C4D-ND	3.53	139.89	132.50
27	A	832	CHL	O1D-CGD-CBD	-3.53	117.25	124.48
27	7	317	CHL	C4D-CHA-C1A	-3.53	116.95	121.25
27	B	818	CHL	CHD-C1D-ND	-3.53	121.21	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	306	CHL	C4D-CHA-C1A	-3.53	116.95	121.25
27	5	325	CHL	CHD-C1D-ND	-3.53	121.21	124.45
29	J	103	LUT	C8-C7-C6	-3.53	117.29	127.20
27	b	312	CHL	CHD-C4C-C3C	-3.53	119.65	124.84
27	5	310	CHL	CHA-C4D-ND	3.53	139.88	132.50
27	B	845	CHL	CHA-C4D-ND	3.53	139.88	132.50
27	A	830	CHL	C4D-CHA-C1A	-3.53	116.96	121.25
27	B	826	CHL	CHD-C1D-ND	-3.52	121.22	124.45
27	B	842	CHL	CHD-C4C-NC	3.52	129.75	124.20
27	4	319	CHL	C2D-C1D-ND	3.52	112.70	110.10
27	7	320	CHL	CGD-CBD-CAD	3.52	122.14	110.73
27	F	309	CHL	CHD-C1D-ND	-3.52	121.22	124.45
27	B	841	CHL	C1C-C2C-C3C	-3.52	103.26	106.96
27	B	848	CHL	CHA-C4D-ND	3.52	139.86	132.50
27	A	839	CHL	C4D-CHA-C1A	-3.52	116.97	121.25
27	a	314	CHL	C4D-CHA-C1A	-3.52	116.97	121.25
27	5	315	CHL	CHA-C4D-ND	3.52	139.86	132.50
27	a	315	CHL	O2D-CGD-O1D	-3.52	116.96	123.84
27	B	836	CHL	CHA-C4D-ND	3.52	139.86	132.50
27	B	838	CHL	CHA-C4D-ND	3.52	139.86	132.50
27	3	310	CHL	CHA-C4D-ND	3.52	139.86	132.50
27	A	825	CHL	O2D-CGD-O1D	-3.52	116.96	123.84
28	7	307	DGD	O6D-C1D-O3G	-3.51	101.66	109.97
27	7	318	CHL	O2D-CGD-O1D	-3.51	116.97	123.84
27	B	824	CHL	CHD-C4C-C3C	-3.51	119.68	124.84
27	6	311	CHL	CHA-C4D-ND	3.51	139.84	132.50
27	b	304	CHL	CHA-C4D-ND	3.51	139.84	132.50
27	B	823	CHL	CHA-C4D-ND	3.51	139.84	132.50
27	6	317	CHL	CHD-C1D-ND	-3.51	121.23	124.45
27	a	309	CHL	CHA-C4D-ND	3.51	139.84	132.50
27	A	845	CHL	CHA-C4D-ND	3.51	139.83	132.50
27	a	309	CHL	CHD-C1D-ND	-3.51	121.23	124.45
27	A	832	CHL	CMC-C2C-C1C	3.51	130.38	125.04
27	B	843	CHL	CHA-C4D-ND	3.51	139.83	132.50
27	6	319	CHL	CAC-C3C-C4C	3.51	129.36	124.81
29	a	302	LUT	C21-C26-C27	-3.51	108.27	112.70
27	5	316	CHL	C4-C3-C5	3.50	121.17	115.27
27	A	836	CHL	CHA-C4D-ND	3.50	139.83	132.50
27	B	820	CHL	C4D-CHA-C1A	-3.50	116.99	121.25
27	6	317	CHL	CHD-C4C-C3C	-3.50	119.69	124.84
27	A	848	CHL	CHA-C4D-ND	3.50	139.82	132.50
27	A	858	CHL	CHA-C4D-ND	3.50	139.82	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	812	CHL	CHD-C4C-C3C	-3.50	119.69	124.84
26	A	815	CL0	C4A-NA-C1A	-3.50	105.13	106.71
27	3	309	CHL	CHA-C4D-ND	3.50	139.82	132.50
27	5	309	CHL	C4-C3-C5	3.50	121.16	115.27
27	A	853	CHL	CHD-C4C-C3C	-3.50	119.70	124.84
27	b	307	CHL	CHA-C4D-ND	3.50	139.81	132.50
27	5	314	CHL	CHA-C4D-ND	3.50	139.81	132.50
27	6	315	CHL	CHA-C4D-ND	3.50	139.81	132.50
27	3	312	CHL	CHD-C1D-ND	-3.50	121.24	124.45
27	5	309	CHL	CHA-C4D-ND	3.50	139.81	132.50
27	b	305	CHL	CHD-C4C-C3C	-3.50	119.70	124.84
27	7	313	CHL	CHD-C1D-ND	-3.50	121.24	124.45
29	5	303	LUT	C30-C31-C32	-3.50	112.31	123.22
27	3	321	CHL	CHA-C4D-ND	3.49	139.81	132.50
27	A	819	CHL	C4D-CHA-C1A	-3.49	117.00	121.25
27	5	323	CHL	CHD-C1D-ND	-3.49	121.24	124.45
27	6	312	CHL	CHD-C4C-C3C	-3.49	119.71	124.84
27	B	813	CHL	CMC-C2C-C1C	3.49	130.36	125.04
27	8	314	CHL	C4D-C3D-CAD	3.49	112.21	108.10
27	6	307	CHL	C4C-C3C-C2C	-3.49	101.81	106.90
27	4	320	CHL	C4D-CHA-C1A	-3.49	117.00	121.25
27	B	830	CHL	CHA-C4D-ND	3.49	139.79	132.50
27	7	320	CHL	C4D-CHA-C1A	-3.49	117.00	121.25
27	a	318	CHL	CGD-CBD-CAD	3.49	122.03	110.73
27	6	320	CHL	CHA-C4D-ND	3.49	139.79	132.50
27	8	316	CHL	CHA-C4D-ND	3.49	139.79	132.50
27	B	849	CHL	CHA-C4D-ND	3.48	139.79	132.50
27	8	314	CHL	CHD-C4C-C3C	-3.48	119.72	124.84
27	6	307	CHL	CHC-C1C-C2C	-3.48	117.08	126.72
27	4	316	CHL	CHD-C4C-C3C	-3.48	119.72	124.84
27	6	305	CHL	CHA-C4D-ND	3.48	139.78	132.50
27	3	319	CHL	CHA-C4D-ND	3.48	139.78	132.50
27	a	313	CHL	CHA-C4D-ND	3.48	139.78	132.50
27	5	318	CHL	C4D-CHA-C1A	-3.48	117.01	121.25
27	8	320	CHL	O1D-CGD-CBD	-3.48	117.36	124.48
22	A	805	BCR	C2-C1-C6	3.48	115.83	110.48
27	3	317	CHL	C4-C3-C5	3.48	121.12	115.27
27	K	207	CHL	CHD-C1D-ND	-3.48	121.26	124.45
27	A	846	CHL	CHC-C1C-C2C	-3.48	117.11	126.72
27	A	844	CHL	C1-C2-C3	-3.48	120.03	126.04
22	7	303	BCR	C2-C1-C6	3.48	115.83	110.48
27	b	310	CHL	C1B-CHB-C4A	-3.47	123.24	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	303	LUT	C40-C33-C34	-3.47	118.06	122.92
27	8	317	CHL	CHA-C4D-ND	3.47	139.76	132.50
27	8	325	CHL	CHA-C4D-ND	3.47	139.76	132.50
27	B	828	CHL	CHA-C4D-ND	3.47	139.76	132.50
27	8	318	CHL	CHA-C4D-ND	3.47	139.76	132.50
27	K	205	CHL	CHD-C4C-C3C	-3.47	119.74	124.84
27	5	307	CHL	CMB-C2B-C3B	3.47	131.16	124.68
27	B	829	CHL	CHA-C4D-ND	3.47	139.75	132.50
27	4	307	CHL	CHA-C4D-ND	3.47	139.75	132.50
27	F	308	CHL	CHA-C4D-ND	3.47	139.75	132.50
29	4	301	LUT	C30-C31-C32	-3.46	112.40	123.22
27	L	304	CHL	CHA-C4D-ND	3.46	139.75	132.50
27	A	851	CHL	CHA-C4D-ND	3.46	139.75	132.50
27	8	312	CHL	O1D-CGD-CBD	-3.46	117.40	124.48
27	a	311	CHL	O2D-CGD-O1D	-3.46	117.07	123.84
27	5	315	CHL	O2D-CGD-O1D	-3.46	117.07	123.84
27	A	843	CHL	C2A-C1A-CHA	-3.46	117.81	123.86
27	A	826	CHL	O2D-CGD-O1D	-3.46	117.07	123.84
27	b	315	CHL	O2D-CGD-O1D	-3.46	117.07	123.84
27	7	317	CHL	O2D-CGD-O1D	-3.46	117.07	123.84
27	a	314	CHL	CHA-C4D-ND	3.46	139.74	132.50
27	5	316	CHL	CAC-C3C-C4C	3.46	129.30	124.81
27	5	311	CHL	CMB-C2B-C3B	3.46	131.15	124.68
27	a	308	CHL	CHD-C1D-ND	-3.46	121.28	124.45
27	A	856	CHL	CHA-C4D-ND	3.46	139.73	132.50
27	6	310	CHL	CHD-C1D-ND	-3.46	121.28	124.45
27	B	826	CHL	CHA-C4D-ND	3.46	139.73	132.50
27	5	316	CHL	C3B-C4B-NB	3.46	113.68	109.21
27	A	819	CHL	CHA-C4D-ND	3.46	139.73	132.50
27	7	316	CHL	CHA-C4D-ND	3.45	139.72	132.50
27	B	848	CHL	C4D-CHA-C1A	-3.45	117.05	121.25
27	5	314	CHL	C4D-CHA-C1A	-3.45	117.05	121.25
27	3	318	CHL	CHA-C4D-ND	3.45	139.72	132.50
27	b	316	CHL	CHD-C4C-C3C	-3.45	119.77	124.84
27	b	314	CHL	CHD-C4C-C3C	-3.45	119.77	124.84
27	a	307	CHL	CHA-C4D-ND	3.45	139.71	132.50
27	b	311	CHL	CHD-C4C-C3C	-3.45	119.77	124.84
27	A	831	CHL	O2D-CGD-O1D	-3.45	117.10	123.84
27	7	323	CHL	C1-C2-C3	-3.45	120.08	126.04
27	A	859	CHL	CHA-C4D-ND	3.45	139.71	132.50
27	a	319	CHL	C4D-CHA-C1A	-3.44	117.06	121.25
27	B	833	CHL	CHA-C4D-ND	3.44	139.70	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	844	CHL	CHA-C4D-ND	3.44	139.70	132.50
27	7	319	CHL	C4D-C3D-CAD	3.44	112.15	108.10
27	5	308	CHL	CHA-C4D-ND	3.44	139.70	132.50
27	B	840	CHL	CHA-C4D-ND	3.44	139.69	132.50
27	B	829	CHL	O1D-CGD-CBD	-3.44	117.45	124.48
27	7	314	CHL	CHA-C4D-ND	3.44	139.69	132.50
27	A	830	CHL	CHA-C4D-ND	3.44	139.69	132.50
27	A	849	CHL	CHA-C4D-ND	3.44	139.69	132.50
27	5	319	CHL	CHD-C4C-C3C	-3.44	119.79	124.84
29	7	304	LUT	C7-C6-C5	-3.44	113.14	121.46
27	A	832	CHL	CHA-C4D-ND	3.44	139.69	132.50
27	B	816	CHL	CHA-C4D-ND	3.43	139.69	132.50
27	a	317	CHL	CHA-C4D-ND	3.43	139.68	132.50
27	4	320	CHL	O1D-CGD-CBD	-3.43	117.46	124.48
27	A	825	CHL	CHA-C4D-ND	3.43	139.68	132.50
27	A	822	CHL	CHA-C4D-ND	3.43	139.68	132.50
27	6	305	CHL	C4D-CHA-C1A	-3.43	117.07	121.25
27	7	318	CHL	O1D-CGD-CBD	-3.43	117.47	124.48
27	4	315	CHL	CHA-C4D-ND	3.43	139.66	132.50
27	B	815	CHL	O2D-CGD-O1D	-3.42	117.14	123.84
27	3	313	CHL	CHA-C4D-ND	3.42	139.66	132.50
27	5	310	CHL	CHD-C4C-NC	3.42	129.59	124.20
29	a	302	LUT	C30-C31-C32	-3.42	112.55	123.22
27	4	312	CHL	CHD-C1D-ND	-3.42	121.31	124.45
27	A	820	CHL	C1C-C2C-C3C	-3.42	103.36	106.96
27	b	305	CHL	CHA-C4D-ND	3.42	139.65	132.50
27	F	308	CHL	CHD-C1D-ND	-3.42	121.31	124.45
27	b	314	CHL	C4D-CHA-C1A	-3.42	117.09	121.25
27	B	827	CHL	CHA-C4D-ND	3.42	139.65	132.50
27	J	106	CHL	CHA-C4D-ND	3.42	139.65	132.50
27	B	826	CHL	O1D-CGD-CBD	-3.42	117.49	124.48
27	4	317	CHL	CHC-C1C-NC	-3.42	119.02	124.20
27	4	310	CHL	CHA-C4D-ND	3.41	139.64	132.50
27	5	318	CHL	CHA-C4D-ND	3.41	139.64	132.50
27	a	308	CHL	CHA-C4D-ND	3.41	139.64	132.50
27	A	837	CHL	CHA-C4D-ND	3.41	139.63	132.50
27	8	315	CHL	CHA-C4D-ND	3.41	139.63	132.50
27	7	323	CHL	C2D-C1D-ND	-3.41	107.59	110.10
27	8	326	CHL	CHA-C4D-ND	3.41	139.63	132.50
27	B	834	CHL	C3D-C2D-C1D	-3.41	101.18	105.83
27	A	835	CHL	CHD-C4C-C3C	-3.41	119.83	124.84
27	K	206	CHL	CHA-C4D-ND	3.41	139.63	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	301	BCR	C36-C18-C17	-3.41	118.15	122.92
27	B	840	CHL	CHD-C4C-NC	3.41	129.57	124.20
27	8	313	CHL	CHA-C4D-ND	3.40	139.62	132.50
27	B	812	CHL	O2D-CGD-O1D	-3.40	117.18	123.84
27	6	306	CHL	O1D-CGD-CBD	-3.40	117.53	124.48
27	A	817	CHL	CHD-C1D-ND	-3.40	121.33	124.45
27	8	314	CHL	CGD-CBD-CAD	3.40	121.74	110.73
22	3	303	BCR	C11-C10-C9	-3.40	122.46	127.31
27	B	811	CHL	CHA-C4D-ND	3.40	139.60	132.50
27	3	314	CHL	CHA-C4D-ND	3.40	139.60	132.50
26	A	815	CL0	CMB-C2B-C3B	3.40	131.03	124.68
27	A	827	CHL	CHA-C4D-ND	3.40	139.60	132.50
27	B	831	CHL	CHA-C4D-ND	3.40	139.60	132.50
27	B	825	CHL	O2D-CGD-O1D	-3.40	117.20	123.84
27	A	844	CHL	CHD-C1D-ND	-3.40	121.33	124.45
27	B	816	CHL	O1D-CGD-CBD	-3.39	117.54	124.48
27	A	817	CHL	CMB-C2B-C3B	3.39	131.03	124.68
27	A	829	CHL	O1D-CGD-CBD	-3.39	117.54	124.48
27	a	313	CHL	O2D-CGD-O1D	-3.39	117.20	123.84
27	B	814	CHL	CHA-C4D-ND	3.39	139.60	132.50
27	B	841	CHL	CHA-C4D-ND	3.39	139.60	132.50
27	A	855	CHL	O2D-CGD-CBD	3.39	117.29	111.27
27	5	322	CHL	C4D-C3D-CAD	3.39	112.09	108.10
27	4	304	CHL	CHA-C4D-ND	3.39	139.59	132.50
27	7	312	CHL	C4D-CHA-C1A	-3.39	117.12	121.25
27	3	308	CHL	CMB-C2B-C3B	3.39	131.02	124.68
27	B	840	CHL	C4D-CHA-C1A	-3.39	117.12	121.25
27	B	839	CHL	CMB-C2B-C3B	3.39	131.02	124.68
27	5	321	CHL	CHA-C4D-ND	3.39	139.59	132.50
29	6	302	LUT	C7-C8-C9	-3.39	121.12	126.23
27	3	316	CHL	C4D-C3D-CAD	3.39	112.09	108.10
27	4	314	CHL	O2D-CGD-O1D	-3.39	117.22	123.84
27	K	207	CHL	CHD-C4C-C3C	-3.39	119.86	124.84
27	6	309	CHL	O2D-CGD-O1D	-3.38	117.22	123.84
27	A	826	CHL	CHA-C4D-ND	3.38	139.58	132.50
27	B	813	CHL	CHA-C4D-ND	3.38	139.58	132.50
30	J	104	LMG	O6-C1-O1	-3.38	101.96	109.97
27	A	829	CHL	CHA-C4D-ND	3.38	139.58	132.50
27	7	322	CHL	O2D-CGD-O1D	-3.38	117.22	123.84
27	B	846	CHL	CHA-C4D-ND	3.38	139.57	132.50
27	5	310	CHL	O1D-CGD-CBD	-3.38	117.57	124.48
27	A	843	CHL	C1B-CHB-C4A	-3.38	123.42	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	320	CHL	CHA-C4D-ND	3.38	139.57	132.50
29	3	305	LUT	C18-C5-C4	-3.38	108.09	114.36
27	4	312	CHL	C4D-C3D-CAD	3.38	112.08	108.10
27	B	839	CHL	CHA-C4D-ND	3.38	139.56	132.50
27	6	314	CHL	CHA-C4D-ND	3.38	139.56	132.50
27	B	829	CHL	C4D-CHA-C1A	-3.37	117.14	121.25
27	a	312	CHL	CHA-C4D-ND	3.37	139.56	132.50
27	B	827	CHL	CHD-C4C-NC	3.37	129.52	124.20
27	5	307	CHL	CHA-C4D-ND	3.37	139.56	132.50
27	A	816	CHL	CHD-C4C-C3C	-3.37	119.88	124.84
27	6	313	CHL	O1D-CGD-CBD	-3.37	117.59	124.48
27	3	315	CHL	CHA-C4D-ND	3.37	139.55	132.50
27	4	307	CHL	O2D-CGD-O1D	-3.37	117.25	123.84
27	K	204	CHL	CHA-C4D-ND	3.37	139.55	132.50
27	a	318	CHL	CHD-C4C-NC	3.37	129.51	124.20
27	4	317	CHL	CBC-CAC-C3C	-3.37	103.15	112.43
27	8	319	CHL	CHA-C4D-ND	3.37	139.54	132.50
27	A	851	CHL	O1D-CGD-CBD	-3.37	117.60	124.48
27	A	842	CHL	CGD-CBD-CAD	3.36	121.63	110.73
27	A	847	CHL	C4-C3-C5	3.36	120.93	115.27
27	A	839	CHL	O1D-CGD-CBD	-3.36	117.60	124.48
27	B	845	CHL	CHD-C4C-NC	3.36	129.50	124.20
27	A	846	CHL	O2D-CGD-O1D	-3.36	117.27	123.84
27	5	323	CHL	C4D-CHA-C1A	-3.36	117.16	121.25
27	K	207	CHL	C4D-C3D-CAD	3.36	112.06	108.10
27	B	820	CHL	C4-C3-C5	3.36	120.92	115.27
27	a	310	CHL	C4D-CHA-C1A	-3.36	117.16	121.25
27	L	303	CHL	C1-C2-C3	-3.36	120.23	126.04
27	8	321	CHL	CHD-C4C-NC	3.36	129.49	124.20
27	B	823	CHL	O1D-CGD-CBD	-3.36	117.62	124.48
27	8	321	CHL	CGD-CBD-CAD	3.36	121.60	110.73
27	A	846	CHL	C1B-CHB-C4A	-3.35	123.47	130.12
27	7	316	CHL	O2D-CGD-O1D	-3.35	117.28	123.84
27	7	311	CHL	CHA-C4D-ND	3.35	139.52	132.50
27	L	304	CHL	CHD-C4C-C3C	-3.35	119.91	124.84
27	5	308	CHL	O1D-CGD-CBD	-3.35	117.63	124.48
27	5	319	CHL	CHD-C1D-ND	-3.35	121.37	124.45
27	7	319	CHL	CHD-C4C-NC	3.35	129.48	124.20
27	4	318	CHL	CHA-C4D-ND	3.35	139.51	132.50
27	6	308	CHL	C1-C2-C3	-3.35	120.25	126.04
27	B	818	CHL	CHA-C4D-ND	3.35	139.51	132.50
27	b	309	CHL	CHA-C4D-ND	3.35	139.51	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	857	CHL	CHA-C4D-ND	3.35	139.50	132.50
33	7	305	XAT	C20-C13-C14	-3.35	118.23	122.92
27	A	818	CHL	CHA-C4D-ND	3.35	139.50	132.50
27	A	850	CHL	C4-C3-C5	3.35	120.90	115.27
27	A	824	CHL	CHA-C4D-ND	3.35	139.50	132.50
27	a	311	CHL	C4-C3-C5	3.35	120.90	115.27
27	A	845	CHL	CHD-C4C-C3C	-3.35	119.92	124.84
22	6	301	BCR	C16-C15-C14	3.34	130.32	123.47
29	5	302	LUT	C30-C31-C32	-3.34	112.78	123.22
27	6	308	CHL	C3D-C4D-ND	3.34	115.64	110.24
29	5	302	LUT	C7-C8-C9	-3.34	121.19	126.23
27	A	823	CHL	CHA-C4D-ND	3.34	139.49	132.50
27	a	318	CHL	C4D-C3D-CAD	3.34	112.03	108.10
29	5	303	LUT	C18-C5-C4	-3.34	108.17	114.36
29	6	302	LUT	C18-C5-C4	-3.34	108.17	114.36
27	8	317	CHL	O2D-CGD-O1D	-3.34	117.31	123.84
27	6	307	CHL	C1-C2-C3	-3.34	120.27	126.04
29	3	305	LUT	C30-C31-C32	-3.34	112.80	123.22
27	b	313	CHL	CHA-C4D-ND	3.34	139.48	132.50
29	J	103	LUT	C21-C26-C27	-3.34	108.48	112.70
27	3	311	CHL	CHA-C4D-ND	3.34	139.48	132.50
27	b	306	CHL	CHA-C4D-ND	3.33	139.47	132.50
27	4	314	CHL	CHD-C4C-NC	3.33	129.45	124.20
27	A	838	CHL	O2D-CGD-O1D	-3.33	117.33	123.84
27	A	821	CHL	CHD-C1D-ND	-3.33	121.40	124.45
29	a	304	LUT	C4-C5-C6	-3.33	113.44	120.85
27	B	842	CHL	CHA-C4D-ND	3.33	139.46	132.50
27	A	833	CHL	CAC-C3C-C4C	3.32	129.12	124.81
29	6	303	LUT	C30-C31-C32	-3.32	112.84	123.22
27	3	311	CHL	O1D-CGD-CBD	-3.32	117.68	124.48
27	A	829	CHL	C4D-CHA-C1A	-3.32	117.20	121.25
29	3	305	LUT	C12-C13-C14	-3.32	113.84	118.94
27	A	833	CHL	C1-C2-C3	-3.32	120.30	126.04
27	A	842	CHL	C1-C2-C3	-3.32	120.30	126.04
27	A	833	CHL	C4D-C3D-CAD	3.32	112.01	108.10
27	b	311	CHL	C4D-C3D-CAD	3.32	112.01	108.10
27	A	850	CHL	CHA-C4D-ND	3.32	139.44	132.50
27	B	817	CHL	CHA-C4D-ND	3.32	139.44	132.50
27	8	311	CHL	O2D-CGD-O1D	-3.32	117.35	123.84
27	6	307	CHL	CAC-C3C-C4C	3.32	129.11	124.81
27	3	318	CHL	C4D-CHA-C1A	-3.32	117.21	121.25
27	B	821	CHL	CHA-C4D-ND	3.32	139.44	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	311	CHL	O2A-CGA-CBA	3.32	122.31	111.91
27	B	848	CHL	O2D-CGD-O1D	-3.31	117.36	123.84
29	b	301	LUT	C10-C11-C12	-3.31	112.88	123.22
27	4	309	CHL	CHD-C1D-ND	-3.31	121.41	124.45
27	a	307	CHL	CMB-C2B-C3B	3.31	130.87	124.68
27	A	834	CHL	O2D-CGD-CBD	3.31	117.15	111.27
27	L	303	CHL	CHC-C1C-C2C	-3.31	117.57	126.72
27	4	308	CHL	C4D-CHA-C1A	-3.31	117.22	121.25
27	b	316	CHL	C4D-C3D-CAD	3.31	111.99	108.10
27	3	319	CHL	O2D-CGD-O1D	-3.31	117.37	123.84
27	8	324	CHL	C4D-C3D-CAD	3.30	111.99	108.10
27	A	838	CHL	C4D-CHA-C1A	-3.30	117.23	121.25
27	A	834	CHL	CHA-C4D-ND	3.30	139.41	132.50
27	7	318	CHL	C4D-CHA-C1A	-3.30	117.23	121.25
27	6	314	CHL	O2D-CGD-O1D	-3.30	117.39	123.84
27	B	817	CHL	CHD-C4C-NC	3.30	129.40	124.20
29	a	302	LUT	C18-C5-C4	-3.30	108.24	114.36
27	3	315	CHL	C4D-CHA-C1A	-3.30	117.23	121.25
27	5	319	CHL	C4D-C3D-CAD	3.30	111.98	108.10
27	A	833	CHL	CHD-C1D-ND	-3.30	121.42	124.45
27	3	320	CHL	C1-C2-C3	-3.30	120.34	126.04
29	8	304	LUT	C7-C6-C5	-3.30	113.48	121.46
27	a	311	CHL	CHD-C4C-NC	3.29	129.40	124.20
27	B	840	CHL	O2A-CGA-CBA	3.29	122.25	111.91
27	4	305	CHL	C4D-CHA-C1A	-3.29	117.24	121.25
27	B	814	CHL	CMB-C2B-C3B	3.29	130.84	124.68
29	6	303	LUT	C10-C11-C12	-3.29	112.95	123.22
27	6	318	CHL	C4D-C3D-CAD	3.29	111.97	108.10
27	7	314	CHL	CHD-C4C-NC	3.29	129.39	124.20
27	3	316	CHL	O2A-CGA-CBA	3.29	122.22	111.91
27	A	842	CHL	CHD-C1D-ND	-3.29	121.43	124.45
27	A	819	CHL	O1D-CGD-CBD	-3.29	117.76	124.48
27	a	315	CHL	C4D-C3D-CAD	3.29	111.97	108.10
27	3	320	CHL	CMC-C2C-C1C	3.29	130.04	125.04
27	A	830	CHL	CMB-C2B-C3B	3.28	130.82	124.68
27	A	848	CHL	CHD-C4C-NC	3.28	129.38	124.20
27	5	313	CHL	C4C-C3C-C2C	-3.28	102.11	106.90
27	4	313	CHL	CHA-C4D-ND	3.28	139.37	132.50
27	4	309	CHL	CHD-C4C-C3C	-3.28	120.02	124.84
27	A	831	CHL	C2A-C1A-CHA	-3.28	118.12	123.86
27	b	316	CHL	CHD-C1D-ND	-3.28	121.44	124.45
27	8	322	CHL	CHA-C4D-ND	3.28	139.36	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	301	LUT	C18-C5-C4	-3.28	108.28	114.36
27	7	321	CHL	C4D-C3D-CAD	3.28	111.96	108.10
27	7	313	CHL	C4D-CHA-C1A	-3.28	117.26	121.25
27	B	850	CHL	CMB-C2B-C3B	3.28	130.81	124.68
27	B	845	CHL	C1-C2-C3	-3.28	121.45	126.75
27	A	847	CHL	O2D-CGD-O1D	-3.28	117.43	123.84
27	6	308	CHL	O2A-CGA-CBA	3.27	122.18	111.91
27	B	825	CHL	CMC-C2C-C1C	3.27	130.02	125.04
27	B	811	CHL	O2D-CGD-O1D	-3.27	117.44	123.84
27	b	315	CHL	CHD-C4C-NC	3.27	129.36	124.20
27	B	818	CHL	CAC-C3C-C4C	3.27	129.05	124.81
27	B	813	CHL	CHD-C4C-NC	3.27	129.36	124.20
27	7	324	CHL	CHA-C4D-ND	3.27	139.34	132.50
27	B	846	CHL	C1-C2-C3	-3.27	120.39	126.04
27	3	321	CHL	CHD-C4C-NC	3.27	129.35	124.20
27	6	318	CHL	CHD-C1D-ND	-3.27	121.45	124.45
22	6	301	BCR	C35-C13-C14	-3.27	118.34	122.92
27	F	309	CHL	C1-C2-C3	-3.27	121.47	126.75
29	6	302	LUT	C35-C15-C14	-3.27	116.78	123.47
27	7	322	CHL	C4D-C3D-CAD	3.26	111.94	108.10
27	6	316	CHL	C4D-C3D-CAD	3.26	111.94	108.10
27	A	847	CHL	CMB-C2B-C3B	3.26	130.78	124.68
27	B	849	CHL	C4D-CHA-C1A	-3.26	117.28	121.25
27	7	319	CHL	CHD-C1D-ND	-3.26	121.46	124.45
27	B	834	CHL	CHD-C4C-NC	3.26	129.34	124.20
27	8	312	CHL	CHA-C4D-ND	3.26	139.32	132.50
27	8	325	CHL	CAA-C2A-C3A	-3.26	103.86	112.78
27	3	316	CHL	CHD-C4C-NC	3.26	129.33	124.20
27	a	315	CHL	O2A-CGA-CBA	3.25	122.12	111.91
27	3	312	CHL	CMB-C2B-C3B	3.25	130.76	124.68
27	3	320	CHL	CHA-C4D-ND	3.25	139.30	132.50
27	4	304	CHL	CMB-C2B-C3B	3.25	130.76	124.68
29	a	304	LUT	C18-C5-C4	-3.25	108.33	114.36
27	4	316	CHL	CHD-C1D-ND	-3.25	121.47	124.45
27	5	308	CHL	CHD-C1D-ND	-3.25	121.47	124.45
27	a	316	CHL	C4D-C3D-CAD	3.25	111.92	108.10
27	A	837	CHL	O1D-CGD-CBD	-3.25	117.84	124.48
27	B	821	CHL	O2D-CGD-O1D	-3.25	117.49	123.84
29	b	303	LUT	C12-C13-C14	3.25	123.92	118.94
27	A	855	CHL	O2A-CGA-CBA	3.25	122.09	111.91
33	7	305	XAT	C15-C35-C34	3.24	130.12	123.47
27	A	848	CHL	C4-C3-C5	3.24	120.73	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	816	CHL	CHA-C4D-ND	3.24	139.28	132.50
27	B	826	CHL	CHD-C4C-NC	3.24	129.31	124.20
29	b	301	LUT	C4-C5-C6	-3.24	113.62	120.85
27	5	325	CHL	CHD-C4C-NC	3.24	129.31	124.20
27	F	308	CHL	O2D-CGD-O1D	-3.24	117.50	123.84
27	4	316	CHL	C4D-C3D-CAD	3.24	111.91	108.10
27	A	854	CHL	CMB-C2B-C3B	3.24	130.74	124.68
27	7	320	CHL	CHD-C4C-NC	3.24	129.31	124.20
27	6	318	CHL	CHD-C4C-NC	3.24	129.30	124.20
27	A	829	CHL	CHD-C4C-NC	3.24	129.30	124.20
27	A	820	CHL	CHA-C4D-ND	3.24	139.27	132.50
29	8	303	LUT	C10-C11-C12	-3.24	113.12	123.22
27	A	842	CHL	C3D-C2D-C1D	-3.23	101.42	105.83
27	3	311	CHL	CHD-C4C-NC	3.23	129.30	124.20
29	3	304	LUT	C8-C7-C6	-3.23	118.13	127.20
27	5	325	CHL	C4D-C3D-CAD	3.23	111.90	108.10
27	b	310	CHL	CHA-C4D-ND	3.23	139.25	132.50
27	A	832	CHL	CHD-C1D-ND	-3.23	121.49	124.45
27	B	849	CHL	C1-C2-C3	-3.23	120.46	126.04
27	8	323	CHL	CMB-C2B-C3B	3.23	130.71	124.68
27	5	315	CHL	CHD-C4C-NC	3.23	129.28	124.20
27	A	819	CHL	CMC-C2C-C1C	3.22	129.95	125.04
27	4	309	CHL	C4D-C3D-CAD	3.22	111.89	108.10
27	5	315	CHL	C1-C2-C3	-3.22	120.47	126.04
27	B	837	CHL	C4-C3-C5	3.22	120.69	115.27
27	7	320	CHL	C4D-C3D-CAD	3.22	111.89	108.10
27	A	844	CHL	CMB-C2B-C3B	3.22	130.70	124.68
33	7	305	XAT	C40-C33-C34	-3.22	118.41	122.92
27	A	851	CHL	CHD-C4C-NC	3.22	129.28	124.20
27	b	306	CHL	O2D-CGD-O1D	-3.22	117.55	123.84
27	8	321	CHL	C4D-C3D-CAD	3.22	111.89	108.10
26	A	815	CL0	CMC-C2C-C1C	3.22	129.94	125.04
27	8	312	CHL	O2A-CGA-CBA	3.22	122.00	111.91
29	8	304	LUT	C30-C31-C32	-3.21	113.19	123.22
29	b	301	LUT	C7-C8-C9	-3.21	121.38	126.23
29	4	302	LUT	C35-C15-C14	-3.21	116.89	123.47
27	B	839	CHL	O2D-CGD-O1D	-3.21	117.56	123.84
27	A	855	CHL	O2D-CGD-O1D	-3.21	117.56	123.84
27	A	859	CHL	O1D-CGD-CBD	-3.21	117.92	124.48
27	b	306	CHL	O1D-CGD-CBD	-3.21	117.92	124.48
29	7	304	LUT	C30-C31-C32	-3.21	113.20	123.22
27	3	321	CHL	O1D-CGD-CBD	-3.21	117.92	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	841	CHL	C3D-C2D-C1D	-3.21	101.45	105.83
29	b	303	LUT	C32-C33-C34	3.21	123.86	118.94
27	A	855	CHL	CHD-C4C-NC	3.20	129.25	124.20
27	A	831	CHL	C1B-CHB-C4A	-3.20	123.78	130.12
27	6	307	CHL	CMB-C2B-C3B	3.20	130.66	124.68
29	F	303	LUT	C21-C26-C27	-3.20	108.66	112.70
27	3	315	CHL	CHD-C4C-NC	3.20	129.25	124.20
27	8	312	CHL	CMB-C2B-C3B	3.20	130.66	124.68
27	7	311	CHL	CHD-C4C-NC	3.20	129.24	124.20
27	b	317	CHL	CHD-C4C-NC	3.20	129.24	124.20
27	a	317	CHL	C4-C3-C5	3.20	120.65	115.27
27	7	319	CHL	C4-C3-C5	3.20	120.65	115.27
27	b	315	CHL	C4D-CHA-C1A	-3.20	117.36	121.25
27	A	843	CHL	C4-C3-C5	3.20	120.65	115.27
27	6	311	CHL	CHD-C4C-NC	3.20	129.24	124.20
27	A	818	CHL	CHD-C4C-NC	3.19	129.24	124.20
27	5	307	CHL	C1-C2-C3	-3.19	120.52	126.04
27	A	856	CHL	C1-C2-C3	-3.19	120.52	126.04
27	B	837	CHL	C2D-C1D-ND	3.19	112.46	110.10
27	A	842	CHL	C4D-C3D-CAD	3.19	111.86	108.10
27	A	822	CHL	O1D-CGD-CBD	-3.19	117.95	124.48
27	b	307	CHL	O2D-CGD-O1D	-3.19	117.60	123.84
27	B	811	CHL	CHD-C4C-NC	3.19	129.23	124.20
27	B	821	CHL	CHD-C4C-NC	3.19	129.23	124.20
27	a	312	CHL	CHD-C4C-NC	3.19	129.23	124.20
27	b	308	CHL	C2D-C1D-ND	-3.19	107.76	110.10
27	A	849	CHL	O1D-CGD-CBD	-3.19	117.97	124.48
27	B	838	CHL	O1D-CGD-CBD	-3.18	117.97	124.48
27	B	851	CHL	O1D-CGD-CBD	-3.18	117.97	124.48
27	4	307	CHL	C4D-CHA-C1A	-3.18	117.38	121.25
27	3	314	CHL	O2D-CGD-O1D	-3.18	117.62	123.84
29	3	304	LUT	C30-C31-C32	-3.18	113.29	123.22
29	b	303	LUT	C8-C9-C10	3.18	123.82	118.94
27	B	850	CHL	C1-C2-C3	-3.18	121.61	126.75
27	5	317	CHL	CHD-C4C-NC	3.18	129.21	124.20
27	5	322	CHL	CHC-C1C-NC	-3.18	119.39	124.20
27	A	841	CHL	CHD-C4C-NC	3.18	129.21	124.20
27	6	308	CHL	C1D-ND-C4D	-3.17	104.08	106.33
27	6	306	CHL	C4D-CHA-C1A	-3.17	117.39	121.25
27	A	843	CHL	CMC-C2C-C1C	3.17	129.87	125.04
27	B	820	CHL	O1D-CGD-CBD	-3.17	117.99	124.48
29	a	302	LUT	C10-C11-C12	-3.17	113.32	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	321	CHL	CHD-C4C-NC	3.17	129.20	124.20
27	B	818	CHL	CHD-C4C-C3C	-3.17	120.18	124.84
27	6	315	CHL	O2D-CGD-O1D	-3.17	117.64	123.84
27	B	825	CHL	CHD-C4C-NC	3.17	129.20	124.20
27	3	317	CHL	C4D-CHA-C1A	-3.17	117.39	121.25
26	A	815	CL0	CHC-C1C-C2C	-3.17	117.96	126.72
27	a	319	CHL	O2D-CGD-O1D	-3.17	117.64	123.84
27	B	812	CHL	O2A-CGA-CBA	3.17	121.85	111.91
27	b	312	CHL	C4D-CHA-C1A	-3.17	117.39	121.25
27	K	204	CHL	C1-C2-C3	-3.17	121.63	126.75
27	A	846	CHL	CAC-C3C-C4C	3.16	128.92	124.81
29	4	302	LUT	C2-C3-C4	3.16	114.63	110.30
29	5	302	LUT	C10-C11-C12	-3.16	113.35	123.22
29	J	103	LUT	C10-C11-C12	-3.16	113.35	123.22
27	5	325	CHL	O2D-CGD-O1D	-3.16	117.66	123.84
27	B	841	CHL	C4D-CHA-C1A	-3.16	117.41	121.25
29	3	305	LUT	C8-C7-C6	-3.15	118.34	127.20
27	6	310	CHL	O1D-CGD-CBD	-3.15	118.03	124.48
27	A	846	CHL	CMB-C2B-C3B	3.15	130.58	124.68
27	7	323	CHL	C6-C5-C3	-3.15	109.46	114.62
34	8	301	SQD	O8-S-C6	3.15	110.76	105.74
29	4	301	LUT	C2-C3-C4	3.15	114.62	110.30
27	F	309	CHL	O1D-CGD-CBD	-3.15	118.04	124.48
27	A	830	CHL	O2D-CGD-O1D	-3.15	117.68	123.84
27	4	304	CHL	CHD-C4C-NC	3.15	129.16	124.20
27	3	308	CHL	CHD-C4C-NC	3.14	129.16	124.20
27	8	321	CHL	CHD-C1D-ND	-3.14	121.56	124.45
29	3	304	LUT	C10-C11-C12	-3.14	113.41	123.22
27	B	844	CHL	CMB-C2B-C3B	3.14	130.56	124.68
29	8	304	LUT	C4-C5-C6	-3.14	113.85	120.85
27	J	106	CHL	CHD-C4C-NC	3.14	129.15	124.20
27	3	317	CHL	O1D-CGD-CBD	-3.14	118.06	124.48
27	4	316	CHL	CHC-C1C-NC	-3.14	119.44	124.20
27	A	846	CHL	CMC-C2C-C1C	3.14	129.82	125.04
27	B	840	CHL	O1D-CGD-CBD	-3.14	118.06	124.48
27	8	325	CHL	O1D-CGD-CBD	-3.14	118.06	124.48
27	4	308	CHL	CHD-C4C-NC	3.14	129.15	124.20
27	B	836	CHL	CMB-C2B-C3B	3.14	130.55	124.68
27	5	317	CHL	C4D-C3D-CAD	3.14	111.79	108.10
27	7	311	CHL	C1-C2-C3	-3.14	120.62	126.04
27	K	205	CHL	C4D-CHA-C1A	-3.14	117.43	121.25
27	4	314	CHL	CMC-C2C-C1C	3.14	129.82	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	308	CHL	CHD-C4C-NC	3.14	129.14	124.20
29	b	301	LUT	C30-C31-C32	-3.14	113.43	123.22
27	A	846	CHL	CHB-C4A-NA	3.13	128.85	124.51
27	B	846	CHL	O1D-CGD-CBD	-3.13	118.07	124.48
27	5	310	CHL	CMC-C2C-C1C	3.13	129.81	125.04
27	b	317	CHL	C4D-C3D-CAD	3.13	111.79	108.10
27	8	313	CHL	CHD-C4C-NC	3.13	129.14	124.20
27	5	307	CHL	CHD-C4C-NC	3.13	129.14	124.20
27	B	828	CHL	C4-C3-C5	3.13	120.54	115.27
29	4	301	LUT	C8-C7-C6	-3.13	118.41	127.20
27	A	832	CHL	CAC-C3C-C4C	3.13	128.87	124.81
27	A	818	CHL	O1D-CGD-CBD	-3.13	118.09	124.48
27	a	314	CHL	O2D-CGD-O1D	-3.12	117.73	123.84
27	6	317	CHL	O1D-CGD-CBD	-3.12	118.09	124.48
27	8	313	CHL	C1-C2-C3	-3.12	121.70	126.75
22	6	301	BCR	C1-C6-C5	-3.12	118.22	122.61
27	A	828	CHL	CMB-C2B-C3B	3.12	130.52	124.68
27	A	836	CHL	CMB-C2B-C3B	3.12	130.52	124.68
29	F	303	LUT	C30-C31-C32	-3.12	113.48	123.22
27	B	851	CHL	C1-C2-C3	-3.12	120.65	126.04
27	6	314	CHL	CHD-C4C-NC	3.12	129.12	124.20
27	A	845	CHL	O1D-CGD-CBD	-3.12	118.10	124.48
27	A	847	CHL	CHD-C4C-NC	3.12	129.12	124.20
27	B	815	CHL	CHD-C4C-NC	3.12	129.12	124.20
27	B	825	CHL	C3D-C2D-C1D	-3.12	101.58	105.83
27	a	314	CHL	CHD-C4C-NC	3.12	129.11	124.20
27	6	316	CHL	CHD-C4C-NC	3.12	129.11	124.20
27	A	858	CHL	O2D-CGD-O1D	-3.12	117.75	123.84
29	5	302	LUT	C8-C7-C6	-3.12	118.45	127.20
27	8	320	CHL	C6-C5-C3	-3.12	109.52	114.62
27	5	313	CHL	C4-C3-C5	3.11	120.51	115.27
27	L	303	CHL	CAC-C3C-C4C	3.11	128.85	124.81
27	8	324	CHL	CHD-C1D-ND	-3.11	121.59	124.45
27	6	306	CHL	O2A-CGA-CBA	3.11	121.67	111.91
27	B	827	CHL	O1D-CGD-CBD	-3.11	118.12	124.48
27	3	317	CHL	CHD-C4C-NC	3.11	129.11	124.20
27	A	820	CHL	CHD-C4C-NC	3.11	129.10	124.20
29	8	304	LUT	C16-C1-C6	-3.11	105.25	110.30
27	A	836	CHL	CHD-C4C-NC	3.11	129.10	124.20
27	5	312	CHL	C1-C2-C3	-3.10	121.73	126.75
27	L	303	CHL	C2A-C1A-CHA	-3.10	118.43	123.86
27	B	850	CHL	C3D-C2D-C1D	-3.10	101.59	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	314	CHL	C3D-C2D-C1D	-3.10	101.59	105.83
27	B	820	CHL	CHD-C4C-NC	3.10	129.09	124.20
27	3	308	CHL	O2A-CGA-CBA	3.10	121.64	111.91
27	a	320	CHL	O2D-CGD-O1D	-3.10	117.77	123.84
28	B	809	DGD	O6D-C1D-O3G	-3.10	102.63	109.97
29	8	303	LUT	C12-C13-C14	-3.10	114.18	118.94
27	a	311	CHL	O1D-CGD-CBD	-3.10	118.14	124.48
29	4	302	LUT	C21-C26-C27	-3.10	108.78	112.70
27	B	830	CHL	O2D-CGD-O1D	-3.10	117.78	123.84
27	A	823	CHL	O1D-CGD-CBD	-3.10	118.15	124.48
27	A	855	CHL	CHA-C4D-ND	3.10	138.98	132.50
27	5	316	CHL	CHB-C4A-NA	3.10	128.79	124.51
27	7	321	CHL	C3D-C2D-C1D	-3.10	101.61	105.83
29	6	302	LUT	C10-C11-C12	-3.10	113.56	123.22
27	A	827	CHL	CHD-C4C-NC	3.09	129.08	124.20
26	A	815	CL0	O2D-CGD-O1D	-3.09	117.79	123.84
27	8	326	CHL	CMB-C2B-C3B	3.09	130.46	124.68
27	5	316	CHL	C1D-ND-C4D	-3.09	104.14	106.33
27	A	857	CHL	O1D-CGD-CBD	-3.09	118.16	124.48
27	5	307	CHL	O2D-CGD-O1D	-3.09	117.80	123.84
27	8	313	CHL	O2D-CGD-O1D	-3.09	117.80	123.84
27	B	837	CHL	CHD-C4C-C3C	-3.09	120.30	124.84
27	K	204	CHL	CHD-C1D-ND	-3.09	121.61	124.45
27	a	317	CHL	O2D-CGD-O1D	-3.09	117.80	123.84
29	a	304	LUT	C30-C31-C32	-3.09	113.58	123.22
27	A	827	CHL	CMB-C2B-C3B	3.09	130.45	124.68
27	3	309	CHL	CHD-C4C-NC	3.09	129.07	124.20
27	A	823	CHL	CHD-C4C-NC	3.09	129.06	124.20
27	B	851	CHL	CHD-C4C-NC	3.09	129.06	124.20
27	A	825	CHL	O1D-CGD-CBD	-3.08	118.17	124.48
27	A	842	CHL	O2D-CGD-O1D	-3.08	117.81	123.84
27	A	824	CHL	C4D-CHA-C1A	-3.08	117.50	121.25
22	7	303	BCR	C28-C27-C26	-3.08	108.57	114.08
27	3	320	CHL	O2A-CGA-CBA	3.08	121.58	111.91
27	A	849	CHL	C4D-CHA-C1A	-3.08	117.50	121.25
27	6	319	CHL	C2D-C1D-ND	3.08	112.37	110.10
27	A	844	CHL	CHD-C4C-NC	3.08	129.06	124.20
27	a	307	CHL	CHD-C4C-NC	3.08	129.06	124.20
26	A	815	CL0	C4-C3-C5	3.08	120.45	115.27
27	3	316	CHL	C3D-C2D-C1D	-3.08	101.63	105.83
27	5	307	CHL	O2A-CGA-CBA	3.08	121.56	111.91
27	b	308	CHL	C3C-C4C-NC	3.08	114.02	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	815	CHL	C3D-C2D-C1D	-3.07	101.64	105.83
27	3	316	CHL	O1D-CGD-CBD	-3.07	118.19	124.48
27	8	322	CHL	O2A-CGA-CBA	3.07	121.55	111.91
27	B	837	CHL	CMB-C2B-C3B	3.07	130.43	124.68
27	8	322	CHL	O2D-CGD-O1D	-3.07	117.83	123.84
29	4	301	LUT	C3-C4-C5	3.07	117.97	111.85
27	A	857	CHL	CMB-C2B-C3B	3.07	130.42	124.68
27	4	304	CHL	CMC-C2C-C1C	3.07	129.71	125.04
27	5	316	CHL	C6-C5-C3	-3.07	105.41	113.45
27	3	314	CHL	C4-C3-C5	3.07	120.43	115.27
27	B	832	CHL	CHD-C1D-ND	-3.07	121.64	124.45
22	B	806	BCR	C15-C14-C13	-3.06	122.94	127.31
27	A	846	CHL	C4C-C3C-C2C	-3.06	102.43	106.90
27	L	303	CHL	CMB-C2B-C3B	3.06	130.41	124.68
27	A	854	CHL	CHD-C4C-NC	3.06	129.03	124.20
27	a	319	CHL	O2A-CGA-CBA	3.06	121.51	111.91
27	b	308	CHL	CMA-C3A-C4A	-3.06	103.55	111.77
29	b	301	LUT	C8-C7-C6	-3.06	118.61	127.20
27	7	311	CHL	CMB-C2B-C3B	3.06	130.40	124.68
27	B	818	CHL	O2D-CGD-O1D	-3.06	117.86	123.84
27	8	316	CHL	CHD-C4C-NC	3.06	129.02	124.20
27	5	313	CHL	CMB-C2B-C3B	3.06	130.40	124.68
27	A	830	CHL	O2A-CGA-CBA	3.06	121.50	111.91
29	J	103	LUT	C17-C1-C6	-3.06	105.34	110.30
27	6	320	CHL	CHD-C4C-NC	3.05	129.02	124.20
20	B	801	PQN	C11-C3-C4	-3.05	115.23	118.50
27	A	854	CHL	C4-C3-C5	3.05	120.41	115.27
27	5	308	CHL	CHD-C4C-NC	3.05	129.01	124.20
29	8	303	LUT	C2-C3-C4	3.05	114.48	110.30
27	4	309	CHL	C4D-CHA-C1A	-3.05	117.54	121.25
27	6	320	CHL	O2D-CGD-O1D	-3.05	117.88	123.84
27	A	840	CHL	CHC-C1C-NC	-3.05	119.58	124.20
27	B	835	CHL	O2D-CGD-O1D	-3.05	117.88	123.84
27	B	832	CHL	C1-C2-C3	-3.05	120.77	126.04
27	A	831	CHL	CHC-C1C-C2C	-3.05	118.30	126.72
27	A	828	CHL	C4-C3-C5	3.04	120.39	115.27
27	6	317	CHL	C4D-C3D-CAD	3.04	111.68	108.10
27	B	835	CHL	CHD-C1D-ND	-3.04	121.66	124.45
27	7	316	CHL	C4C-C3C-C2C	-3.04	104.28	107.07
27	A	829	CHL	C1-C2-C3	-3.04	120.78	126.04
27	A	820	CHL	CMC-C2C-C1C	3.04	129.67	125.04
27	A	834	CHL	CHD-C4C-NC	3.04	129.00	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	818	CHL	C4-C3-C5	3.04	120.39	115.27
27	a	312	CHL	C1-C2-C3	-3.04	121.83	126.75
28	B	809	DGD	O5D-C6D-C5D	-3.04	103.42	109.05
27	A	841	CHL	C4-C3-C5	3.04	120.39	115.27
27	a	315	CHL	CHD-C4C-NC	3.04	128.99	124.20
27	B	849	CHL	O2D-CGD-O1D	-3.04	117.89	123.84
27	5	321	CHL	CHD-C4C-NC	3.04	128.99	124.20
27	b	309	CHL	C1B-CHB-C4A	-3.04	124.10	130.12
29	4	301	LUT	C10-C11-C12	-3.04	113.74	123.22
27	a	316	CHL	CHD-C4C-NC	3.03	128.99	124.20
27	4	318	CHL	CHD-C4C-NC	3.03	128.98	124.20
27	A	857	CHL	CAC-C3C-C4C	3.03	128.75	124.81
27	A	835	CHL	CHD-C1D-ND	-3.03	121.67	124.45
27	4	307	CHL	CHD-C4C-NC	3.03	128.98	124.20
29	3	304	LUT	C35-C15-C14	-3.03	117.27	123.47
27	4	319	CHL	CHD-C4C-NC	3.03	128.98	124.20
27	7	319	CHL	C3D-C2D-C1D	-3.03	101.70	105.83
27	6	306	CHL	CHD-C4C-NC	3.03	128.97	124.20
27	A	853	CHL	C4-C3-C5	3.03	120.36	115.27
27	a	319	CHL	CHD-C4C-NC	3.03	128.97	124.20
27	6	317	CHL	CGD-CBD-CAD	3.03	120.53	110.73
27	A	832	CHL	CHD-C4C-NC	3.02	128.97	124.20
27	B	812	CHL	C1C-C2C-C3C	-3.02	103.78	106.96
27	5	317	CHL	C3D-C2D-C1D	-3.02	101.71	105.83
27	8	326	CHL	O2D-CGD-O1D	-3.02	117.93	123.84
27	B	841	CHL	C3D-C2D-C1D	-3.02	101.71	105.83
27	A	834	CHL	CMB-C2B-C3B	3.02	130.33	124.68
27	7	313	CHL	O2D-CGD-O1D	-3.02	117.94	123.84
27	8	326	CHL	C3D-C2D-C1D	-3.02	101.71	105.83
27	L	303	CHL	C4-C3-C5	3.02	120.35	115.27
27	B	845	CHL	C3D-C2D-C1D	-3.02	101.71	105.83
29	6	302	LUT	C8-C7-C6	-3.02	118.73	127.20
29	3	304	LUT	C18-C5-C4	-3.02	108.77	114.36
27	8	319	CHL	CMB-C2B-C3B	3.02	130.32	124.68
27	B	841	CHL	CHD-C4C-NC	3.02	128.96	124.20
27	8	325	CHL	O2A-CGA-CBA	3.02	121.37	111.91
27	8	323	CHL	CHC-C1C-NC	-3.01	119.63	124.20
27	6	307	CHL	O2D-CGD-O1D	-3.01	117.94	123.84
27	B	834	CHL	CMB-C2B-C3B	3.01	130.32	124.68
27	4	311	CHL	O2D-CGD-O1D	-3.01	117.95	123.84
27	B	829	CHL	CHD-C4C-NC	3.01	128.95	124.20
27	5	323	CHL	CHD-C4C-NC	3.01	128.95	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	318	CHL	C4-C3-C5	3.01	120.34	115.27
27	B	836	CHL	O2D-CGD-O1D	-3.01	117.95	123.84
29	4	302	LUT	C10-C11-C12	-3.01	113.82	123.22
27	8	311	CHL	CHD-C4C-NC	3.01	128.95	124.20
27	B	812	CHL	CMB-C2B-C3B	3.01	130.31	124.68
27	4	320	CHL	CAA-CBA-CGA	-3.01	104.46	113.25
27	b	307	CHL	CHD-C4C-NC	3.01	128.94	124.20
27	4	311	CHL	O1D-CGD-CBD	-3.01	118.33	124.48
27	5	314	CHL	CHD-C4C-NC	3.01	128.94	124.20
27	8	321	CHL	C3D-C2D-C1D	-3.01	101.73	105.83
27	B	811	CHL	C4-C3-C5	3.01	120.33	115.27
27	5	316	CHL	C3D-C4D-ND	3.00	115.10	110.24
27	B	843	CHL	CHD-C4C-NC	3.00	128.93	124.20
27	8	316	CHL	CMB-C2B-C3B	3.00	130.29	124.68
27	A	826	CHL	C4-C3-C5	3.00	120.31	115.27
27	5	320	CHL	O2D-CGD-O1D	-3.00	117.98	123.84
27	7	322	CHL	CHD-C1D-ND	-3.00	121.70	124.45
27	a	307	CHL	CMC-C2C-C1C	3.00	129.60	125.04
29	a	302	LUT	C8-C7-C6	-3.00	118.79	127.20
27	3	308	CHL	O2D-CGD-O1D	-3.00	117.98	123.84
27	3	319	CHL	CHD-C4C-NC	3.00	128.92	124.20
27	4	310	CHL	O2D-CGD-O1D	-3.00	117.98	123.84
27	4	314	CHL	C4D-CHA-C1A	-3.00	117.60	121.25
27	A	852	CHL	C3D-C2D-C1D	-2.99	101.74	105.83
27	3	318	CHL	CHD-C4C-NC	2.99	128.92	124.20
27	4	312	CHL	O2A-CGA-CBA	2.99	121.30	111.91
27	6	307	CHL	C4-C3-C5	2.99	120.31	115.27
22	6	301	BCR	C19-C18-C17	2.99	123.53	118.94
27	4	309	CHL	O2D-CGD-O1D	-2.99	117.99	123.84
27	B	842	CHL	O1D-CGD-CBD	-2.99	118.36	124.48
27	8	322	CHL	C3D-C2D-C1D	-2.99	101.75	105.83
27	8	317	CHL	CHD-C4C-NC	2.99	128.91	124.20
27	A	817	CHL	C1-C2-C3	-2.99	120.87	126.04
27	b	316	CHL	O2D-CGD-O1D	-2.99	118.00	123.84
27	a	313	CHL	CHD-C4C-NC	2.99	128.91	124.20
27	5	322	CHL	CHD-C4C-NC	2.99	128.91	124.20
27	A	830	CHL	C4-C3-C5	2.98	120.29	115.27
29	J	103	LUT	C18-C5-C4	-2.98	108.83	114.36
27	6	317	CHL	C3D-C2D-C1D	-2.98	101.76	105.83
27	b	317	CHL	C3D-C2D-C1D	-2.98	101.76	105.83
26	A	815	CL0	C1-C2-C3	-2.98	120.89	126.04
27	A	841	CHL	CMD-C2D-C1D	2.98	129.97	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	308	CHL	C3D-C2D-C1D	-2.98	101.76	105.83
27	4	313	CHL	CHB-C4A-NA	2.98	128.63	124.51
27	B	845	CHL	CMB-C2B-C3B	2.98	130.25	124.68
27	a	318	CHL	CHD-C1D-ND	-2.98	121.72	124.45
27	A	821	CHL	C3D-C2D-C1D	-2.98	101.77	105.83
27	B	847	CHL	CHD-C4C-NC	2.98	128.90	124.20
29	5	303	LUT	C17-C1-C6	-2.98	105.47	110.30
27	8	320	CHL	CHD-C4C-NC	2.98	128.90	124.20
27	4	319	CHL	CHA-C4D-ND	2.98	138.73	132.50
27	A	820	CHL	CHB-C4A-NA	2.98	128.63	124.51
27	A	844	CHL	O2D-CGD-O1D	-2.97	118.02	123.84
34	8	301	SQD	O7-S-C6	2.97	110.47	106.94
27	B	812	CHL	CHA-C4D-ND	2.97	138.72	132.50
27	3	319	CHL	C1-C2-C3	-2.97	120.90	126.04
27	6	319	CHL	CHD-C4C-C3C	-2.97	120.47	124.84
27	B	839	CHL	O2A-CGA-CBA	2.97	121.24	111.91
29	F	303	LUT	C10-C11-C12	-2.97	113.94	123.22
27	a	310	CHL	CHD-C4C-NC	2.97	128.88	124.20
26	A	815	CL0	C1B-CHB-C4A	-2.97	124.24	130.12
29	3	304	LUT	C7-C8-C9	-2.97	121.75	126.23
27	A	835	CHL	CAC-C3C-C4C	2.97	128.66	124.81
27	A	831	CHL	C4-C3-C5	2.97	120.27	115.27
27	6	306	CHL	O2D-CGD-O1D	-2.97	118.03	123.84
27	3	317	CHL	C3D-C2D-C1D	-2.97	101.78	105.83
27	3	320	CHL	CMB-C2B-C3B	2.97	130.23	124.68
27	B	816	CHL	C3D-C2D-C1D	-2.96	101.78	105.83
27	A	830	CHL	CHD-C4C-NC	2.96	128.88	124.20
27	5	318	CHL	CHD-C4C-NC	2.96	128.88	124.20
27	3	310	CHL	C4D-CHA-C1A	-2.96	117.64	121.25
27	B	821	CHL	CMB-C2B-C3B	2.96	130.22	124.68
27	B	812	CHL	C1-C2-C3	-2.96	120.92	126.04
27	6	316	CHL	O1D-CGD-CBD	-2.96	118.43	124.48
27	8	322	CHL	C1-C2-C3	-2.96	121.96	126.75
27	5	313	CHL	O2A-CGA-CBA	2.96	121.19	111.91
27	B	812	CHL	C3D-C2D-C1D	-2.96	101.79	105.83
22	J	102	BCR	C24-C23-C22	-2.96	121.76	126.23
27	B	835	CHL	O1D-CGD-CBD	-2.96	118.43	124.48
27	A	817	CHL	CAC-C3C-C4C	2.96	128.65	124.81
27	A	820	CHL	C4-C3-C5	2.96	120.25	115.27
27	5	309	CHL	CHD-C4C-NC	2.96	128.86	124.20
22	6	301	BCR	C8-C9-C10	2.96	123.48	118.94
27	5	311	CHL	CHD-C4C-NC	2.95	128.86	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	8	303	LUT	C8-C7-C6	-2.95	118.91	127.20
27	6	315	CHL	CHD-C4C-NC	2.95	128.85	124.20
27	B	814	CHL	O2A-CGA-CBA	2.95	121.17	111.91
27	A	837	CHL	C3D-C2D-C1D	-2.95	101.80	105.83
27	b	311	CHL	C3D-C2D-C1D	-2.95	101.80	105.83
27	B	816	CHL	CAC-C3C-C4C	2.95	128.64	124.81
27	A	833	CHL	C3D-C2D-C1D	-2.95	101.80	105.83
27	A	840	CHL	CMB-C2B-C3B	2.95	130.20	124.68
27	6	312	CHL	CHC-C1C-NC	-2.95	119.73	124.20
27	A	857	CHL	CHD-C4C-NC	2.95	128.85	124.20
27	A	848	CHL	O1D-CGD-CBD	-2.95	118.45	124.48
27	7	319	CHL	CGD-CBD-CAD	2.95	120.29	110.73
27	5	314	CHL	O2D-CGD-O1D	-2.95	118.07	123.84
27	A	817	CHL	CHA-C4D-ND	2.95	138.67	132.50
27	6	306	CHL	CMC-C2C-C1C	2.95	129.53	125.04
27	6	311	CHL	CMC-C2C-C1C	2.95	129.53	125.04
27	A	816	CHL	CAC-C3C-C4C	2.95	128.63	124.81
27	b	306	CHL	C1D-CHD-C4C	-2.95	119.70	126.06
27	a	320	CHL	CHD-C4C-NC	2.95	128.84	124.20
27	7	316	CHL	CHD-C4C-NC	2.95	128.84	124.20
26	A	815	CL0	CHB-C4A-NA	2.94	128.58	124.51
27	5	313	CHL	C2A-C1A-CHA	-2.94	118.71	123.86
27	a	317	CHL	CHC-C1C-NC	-2.94	119.74	124.20
27	6	319	CHL	CHC-C1C-NC	-2.94	119.74	124.20
27	8	316	CHL	C4-C3-C5	2.94	120.22	115.27
27	7	320	CHL	O1D-CGD-CBD	-2.94	118.47	124.48
27	A	822	CHL	CHD-C4C-NC	2.94	128.83	124.20
27	B	823	CHL	CHD-C4C-NC	2.94	128.83	124.20
27	4	308	CHL	C3D-C2D-C1D	-2.94	101.82	105.83
27	F	308	CHL	CHD-C4C-NC	2.94	128.83	124.20
27	5	311	CHL	CMC-C2C-C1C	2.94	129.51	125.04
27	B	825	CHL	CHC-C1C-NC	-2.94	119.75	124.20
27	4	312	CHL	CHD-C4C-NC	2.94	128.83	124.20
27	7	315	CHL	CMB-C2B-C3B	2.94	130.17	124.68
27	A	821	CHL	O1D-CGD-CBD	-2.94	118.48	124.48
27	6	308	CHL	O2D-CGD-O1D	-2.94	118.10	123.84
29	b	301	LUT	C35-C15-C14	-2.93	117.46	123.47
27	7	318	CHL	CHD-C4C-NC	2.93	128.83	124.20
27	7	315	CHL	CHD-C4C-NC	2.93	128.83	124.20
27	A	845	CHL	C1-C2-C3	-2.93	120.97	126.04
27	5	316	CHL	CMB-C2B-C3B	2.93	130.16	124.68
29	8	304	LUT	C22-C23-C24	2.93	115.08	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	318	CHL	C3D-C2D-C1D	-2.93	101.83	105.83
27	B	813	CHL	C4-C3-C5	2.93	120.19	115.27
27	A	819	CHL	CMB-C2B-C3B	2.93	130.15	124.68
27	3	314	CHL	CHD-C4C-NC	2.93	128.81	124.20
27	8	318	CHL	CHD-C4C-NC	2.93	128.81	124.20
27	b	310	CHL	CHD-C4C-NC	2.93	128.81	124.20
27	A	859	CHL	CHD-C4C-NC	2.92	128.81	124.20
27	B	849	CHL	CHD-C4C-NC	2.92	128.81	124.20
27	L	303	CHL	O2D-CGD-O1D	-2.92	118.12	123.84
27	A	843	CHL	CAC-C3C-C2C	2.92	132.53	127.53
27	4	306	CHL	CAC-C3C-C4C	2.92	128.60	124.81
27	8	324	CHL	CHD-C4C-NC	2.92	128.81	124.20
27	B	831	CHL	CAC-C3C-C4C	2.92	128.60	124.81
27	B	826	CHL	C1-C2-C3	-2.92	122.03	126.75
27	3	313	CHL	C1-C2-C3	-2.92	121.00	126.04
27	8	319	CHL	CHD-C4C-NC	2.92	128.80	124.20
27	A	825	CHL	O2A-CGA-CBA	2.92	121.06	111.91
27	8	315	CHL	C3D-C2D-C1D	-2.92	101.85	105.83
29	F	303	LUT	C1-C6-C7	-2.92	107.52	115.78
27	4	307	CHL	CMB-C2B-C3B	2.92	130.14	124.68
27	B	841	CHL	C4-C3-C5	2.92	120.18	115.27
27	7	311	CHL	C3D-C2D-C1D	-2.92	101.85	105.83
27	8	314	CHL	C3D-C2D-C1D	-2.92	101.85	105.83
33	7	305	XAT	C12-C13-C14	2.92	123.42	118.94
22	6	301	BCR	C12-C13-C14	2.91	123.41	118.94
27	A	830	CHL	O1D-CGD-CBD	-2.91	118.52	124.48
27	A	849	CHL	C3D-C2D-C1D	-2.91	101.85	105.83
27	7	320	CHL	C3D-C2D-C1D	-2.91	101.86	105.83
27	4	313	CHL	CHC-C1C-NC	-2.91	119.78	124.20
27	K	206	CHL	CHD-C4C-NC	2.91	128.79	124.20
27	7	322	CHL	CHD-C4C-NC	2.91	128.79	124.20
27	A	827	CHL	C4-C3-C5	2.91	120.17	115.27
27	b	304	CHL	CHC-C1C-NC	-2.91	119.79	124.20
27	B	845	CHL	O2A-CGA-CBA	2.91	121.04	111.91
27	8	312	CHL	O2D-CGD-O1D	-2.91	118.15	123.84
27	B	819	CHL	CHD-C4C-NC	2.91	128.79	124.20
27	A	833	CHL	CHD-C4C-C3C	-2.91	120.56	124.84
29	a	302	LUT	C21-C26-C25	2.91	116.63	111.42
27	4	312	CHL	O2D-CGD-O1D	-2.91	118.15	123.84
27	4	311	CHL	CHD-C4C-NC	2.91	128.79	124.20
27	3	316	CHL	CMD-C2D-C1D	2.91	129.84	124.71
27	b	315	CHL	O2A-CGA-CBA	2.91	121.03	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	318	CHL	C4D-CHA-C1A	-2.91	117.71	121.25
27	A	857	CHL	C3D-C2D-C1D	-2.91	101.86	105.83
27	A	819	CHL	C3D-C2D-C1D	-2.91	101.86	105.83
27	A	820	CHL	CMB-C2B-C3B	2.90	130.11	124.68
27	b	314	CHL	CAC-C3C-C4C	2.90	128.58	124.81
27	A	839	CHL	CHD-C4C-NC	2.90	128.78	124.20
27	5	312	CHL	CHD-C4C-NC	2.90	128.78	124.20
27	8	320	CHL	C4-C3-C5	2.90	120.16	115.27
27	A	842	CHL	C2D-C1D-ND	2.90	112.24	110.10
27	B	840	CHL	CMB-C2B-C3B	2.90	130.11	124.68
27	A	836	CHL	C4-C3-C5	2.90	120.15	115.27
27	5	311	CHL	CHC-C1C-NC	-2.90	119.80	124.20
27	B	834	CHL	C1-C2-C3	-2.90	121.03	126.04
27	6	316	CHL	C3D-C2D-C1D	-2.90	101.87	105.83
27	A	824	CHL	C3D-C2D-C1D	-2.90	101.87	105.83
27	A	816	CHL	CHC-C1C-NC	-2.90	119.80	124.20
27	B	838	CHL	C4-C3-C5	2.90	120.15	115.27
27	B	826	CHL	CHC-C1C-NC	-2.90	119.81	124.20
27	5	318	CHL	CAA-CBA-CGA	-2.90	104.79	113.25
27	A	842	CHL	C4-C3-C5	2.90	120.14	115.27
27	5	310	CHL	C4-C3-C5	2.90	120.14	115.27
27	B	814	CHL	CHD-C4C-NC	2.89	128.76	124.20
27	a	315	CHL	C3D-C2D-C1D	-2.89	101.88	105.83
27	A	832	CHL	CHC-C1C-NC	-2.89	119.81	124.20
27	K	204	CHL	CHC-C1C-NC	-2.89	119.82	124.20
27	7	313	CHL	C4-C3-C5	2.89	120.13	115.27
27	B	825	CHL	O1D-CGD-CBD	-2.89	118.57	124.48
27	a	309	CHL	CHD-C4C-NC	2.89	128.76	124.20
27	B	851	CHL	CMC-C2C-C1C	2.89	129.44	125.04
27	6	305	CHL	CHD-C4C-NC	2.89	128.76	124.20
27	5	311	CHL	C3D-C2D-C1D	-2.89	101.89	105.83
27	A	827	CHL	O1D-CGD-CBD	-2.89	118.57	124.48
27	B	815	CHL	C11-C12-C13	-2.89	106.59	115.92
27	4	304	CHL	C3D-C2D-C1D	-2.89	101.89	105.83
27	A	822	CHL	CMB-C2B-C3B	2.89	130.08	124.68
27	A	832	CHL	CMB-C2B-C3B	2.89	130.08	124.68
27	A	825	CHL	CHD-C4C-NC	2.89	128.75	124.20
27	5	309	CHL	O2D-CGD-O1D	-2.89	118.20	123.84
27	3	318	CHL	O2D-CGD-O1D	-2.88	118.20	123.84
27	5	308	CHL	CHC-C1C-NC	-2.88	119.83	124.20
27	5	319	CHL	CHC-C1C-NC	-2.88	119.83	124.20
29	J	103	LUT	C30-C31-C32	-2.88	114.22	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	317	CHL	C3D-C2D-C1D	-2.88	101.90	105.83
27	3	310	CHL	CHD-C4C-NC	2.88	128.75	124.20
27	5	319	CHL	O2D-CGD-O1D	-2.88	118.20	123.84
27	A	840	CHL	CHD-C1D-ND	-2.88	121.81	124.45
27	8	314	CHL	O2D-CGD-O1D	-2.88	118.21	123.84
27	b	304	CHL	O2D-CGD-O1D	-2.88	118.21	123.84
27	3	316	CHL	C4-C3-C5	2.88	120.11	115.27
27	A	838	CHL	CMB-C2B-C3B	2.88	130.06	124.68
27	a	307	CHL	O2A-CGA-CBA	2.88	120.94	111.91
27	5	318	CHL	C4-C3-C5	2.88	120.11	115.27
27	A	822	CHL	CMC-C2C-C1C	2.88	129.42	125.04
27	7	322	CHL	C4-C3-C5	2.88	120.11	115.27
27	A	852	CHL	CMB-C2B-C3B	2.88	130.06	124.68
27	A	820	CHL	C3D-C2D-C1D	-2.88	101.91	105.83
27	A	834	CHL	C1-C2-C3	-2.88	121.07	126.04
27	B	842	CHL	C1-C2-C3	-2.87	121.07	126.04
27	A	826	CHL	CHD-C4C-NC	2.87	128.73	124.20
27	A	824	CHL	C4-C3-C5	2.87	120.11	115.27
27	A	837	CHL	CHD-C4C-NC	2.87	128.73	124.20
27	4	310	CHL	CHD-C4C-NC	2.87	128.73	124.20
27	A	844	CHL	C4-C3-C5	2.87	120.10	115.27
27	8	324	CHL	C3D-C2D-C1D	-2.87	101.91	105.83
27	a	310	CHL	CMC-C2C-C1C	2.87	129.41	125.04
27	B	844	CHL	O1D-CGD-CBD	-2.87	118.61	124.48
27	A	838	CHL	O1D-CGD-CBD	-2.87	118.61	124.48
29	4	301	LUT	C22-C23-C24	2.87	115.01	111.74
27	B	844	CHL	CHD-C4C-NC	2.87	128.73	124.20
29	J	103	LUT	C1-C6-C5	-2.87	118.57	122.61
27	b	313	CHL	O2D-CGD-O1D	-2.87	118.23	123.84
27	b	313	CHL	CHD-C4C-NC	2.87	128.72	124.20
27	4	308	CHL	CHC-C1C-NC	-2.86	119.86	124.20
27	a	307	CHL	C3D-C2D-C1D	-2.86	101.92	105.83
27	3	320	CHL	C3D-C2D-C1D	-2.86	101.92	105.83
27	8	325	CHL	CHD-C4C-NC	2.86	128.72	124.20
27	4	318	CHL	O2D-CGD-O1D	-2.86	118.24	123.84
27	F	309	CHL	CHD-C4C-NC	2.86	128.72	124.20
27	3	310	CHL	O2D-CGD-O1D	-2.86	118.24	123.84
27	B	813	CHL	C3D-C2D-C1D	-2.86	101.93	105.83
27	7	314	CHL	CMB-C2B-C3B	2.86	130.03	124.68
27	6	312	CHL	C3D-C2D-C1D	-2.86	101.93	105.83
27	6	319	CHL	CMB-C2B-C3B	2.86	130.03	124.68
27	8	316	CHL	C3D-C2D-C1D	-2.86	101.93	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	840	CHL	C3D-C2D-C1D	-2.86	101.93	105.83
27	4	307	CHL	C3D-C2D-C1D	-2.86	101.93	105.83
27	3	308	CHL	C1-C2-C3	-2.86	121.10	126.04
27	B	818	CHL	C3D-C2D-C1D	-2.86	101.93	105.83
27	6	318	CHL	C3D-C2D-C1D	-2.86	101.93	105.83
27	A	850	CHL	O1D-CGD-CBD	-2.86	118.64	124.48
27	8	319	CHL	C3D-C2D-C1D	-2.86	101.93	105.83
27	3	310	CHL	O2A-CGA-CBA	2.85	120.87	111.91
27	7	313	CHL	O1D-CGD-CBD	-2.85	118.64	124.48
27	4	317	CHL	C3D-C2D-C1D	-2.85	101.94	105.83
27	A	853	CHL	CAC-C3C-C4C	2.85	128.51	124.81
27	7	322	CHL	C4D-CHA-C1A	-2.85	117.78	121.25
27	A	850	CHL	CHD-C4C-NC	2.85	128.70	124.20
27	A	833	CHL	C4-C3-C5	2.85	120.07	115.27
27	A	855	CHL	O1D-CGD-CBD	-2.85	118.65	124.48
27	6	309	CHL	CHD-C4C-NC	2.85	128.69	124.20
27	8	313	CHL	CHC-C1C-NC	-2.85	119.88	124.20
27	A	854	CHL	O2A-CGA-CBA	2.85	120.84	111.91
27	6	310	CHL	CHC-C1C-NC	-2.85	119.88	124.20
27	A	842	CHL	CHD-C4C-NC	2.85	128.69	124.20
27	A	822	CHL	O2A-CGA-CBA	2.85	120.84	111.91
27	B	835	CHL	C1-O2A-CGA	2.85	123.91	116.44
27	5	310	CHL	C3D-C2D-C1D	-2.85	101.95	105.83
27	B	827	CHL	C3D-C2D-C1D	-2.85	101.95	105.83
27	a	307	CHL	C1-C2-C3	-2.84	121.12	126.04
27	6	315	CHL	C1-C2-C3	-2.84	122.15	126.75
27	A	816	CHL	CMB-C2B-C3B	2.84	130.00	124.68
27	8	314	CHL	O2A-CGA-CBA	2.84	120.83	111.91
27	8	317	CHL	C1-C2-C3	-2.84	121.13	126.04
27	A	858	CHL	CAA-C2A-C3A	-2.84	105.00	112.78
27	A	836	CHL	C3D-C2D-C1D	-2.84	101.95	105.83
27	B	839	CHL	CHD-C4C-NC	2.84	128.68	124.20
27	a	311	CHL	C3D-C2D-C1D	-2.84	101.95	105.83
27	B	823	CHL	C3D-C2D-C1D	-2.84	101.96	105.83
27	B	831	CHL	C3D-C2D-C1D	-2.84	101.96	105.83
27	4	312	CHL	C3D-C2D-C1D	-2.84	101.96	105.83
27	B	830	CHL	CHD-C4C-NC	2.84	128.68	124.20
27	3	316	CHL	CHC-C1C-NC	-2.84	119.90	124.20
27	5	317	CHL	CHC-C1C-NC	-2.84	119.90	124.20
27	B	814	CHL	C3D-C2D-C1D	-2.84	101.96	105.83
27	B	837	CHL	CMD-C2D-C1D	2.84	129.71	124.71
27	b	316	CHL	CHD-C4C-NC	2.83	128.67	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	322	CHL	C3D-C2D-C1D	-2.83	101.96	105.83
27	B	850	CHL	CHD-C4C-NC	2.83	128.67	124.20
27	3	313	CHL	CHD-C4C-NC	2.83	128.67	124.20
27	8	312	CHL	C3D-C2D-C1D	-2.83	101.97	105.83
27	B	832	CHL	C4-C3-C5	2.83	120.03	115.27
27	b	315	CHL	C3D-C2D-C1D	-2.83	101.97	105.83
27	8	312	CHL	CHD-C4C-NC	2.83	128.66	124.20
27	A	859	CHL	C3D-C2D-C1D	-2.83	101.97	105.83
27	A	824	CHL	CMB-C2B-C3B	2.83	129.97	124.68
27	B	833	CHL	CHD-C4C-NC	2.83	128.66	124.20
27	L	304	CHL	CHC-C1C-NC	-2.83	119.91	124.20
27	5	317	CHL	O1D-CGD-CBD	-2.83	118.70	124.48
27	7	320	CHL	CHC-C1C-NC	-2.83	119.91	124.20
27	K	204	CHL	CHD-C4C-NC	2.83	128.66	124.20
27	A	859	CHL	C4-C3-C5	2.83	120.03	115.27
27	B	841	CHL	C1-C2-C3	-2.83	121.16	126.04
27	B	817	CHL	O2A-CGA-CBA	2.83	120.78	111.91
27	5	310	CHL	CHC-C1C-NC	-2.82	119.92	124.20
27	6	317	CHL	CHD-C4C-NC	2.82	128.65	124.20
27	A	816	CHL	O1D-CGD-CBD	-2.82	118.71	124.48
27	6	310	CHL	CHD-C4C-NC	2.82	128.65	124.20
27	A	854	CHL	C3D-C2D-C1D	-2.82	101.98	105.83
27	5	316	CHL	O2A-CGA-CBA	2.82	120.76	111.91
27	B	824	CHL	CAC-C3C-C4C	2.82	128.47	124.81
28	7	307	DGD	CDB-CCB-CBB	-2.82	100.11	114.42
22	K	202	BCR	C27-C26-C25	2.82	126.83	122.73
22	M	102	BCR	C15-C16-C17	-2.82	117.70	123.47
27	B	848	CHL	CHD-C4C-NC	2.82	128.65	124.20
27	a	310	CHL	C3D-C2D-C1D	-2.82	101.98	105.83
27	a	316	CHL	C3D-C2D-C1D	-2.82	101.98	105.83
28	B	809	DGD	CDB-CCB-CBB	-2.82	100.12	114.42
27	a	311	CHL	CMB-C2B-C3B	2.82	129.95	124.68
27	A	821	CHL	CHC-C1C-NC	-2.82	119.93	124.20
22	B	802	BCR	C27-C26-C25	2.82	126.82	122.73
27	b	308	CHL	CHC-C1C-NC	-2.82	119.93	124.20
27	7	314	CHL	C3D-C2D-C1D	-2.82	101.99	105.83
27	8	314	CHL	CHC-C1C-NC	-2.82	119.93	124.20
27	b	315	CHL	CHC-C1C-NC	-2.82	119.93	124.20
27	A	856	CHL	CHD-C4C-NC	2.81	128.64	124.20
27	6	320	CHL	C3D-C2D-C1D	-2.81	101.99	105.83
27	A	818	CHL	CAC-C3C-C4C	2.81	128.46	124.81
27	b	310	CHL	CAC-C3C-C4C	2.81	128.46	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	305	CHL	CHD-C4C-NC	2.81	128.64	124.20
27	A	817	CHL	O2A-CGA-CBA	2.81	120.73	111.91
27	7	317	CHL	CHD-C4C-NC	2.81	128.63	124.20
27	b	308	CHL	CHD-C1D-C2D	2.81	131.38	125.48
27	5	325	CHL	C3D-C2D-C1D	-2.81	102.00	105.83
27	6	318	CHL	CHC-C1C-NC	-2.81	119.94	124.20
27	A	832	CHL	C3D-C2D-C1D	-2.81	102.00	105.83
27	4	308	CHL	C1-C2-C3	-2.81	121.19	126.04
27	A	822	CHL	C4-C3-C5	2.81	120.00	115.27
27	a	318	CHL	C3D-C2D-C1D	-2.81	102.00	105.83
27	7	313	CHL	CAC-C3C-C4C	2.81	128.45	124.81
27	4	304	CHL	O2A-CGA-CBA	2.81	120.72	111.91
27	B	815	CHL	C4-C3-C5	2.80	119.99	115.27
27	A	827	CHL	CMC-C2C-C1C	2.80	129.31	125.04
27	A	824	CHL	CHD-C4C-NC	2.80	128.62	124.20
27	B	828	CHL	CHD-C4C-NC	2.80	128.62	124.20
27	B	838	CHL	CHD-C4C-NC	2.80	128.62	124.20
27	A	840	CHL	C3D-C2D-C1D	-2.80	102.01	105.83
27	A	852	CHL	CHD-C4C-NC	2.80	128.62	124.20
27	5	323	CHL	C1-C2-C3	-2.80	121.20	126.04
27	B	829	CHL	C3D-C2D-C1D	-2.80	102.01	105.83
27	8	315	CHL	CHC-C1C-NC	-2.80	119.96	124.20
27	A	824	CHL	O1D-CGD-CBD	-2.80	118.76	124.48
27	A	841	CHL	C2D-C1D-ND	2.80	112.17	110.10
27	A	817	CHL	C4-C3-C5	2.80	119.98	115.27
27	B	846	CHL	CHD-C4C-NC	2.80	128.61	124.20
27	B	819	CHL	C3D-C2D-C1D	-2.80	102.02	105.83
27	A	821	CHL	CHD-C4C-NC	2.80	128.61	124.20
27	a	318	CHL	CHC-C1C-NC	-2.79	119.97	124.20
27	A	823	CHL	C3D-C2D-C1D	-2.79	102.02	105.83
26	A	815	CL0	C4C-C3C-C2C	-2.79	102.83	106.90
27	B	843	CHL	CHC-C1C-NC	-2.79	119.97	124.20
27	B	849	CHL	C3D-C2D-C1D	-2.79	102.02	105.83
27	4	314	CHL	CMD-C2D-C1D	2.79	129.63	124.71
27	L	303	CHL	CMC-C2C-C1C	2.79	129.29	125.04
27	5	307	CHL	C3D-C2D-C1D	-2.79	102.02	105.83
22	B	802	BCR	C7-C8-C9	-2.79	122.02	126.23
27	K	207	CHL	C3D-C2D-C1D	-2.79	102.02	105.83
27	4	316	CHL	C4D-CHA-C1A	-2.79	117.85	121.25
27	K	207	CHL	CHD-C4C-NC	2.79	128.60	124.20
27	a	309	CHL	O1D-CGD-CBD	-2.79	118.78	124.48
27	B	815	CHL	C1-C2-C3	-2.79	121.22	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	311	CHL	C4-C3-C5	2.79	119.96	115.27
27	B	839	CHL	C3D-C2D-C1D	-2.79	102.03	105.83
27	b	309	CHL	CHD-C4C-NC	2.79	128.59	124.20
27	3	309	CHL	CHC-C1C-NC	-2.79	119.98	124.20
27	B	836	CHL	CAC-C3C-C4C	2.78	128.42	124.81
27	A	830	CHL	C3D-C2D-C1D	-2.78	102.03	105.83
27	B	821	CHL	C4-C3-C5	2.78	119.95	115.27
27	a	308	CHL	CHC-C1C-NC	-2.78	119.98	124.20
27	6	310	CHL	C4-C3-C5	2.78	119.95	115.27
27	a	314	CHL	C3D-C2D-C1D	-2.78	102.03	105.83
27	A	828	CHL	C3D-C2D-C1D	-2.78	102.03	105.83
27	5	319	CHL	C3D-C2D-C1D	-2.78	102.03	105.83
27	B	819	CHL	C4-C3-C5	2.78	119.95	115.27
27	a	307	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
27	8	313	CHL	O1D-CGD-CBD	-2.78	118.79	124.48
27	b	311	CHL	O2D-CGD-O1D	-2.78	118.40	123.84
27	6	313	CHL	CAC-C3C-C4C	2.78	128.42	124.81
27	A	818	CHL	C4-C3-C5	2.78	119.95	115.27
27	B	834	CHL	C4-C3-C5	2.78	119.95	115.27
30	J	101	LMG	O6-C1-O1	-2.78	103.39	109.97
27	A	849	CHL	C4-C3-C5	2.78	119.94	115.27
27	B	845	CHL	CMC-C2C-C1C	2.78	129.27	125.04
27	8	317	CHL	O2A-CGA-CBA	2.78	120.62	111.91
27	A	856	CHL	CAC-C3C-C4C	2.78	128.41	124.81
27	8	315	CHL	CMB-C2B-C3B	2.78	129.87	124.68
27	A	820	CHL	O2A-CGA-CBA	2.78	120.62	111.91
27	8	311	CHL	C3D-C2D-C1D	-2.78	102.04	105.83
27	b	311	CHL	CHD-C4C-NC	2.77	128.58	124.20
27	8	314	CHL	C4-C3-C5	2.77	119.94	115.27
27	4	305	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
27	5	313	CHL	CMC-C2C-C1C	2.77	129.26	125.04
27	4	309	CHL	CHD-C4C-NC	2.77	128.57	124.20
27	3	319	CHL	CHC-C1C-NC	-2.77	120.00	124.20
27	3	315	CHL	C3D-C2D-C1D	-2.77	102.05	105.83
27	5	313	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
27	B	823	CHL	C4-C3-C5	2.77	119.93	115.27
27	7	321	CHL	CMB-C2B-C3B	2.77	129.86	124.68
27	4	308	CHL	CMC-C2C-C1C	2.77	129.25	125.04
27	A	839	CHL	C3D-C2D-C1D	-2.77	102.05	105.83
27	K	204	CHL	CMC-C2C-C1C	2.77	129.25	125.04
27	A	858	CHL	CHD-C4C-NC	2.77	128.56	124.20
27	6	306	CHL	CAC-C3C-C4C	2.77	128.40	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	847	CHL	C3D-C2D-C1D	-2.77	102.06	105.83
27	7	315	CHL	C3D-C2D-C1D	-2.76	102.06	105.83
27	B	842	CHL	C3D-C2D-C1D	-2.76	102.06	105.83
27	F	308	CHL	O1D-CGD-CBD	-2.76	118.83	124.48
27	B	811	CHL	C3D-C2D-C1D	-2.76	102.06	105.83
27	b	307	CHL	C3D-C2D-C1D	-2.76	102.06	105.83
27	7	319	CHL	O2D-CGD-O1D	-2.76	118.44	123.84
27	6	308	CHL	C2A-C1A-CHA	-2.76	119.03	123.86
27	6	312	CHL	CAC-C3C-C4C	2.76	128.39	124.81
27	A	856	CHL	O2D-CGD-O1D	-2.76	118.44	123.84
27	4	304	CHL	O2D-CGD-O1D	-2.76	118.44	123.84
27	3	312	CHL	O1D-CGD-CBD	-2.76	118.84	124.48
27	a	309	CHL	CHC-C1C-NC	-2.76	120.02	124.20
27	b	305	CHL	CAC-C3C-C4C	2.76	128.39	124.81
27	6	305	CHL	C3D-C2D-C1D	-2.76	102.07	105.83
27	B	822	CHL	C1-C2-C3	-2.76	121.28	126.04
27	7	312	CHL	C3D-C2D-C1D	-2.76	102.07	105.83
27	3	319	CHL	C4-C3-C5	2.76	119.91	115.27
27	4	306	CHL	CMD-C2D-C1D	2.76	129.57	124.71
27	3	318	CHL	C3D-C2D-C1D	-2.76	102.07	105.83
27	A	817	CHL	CHD-C4C-NC	2.75	128.54	124.20
27	4	306	CHL	O2D-CGD-O1D	-2.75	118.45	123.84
27	b	311	CHL	CHC-C1C-NC	-2.75	120.03	124.20
27	b	312	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
27	6	313	CHL	CHD-C4C-NC	2.75	128.54	124.20
27	4	307	CHL	CHC-C1C-NC	-2.75	120.03	124.20
27	B	851	CHL	C3D-C2D-C1D	-2.75	102.08	105.83
27	a	318	CHL	O2A-CGA-CBA	2.75	120.53	111.91
27	6	310	CHL	C3D-C2D-C1D	-2.75	102.08	105.83
27	A	829	CHL	C3D-C2D-C1D	-2.75	102.08	105.83
27	4	316	CHL	C3D-C2D-C1D	-2.75	102.08	105.83
29	4	302	LUT	C7-C6-C5	-2.75	114.81	121.46
27	7	317	CHL	CHC-C1C-NC	-2.75	120.04	124.20
27	5	314	CHL	C3D-C2D-C1D	-2.75	102.08	105.83
27	B	813	CHL	CHC-C1C-NC	-2.74	120.04	124.20
27	7	311	CHL	CAC-C3C-C4C	2.74	128.37	124.81
27	3	310	CHL	C3D-C2D-C1D	-2.74	102.09	105.83
27	6	306	CHL	C3D-C2D-C1D	-2.74	102.09	105.83
27	B	843	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
27	B	848	CHL	C3D-C2D-C1D	-2.74	102.09	105.83
27	A	854	CHL	O1D-CGD-CBD	-2.74	118.88	124.48
24	A	812	LHG	O8-C23-C24	2.74	120.51	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	843	CHL	CHC-C1C-C2C	-2.74	119.14	126.72
27	4	316	CHL	CHD-C4C-NC	2.74	128.52	124.20
27	B	824	CHL	C3D-C2D-C1D	-2.74	102.09	105.83
27	8	324	CHL	CED-O2D-CGD	2.74	122.13	115.94
27	a	318	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
27	8	323	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
27	B	827	CHL	CMC-C2C-C1C	2.74	129.21	125.04
27	4	315	CHL	CHC-C1C-NC	-2.74	120.05	124.20
27	A	856	CHL	C4-C3-C5	2.74	119.88	115.27
27	4	306	CHL	CHD-C4C-NC	2.74	128.51	124.20
27	A	841	CHL	CMB-C2B-C3B	2.74	129.80	124.68
27	F	309	CHL	C3D-C2D-C1D	-2.74	102.10	105.83
27	7	312	CHL	C1D-CHD-C4C	-2.74	120.16	126.06
27	4	306	CHL	CHC-C1C-NC	-2.73	120.05	124.20
27	6	318	CHL	C4D-CHA-C1A	-2.73	117.92	121.25
27	a	320	CHL	CAC-C3C-C4C	2.73	128.36	124.81
33	7	305	XAT	C32-C33-C34	2.73	123.14	118.94
27	B	832	CHL	CHD-C4C-NC	2.73	128.51	124.20
22	L	302	BCR	C15-C16-C17	-2.73	117.87	123.47
27	A	855	CHL	C3D-C2D-C1D	-2.73	102.10	105.83
27	a	314	CHL	O1D-CGD-CBD	-2.73	118.89	124.48
27	5	325	CHL	C4D-CHA-C1A	-2.73	117.92	121.25
27	4	318	CHL	C1B-CHB-C4A	-2.73	124.71	130.12
27	6	315	CHL	CHC-C1C-NC	-2.73	120.06	124.20
27	a	315	CHL	CED-O2D-CGD	2.73	122.11	115.94
27	6	313	CHL	O2A-CGA-CBA	2.73	120.48	111.91
27	B	828	CHL	C3D-C2D-C1D	-2.73	102.10	105.83
27	5	322	CHL	C3D-C2D-C1D	-2.73	102.10	105.83
27	a	313	CHL	C1-C2-C3	-2.73	121.32	126.04
29	5	302	LUT	C18-C5-C4	-2.73	109.30	114.36
27	B	833	CHL	CMB-C2B-C3B	2.73	129.79	124.68
27	A	816	CHL	C4-C3-C5	2.73	119.86	115.27
27	a	309	CHL	CAC-C3C-C4C	2.73	128.35	124.81
27	b	306	CHL	CHD-C4C-NC	2.73	128.50	124.20
27	b	315	CHL	CMB-C2B-C3B	2.73	129.78	124.68
27	A	817	CHL	CHC-C1C-NC	-2.73	120.06	124.20
27	A	817	CHL	C3D-C2D-C1D	-2.73	102.11	105.83
27	4	320	CHL	CHC-C1C-NC	-2.73	120.06	124.20
27	5	318	CHL	C3D-C2D-C1D	-2.73	102.11	105.83
27	A	855	CHL	C1-C2-C3	-2.73	121.33	126.04
27	8	313	CHL	CMC-C2C-C1C	2.73	129.19	125.04
27	6	311	CHL	CAC-C3C-C4C	2.73	128.35	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	835	CHL	CHC-C1C-NC	-2.73	120.07	124.20
27	A	830	CHL	C1-C2-C3	-2.73	121.33	126.04
27	6	314	CHL	CHC-C1C-NC	-2.72	120.07	124.20
27	B	830	CHL	O1D-CGD-CBD	-2.72	118.91	124.48
27	B	835	CHL	CAC-C3C-C4C	2.72	128.34	124.81
27	3	311	CHL	C3D-C2D-C1D	-2.72	102.11	105.83
27	7	315	CHL	O2D-CGD-O1D	-2.72	117.91	124.09
22	3	301	BCR	C11-C10-C9	-2.72	123.42	127.31
27	A	842	CHL	O2A-CGA-CBA	2.72	120.45	111.91
30	7	301	LMG	O6-C1-O1	-2.72	103.53	109.97
27	A	837	CHL	CMB-C2B-C3B	2.72	129.77	124.68
27	4	310	CHL	CHC-C1C-NC	-2.72	120.07	124.20
27	A	838	CHL	C3D-C2D-C1D	-2.72	102.12	105.83
27	5	319	CHL	CHD-C4C-NC	2.72	128.49	124.20
27	8	318	CHL	C3D-C2D-C1D	-2.72	102.12	105.83
27	K	204	CHL	O2A-CGA-CBA	2.72	120.44	111.91
27	b	316	CHL	C3D-C2D-C1D	-2.72	102.12	105.83
27	A	824	CHL	CAC-C3C-C4C	2.72	128.34	124.81
27	3	319	CHL	O2A-CGA-CBA	2.72	120.44	111.91
27	a	316	CHL	C1B-CHB-C4A	-2.72	124.73	130.12
27	3	311	CHL	O2A-CGA-CBA	2.72	120.43	111.91
27	B	841	CHL	O2A-CGA-CBA	2.71	120.42	111.91
27	8	325	CHL	C3D-C2D-C1D	-2.71	102.13	105.83
27	b	317	CHL	O2A-CGA-CBA	2.71	120.42	111.91
27	A	858	CHL	C3D-C2D-C1D	-2.71	102.13	105.83
29	a	302	LUT	C17-C1-C6	-2.71	105.90	110.30
27	A	852	CHL	CED-O2D-CGD	2.71	122.07	115.94
27	F	308	CHL	CHC-C1C-NC	-2.71	120.09	124.20
27	3	321	CHL	CHC-C1C-NC	-2.71	120.09	124.20
27	7	322	CHL	O2A-CGA-CBA	2.71	120.42	111.91
27	B	818	CHL	C3B-C4B-NB	2.71	112.72	109.21
27	B	833	CHL	CAC-C3C-C4C	2.71	128.33	124.81
27	B	821	CHL	C3D-C2D-C1D	-2.71	102.13	105.83
27	B	834	CHL	CMD-C2D-C1D	2.71	129.49	124.71
27	F	309	CHL	CHC-C1C-NC	-2.71	120.09	124.20
27	B	825	CHL	CMB-C2B-C3B	2.71	129.75	124.68
29	8	303	LUT	C30-C31-C32	-2.71	114.77	123.22
27	6	314	CHL	C3D-C2D-C1D	-2.71	102.14	105.83
27	5	320	CHL	CHD-C4C-NC	2.71	128.47	124.20
27	6	310	CHL	CMC-C2C-C1C	2.71	129.16	125.04
27	B	835	CHL	C4-C3-C5	2.71	119.83	115.27
27	b	305	CHL	O1D-CGD-CBD	-2.71	118.94	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	837	CHL	CAC-C3C-C4C	2.71	128.32	124.81
27	A	826	CHL	CMB-C2B-C3B	2.71	129.74	124.68
27	A	855	CHL	C4-C3-C5	2.71	119.82	115.27
27	4	317	CHL	CHD-C4C-C3C	-2.71	120.86	124.84
27	A	825	CHL	C3D-C2D-C1D	-2.71	102.14	105.83
27	B	841	CHL	CAC-C3C-C4C	2.71	128.32	124.81
27	A	846	CHL	O2A-CGA-CBA	2.71	120.40	111.91
27	A	822	CHL	C3D-C2D-C1D	-2.70	102.14	105.83
27	8	315	CHL	C4-C3-C5	2.70	119.82	115.27
27	6	307	CHL	CMC-C2C-C1C	2.70	129.16	125.04
27	6	309	CHL	O2A-CGA-CBA	2.70	120.39	111.91
27	7	317	CHL	C4-C3-C5	2.70	119.82	115.27
27	b	306	CHL	CMB-C2B-C3B	2.70	129.74	124.68
27	b	314	CHL	O2D-CGD-O1D	-2.70	118.55	123.84
27	7	319	CHL	C4D-CHA-C1A	-2.70	117.96	121.25
27	8	323	CHL	CHA-C4D-ND	2.70	138.15	132.50
27	5	315	CHL	O2A-CGA-CBA	2.70	120.38	111.91
27	7	323	CHL	CHA-C4D-ND	2.70	138.15	132.50
27	b	313	CHL	CHC-C1C-NC	-2.70	120.11	124.20
27	3	312	CHL	O2A-CGA-CBA	2.70	120.38	111.91
27	3	313	CHL	O1D-CGD-CBD	-2.70	118.96	124.48
27	A	818	CHL	CMB-C2B-C3B	2.70	129.73	124.68
27	7	324	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
27	B	842	CHL	CMC-C2C-C1C	2.70	129.15	125.04
27	K	207	CHL	O2D-CGD-O1D	-2.70	118.56	123.84
27	B	835	CHL	CMB-C2B-C3B	2.69	129.72	124.68
27	5	323	CHL	C3D-C2D-C1D	-2.69	102.16	105.83
27	B	827	CHL	C1-C2-C3	-2.69	121.39	126.04
29	8	304	LUT	C10-C11-C12	-2.69	114.81	123.22
27	L	304	CHL	CMB-C2B-C3B	2.69	129.72	124.68
27	A	842	CHL	C2C-C3C-C4C	-2.69	104.57	106.49
27	A	848	CHL	C1-C2-C3	-2.69	121.39	126.04
27	6	312	CHL	CMB-C2B-C3B	2.69	129.71	124.68
22	5	301	BCR	C27-C26-C25	2.69	126.64	122.73
27	7	314	CHL	C4-C3-C5	2.69	119.79	115.27
27	b	316	CHL	C4D-CHA-C1A	-2.69	117.98	121.25
27	3	314	CHL	C3D-C2D-C1D	-2.69	102.16	105.83
27	6	309	CHL	C3D-C2D-C1D	-2.69	102.16	105.83
27	A	818	CHL	C3D-C2D-C1D	-2.69	102.16	105.83
27	K	205	CHL	O1D-CGD-CBD	-2.69	118.98	124.48
27	7	324	CHL	CHD-C4C-NC	2.69	128.44	124.20
27	5	323	CHL	C4-C3-C5	2.69	119.79	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	205	CHL	C3D-C2D-C1D	-2.69	102.17	105.83
27	7	322	CHL	O1D-CGD-CBD	-2.69	118.99	124.48
27	5	313	CHL	C1-C2-C3	-2.69	121.40	126.04
27	A	826	CHL	C3D-C2D-C1D	-2.69	102.17	105.83
27	6	307	CHL	CHB-C4A-NA	2.69	128.22	124.51
27	b	304	CHL	CHD-C4C-NC	2.68	128.43	124.20
27	A	837	CHL	C4-C3-C5	2.68	119.79	115.27
27	3	316	CHL	C4D-CHA-C1A	-2.68	117.98	121.25
27	A	856	CHL	O2A-CGA-CBA	2.68	120.33	111.91
27	B	839	CHL	CAC-C3C-C4C	2.68	128.29	124.81
27	A	819	CHL	C4-C3-C5	2.68	119.78	115.27
27	4	312	CHL	C4D-CHA-C1A	-2.68	117.98	121.25
27	6	311	CHL	C3D-C2D-C1D	-2.68	102.17	105.83
27	7	313	CHL	CHD-C4C-NC	2.68	128.43	124.20
27	4	310	CHL	C3D-C2D-C1D	-2.68	102.17	105.83
27	4	315	CHL	C3D-C2D-C1D	-2.68	102.17	105.83
27	8	314	CHL	CHD-C4C-NC	2.68	128.43	124.20
22	B	802	BCR	C11-C10-C9	-2.68	123.48	127.31
27	7	319	CHL	O2A-CGA-CBA	2.68	120.32	111.91
27	B	837	CHL	CHC-C1C-NC	-2.68	120.14	124.20
27	B	851	CHL	CAC-C3C-C4C	2.68	128.29	124.81
27	b	306	CHL	C3D-C2D-C1D	-2.68	102.17	105.83
27	B	824	CHL	C4-C3-C5	2.68	119.78	115.27
27	8	315	CHL	CAC-C3C-C4C	2.68	128.28	124.81
27	B	831	CHL	O1D-CGD-CBD	-2.68	119.00	124.48
27	6	317	CHL	CHC-C1C-NC	-2.68	120.14	124.20
27	a	309	CHL	CMC-C2C-C1C	2.68	129.12	125.04
27	7	323	CHL	CHD-C1D-C2D	2.68	131.09	125.48
27	4	306	CHL	C4-C3-C5	2.68	119.77	115.27
27	7	312	CHL	O2D-CGD-O1D	-2.68	118.61	123.84
24	8	305	LHG	O8-C23-C24	2.68	120.31	111.91
27	4	311	CHL	O2A-CGA-CBA	2.68	120.31	111.91
27	b	314	CHL	C3D-C2D-C1D	-2.68	102.18	105.83
29	F	303	LUT	C4-C5-C6	-2.68	114.89	120.85
27	A	821	CHL	O2A-CGA-CBA	2.68	120.30	111.91
27	5	322	CHL	C4D-CHA-C1A	-2.67	117.99	121.25
27	5	313	CHL	CHC-C1C-C2C	-2.67	119.32	126.72
27	A	838	CHL	C4-C3-C5	2.67	119.77	115.27
22	8	302	BCR	C15-C16-C17	-2.67	118.00	123.47
27	A	830	CHL	CAC-C3C-C4C	2.67	128.28	124.81
27	A	839	CHL	CAC-C3C-C4C	2.67	128.28	124.81
27	A	851	CHL	C3D-C2D-C1D	-2.67	102.18	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	835	CHL	C3D-C2D-C1D	-2.67	102.18	105.83
27	B	851	CHL	C4-C3-C5	2.67	119.77	115.27
27	8	321	CHL	C2C-C3C-C4C	-2.67	104.58	106.49
27	7	313	CHL	C3D-C2D-C1D	-2.67	102.19	105.83
29	6	303	LUT	C1-C6-C7	-2.67	108.22	115.78
27	B	826	CHL	C3D-C2D-C1D	-2.67	102.19	105.83
27	b	311	CHL	CHD-C1D-ND	-2.67	122.00	124.45
27	a	310	CHL	C4-C3-C5	2.67	119.76	115.27
27	4	317	CHL	CHA-C4D-ND	2.67	138.08	132.50
27	8	321	CHL	C2D-C1D-ND	2.67	112.07	110.10
27	B	833	CHL	C1-O2A-CGA	2.67	123.44	116.44
27	A	845	CHL	C3D-C2D-C1D	-2.67	102.19	105.83
27	a	319	CHL	C3D-C2D-C1D	-2.67	102.19	105.83
27	A	819	CHL	CHC-C1C-NC	-2.67	120.16	124.20
27	A	859	CHL	CMB-C2B-C3B	2.67	129.67	124.68
27	A	853	CHL	CHD-C4C-NC	2.67	128.41	124.20
27	8	319	CHL	O2A-CGA-CBA	2.67	120.28	111.91
27	A	834	CHL	C3D-C2D-C1D	-2.66	102.19	105.83
27	A	848	CHL	C3D-C2D-C1D	-2.66	102.20	105.83
27	3	309	CHL	C3D-C2D-C1D	-2.66	102.20	105.83
27	6	311	CHL	CMB-C2B-C3B	2.66	129.66	124.68
29	4	301	LUT	C18-C5-C4	-2.66	109.42	114.36
27	B	846	CHL	O2A-CGA-CBA	2.66	120.26	111.91
27	4	314	CHL	O1D-CGD-CBD	-2.66	119.04	124.48
27	A	838	CHL	CHD-C4C-NC	2.66	128.40	124.20
27	B	851	CHL	CHC-C1C-NC	-2.66	120.17	124.20
27	3	312	CHL	C3D-C2D-C1D	-2.66	102.20	105.83
27	K	205	CHL	C1D-CHD-C4C	-2.66	120.32	126.06
27	5	320	CHL	CHC-C1C-NC	-2.66	120.17	124.20
27	3	312	CHL	CHD-C4C-NC	2.66	128.39	124.20
27	b	313	CHL	C3D-C2D-C1D	-2.66	102.20	105.83
27	3	314	CHL	CMC-C2C-C1C	2.66	129.09	125.04
27	3	312	CHL	C4-C3-C5	2.66	119.74	115.27
27	A	842	CHL	C1D-CHD-C4C	-2.66	120.33	126.06
27	a	310	CHL	CAC-C3C-C4C	2.66	128.26	124.81
27	6	319	CHL	C1B-CHB-C4A	-2.66	124.86	130.12
27	4	320	CHL	C3D-C2D-C1D	-2.66	102.21	105.83
27	A	854	CHL	CHC-C1C-NC	-2.66	120.17	124.20
27	8	311	CHL	CHC-C1C-NC	-2.66	120.17	124.20
27	A	822	CHL	CAC-C3C-C4C	2.66	128.25	124.81
22	5	301	BCR	C11-C10-C9	-2.65	123.52	127.31
27	A	850	CHL	CMB-C2B-C3B	2.65	129.64	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	849	CHL	CHD-C4C-NC	2.65	128.38	124.20
27	a	320	CHL	C3D-C2D-C1D	-2.65	102.21	105.83
27	4	320	CHL	C1-C2-C3	-2.65	122.46	126.75
27	8	320	CHL	C3D-C2D-C1D	-2.65	102.21	105.83
27	B	830	CHL	C1-C2-C3	-2.65	121.46	126.04
27	B	820	CHL	C3D-C2D-C1D	-2.65	102.22	105.83
27	B	844	CHL	C4-C3-C5	2.65	119.73	115.27
27	4	305	CHL	C3D-C2D-C1D	-2.65	102.22	105.83
27	B	838	CHL	CMB-C2B-C3B	2.65	129.63	124.68
27	a	314	CHL	CMD-C2D-C1D	2.65	129.38	124.71
27	4	308	CHL	O2A-CGA-CBA	2.65	120.22	111.91
27	4	306	CHL	CMC-C2C-C1C	2.65	129.07	125.04
27	a	311	CHL	CMD-C2D-C1D	2.65	129.38	124.71
27	B	846	CHL	CHC-C1C-NC	-2.65	120.19	124.20
27	A	827	CHL	C3D-C2D-C1D	-2.65	102.22	105.83
27	a	317	CHL	C3D-C2D-C1D	-2.65	102.22	105.83
27	B	819	CHL	O2A-CGA-CBA	2.65	120.21	111.91
29	6	302	LUT	C22-C23-C24	2.65	114.75	111.74
27	5	315	CHL	C3D-C2D-C1D	-2.65	102.22	105.83
27	b	304	CHL	C3D-C2D-C1D	-2.65	102.22	105.83
27	A	858	CHL	O2A-CGA-CBA	2.65	120.21	111.91
27	B	817	CHL	C3D-C2D-C1D	-2.65	102.22	105.83
27	B	822	CHL	C3D-C2D-C1D	-2.65	102.22	105.83
27	6	308	CHL	C4-C3-C5	2.64	119.72	115.27
27	A	842	CHL	CHC-C1C-NC	-2.64	120.19	124.20
27	A	849	CHL	CMD-C2D-C1D	2.64	129.37	124.71
24	7	302	LHG	O8-C23-C24	2.64	120.20	111.91
27	A	823	CHL	C4-C3-C5	2.64	119.72	115.27
27	B	836	CHL	CHD-C4C-NC	2.64	128.37	124.20
27	6	318	CHL	O2D-CGD-O1D	-2.64	118.67	123.84
27	4	311	CHL	C3D-C2D-C1D	-2.64	102.23	105.83
27	3	319	CHL	O1D-CGD-CBD	-2.64	119.08	124.48
27	b	309	CHL	O2D-CGD-O1D	-2.64	118.68	123.84
27	A	827	CHL	CHC-C1C-NC	-2.64	120.20	124.20
27	A	828	CHL	CHD-C4C-NC	2.64	128.36	124.20
27	B	835	CHL	CMC-C2C-C1C	2.64	129.06	125.04
27	B	834	CHL	O2A-CGA-CBA	2.64	120.19	111.91
27	4	304	CHL	O1D-CGD-CBD	-2.64	119.09	124.48
27	8	313	CHL	C3D-C2D-C1D	-2.64	102.23	105.83
27	b	312	CHL	C3D-C2D-C1D	-2.64	102.23	105.83
27	B	835	CHL	CHD-C4C-NC	2.64	128.36	124.20
27	A	835	CHL	C3D-C2D-C1D	-2.64	102.23	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	304	CHL	C3D-C2D-C1D	-2.64	102.23	105.83
27	A	848	CHL	O2A-CGA-CBA	2.64	120.18	111.91
27	A	825	CHL	CMB-C2B-C3B	2.64	129.61	124.68
27	6	314	CHL	O1D-CGD-CBD	-2.64	119.09	124.48
27	b	309	CHL	CHC-C1C-NC	-2.64	120.20	124.20
27	B	842	CHL	C4-C3-C5	2.64	119.70	115.27
27	A	816	CHL	C3D-C2D-C1D	-2.64	102.23	105.83
27	5	312	CHL	C3D-C2D-C1D	-2.64	102.23	105.83
27	A	832	CHL	O2A-CGA-CBA	2.64	120.18	111.91
27	5	320	CHL	C3D-C2D-C1D	-2.64	102.23	105.83
27	A	821	CHL	C1-C2-C3	-2.63	121.49	126.04
27	8	321	CHL	O2A-CGA-CBA	2.63	120.17	111.91
27	A	820	CHL	C1-C2-C3	-2.63	121.49	126.04
27	6	306	CHL	C1-C2-C3	-2.63	121.49	126.04
27	B	844	CHL	C3D-C2D-C1D	-2.63	102.24	105.83
27	K	204	CHL	C3D-C2D-C1D	-2.63	102.24	105.83
27	a	309	CHL	C3D-C2D-C1D	-2.63	102.24	105.83
27	F	309	CHL	CMC-C2C-C1C	2.63	129.05	125.04
27	B	824	CHL	CMB-C2B-C3B	2.63	129.60	124.68
27	a	316	CHL	C4D-CHA-C1A	-2.63	118.05	121.25
27	8	317	CHL	C4-C3-C5	2.63	119.69	115.27
27	3	320	CHL	CAC-C3C-C4C	2.63	128.22	124.81
27	a	313	CHL	CHC-C1C-NC	-2.63	120.22	124.20
27	B	821	CHL	CMC-C2C-C1C	2.62	129.04	125.04
27	A	850	CHL	CHC-C1C-NC	-2.62	120.22	124.20
24	b	302	LHG	O8-C23-C24	2.62	120.14	111.91
27	L	303	CHL	O2A-CGA-CBA	2.62	120.14	111.91
27	a	313	CHL	CMB-C2B-C3B	2.62	129.59	124.68
22	A	805	BCR	C28-C27-C26	-2.62	109.39	114.08
27	K	205	CHL	CMD-C2D-C1D	2.62	129.33	124.71
27	8	324	CHL	CHC-C1C-NC	-2.62	120.23	124.20
27	6	305	CHL	CMC-C2C-C1C	2.62	129.03	125.04
27	B	826	CHL	O2A-CGA-CBA	2.62	120.13	111.91
27	8	321	CHL	CHC-C1C-NC	-2.62	120.23	124.20
29	5	302	LUT	C4-C5-C6	-2.62	115.01	120.85
27	b	312	CHL	CHD-C4C-NC	2.62	128.33	124.20
22	K	202	BCR	C24-C23-C22	-2.62	122.28	126.23
27	6	313	CHL	C3D-C2D-C1D	-2.62	102.26	105.83
24	B	808	LHG	C11-C10-C9	-2.62	101.13	114.42
27	A	852	CHL	CMD-C2D-C1D	2.62	129.33	124.71
27	B	846	CHL	C4-C3-C5	2.62	119.68	115.27
27	B	839	CHL	C1-C2-C3	-2.62	121.52	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	324	CHL	C4D-CHA-C1A	-2.62	118.06	121.25
27	4	309	CHL	CAC-C3C-C4C	2.62	128.21	124.81
27	7	318	CHL	CMC-C2C-C1C	2.62	129.02	125.04
27	3	314	CHL	CAC-C3C-C4C	2.62	128.20	124.81
27	B	848	CHL	C4-C3-C5	2.62	119.67	115.27
27	B	818	CHL	O2A-CGA-CBA	2.62	120.11	111.91
27	A	829	CHL	CMB-C2B-C3B	2.62	129.57	124.68
27	B	822	CHL	CMB-C2B-C3B	2.61	129.57	124.68
27	a	310	CHL	CHC-C1C-NC	-2.61	120.24	124.20
27	B	846	CHL	C3D-C2D-C1D	-2.61	102.26	105.83
27	a	313	CHL	C3D-C2D-C1D	-2.61	102.26	105.83
34	8	301	SQD	O48-C23-C24	2.61	120.11	111.91
27	A	841	CHL	C2C-C3C-C4C	-2.61	104.63	106.49
27	B	846	CHL	CMC-C2C-C1C	2.61	129.02	125.04
27	B	841	CHL	C1D-CHD-C4C	-2.61	120.42	126.06
27	5	323	CHL	CHC-C1C-NC	-2.61	120.24	124.20
27	K	207	CHL	CAC-C3C-C4C	2.61	128.20	124.81
27	A	856	CHL	C3D-C2D-C1D	-2.61	102.27	105.83
27	7	323	CHL	O2D-CGD-O1D	-2.61	118.73	123.84
27	A	838	CHL	O2A-CGA-CBA	2.61	120.10	111.91
22	M	102	BCR	C15-C14-C13	-2.61	123.58	127.31
27	B	815	CHL	O2A-CGA-CBA	2.61	120.10	111.91
27	4	314	CHL	CHC-C1C-NC	-2.61	120.24	124.20
27	B	851	CHL	CMB-C2B-C3B	2.61	129.56	124.68
27	6	308	CHL	CHB-C4A-NA	2.61	128.12	124.51
27	B	842	CHL	O2A-CGA-CBA	2.61	120.09	111.91
29	3	304	LUT	C4-C5-C6	-2.61	115.03	120.85
27	B	820	CHL	CMB-C2B-C3B	2.61	129.56	124.68
27	a	307	CHL	CHC-C1C-NC	-2.61	120.25	124.20
27	A	831	CHL	O2A-CGA-CBA	2.61	120.09	111.91
27	a	317	CHL	CMB-C2B-C3B	2.61	129.55	124.68
27	a	311	CHL	O2A-CGA-CBA	2.60	120.08	111.91
27	B	844	CHL	C1-C2-C3	-2.60	121.54	126.04
27	4	317	CHL	CHA-C1A-NA	-2.60	120.43	126.40
27	5	315	CHL	CHC-C1C-NC	-2.60	120.25	124.20
27	b	316	CHL	C1B-CHB-C4A	-2.60	124.96	130.12
29	a	302	LUT	C4-C5-C6	-2.60	115.05	120.85
27	5	314	CHL	CHC-C1C-NC	-2.60	120.25	124.20
27	b	316	CHL	CHC-C1C-NC	-2.60	120.25	124.20
27	8	316	CHL	CMD-C2D-C1D	2.60	129.30	124.71
27	B	844	CHL	CAC-C3C-C4C	2.60	128.19	124.81
27	A	823	CHL	C1-C2-C3	-2.60	121.54	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	308	CHL	C3D-C2D-C1D	-2.60	102.28	105.83
27	8	321	CHL	C4D-CHA-C1A	-2.60	118.09	121.25
27	B	826	CHL	CMC-C2C-C1C	2.60	129.00	125.04
27	7	317	CHL	CMB-C2B-C3B	2.60	129.54	124.68
27	6	308	CHL	OMC-CMC-C2C	-2.60	119.81	125.69
29	7	304	LUT	C4-C5-C6	-2.60	115.06	120.85
27	8	313	CHL	C1-O2A-CGA	2.60	123.26	116.44
27	b	316	CHL	O2A-CGA-CBA	2.60	120.06	111.91
27	5	322	CHL	CHD-C1D-ND	-2.60	122.07	124.45
29	6	303	LUT	C3-C4-C5	2.60	117.03	111.85
27	7	311	CHL	CMC-C2C-C1C	2.60	128.99	125.04
27	4	320	CHL	CHD-C4C-NC	2.59	128.29	124.20
27	B	844	CHL	CMD-C2D-C1D	2.59	129.28	124.71
27	B	812	CHL	O1D-CGD-CBD	-2.59	119.18	124.48
24	A	811	LHG	O8-C23-C24	2.59	120.05	111.91
27	A	823	CHL	CMC-C2C-C1C	2.59	128.99	125.04
27	B	831	CHL	CMB-C2B-C3B	2.59	129.53	124.68
27	A	841	CHL	C1-O2A-CGA	2.59	123.25	116.44
27	7	321	CHL	C2D-C1D-ND	2.59	112.01	110.10
27	4	318	CHL	C3D-C2D-C1D	-2.59	102.30	105.83
29	J	103	LUT	C3-C4-C5	2.59	117.01	111.85
27	J	106	CHL	O2D-CGD-O1D	-2.59	118.77	123.84
27	8	314	CHL	CHD-C1D-ND	-2.59	122.07	124.45
27	a	319	CHL	CMD-C2D-C1D	2.59	129.28	124.71
27	4	309	CHL	C3D-C2D-C1D	-2.59	102.30	105.83
22	3	302	BCR	C7-C8-C9	-2.59	122.32	126.23
27	A	849	CHL	CAC-C3C-C4C	2.59	128.17	124.81
27	7	314	CHL	O2A-CGA-CBA	2.59	120.03	111.91
27	B	849	CHL	CAC-C3C-C4C	2.59	128.17	124.81
27	7	312	CHL	CHC-C1C-NC	-2.59	120.28	124.20
27	4	307	CHL	CMC-C2C-C1C	2.59	128.98	125.04
27	3	308	CHL	CHC-C1C-NC	-2.59	120.28	124.20
27	a	311	CHL	C4-C3-C2	-2.59	117.04	123.68
27	B	829	CHL	C4-C3-C5	2.59	119.62	115.27
27	4	304	CHL	CHC-C1C-NC	-2.59	120.28	124.20
27	5	322	CHL	O2D-CGD-O1D	-2.58	118.78	123.84
27	6	315	CHL	O1D-CGD-CBD	-2.58	119.19	124.48
27	B	815	CHL	CMC-C2C-C1C	2.58	128.97	125.04
27	4	319	CHL	CMB-C2B-C3B	2.58	129.51	124.68
27	5	323	CHL	O2A-CGA-CBA	2.58	120.01	111.91
27	B	813	CHL	CMB-C2B-C3B	2.58	129.51	124.68
22	K	203	BCR	C24-C23-C22	-2.58	122.33	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	311	CHL	CMD-C2D-C1D	2.58	129.26	124.71
27	F	309	CHL	O2A-CGA-CBA	2.58	120.01	111.91
27	A	840	CHL	CHD-C4C-NC	2.58	128.27	124.20
27	8	317	CHL	C3D-C2D-C1D	-2.58	102.31	105.83
27	B	849	CHL	CMB-C2B-C3B	2.58	129.50	124.68
24	b	302	LHG	C11-C10-C9	-2.58	101.33	114.42
27	K	206	CHL	CED-O2D-CGD	2.58	121.77	115.94
27	J	106	CHL	C3D-C2D-C1D	-2.58	102.31	105.83
27	B	850	CHL	CED-O2D-CGD	2.58	121.77	115.94
27	B	847	CHL	C3D-C2D-C1D	-2.58	102.31	105.83
27	B	829	CHL	CMC-C2C-C1C	2.58	128.96	125.04
27	A	823	CHL	CAC-C3C-C4C	2.58	128.15	124.81
27	b	304	CHL	CMC-C2C-C1C	2.58	128.96	125.04
27	B	832	CHL	CMD-C2D-C1D	2.58	129.25	124.71
27	7	316	CHL	C3D-C2D-C1D	-2.57	102.32	105.83
27	7	323	CHL	O2A-CGA-CBA	2.57	119.99	111.91
27	5	317	CHL	CMB-C2B-C3B	2.57	129.49	124.68
27	B	831	CHL	CHD-C4C-NC	2.57	128.26	124.20
27	4	305	CHL	CHD-C4C-NC	2.57	128.26	124.20
27	B	828	CHL	C1-C2-C3	-2.57	121.59	126.04
27	B	847	CHL	O2A-CGA-CBA	2.57	119.98	111.91
27	8	323	CHL	C2D-C1D-ND	-2.57	108.21	110.10
27	5	309	CHL	C3D-C2D-C1D	-2.57	102.33	105.83
27	B	831	CHL	CED-O2D-CGD	2.57	121.75	115.94
27	4	313	CHL	O2D-CGD-O1D	-2.57	118.82	123.84
27	a	315	CHL	CMD-C2D-C1D	2.57	129.24	124.71
29	3	305	LUT	C10-C11-C12	-2.57	115.20	123.22
27	6	312	CHL	CMC-C2C-C1C	2.57	128.95	125.04
29	3	305	LUT	C1-C6-C7	-2.57	108.52	115.78
27	A	823	CHL	CMD-C2D-C1D	2.57	129.24	124.71
27	B	831	CHL	CMC-C2C-C1C	2.57	128.95	125.04
27	7	316	CHL	O1D-CGD-CBD	-2.57	119.23	124.48
27	5	311	CHL	CMD-C2D-C1D	2.57	129.23	124.71
27	3	314	CHL	CHC-C1C-NC	-2.56	120.31	124.20
27	b	307	CHL	O2A-CGA-CBA	2.56	119.96	111.91
27	A	847	CHL	CMC-C2C-C1C	2.56	128.94	125.04
22	A	804	BCR	C15-C14-C13	-2.56	123.65	127.31
27	A	831	CHL	CHB-C4A-NA	2.56	128.06	124.51
27	8	312	CHL	CHC-C1C-NC	-2.56	120.31	124.20
22	8	302	BCR	C2-C1-C6	2.56	114.43	110.48
27	5	315	CHL	CMD-C2D-C1D	2.56	129.23	124.71
27	B	838	CHL	CAC-C3C-C4C	2.56	128.13	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	313	CHL	CAC-C3C-C4C	2.56	128.13	124.81
27	3	310	CHL	CMB-C2B-C3B	2.56	129.47	124.68
27	4	315	CHL	CHD-C4C-NC	2.56	128.24	124.20
27	3	313	CHL	O2A-CGA-CBA	2.56	119.94	111.91
27	A	823	CHL	CMB-C2B-C3B	2.56	129.47	124.68
27	A	852	CHL	CHC-C1C-NC	-2.56	120.32	124.20
27	A	826	CHL	CHC-C1C-NC	-2.56	120.32	124.20
27	A	856	CHL	CMB-C2B-C3B	2.56	129.47	124.68
27	b	310	CHL	C3D-C2D-C1D	-2.56	102.34	105.83
27	8	312	CHL	CMC-C2C-C1C	2.56	128.94	125.04
22	3	301	BCR	C15-C14-C13	-2.56	123.66	127.31
27	5	308	CHL	C3D-C2D-C1D	-2.56	102.34	105.83
27	b	309	CHL	C3D-C2D-C1D	-2.56	102.34	105.83
27	5	321	CHL	CHC-C1C-NC	-2.56	120.32	124.20
22	B	805	BCR	C15-C16-C17	-2.56	118.23	123.47
27	B	838	CHL	C3D-C2D-C1D	-2.56	102.34	105.83
27	a	316	CHL	O2A-CGA-CBA	2.56	119.93	111.91
27	4	313	CHL	C2C-C1C-NC	2.56	112.37	109.97
27	4	306	CHL	C3D-C2D-C1D	-2.56	102.34	105.83
27	A	830	CHL	CMD-C2D-C1D	2.55	129.22	124.71
27	5	309	CHL	CMD-C2D-C1D	2.55	129.21	124.71
27	4	304	CHL	C1-C2-C3	-2.55	121.63	126.04
27	4	304	CHL	CAC-C3C-C4C	2.55	128.12	124.81
22	3	303	BCR	C15-C14-C13	-2.55	123.67	127.31
27	4	315	CHL	CMC-C2C-C1C	2.55	128.93	125.04
27	B	822	CHL	O2A-CGA-CBA	2.55	119.92	111.91
27	B	814	CHL	CHB-C4A-NA	2.55	128.04	124.51
27	a	309	CHL	C4-C3-C5	2.55	119.56	115.27
27	B	836	CHL	C3D-C2D-C1D	-2.55	102.35	105.83
27	b	311	CHL	C4D-CHA-C1A	-2.55	118.14	121.25
27	B	822	CHL	C4-C3-C5	2.55	119.56	115.27
27	4	315	CHL	C1D-CHD-C4C	-2.55	120.56	126.06
27	A	849	CHL	O2A-CGA-CBA	2.55	119.91	111.91
27	a	317	CHL	CHD-C4C-NC	2.55	128.22	124.20
27	A	831	CHL	CAC-C3C-C2C	2.55	131.89	127.53
27	B	833	CHL	C3D-C2D-C1D	-2.55	102.35	105.83
27	a	320	CHL	CMC-C2C-C1C	2.55	128.92	125.04
27	6	317	CHL	CMD-C2D-C1D	2.55	129.20	124.71
27	B	825	CHL	CAC-C3C-C4C	2.55	128.11	124.81
27	6	313	CHL	CMC-C2C-C1C	2.55	128.91	125.04
27	B	814	CHL	CMD-C2D-C1D	2.54	129.20	124.71
27	3	315	CHL	C1-C2-C3	-2.54	121.64	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	824	CHL	O2A-CGA-CBA	2.54	119.89	111.91
27	3	321	CHL	C3D-C2D-C1D	-2.54	102.36	105.83
27	B	836	CHL	C1-O2A-CGA	2.54	123.12	116.44
27	B	813	CHL	CAC-C3C-C4C	2.54	128.11	124.81
27	B	811	CHL	CMC-C2C-C1C	2.54	128.91	125.04
27	B	843	CHL	C3D-C2D-C1D	-2.54	102.36	105.83
27	8	321	CHL	C4-C3-C5	2.54	119.55	115.27
27	b	315	CHL	CMC-C2C-C1C	2.54	128.91	125.04
27	6	309	CHL	CHC-C1C-NC	-2.54	120.35	124.20
22	K	202	BCR	C15-C16-C17	-2.54	118.27	123.47
27	3	318	CHL	CMC-C2C-C1C	2.54	128.91	125.04
27	7	318	CHL	CHC-C1C-NC	-2.54	120.35	124.20
27	A	854	CHL	CMC-C2C-C1C	2.54	128.91	125.04
27	A	845	CHL	CAC-C3C-C4C	2.54	128.11	124.81
27	4	313	CHL	CHD-C4C-C3C	-2.54	121.11	124.84
27	A	837	CHL	CAC-C3C-C4C	2.54	128.10	124.81
27	8	317	CHL	O1D-CGD-CBD	-2.54	119.29	124.48
27	b	312	CHL	CAC-C3C-C4C	2.54	128.10	124.81
27	A	833	CHL	C4D-CHA-C1A	-2.54	118.16	121.25
27	6	312	CHL	CMD-C2D-C1D	2.54	129.19	124.71
27	6	315	CHL	CMC-C2C-C1C	2.54	128.90	125.04
27	8	316	CHL	O2D-CGD-O1D	-2.54	118.88	123.84
27	6	305	CHL	CMB-C2B-C3B	2.54	129.43	124.68
27	A	825	CHL	CHC-C1C-NC	-2.54	120.35	124.20
27	B	836	CHL	C4-C3-C5	2.54	119.54	115.27
27	7	313	CHL	CHC-C1C-NC	-2.54	120.35	124.20
27	A	853	CHL	CED-O2D-CGD	2.54	121.67	115.94
27	b	317	CHL	O2D-CGD-O1D	-2.54	118.88	123.84
27	A	821	CHL	CMD-C2D-C1D	2.54	129.18	124.71
27	B	816	CHL	CHD-C4C-NC	2.54	128.20	124.20
27	6	312	CHL	CHD-C4C-NC	2.54	128.20	124.20
27	4	312	CHL	CMD-C2D-C1D	2.54	129.18	124.71
27	6	305	CHL	CHC-C1C-NC	-2.54	120.36	124.20
22	L	301	BCR	C15-C16-C17	-2.54	118.28	123.47
27	3	313	CHL	C3D-C2D-C1D	-2.54	102.37	105.83
27	a	308	CHL	C3D-C2D-C1D	-2.53	102.37	105.83
24	A	810	LHG	C11-C10-C9	-2.53	101.56	114.42
27	B	812	CHL	C4-C3-C5	2.53	119.53	115.27
27	4	320	CHL	C1D-CHD-C4C	-2.53	120.59	126.06
27	6	319	CHL	CMD-C2D-C3D	-2.53	121.79	127.61
27	6	305	CHL	CAC-C3C-C4C	2.53	128.10	124.81
27	B	832	CHL	CAC-C3C-C4C	2.53	128.09	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	827	CHL	CMB-C2B-C3B	2.53	129.41	124.68
27	B	845	CHL	O1D-CGD-CBD	-2.53	119.31	124.48
27	K	206	CHL	C3D-C2D-C1D	-2.53	102.38	105.83
27	b	304	CHL	CAC-C3C-C4C	2.53	128.09	124.81
27	B	817	CHL	CHC-C1C-NC	-2.53	120.37	124.20
27	A	826	CHL	O2A-CGA-CBA	2.53	119.84	111.91
27	8	311	CHL	O1D-CGD-CBD	-2.53	119.31	124.48
27	b	314	CHL	CHC-C1C-NC	-2.53	120.37	124.20
27	A	859	CHL	CMC-C2C-C1C	2.53	128.88	125.04
22	K	203	BCR	C27-C26-C25	2.53	126.40	122.73
22	3	303	BCR	C27-C26-C25	2.53	126.40	122.73
27	8	323	CHL	C4C-C3C-C2C	-2.52	103.22	106.90
27	b	315	CHL	C4-C3-C5	2.52	119.52	115.27
27	A	853	CHL	O2A-CGA-CBA	2.52	119.82	111.91
27	B	827	CHL	O2A-CGA-CBA	2.52	119.82	111.91
27	A	856	CHL	CMC-C2C-C1C	2.52	128.88	125.04
27	7	323	CHL	C4-C3-C5	2.52	119.51	115.27
29	8	304	LUT	C36-C21-C26	2.52	113.36	109.55
27	5	320	CHL	C1B-CHB-C4A	-2.52	125.12	130.12
22	3	302	BCR	C11-C10-C9	-2.52	123.71	127.31
27	B	825	CHL	C4-C3-C5	2.52	119.51	115.27
27	A	817	CHL	O1D-CGD-CBD	-2.52	119.33	124.48
27	6	305	CHL	CMD-C2D-C1D	2.52	129.15	124.71
27	A	858	CHL	O1D-CGD-CBD	-2.52	119.33	124.48
27	b	317	CHL	C4D-CHA-C1A	-2.52	118.19	121.25
27	A	842	CHL	CMB-C2B-C3B	2.52	129.39	124.68
27	A	835	CHL	CHC-C1C-NC	-2.52	120.39	124.20
27	a	315	CHL	C4-C3-C5	2.52	119.50	115.27
27	8	316	CHL	O2A-CGA-CBA	2.52	119.80	111.91
27	B	832	CHL	CMB-C2B-C3B	2.52	129.38	124.68
24	A	812	LHG	C11-C10-C9	-2.52	101.65	114.42
27	A	853	CHL	C3D-C2D-C1D	-2.51	102.40	105.83
27	4	319	CHL	C3D-C2D-C1D	-2.51	102.40	105.83
27	7	319	CHL	CMD-C2D-C1D	2.51	129.15	124.71
22	M	102	BCR	C27-C26-C25	2.51	126.38	122.73
27	6	310	CHL	CAC-C3C-C4C	2.51	128.07	124.81
27	B	811	CHL	CHC-C1C-NC	-2.51	120.39	124.20
27	a	308	CHL	CED-O2D-CGD	2.51	121.62	115.94
27	b	304	CHL	C1B-CHB-C4A	-2.51	125.14	130.12
27	5	321	CHL	C3D-C2D-C1D	-2.51	102.41	105.83
27	4	315	CHL	CMB-C2B-C3B	2.51	129.38	124.68
27	5	314	CHL	CMC-C2C-C1C	2.51	128.86	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	831	CHL	C1-C2-C3	-2.51	121.70	126.04
27	B	820	CHL	O2A-CGA-CBA	2.51	119.78	111.91
26	A	815	CL0	C1-O2A-CGA	2.51	123.03	116.44
27	A	817	CHL	CMC-C2C-C1C	2.51	128.86	125.04
27	5	317	CHL	C4D-CHA-C1A	-2.51	118.20	121.25
27	B	842	CHL	CHC-C1C-NC	-2.51	120.40	124.20
27	6	315	CHL	C3D-C2D-C1D	-2.51	102.41	105.83
27	B	846	CHL	CAC-C3C-C4C	2.51	128.06	124.81
24	5	324	LHG	O8-C23-C24	2.51	119.77	111.91
27	8	319	CHL	CAC-C3C-C4C	2.50	128.06	124.81
27	7	316	CHL	C1-C2-C3	-2.50	121.71	126.04
27	3	308	CHL	C4-C3-C5	2.50	119.48	115.27
27	B	817	CHL	CHB-C4A-NA	2.50	127.97	124.51
27	3	318	CHL	CHC-C1C-NC	-2.50	120.41	124.20
27	K	205	CHL	CHD-C4C-NC	2.50	128.15	124.20
22	B	805	BCR	C27-C26-C25	2.50	126.36	122.73
27	5	318	CHL	CMD-C2D-C1D	2.50	129.12	124.71
27	B	815	CHL	CMB-C2B-C3B	2.50	129.36	124.68
27	5	310	CHL	CMB-C2B-C3B	2.50	129.36	124.68
27	L	304	CHL	CED-O2D-CGD	2.50	121.59	115.94
27	B	819	CHL	CMB-C2B-C3B	2.50	129.36	124.68
27	6	320	CHL	CHC-C1C-NC	-2.50	120.41	124.20
27	6	307	CHL	O2A-CGA-CBA	2.50	119.75	111.91
29	4	301	LUT	C1-C6-C7	-2.50	108.70	115.78
27	5	313	CHL	CAC-C3C-C4C	2.50	128.05	124.81
27	a	312	CHL	CMD-C2D-C1D	2.50	129.12	124.71
27	4	313	CHL	C4C-C3C-C2C	-2.50	103.26	106.90
27	4	316	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
22	3	303	BCR	C2-C1-C6	2.50	114.33	110.48
22	3	301	BCR	C15-C16-C17	-2.50	118.36	123.47
27	3	316	CHL	CED-O2D-CGD	2.50	121.58	115.94
27	3	311	CHL	C4-C3-C5	2.50	119.47	115.27
27	A	829	CHL	O2A-CGA-CBA	2.50	119.74	111.91
27	A	828	CHL	CAC-C3C-C4C	2.49	128.05	124.81
27	J	106	CHL	CHC-C1C-NC	-2.49	120.42	124.20
27	5	319	CHL	C4D-CHA-C1A	-2.49	118.21	121.25
27	6	320	CHL	O1D-CGD-CBD	-2.49	119.38	124.48
27	A	834	CHL	O2A-CGA-CBA	2.49	119.73	111.91
27	B	833	CHL	CMD-C2D-C1D	2.49	129.11	124.71
27	4	318	CHL	CMD-C2D-C1D	2.49	129.11	124.71
27	6	308	CHL	O2A-CGA-O1A	-2.49	117.30	123.59
27	4	318	CHL	O1D-CGD-CBD	-2.49	119.38	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	315	CHL	CHC-C1C-NC	-2.49	120.42	124.20
27	B	819	CHL	CMD-C2D-C1D	2.49	129.11	124.71
27	5	320	CHL	O1D-CGD-CBD	-2.49	119.38	124.48
27	8	323	CHL	O2A-CGA-CBA	2.49	119.73	111.91
23	A	808	LMT	C1'-O5'-C5'	-2.49	108.80	113.69
27	7	319	CHL	C2D-C1D-ND	2.49	111.94	110.10
27	7	315	CHL	CMC-C2C-C1C	2.49	128.83	125.04
27	A	841	CHL	C4D-CHA-C1A	-2.49	118.22	121.25
27	A	826	CHL	CMD-C2D-C1D	2.49	129.10	124.71
27	4	307	CHL	C1-C2-C3	-2.49	121.74	126.04
27	6	306	CHL	CHC-C1C-NC	-2.49	120.42	124.20
27	B	814	CHL	CAC-C3C-C4C	2.49	128.04	124.81
27	B	820	CHL	C1-C2-C3	-2.49	121.74	126.04
27	5	322	CHL	O1D-CGD-CBD	-2.49	119.39	124.48
27	A	845	CHL	CMB-C2B-C3B	2.49	129.33	124.68
27	3	310	CHL	C4-C3-C5	2.49	119.46	115.27
27	A	847	CHL	O1D-CGD-CBD	-2.49	119.39	124.48
27	A	855	CHL	CHB-C4A-NA	2.49	127.95	124.51
27	A	821	CHL	CMC-C2C-C1C	2.49	128.82	125.04
27	8	322	CHL	CMB-C2B-C3B	2.49	129.33	124.68
27	b	314	CHL	CHD-C4C-NC	2.49	128.12	124.20
27	8	316	CHL	CMC-C2C-C1C	2.49	128.82	125.04
27	3	309	CHL	CMB-C2B-C3B	2.49	129.33	124.68
27	B	815	CHL	CMD-C2D-C1D	2.49	129.09	124.71
27	7	318	CHL	CAC-C3C-C4C	2.48	128.03	124.81
27	A	855	CHL	CED-O2D-CGD	2.48	121.56	115.94
27	a	310	CHL	CMB-C2B-C3B	2.48	129.33	124.68
27	A	835	CHL	CHD-C4C-NC	2.48	128.12	124.20
22	K	202	BCR	C15-C14-C13	-2.48	123.77	127.31
29	b	301	LUT	C22-C23-C24	2.48	114.57	111.74
27	4	307	CHL	C4-C3-C5	2.48	119.45	115.27
27	b	308	CHL	CMC-C2C-C1C	-2.48	121.26	125.04
27	a	308	CHL	CMC-C2C-C1C	2.48	128.82	125.04
27	A	839	CHL	CED-O2D-CGD	2.48	121.55	115.94
27	3	319	CHL	CMC-C2C-C1C	2.48	128.82	125.04
27	B	848	CHL	CHC-C1C-NC	-2.48	120.44	124.20
27	B	849	CHL	CMC-C2C-C1C	2.48	128.82	125.04
27	B	812	CHL	C1D-CHD-C4C	-2.48	120.71	126.06
27	B	830	CHL	CMD-C2D-C1D	2.48	129.09	124.71
27	a	312	CHL	CHC-C1C-NC	-2.48	120.44	124.20
29	4	302	LUT	C30-C31-C32	-2.48	115.48	123.22
27	F	308	CHL	CMC-C2C-C1C	2.48	128.81	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	845	CHL	CHC-C1C-NC	-2.48	120.44	124.20
27	7	321	CHL	CMD-C2D-C1D	2.48	129.08	124.71
27	B	838	CHL	CHC-C1C-NC	-2.48	120.44	124.20
27	6	313	CHL	CHC-C1C-NC	-2.48	120.44	124.20
27	4	315	CHL	CAC-C3C-C4C	2.48	128.02	124.81
27	5	313	CHL	CAA-CBA-CGA	-2.48	106.02	113.25
27	6	311	CHL	CED-O2D-CGD	2.48	121.54	115.94
27	B	816	CHL	CHC-C1C-NC	-2.48	120.45	124.20
27	4	308	CHL	CMD-C2D-C1D	2.48	129.08	124.71
27	B	847	CHL	CMC-C2C-C1C	2.48	128.81	125.04
27	A	839	CHL	C4-C3-C5	2.47	119.43	115.27
29	8	304	LUT	C12-C13-C14	-2.47	115.14	118.94
27	5	321	CHL	CMC-C2C-C1C	2.47	128.81	125.04
27	B	822	CHL	C4C-C3C-C2C	-2.47	103.29	106.90
27	7	322	CHL	CHC-C1C-NC	-2.47	120.45	124.20
27	7	322	CHL	C1-O2A-CGA	2.47	122.93	116.44
27	8	316	CHL	C1-C2-C3	-2.47	121.77	126.04
27	A	822	CHL	CHC-C1C-NC	-2.47	120.45	124.20
27	b	316	CHL	O1D-CGD-CBD	-2.47	119.42	124.48
27	K	207	CHL	CMD-C2D-C1D	2.47	129.07	124.71
27	7	316	CHL	CMB-C2B-C3B	2.47	129.30	124.68
27	a	312	CHL	C3D-C2D-C1D	-2.47	102.46	105.83
27	6	320	CHL	CMC-C2C-C1C	2.47	128.80	125.04
27	8	326	CHL	C3B-C4B-NB	2.47	112.41	109.21
22	8	302	BCR	C15-C14-C13	-2.47	123.78	127.31
27	4	308	CHL	O2D-CGD-O1D	-2.47	119.00	123.84
27	A	823	CHL	O2A-CGA-CBA	2.47	119.67	111.91
27	L	303	CHL	C11-C10-C8	-2.47	107.93	115.92
27	b	313	CHL	O1D-CGD-CBD	-2.47	119.43	124.48
27	b	307	CHL	O1D-CGD-CBD	-2.47	119.43	124.48
27	6	316	CHL	C2C-C3C-C4C	-2.47	104.73	106.49
27	6	320	CHL	CMB-C2B-C3B	2.47	129.30	124.68
27	A	849	CHL	CMB-C2B-C3B	2.47	129.30	124.68
22	3	301	BCR	C27-C26-C25	2.47	126.32	122.73
27	B	821	CHL	CHC-C1C-NC	-2.47	120.46	124.20
27	B	847	CHL	C4-C3-C5	2.47	119.42	115.27
27	4	307	CHL	O2A-CGA-CBA	2.47	119.65	111.91
27	5	320	CHL	CMD-C2D-C1D	2.47	129.06	124.71
22	A	803	BCR	C27-C26-C25	2.47	126.31	122.73
27	a	319	CHL	O1D-CGD-CBD	-2.47	119.44	124.48
27	5	313	CHL	CHC-C1C-NC	-2.47	120.46	124.20
27	B	832	CHL	C3D-C2D-C1D	-2.47	102.47	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	837	CHL	CMC-C2C-C1C	2.47	128.79	125.04
27	4	305	CHL	C1D-CHD-C4C	-2.47	120.74	126.06
27	A	857	CHL	CMC-C2C-C1C	2.47	128.79	125.04
27	A	851	CHL	CMB-C2B-C3B	2.47	129.29	124.68
27	4	311	CHL	CHC-C1C-NC	-2.46	120.46	124.20
27	A	850	CHL	C1-C2-C3	-2.46	121.78	126.04
27	4	313	CHL	C3B-C4B-NB	2.46	112.39	109.21
27	7	312	CHL	CMC-C2C-C1C	2.46	128.79	125.04
27	B	821	CHL	CAC-C3C-C4C	2.46	128.00	124.81
27	5	309	CHL	O1D-CGD-CBD	-2.46	119.45	124.48
27	5	312	CHL	CHC-C1C-NC	-2.46	120.47	124.20
27	6	311	CHL	O2A-CGA-CBA	2.46	119.63	111.91
27	B	812	CHL	C4C-C3C-C2C	-2.46	103.31	106.90
27	6	320	CHL	CMD-C2D-C1D	2.46	129.05	124.71
22	L	302	BCR	C15-C14-C13	-2.46	123.80	127.31
22	B	807	BCR	C27-C26-C25	2.46	126.30	122.73
29	8	303	LUT	C35-C15-C14	-2.46	118.44	123.47
27	B	840	CHL	C4-C3-C5	2.46	119.41	115.27
27	a	307	CHL	CAC-C3C-C4C	2.46	128.00	124.81
27	8	325	CHL	C4-C3-C5	2.46	119.41	115.27
27	4	304	CHL	C4-C3-C5	2.46	119.41	115.27
27	3	311	CHL	CMD-C2D-C1D	2.46	129.04	124.71
27	A	853	CHL	C2A-C1A-CHA	-2.46	119.56	123.86
27	B	837	CHL	O1D-CGD-CBD	-2.46	119.46	124.48
27	3	317	CHL	C1-C2-C3	-2.46	121.79	126.04
27	5	317	CHL	C2D-C1D-ND	2.46	111.91	110.10
27	6	318	CHL	C2D-C1D-ND	2.46	111.91	110.10
27	A	816	CHL	CMC-C2C-C1C	2.46	128.78	125.04
24	A	810	LHG	C20-C19-C18	-2.46	101.96	114.42
27	B	813	CHL	CMD-C2D-C1D	2.45	129.04	124.71
27	B	825	CHL	CMD-C2D-C1D	2.45	129.04	124.71
27	3	314	CHL	C1-C2-C3	-2.45	121.80	126.04
27	A	852	CHL	C3B-C4B-NB	2.45	112.38	109.21
29	7	304	LUT	C18-C5-C4	-2.45	109.81	114.36
27	7	324	CHL	C3D-C2D-C1D	-2.45	102.48	105.83
27	B	818	CHL	CHC-C1C-NC	-2.45	120.48	124.20
27	B	820	CHL	CMC-C2C-C1C	2.45	128.78	125.04
27	A	837	CHL	O2A-CGA-CBA	2.45	119.61	111.91
27	B	819	CHL	CHC-C1C-NC	-2.45	120.48	124.20
27	8	318	CHL	CHC-C1C-NC	-2.45	120.48	124.20
27	5	307	CHL	CMC-C2C-C1C	2.45	128.78	125.04
22	8	302	BCR	C27-C26-C25	2.45	126.29	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	855	CHL	CMC-C2C-C1C	2.45	128.77	125.04
27	B	840	CHL	C1-C2-C3	-2.45	121.80	126.04
27	A	818	CHL	C1-C2-C3	-2.45	121.80	126.04
22	K	203	BCR	C3-C4-C5	-2.45	109.70	114.08
27	4	320	CHL	CMC-C2C-C1C	2.45	128.77	125.04
27	B	827	CHL	CMD-C2D-C1D	2.45	129.03	124.71
27	5	320	CHL	CAC-C3C-C4C	2.45	127.99	124.81
27	5	308	CHL	CMC-C2C-C1C	2.45	128.77	125.04
27	A	840	CHL	C1-C2-C3	-2.45	121.81	126.04
27	5	321	CHL	O1D-CGD-CBD	-2.45	119.47	124.48
27	A	846	CHL	C5-C3-C4	2.45	120.01	114.60
27	B	826	CHL	CMB-C2B-C3B	2.45	129.26	124.68
27	b	307	CHL	CMD-C2D-C1D	2.45	129.03	124.71
27	4	305	CHL	CHC-C1C-NC	-2.45	120.49	124.20
27	A	850	CHL	CAC-C3C-C4C	2.45	127.98	124.81
27	a	317	CHL	O1D-CGD-CBD	-2.45	119.48	124.48
27	B	837	CHL	C1-O2A-CGA	2.44	122.86	116.44
24	B	808	LHG	O8-C23-C24	2.44	119.58	111.91
27	a	315	CHL	CHC-C1C-NC	-2.44	120.50	124.20
27	A	840	CHL	CMC-C2C-C1C	2.44	128.76	125.04
27	8	314	CHL	CMD-C2D-C1D	2.44	129.02	124.71
27	b	305	CHL	CHC-C1C-NC	-2.44	120.50	124.20
27	B	846	CHL	CED-O2D-CGD	2.44	121.46	115.94
27	F	309	CHL	CAC-C3C-C4C	2.44	127.98	124.81
27	A	848	CHL	CHC-C1C-NC	-2.44	120.50	124.20
27	6	311	CHL	CHC-C1C-NC	-2.44	120.50	124.20
29	4	301	LUT	C36-C21-C26	2.44	113.24	109.55
27	A	816	CHL	CHD-C4C-NC	2.44	128.05	124.20
27	B	824	CHL	CHD-C4C-NC	2.44	128.05	124.20
27	7	312	CHL	CHD-C4C-NC	2.44	128.05	124.20
27	B	815	CHL	CHC-C1C-NC	-2.44	120.50	124.20
27	b	312	CHL	CHC-C1C-NC	-2.44	120.50	124.20
27	6	315	CHL	CED-O2D-CGD	2.44	121.46	115.94
27	L	304	CHL	CHD-C4C-NC	2.44	128.05	124.20
27	8	314	CHL	CMB-C2B-C3B	2.44	129.25	124.68
27	A	851	CHL	CHC-C1C-NC	-2.44	120.50	124.20
27	b	312	CHL	CMD-C2D-C1D	2.44	129.01	124.71
27	B	816	CHL	C4-C3-C5	2.44	119.38	115.27
27	6	306	CHL	CMB-C2B-C3B	2.44	129.24	124.68
27	B	829	CHL	C1-C2-C3	-2.44	121.83	126.04
27	A	833	CHL	CHC-C1C-NC	-2.44	120.50	124.20
27	A	858	CHL	CHC-C1C-NC	-2.44	120.50	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	817	CHL	C4-C3-C5	2.44	119.37	115.27
27	5	320	CHL	CMB-C2B-C3B	2.44	129.24	124.68
27	A	839	CHL	C1-C2-C3	-2.44	121.83	126.04
27	6	310	CHL	CMD-C2D-C1D	2.44	129.01	124.71
27	7	315	CHL	CMD-C2D-C1D	2.44	129.01	124.71
27	A	843	CHL	O2D-CGD-O1D	-2.44	119.08	123.84
22	A	803	BCR	C24-C23-C22	-2.44	122.55	126.23
27	A	853	CHL	O1D-CGD-CBD	-2.44	119.50	124.48
27	A	833	CHL	C1-O2A-CGA	2.44	122.83	116.44
27	5	325	CHL	CED-O2D-CGD	2.44	121.44	115.94
27	A	833	CHL	CHD-C4C-NC	2.43	128.04	124.20
27	5	318	CHL	CMB-C2B-C3B	2.43	129.23	124.68
27	A	856	CHL	CHC-C1C-NC	-2.43	120.51	124.20
27	3	321	CHL	CMB-C2B-C3B	2.43	129.23	124.68
27	B	850	CHL	CMD-C2D-C1D	2.43	129.00	124.71
24	7	306	LHG	C11-C10-C9	-2.43	102.08	114.42
27	B	829	CHL	CMB-C2B-C3B	2.43	129.23	124.68
27	B	812	CHL	CHD-C4C-NC	2.43	128.04	124.20
27	5	313	CHL	C6-C7-C8	-2.43	108.06	115.92
27	8	320	CHL	C1-C2-C3	-2.43	121.84	126.04
26	A	815	CL0	O2A-CGA-CBA	2.43	119.53	111.91
27	B	829	CHL	CHC-C1C-NC	-2.43	120.52	124.20
27	B	823	CHL	C1D-CHD-C4C	-2.43	120.82	126.06
27	5	315	CHL	CMC-C2C-C1C	2.43	128.74	125.04
27	3	317	CHL	CMB-C2B-C3B	2.43	129.22	124.68
27	8	325	CHL	CHC-C1C-NC	-2.43	120.52	124.20
27	5	316	CHL	OMC-CMC-C2C	-2.43	120.20	125.69
27	B	830	CHL	C3D-C2D-C1D	-2.43	102.52	105.83
27	3	314	CHL	O1D-CGD-CBD	-2.43	119.52	124.48
27	6	316	CHL	C2D-C1D-ND	2.43	111.89	110.10
27	A	844	CHL	CAC-C3C-C4C	2.43	127.96	124.81
29	5	302	LUT	C17-C1-C6	-2.43	106.36	110.30
27	B	823	CHL	CMD-C2D-C1D	2.43	128.99	124.71
27	b	317	CHL	C1D-CHD-C4C	-2.43	120.83	126.06
27	A	835	CHL	O2A-CGA-CBA	2.43	119.52	111.91
27	3	314	CHL	CMB-C2B-C3B	2.42	129.22	124.68
27	A	849	CHL	C1D-CHD-C4C	-2.42	120.83	126.06
27	3	318	CHL	CMB-C2B-C3B	2.42	129.21	124.68
24	A	811	LHG	C11-C10-C9	-2.42	102.12	114.42
27	4	311	CHL	CMD-C2D-C1D	2.42	128.98	124.71
27	B	830	CHL	O2A-CGA-CBA	2.42	119.51	111.91
27	B	824	CHL	C1D-CHD-C4C	-2.42	120.83	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	822	CHL	CMD-C2D-C1D	2.42	128.98	124.71
27	5	317	CHL	CMD-C2D-C1D	2.42	128.98	124.71
27	A	851	CHL	CMD-C2D-C1D	2.42	128.98	124.71
27	A	843	CHL	CHB-C4A-NA	2.42	127.86	124.51
27	A	852	CHL	C1-O2A-CGA	2.42	122.80	116.44
27	5	309	CHL	CHC-C1C-NC	-2.42	120.53	124.20
27	B	830	CHL	C4-C3-C5	2.42	119.34	115.27
27	B	816	CHL	CMC-C2C-C1C	2.42	128.72	125.04
27	A	823	CHL	CHC-C1C-NC	-2.42	120.53	124.20
27	4	306	CHL	O2A-CGA-CBA	2.42	119.50	111.91
27	4	311	CHL	CMC-C2C-C1C	2.42	128.72	125.04
27	B	850	CHL	CHC-C1C-NC	-2.42	120.53	124.20
22	A	804	BCR	C24-C23-C22	-2.42	122.58	126.23
27	B	822	CHL	CHD-C4C-NC	2.42	128.01	124.20
29	3	305	LUT	C2-C3-C4	2.42	113.61	110.30
27	B	811	CHL	O1D-CGD-CBD	-2.42	119.54	124.48
27	6	310	CHL	O2A-CGA-CBA	2.42	119.49	111.91
27	4	308	CHL	C1D-CHD-C4C	-2.42	120.84	126.06
27	A	818	CHL	O2A-CGA-CBA	2.42	119.49	111.91
27	B	849	CHL	C4-C3-C5	2.42	119.34	115.27
27	8	313	CHL	O2A-CGA-CBA	2.42	119.49	111.91
27	8	315	CHL	O2A-CGA-CBA	2.42	119.49	111.91
27	6	307	CHL	CMD-C2D-C3D	-2.42	122.06	127.61
27	a	313	CHL	CED-O2D-CGD	2.41	121.40	115.94
27	A	845	CHL	CHC-C1C-NC	-2.41	120.54	124.20
27	8	312	CHL	CAC-C3C-C4C	2.41	127.94	124.81
27	8	325	CHL	CMC-C2C-C1C	2.41	128.72	125.04
27	b	305	CHL	C3D-C2D-C1D	-2.41	102.54	105.83
22	5	301	BCR	C24-C23-C22	-2.41	122.59	126.23
27	4	315	CHL	O2A-CGA-CBA	2.41	119.48	111.91
27	B	842	CHL	CMD-C2D-C1D	2.41	128.97	124.71
27	6	315	CHL	CMD-C2D-C1D	2.41	128.97	124.71
27	a	311	CHL	CMC-C2C-C1C	2.41	128.71	125.04
27	5	312	CHL	CMD-C2D-C1D	2.41	128.96	124.71
27	6	308	CHL	CMD-C2D-C3D	-2.41	122.07	127.61
24	7	306	LHG	O8-C23-C24	2.41	119.47	111.91
27	K	205	CHL	CMB-C2B-C3B	2.41	129.19	124.68
27	5	307	CHL	CHC-C1C-NC	-2.41	120.55	124.20
27	3	312	CHL	C3B-C4B-NB	2.41	112.33	109.21
27	a	308	CHL	CMB-C2B-C3B	2.41	129.19	124.68
27	7	316	CHL	CMC-C2C-C1C	2.41	128.71	125.04
24	8	305	LHG	C11-C10-C9	-2.41	102.20	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	323	CHL	C5-C3-C4	2.41	119.92	114.60
27	A	858	CHL	C4-C3-C2	-2.41	117.50	123.68
27	4	311	CHL	CAC-C3C-C4C	2.41	127.93	124.81
27	A	819	CHL	C1-O2A-CGA	2.41	122.76	116.44
27	A	829	CHL	C4-C3-C5	2.41	119.32	115.27
27	A	816	CHL	O2A-CGA-CBA	2.41	119.46	111.91
27	a	310	CHL	O2A-CGA-CBA	2.41	119.46	111.91
27	B	840	CHL	CMC-C2C-C1C	2.41	128.70	125.04
27	8	324	CHL	CMD-C2D-C1D	2.41	128.95	124.71
27	A	825	CHL	C4-C3-C5	2.41	119.32	115.27
30	a	301	LMG	C38-C37-C36	-2.41	102.22	114.42
27	b	310	CHL	O1D-CGD-CBD	-2.40	119.56	124.48
27	5	321	CHL	CAC-C3C-C4C	2.40	127.93	124.81
27	A	850	CHL	C3D-C2D-C1D	-2.40	102.55	105.83
27	8	311	CHL	CMC-C2C-C1C	2.40	128.70	125.04
27	B	818	CHL	C1-C2-C3	-2.40	121.89	126.04
27	7	313	CHL	CMC-C2C-C1C	2.40	128.70	125.04
27	a	314	CHL	CMB-C2B-C3B	2.40	129.17	124.68
27	A	827	CHL	C1-O2A-CGA	2.40	122.74	116.44
27	B	830	CHL	CHC-C1C-NC	-2.40	120.56	124.20
22	3	303	BCR	C24-C23-C22	-2.40	122.61	126.23
27	L	304	CHL	CMD-C2D-C1D	2.40	128.94	124.71
27	7	320	CHL	CAA-CBA-CGA	-2.40	106.24	113.25
22	8	302	BCR	C11-C10-C9	-2.40	123.89	127.31
27	4	313	CHL	C1C-C2C-C3C	-2.40	104.43	106.96
27	7	322	CHL	CMD-C2D-C1D	2.40	128.94	124.71
27	5	318	CHL	C1D-CHD-C4C	-2.40	120.88	126.06
27	B	827	CHL	C4-C3-C5	2.40	119.31	115.27
27	6	313	CHL	CMD-C2D-C1D	2.40	128.94	124.71
27	B	816	CHL	CMB-C2B-C3B	2.40	129.16	124.68
27	5	323	CHL	C3B-C4B-NB	2.40	112.31	109.21
27	b	311	CHL	CAC-C3C-C4C	2.40	127.92	124.81
22	B	804	BCR	C27-C26-C25	2.40	126.21	122.73
27	B	840	CHL	CMD-C2D-C1D	2.40	128.94	124.71
27	K	207	CHL	CHC-C1C-NC	-2.40	120.57	124.20
27	3	320	CHL	CAA-C2A-C1A	-2.40	104.12	111.97
27	A	827	CHL	O2A-CGA-CBA	2.40	119.43	111.91
27	b	316	CHL	CMD-C2D-C1D	2.40	128.94	124.71
27	A	855	CHL	CAC-C3C-C4C	2.40	127.92	124.81
27	B	831	CHL	CHC-C1C-NC	-2.40	120.57	124.20
27	3	310	CHL	O1D-CGD-CBD	-2.39	119.58	124.48
27	B	821	CHL	O2A-CGA-CBA	2.39	119.42	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	313	CHL	O2A-CGA-CBA	2.39	119.42	111.91
27	B	829	CHL	O2A-CGA-CBA	2.39	119.42	111.91
27	A	850	CHL	O2A-CGA-CBA	2.39	119.42	111.91
27	B	844	CHL	O2A-CGA-CBA	2.39	119.42	111.91
27	7	318	CHL	CMD-C2D-C1D	2.39	128.93	124.71
22	B	802	BCR	C24-C23-C22	-2.39	122.62	126.23
27	5	307	CHL	C1D-CHD-C4C	-2.39	120.90	126.06
27	A	852	CHL	CAC-C3C-C4C	2.39	127.91	124.81
27	4	320	CHL	CED-O2D-CGD	2.39	121.35	115.94
27	a	309	CHL	C1-C2-C3	-2.39	121.91	126.04
27	5	320	CHL	CMC-C2C-C1C	2.39	128.68	125.04
27	4	312	CHL	CHC-C1C-NC	-2.39	120.58	124.20
27	A	843	CHL	CAA-CBA-CGA	-2.39	106.27	113.25
27	b	317	CHL	CMD-C2D-C1D	2.39	128.93	124.71
27	A	859	CHL	CAC-C3C-C4C	2.39	127.91	124.81
27	B	823	CHL	C1-C2-C3	-2.39	121.91	126.04
27	7	316	CHL	CHC-C1C-NC	-2.39	120.58	124.20
27	a	313	CHL	O1D-CGD-CBD	-2.39	119.60	124.48
27	8	319	CHL	CHC-C1C-NC	-2.39	120.58	124.20
27	8	325	CHL	CAC-C3C-C4C	2.39	127.91	124.81
27	4	314	CHL	CMB-C2B-C3B	2.39	129.14	124.68
27	b	314	CHL	CMB-C2B-C3B	2.39	129.14	124.68
27	A	844	CHL	C3D-C2D-C1D	-2.39	102.58	105.83
27	A	850	CHL	CMC-C2C-C1C	2.38	128.67	125.04
24	A	810	LHG	C18-C17-C16	-2.38	102.32	114.42
27	a	315	CHL	C4D-CHA-C1A	-2.38	118.35	121.25
27	3	318	CHL	CAC-C3C-C4C	2.38	127.90	124.81
27	6	315	CHL	CAC-C3C-C4C	2.38	127.90	124.81
27	a	320	CHL	CMD-C2D-C1D	2.38	128.91	124.71
27	8	311	CHL	CMD-C2D-C1D	2.38	128.91	124.71
27	3	311	CHL	CHB-C4A-NA	2.38	127.81	124.51
27	3	317	CHL	CAC-C3C-C4C	2.38	127.90	124.81
27	A	846	CHL	CBC-CAC-C3C	-2.38	105.87	112.43
27	b	314	CHL	CMD-C2D-C1D	2.38	128.91	124.71
29	5	302	LUT	C1-C6-C7	-2.38	109.04	115.78
27	B	828	CHL	CAC-C3C-C4C	2.38	127.90	124.81
27	5	314	CHL	CAC-C3C-C4C	2.38	127.90	124.81
27	A	851	CHL	CMC-C2C-C1C	2.38	128.66	125.04
27	a	316	CHL	C2C-C3C-C4C	-2.38	104.79	106.49
24	8	305	LHG	C20-C19-C18	-2.38	102.35	114.42
27	B	841	CHL	CMB-C2B-C3B	2.38	129.13	124.68
27	A	845	CHL	C4-C3-C5	2.38	119.27	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	824	CHL	O2A-CGA-CBA	2.38	119.36	111.91
27	a	309	CHL	O2A-CGA-CBA	2.38	119.36	111.91
27	b	312	CHL	CMC-C2C-C1C	2.37	128.66	125.04
27	3	311	CHL	CMB-C2B-C3B	2.37	129.12	124.68
27	6	319	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
27	5	312	CHL	C5-C3-C4	2.37	119.85	114.60
27	A	819	CHL	CMD-C2D-C1D	2.37	128.90	124.71
27	A	825	CHL	CMC-C2C-C1C	2.37	128.65	125.04
27	a	313	CHL	CMC-C2C-C1C	2.37	128.65	125.04
27	8	322	CHL	CMD-C2D-C1D	2.37	128.90	124.71
27	B	843	CHL	O1D-CGD-CBD	-2.37	119.63	124.48
27	B	842	CHL	CMB-C2B-C3B	2.37	129.12	124.68
27	3	312	CHL	CHC-C1C-NC	-2.37	120.60	124.20
27	b	308	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
27	A	821	CHL	CMB-C2B-C3B	2.37	129.12	124.68
27	3	317	CHL	CMD-C2D-C1D	2.37	128.89	124.71
27	8	313	CHL	C5-C3-C4	2.37	119.84	114.60
27	7	316	CHL	C4-C3-C5	2.37	119.26	115.27
27	a	312	CHL	CED-O2D-CGD	2.37	121.30	115.94
27	b	314	CHL	CMC-C2C-C1C	2.37	128.65	125.04
27	B	816	CHL	CED-O2D-CGD	2.37	121.30	115.94
27	A	826	CHL	CAC-C3C-C4C	2.37	127.89	124.81
27	B	843	CHL	CMC-C2C-C1C	2.37	128.65	125.04
27	5	325	CHL	CHC-C1C-NC	-2.37	120.61	124.20
27	A	822	CHL	CMD-C2D-C1D	2.37	128.89	124.71
27	B	832	CHL	CHC-C1C-NC	-2.37	120.61	124.20
27	B	849	CHL	CHC-C1C-NC	-2.37	120.61	124.20
27	B	818	CHL	CHD-C4C-NC	2.37	127.94	124.20
27	B	847	CHL	CMD-C2D-C1D	2.37	128.89	124.71
27	B	839	CHL	C4-C3-C5	2.37	119.25	115.27
27	A	857	CHL	C3B-C4B-NB	2.37	112.27	109.21
24	7	302	LHG	C20-C19-C18	-2.37	102.41	114.42
27	5	309	CHL	CAC-C3C-C4C	2.37	127.88	124.81
27	A	833	CHL	CMB-C2B-C3B	2.37	129.10	124.68
27	A	847	CHL	CMD-C2D-C1D	2.37	128.88	124.71
27	6	311	CHL	C1-C2-C3	-2.37	121.95	126.04
27	8	312	CHL	O2A-CGA-O1A	-2.37	117.62	123.59
27	A	855	CHL	CMB-C2B-C3B	2.37	129.10	124.68
27	4	304	CHL	CMD-C2D-C1D	2.36	128.88	124.71
27	A	857	CHL	CED-O2D-CGD	2.36	121.28	115.94
27	7	324	CHL	CHC-C1C-NC	-2.36	120.62	124.20
27	3	316	CHL	O2A-CGA-O1A	-2.36	117.63	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	318	CHL	CMD-C2D-C1D	2.36	128.88	124.71
22	B	803	BCR	C15-C16-C17	-2.36	118.64	123.47
22	6	301	BCR	C23-C22-C21	2.36	122.56	118.94
27	b	311	CHL	CED-O2D-CGD	2.36	121.28	115.94
27	a	314	CHL	CMC-C2C-C1C	2.36	128.63	125.04
27	3	316	CHL	C2D-C1D-ND	2.36	111.84	110.10
22	A	806	BCR	C11-C10-C9	-2.36	123.94	127.31
27	a	312	CHL	C5-C3-C4	2.36	119.81	114.60
27	4	310	CHL	C1B-CHB-C4A	-2.36	125.44	130.12
22	B	804	BCR	C24-C23-C22	-2.36	122.67	126.23
27	A	840	CHL	CAC-C3C-C4C	2.36	127.87	124.81
27	A	840	CHL	C4-C3-C5	2.36	119.24	115.27
27	6	318	CHL	CMB-C2B-C3B	2.36	129.09	124.68
27	6	307	CHL	CBA-CAA-C2A	-2.36	106.90	113.86
27	5	323	CHL	CED-O2D-CGD	2.36	121.27	115.94
27	A	845	CHL	C3B-C4B-NB	2.36	112.26	109.21
27	a	317	CHL	C1D-CHD-C4C	-2.36	120.97	126.06
27	a	310	CHL	CMD-C2D-C1D	2.36	128.87	124.71
27	A	826	CHL	CMC-C2C-C1C	2.35	128.62	125.04
27	a	307	CHL	C4-C3-C5	2.35	119.23	115.27
27	4	320	CHL	CMD-C2D-C1D	2.35	128.86	124.71
27	6	309	CHL	C3D-C4D-CHA	-2.35	107.34	112.72
22	3	302	BCR	C15-C16-C17	-2.35	118.65	123.47
27	A	824	CHL	C3B-C4B-NB	2.35	112.25	109.21
27	B	833	CHL	CMC-C2C-C1C	2.35	128.62	125.04
27	8	314	CHL	C2C-C3C-C4C	-2.35	104.81	106.49
27	3	308	CHL	CMD-C2D-C1D	2.35	128.86	124.71
27	B	820	CHL	CHC-C1C-NC	-2.35	120.63	124.20
27	a	320	CHL	O1D-CGD-CBD	-2.35	119.67	124.48
28	B	809	DGD	C3G-C2G-C1G	-2.35	106.23	111.79
27	B	814	CHL	C4-C3-C5	2.35	119.22	115.27
27	3	310	CHL	CHC-C1C-NC	-2.35	120.64	124.20
27	8	313	CHL	CAC-C3C-C4C	2.35	127.86	124.81
27	B	825	CHL	C3D-C4D-CHA	-2.35	107.35	112.72
27	7	314	CHL	CMC-C2C-C1C	2.35	128.62	125.04
22	B	803	BCR	C27-C26-C25	2.35	126.14	122.73
29	a	304	LUT	C21-C26-C27	-2.35	109.73	112.70
27	A	859	CHL	CHC-C1C-NC	-2.35	120.64	124.20
27	5	316	CHL	C2A-C1A-CHA	-2.35	119.75	123.86
27	5	312	CHL	CAC-C3C-C4C	2.35	127.86	124.81
27	b	317	CHL	C2D-C1D-ND	2.35	111.83	110.10
27	B	820	CHL	CMD-C2D-C1D	2.35	128.85	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	320	CHL	CHC-C1C-NC	-2.35	120.64	124.20
27	5	314	CHL	CMB-C2B-C3B	2.35	129.07	124.68
27	3	319	CHL	C3D-C2D-C1D	-2.35	102.63	105.83
27	A	841	CHL	CAC-C3C-C4C	2.35	127.85	124.81
22	B	806	BCR	C11-C10-C9	-2.35	123.96	127.31
27	3	311	CHL	C1-C2-C3	-2.35	121.99	126.04
27	B	827	CHL	CHC-C1C-NC	-2.35	120.64	124.20
27	A	828	CHL	O2A-CGA-CBA	2.35	119.27	111.91
27	B	811	CHL	CED-O2D-CGD	2.34	121.24	115.94
27	A	838	CHL	CAC-C3C-C4C	2.34	127.85	124.81
27	B	816	CHL	O2A-CGA-CBA	2.34	119.27	111.91
27	A	822	CHL	CED-O2D-CGD	2.34	121.24	115.94
27	8	322	CHL	C1D-CHD-C4C	-2.34	121.00	126.06
27	A	828	CHL	CMD-C2D-C1D	2.34	128.84	124.71
27	B	824	CHL	C4-C3-C2	-2.34	117.67	123.68
27	4	317	CHL	CMB-C2B-C1B	2.34	132.06	128.46
27	A	856	CHL	CMD-C2D-C1D	2.34	128.84	124.71
22	A	806	BCR	C28-C27-C26	-2.34	109.89	114.08
27	B	825	CHL	O2A-CGA-CBA	2.34	119.26	111.91
27	A	847	CHL	CHC-C1C-NC	-2.34	120.65	124.20
27	4	309	CHL	CHC-C1C-NC	-2.34	120.65	124.20
27	B	841	CHL	C4C-C3C-C2C	-2.34	103.48	106.90
27	6	314	CHL	CMC-C2C-C1C	2.34	128.60	125.04
27	A	831	CHL	C6-C5-C3	-2.34	107.31	113.45
27	7	314	CHL	CMD-C2D-C1D	2.34	128.84	124.71
27	B	845	CHL	CMD-C2D-C1D	2.34	128.84	124.71
27	5	317	CHL	C1D-CHD-C4C	-2.34	121.01	126.06
27	5	311	CHL	CED-O2D-CGD	2.34	121.23	115.94
27	3	310	CHL	CMD-C2D-C1D	2.34	128.84	124.71
27	5	313	CHL	C2A-C3A-C4A	-2.34	98.09	101.87
27	7	311	CHL	O2A-CGA-O1A	-2.34	117.69	123.59
27	B	845	CHL	C5-C3-C4	2.34	119.77	114.60
27	a	319	CHL	CMB-C2B-C3B	2.34	129.05	124.68
27	4	319	CHL	CMD-C2D-C1D	2.34	128.83	124.71
27	8	314	CHL	CAC-C3C-C4C	2.34	127.84	124.81
27	B	837	CHL	O2A-CGA-CBA	2.34	119.24	111.91
27	6	307	CHL	C3D-C4D-CHA	-2.34	107.38	112.72
28	B	809	DGD	CFB-CEB-CDB	-2.34	102.56	114.42
24	5	324	LHG	C11-C10-C9	-2.34	102.57	114.42
29	b	301	LUT	C36-C21-C26	2.33	113.08	109.55
27	3	315	CHL	O2A-CGA-CBA	2.33	119.23	111.91
27	b	308	CHL	O2A-CGA-CBA	2.33	121.46	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	314	CHL	CMD-C2D-C1D	2.33	128.82	124.71
27	4	310	CHL	CMB-C2B-C3B	2.33	129.04	124.68
27	A	843	CHL	C16-C17-C18	-2.33	104.99	115.98
27	B	817	CHL	C3B-C4B-NB	2.33	112.23	109.21
27	b	312	CHL	CMB-C2B-C3B	2.33	129.04	124.68
27	A	859	CHL	O2A-CGA-CBA	2.33	119.23	111.91
28	7	307	DGD	CFB-CEB-CDB	-2.33	102.59	114.42
27	a	316	CHL	CHC-C1C-NC	-2.33	120.67	124.20
27	5	319	CHL	CMD-C2D-C1D	2.33	128.82	124.71
27	7	313	CHL	CMD-C2D-C1D	2.33	128.82	124.71
27	B	823	CHL	O2A-CGA-CBA	2.33	119.22	111.91
27	A	858	CHL	CAC-C3C-C4C	2.33	127.83	124.81
27	6	306	CHL	O2A-CGA-O1A	-2.33	117.71	123.59
27	5	315	CHL	O1D-CGD-CBD	-2.33	119.72	124.48
24	A	810	LHG	O8-C23-C24	2.33	119.22	111.91
27	A	837	CHL	C1-C2-C3	-2.33	122.01	126.04
27	8	319	CHL	CMD-C2D-C1D	2.33	128.82	124.71
27	a	317	CHL	O2A-CGA-CBA	2.33	119.22	111.91
27	3	319	CHL	CMB-C2B-C3B	2.33	129.03	124.68
27	5	310	CHL	CMD-C2D-C1D	2.33	128.82	124.71
24	7	302	LHG	C11-C10-C9	-2.33	102.61	114.42
27	4	314	CHL	CAC-C3C-C4C	2.33	127.83	124.81
27	A	835	CHL	CMD-C2D-C1D	2.33	128.81	124.71
27	7	320	CHL	CMD-C2D-C1D	2.33	128.81	124.71
27	3	315	CHL	CMB-C2B-C3B	2.33	129.03	124.68
27	B	833	CHL	C4-C3-C5	2.33	119.18	115.27
27	5	311	CHL	CBC-CAC-C3C	-2.33	106.02	112.43
27	4	315	CHL	CMD-C2D-C1D	2.32	128.81	124.71
27	b	310	CHL	CMD-C2D-C1D	2.32	128.81	124.71
27	A	838	CHL	CMD-C2D-C1D	2.32	128.81	124.71
27	J	106	CHL	CMC-C2C-C1C	2.32	128.58	125.04
33	7	305	XAT	C28-C29-C30	2.32	122.51	118.94
27	7	314	CHL	C1-C2-C3	-2.32	122.02	126.04
27	5	312	CHL	CMC-C2C-C1C	2.32	128.58	125.04
27	6	320	CHL	CAC-C3C-C4C	2.32	127.82	124.81
22	M	102	BCR	C24-C23-C22	-2.32	122.73	126.23
22	I	801	BCR	C33-C5-C6	-2.32	121.92	124.53
22	8	302	BCR	C24-C23-C22	-2.32	122.73	126.23
27	a	314	CHL	CAC-C3C-C4C	2.32	127.82	124.81
27	b	306	CHL	CMD-C2D-C1D	2.32	128.80	124.71
27	A	848	CHL	CMC-C2C-C1C	2.32	128.57	125.04
27	B	834	CHL	C1D-CHD-C4C	-2.32	121.05	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	805	BCR	C15-C14-C13	-2.32	124.00	127.31
27	A	846	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
27	A	843	CHL	C11-C12-C13	-2.32	108.42	115.92
27	6	315	CHL	O2A-CGA-CBA	2.32	119.19	111.91
27	a	312	CHL	CMB-C2B-C3B	2.32	129.02	124.68
27	B	844	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
27	8	314	CHL	CHA-C4D-ND	2.32	137.35	132.50
22	B	804	BCR	C15-C16-C17	-2.32	118.72	123.47
27	A	820	CHL	C7-C6-C5	-2.32	107.06	113.36
27	3	309	CHL	CMD-C2D-C1D	2.32	128.80	124.71
27	B	836	CHL	C3B-C4B-NB	2.32	112.21	109.21
27	A	833	CHL	CMD-C2D-C1D	2.32	128.80	124.71
27	8	321	CHL	CMD-C2D-C1D	2.32	128.80	124.71
27	A	839	CHL	CMB-C2B-C3B	2.32	129.01	124.68
27	A	823	CHL	C6-C5-C3	-2.32	107.38	113.45
27	A	836	CHL	O2A-CGA-CBA	2.32	119.17	111.91
24	A	812	LHG	C20-C19-C18	-2.32	102.67	114.42
27	b	310	CHL	CMC-C2C-C1C	2.31	128.56	125.04
27	5	325	CHL	CMB-C2B-C3B	2.31	129.01	124.68
27	a	320	CHL	CHC-C1C-NC	-2.31	120.69	124.20
27	8	316	CHL	CHC-C1C-NC	-2.31	120.69	124.20
33	7	305	XAT	C8-C9-C10	2.31	122.49	118.94
27	b	305	CHL	CMC-C2C-C1C	2.31	128.56	125.04
27	8	311	CHL	CMB-C2B-C3B	2.31	129.01	124.68
27	b	306	CHL	CAC-C3C-C4C	2.31	127.81	124.81
27	F	309	CHL	CMB-C2B-C3B	2.31	129.00	124.68
27	8	320	CHL	CMC-C2C-C1C	2.31	128.56	125.04
27	A	835	CHL	CMB-C2B-C3B	2.31	129.00	124.68
27	A	839	CHL	CMD-C2D-C1D	2.31	128.79	124.71
27	B	815	CHL	O1D-CGD-CBD	-2.31	119.75	124.48
27	6	318	CHL	CMD-C2D-C1D	2.31	128.79	124.71
27	4	312	CHL	CAC-C3C-C4C	2.31	127.81	124.81
27	5	310	CHL	CAC-C3C-C4C	2.31	127.81	124.81
27	8	317	CHL	CMB-C2B-C3B	2.31	129.00	124.68
27	B	849	CHL	O2A-CGA-CBA	2.31	119.16	111.91
27	B	850	CHL	C5-C3-C4	2.31	119.71	114.60
27	B	830	CHL	CAC-C3C-C4C	2.31	127.81	124.81
27	B	817	CHL	C1D-CHD-C4C	-2.31	121.08	126.06
27	4	307	CHL	O1D-CGD-CBD	-2.31	119.76	124.48
27	7	323	CHL	CMB-C2B-C3B	2.31	129.00	124.68
27	A	821	CHL	C4-C3-C5	2.31	119.16	115.27
27	A	818	CHL	C2A-C1A-CHA	-2.31	119.82	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	837	CHL	C3D-C4D-CHA	-2.31	107.44	112.72
27	B	811	CHL	C1-C2-C3	-2.31	122.05	126.04
27	B	817	CHL	C1-C2-C3	-2.31	122.05	126.04
27	B	840	CHL	O2A-CGA-O1A	-2.31	117.77	123.59
27	7	323	CHL	CHD-C4C-NC	2.31	127.84	124.20
27	b	307	CHL	CHC-C1C-NC	-2.31	120.70	124.20
27	3	318	CHL	O2A-CGA-CBA	2.31	119.14	111.91
27	B	823	CHL	CHC-C1C-NC	-2.30	120.71	124.20
27	A	834	CHL	C3B-C4B-NB	2.30	112.19	109.21
27	3	312	CHL	CAC-C3C-C4C	2.30	127.80	124.81
27	A	837	CHL	CHC-C1C-NC	-2.30	120.71	124.20
27	8	320	CHL	CMB-C2B-C3B	2.30	128.99	124.68
27	A	836	CHL	CMD-C2D-C1D	2.30	128.77	124.71
27	b	307	CHL	C1-C2-C3	-2.30	122.06	126.04
27	A	818	CHL	CMC-C2C-C1C	2.30	128.54	125.04
27	5	325	CHL	C2D-C1D-ND	2.30	111.80	110.10
27	A	828	CHL	C4C-C3C-C2C	-2.30	103.54	106.90
27	B	838	CHL	CMC-C2C-C1C	2.30	128.54	125.04
29	3	304	LUT	C1-C6-C7	-2.30	109.27	115.78
29	8	303	LUT	C1-C6-C7	-2.30	109.27	115.78
27	A	833	CHL	C2C-C3C-C4C	-2.30	104.85	106.49
27	K	205	CHL	CAC-C3C-C4C	2.30	127.79	124.81
27	7	320	CHL	CHD-C1D-ND	-2.30	122.34	124.45
27	A	820	CHL	CMD-C2D-C1D	2.30	128.76	124.71
27	7	320	CHL	C2C-C3C-C4C	-2.30	104.85	106.49
27	6	316	CHL	CMD-C2D-C1D	2.30	128.76	124.71
27	8	314	CHL	C2D-C1D-ND	2.30	111.80	110.10
27	5	309	CHL	C1-O2A-CGA	2.30	122.47	116.44
27	a	320	CHL	CMB-C2B-C3B	2.30	128.97	124.68
27	5	313	CHL	CMD-C2D-C3D	-2.30	122.33	127.61
22	3	303	BCR	C3-C4-C5	-2.30	109.98	114.08
27	B	838	CHL	CMD-C2D-C1D	2.30	128.76	124.71
27	4	308	CHL	CMB-C2B-C3B	2.30	128.97	124.68
27	B	821	CHL	C3B-C4B-NB	2.29	112.18	109.21
27	b	315	CHL	C3D-C4D-CHA	-2.29	107.47	112.72
27	A	853	CHL	C3D-C4D-CHA	-2.29	107.47	112.72
22	A	807	BCR	C27-C26-C25	2.29	126.06	122.73
27	3	313	CHL	C3B-C4B-NB	2.29	112.18	109.21
27	A	845	CHL	CHD-C4C-NC	2.29	127.82	124.20
27	B	828	CHL	CMB-C2B-C3B	2.29	128.97	124.68
22	B	802	BCR	C33-C5-C6	-2.29	121.95	124.53
27	3	321	CHL	CMC-C2C-C1C	2.29	128.53	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	305	CHL	C3D-C4D-CHA	-2.29	107.48	112.72
27	B	847	CHL	CMB-C2B-C3B	2.29	128.97	124.68
27	3	312	CHL	C1-C2-C3	-2.29	122.08	126.04
27	a	316	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
27	B	822	CHL	CHC-C1C-NC	-2.29	120.73	124.20
27	b	317	CHL	CHC-C1C-NC	-2.29	120.73	124.20
27	8	323	CHL	CAA-CBA-CGA	-2.29	106.56	113.25
27	8	325	CHL	CMD-C2D-C1D	2.29	128.75	124.71
27	3	309	CHL	CMC-C2C-C1C	2.29	128.53	125.04
27	4	308	CHL	O1D-CGD-CBD	-2.29	119.80	124.48
27	A	829	CHL	CHC-C1C-NC	-2.29	120.73	124.20
27	B	814	CHL	CHC-C1C-NC	-2.29	120.73	124.20
30	7	301	LMG	O3-C3-C2	-2.29	105.05	110.35
27	A	859	CHL	C1D-CHD-C4C	-2.29	121.12	126.06
27	5	318	CHL	C2A-C1A-CHA	-2.29	119.86	123.86
27	8	317	CHL	CHC-C1C-NC	-2.29	120.73	124.20
27	7	317	CHL	C1-C2-C3	-2.29	122.08	126.04
27	7	319	CHL	CMB-C2B-C3B	2.29	128.96	124.68
27	B	844	CHL	CMC-C2C-C1C	2.29	128.52	125.04
27	6	315	CHL	C5-C3-C4	2.29	119.66	114.60
27	A	832	CHL	C4-C3-C2	-2.29	117.81	123.68
27	b	304	CHL	O1D-CGD-CBD	-2.29	119.80	124.48
27	a	315	CHL	CAC-C3C-C4C	2.29	127.78	124.81
27	a	309	CHL	CMD-C2D-C1D	2.29	128.74	124.71
27	A	834	CHL	CHC-C1C-NC	-2.29	120.73	124.20
27	7	317	CHL	C1-O2A-CGA	2.29	122.44	116.44
27	B	851	CHL	CMD-C2D-C1D	2.29	128.74	124.71
27	5	313	CHL	CHB-C4A-NA	2.29	127.67	124.51
27	5	312	CHL	O2A-CGA-CBA	2.29	119.08	111.91
27	7	317	CHL	CMC-C2C-C1C	2.29	128.52	125.04
27	4	314	CHL	C3D-C4D-CHA	-2.29	107.50	112.72
27	a	307	CHL	CMD-C2D-C1D	2.28	128.74	124.71
27	8	322	CHL	O1D-CGD-CBD	-2.28	119.81	124.48
27	A	852	CHL	CMC-C2C-C1C	2.28	128.52	125.04
27	3	318	CHL	CMD-C2D-C1D	2.28	128.74	124.71
27	B	844	CHL	C3D-C4D-CHA	-2.28	107.50	112.72
27	3	313	CHL	CMB-C2B-C3B	2.28	128.95	124.68
27	6	310	CHL	C1-C2-C3	-2.28	122.09	126.04
27	B	834	CHL	C4C-C3C-C2C	-2.28	103.57	106.90
27	b	313	CHL	CMB-C2B-C3B	2.28	128.95	124.68
27	A	847	CHL	CAC-C3C-C4C	2.28	127.77	124.81
27	5	323	CHL	CMC-C2C-C1C	2.28	128.51	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	858	CHL	CMB-C2B-C3B	2.28	128.95	124.68
27	b	307	CHL	CMC-C2C-C1C	2.28	128.51	125.04
27	3	315	CHL	CMD-C2D-C1D	2.28	128.73	124.71
22	A	804	BCR	C11-C10-C9	-2.28	124.06	127.31
27	6	314	CHL	CMB-C2B-C3B	2.28	128.94	124.68
27	4	304	CHL	C1D-CHD-C4C	-2.28	121.14	126.06
27	B	849	CHL	CMD-C2D-C1D	2.28	128.73	124.71
27	7	323	CHL	C3D-C2D-C1D	-2.28	102.72	105.83
27	b	309	CHL	CMB-C2B-C3B	2.28	128.94	124.68
27	b	316	CHL	CMB-C2B-C3B	2.28	128.94	124.68
29	a	304	LUT	C1-C6-C7	-2.28	109.33	115.78
22	3	301	BCR	C2-C1-C6	2.28	113.99	110.48
27	A	856	CHL	C6-C5-C3	-2.28	107.48	113.45
27	A	846	CHL	CAA-CBA-CGA	-2.28	106.59	113.25
27	b	309	CHL	CMD-C2D-C1D	2.28	128.73	124.71
27	b	308	CHL	C4C-C3C-C2C	-2.28	103.58	106.90
27	B	824	CHL	C3B-C4B-NB	2.28	112.15	109.21
27	B	823	CHL	CMB-C2B-C3B	2.28	128.94	124.68
22	B	806	BCR	C31-C1-C6	2.28	113.99	110.30
27	A	828	CHL	C3B-C4B-NB	2.28	112.15	109.21
27	b	313	CHL	C1D-CHD-C4C	-2.28	121.15	126.06
27	7	315	CHL	CAC-C3C-C4C	2.28	127.76	124.81
27	a	316	CHL	CMD-C2D-C1D	2.27	128.72	124.71
27	6	315	CHL	CMB-C2B-C3B	2.27	128.93	124.68
27	b	304	CHL	CMB-C2B-C3B	2.27	128.93	124.68
27	B	839	CHL	O1D-CGD-CBD	-2.27	119.83	124.48
27	a	319	CHL	CHC-C1C-NC	-2.27	120.75	124.20
29	6	303	LUT	C8-C7-C6	-2.27	120.82	127.20
27	b	306	CHL	CHC-C1C-NC	-2.27	120.76	124.20
22	L	302	BCR	C33-C5-C6	-2.27	121.98	124.53
27	7	323	CHL	C3C-C4C-NC	2.27	113.12	110.57
27	6	306	CHL	CMD-C2D-C1D	2.27	128.71	124.71
27	8	321	CHL	CMB-C2B-C3B	2.27	128.92	124.68
27	b	311	CHL	CHA-C4D-ND	2.27	137.25	132.50
27	A	840	CHL	CMD-C2D-C1D	2.27	128.71	124.71
27	5	315	CHL	CMB-C2B-C3B	2.27	128.92	124.68
27	B	819	CHL	C1D-CHD-C4C	-2.27	121.16	126.06
27	a	316	CHL	C2D-C1D-ND	2.27	111.78	110.10
27	K	206	CHL	CHC-C1C-NC	-2.27	120.76	124.20
27	A	858	CHL	CMC-C2C-C1C	2.27	128.49	125.04
27	8	323	CHL	CMD-C2D-C3D	-2.27	122.40	127.61
22	A	805	BCR	C3-C4-C5	-2.27	110.03	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	311	CHL	CAC-C3C-C4C	2.27	127.75	124.81
27	A	855	CHL	CHC-C1C-NC	-2.27	120.77	124.20
27	6	317	CHL	CAC-C3C-C4C	2.27	127.75	124.81
30	a	301	LMG	O6-C1-O1	-2.27	104.61	109.97
27	A	824	CHL	CMD-C2D-C1D	2.27	128.71	124.71
22	8	302	BCR	C3-C4-C5	-2.27	110.03	114.08
27	7	324	CHL	CMB-C2B-C3B	2.27	128.92	124.68
27	B	817	CHL	CMD-C2D-C1D	2.27	128.71	124.71
27	F	309	CHL	CMD-C2D-C1D	2.27	128.71	124.71
27	5	311	CHL	C3B-C4B-NB	2.26	112.14	109.21
27	A	842	CHL	CHA-C4D-ND	2.26	137.24	132.50
27	7	321	CHL	CHC-C1C-NC	-2.26	120.77	124.20
27	8	324	CHL	C2D-C1D-ND	2.26	111.77	110.10
27	5	325	CHL	CMD-C2D-C1D	2.26	128.70	124.71
27	7	316	CHL	O2A-CGA-CBA	2.26	119.01	111.91
27	4	305	CHL	CMD-C2D-C1D	2.26	128.70	124.71
27	3	316	CHL	CMB-C2B-C3B	2.26	128.91	124.68
22	A	804	BCR	C27-C26-C25	2.26	126.02	122.73
29	a	302	LUT	C1-C6-C7	-2.26	109.38	115.78
27	B	826	CHL	C5-C3-C4	2.26	119.60	114.60
22	B	803	BCR	C33-C5-C6	-2.26	121.99	124.53
27	a	319	CHL	C5-C3-C4	2.26	119.60	114.60
27	6	307	CHL	C4D-C3D-CAD	2.26	110.76	108.10
27	b	307	CHL	CMB-C2B-C3B	2.26	128.91	124.68
27	8	315	CHL	C1-C2-C3	-2.26	122.14	126.04
27	7	314	CHL	CHC-C1C-NC	-2.26	120.78	124.20
27	B	837	CHL	CHD-C4C-NC	2.26	127.76	124.20
27	A	818	CHL	C3B-C4B-NB	2.26	112.13	109.21
27	5	313	CHL	C3D-C4D-CHA	-2.26	107.56	112.72
27	A	829	CHL	CMD-C2D-C1D	2.26	128.69	124.71
27	A	828	CHL	CED-O2D-CGD	2.26	121.04	115.94
27	A	848	CHL	CMD-C2D-C1D	2.26	128.69	124.71
27	5	313	CHL	C4D-C3D-CAD	2.26	110.76	108.10
27	b	306	CHL	CMC-C2C-C1C	2.26	128.48	125.04
27	B	811	CHL	C1-O2A-CGA	2.26	122.37	116.44
27	A	820	CHL	C1D-CHD-C4C	-2.26	121.19	126.06
27	6	309	CHL	C1D-CHD-C4C	-2.26	121.19	126.06
27	A	859	CHL	C1-C2-C3	-2.26	122.14	126.04
27	b	310	CHL	CED-O2D-CGD	2.26	121.04	115.94
22	F	301	BCR	C24-C23-C22	-2.26	122.83	126.23
27	B	850	CHL	C1D-CHD-C4C	-2.25	121.19	126.06
27	B	839	CHL	CMD-C2D-C1D	2.25	128.69	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	320	CHL	CMD-C2D-C1D	2.25	128.69	124.71
27	4	305	CHL	CAC-C3C-C4C	2.25	127.73	124.81
27	A	838	CHL	C1-C2-C3	-2.25	122.14	126.04
27	a	310	CHL	C1-C2-C3	-2.25	122.15	126.04
27	A	848	CHL	CMB-C2B-C3B	2.25	128.89	124.68
27	B	830	CHL	C3D-C4D-CHA	-2.25	107.57	112.72
27	A	840	CHL	C3B-C4B-NB	2.25	112.12	109.21
27	a	311	CHL	CHC-C1C-NC	-2.25	120.79	124.20
22	5	301	BCR	C2-C1-C6	2.25	113.94	110.48
27	K	206	CHL	CMD-C2D-C1D	2.25	128.68	124.71
27	4	309	CHL	CMD-C2D-C1D	2.25	128.68	124.71
27	5	310	CHL	O2A-CGA-CBA	2.25	118.97	111.91
27	7	319	CHL	CHC-C1C-NC	-2.25	120.79	124.20
27	b	311	CHL	C2D-C1D-ND	2.25	111.76	110.10
22	L	302	BCR	C27-C26-C25	2.25	126.00	122.73
27	b	305	CHL	CMD-C2D-C1D	2.25	128.68	124.71
27	5	317	CHL	O2A-CGA-CBA	2.25	121.11	112.23
24	B	808	LHG	C27-C26-C25	-2.25	103.02	114.42
27	a	312	CHL	CMC-C2C-C1C	2.25	128.46	125.04
30	a	301	LMG	O3-C3-C2	-2.25	105.16	110.35
27	A	826	CHL	O1D-CGD-CBD	-2.25	119.89	124.48
22	7	303	BCR	C15-C16-C17	-2.25	118.87	123.47
27	B	830	CHL	CMB-C2B-C3B	2.25	128.88	124.68
27	a	320	CHL	CED-O2D-CGD	2.25	121.02	115.94
27	5	322	CHL	CMD-C2D-C1D	2.24	128.67	124.71
27	B	812	CHL	O2A-CGA-O1A	-2.24	117.93	123.59
28	B	809	DGD	CBB-CAB-C9B	-2.24	103.03	114.42
27	4	316	CHL	CMD-C2D-C1D	2.24	128.67	124.71
27	A	818	CHL	CMD-C2D-C1D	2.24	128.67	124.71
27	4	308	CHL	C4-C3-C5	2.24	119.05	115.27
27	6	317	CHL	C1D-CHD-C4C	-2.24	121.22	126.06
27	B	818	CHL	O1D-CGD-CBD	-2.24	119.89	124.48
27	a	315	CHL	C2D-C1D-ND	2.24	111.76	110.10
22	A	805	BCR	C15-C16-C17	-2.24	118.88	123.47
27	3	320	CHL	C2A-C1A-CHA	-2.24	119.94	123.86
27	B	840	CHL	CHC-C1C-NC	-2.24	120.80	124.20
27	5	323	CHL	CAC-C3C-C4C	2.24	127.72	124.81
27	B	832	CHL	CMC-C2C-C1C	2.24	128.45	125.04
27	A	857	CHL	CHC-C1C-NC	-2.24	120.80	124.20
27	A	842	CHL	CMD-C2D-C1D	2.24	128.66	124.71
27	3	318	CHL	C1-O2A-CGA	2.24	122.32	116.44
27	7	311	CHL	C4-C3-C5	2.24	119.04	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	315	CHL	O1D-CGD-CBD	-2.24	119.90	124.48
27	A	853	CHL	CMB-C2B-C3B	2.24	128.87	124.68
27	8	315	CHL	CMD-C2D-C1D	2.24	128.66	124.71
22	A	806	BCR	C16-C15-C14	-2.24	118.89	123.47
27	B	813	CHL	C1-C2-C3	-2.24	122.17	126.04
27	6	311	CHL	CMD-C2D-C1D	2.24	128.66	124.71
27	A	839	CHL	CMC-C2C-C1C	2.24	128.45	125.04
27	F	309	CHL	C5-C3-C4	2.24	119.54	114.60
27	b	314	CHL	O1D-CGD-CBD	-2.23	119.91	124.48
27	A	848	CHL	C3D-C4D-CHA	-2.23	107.61	112.72
27	4	311	CHL	C3D-C4D-CHA	-2.23	107.61	112.72
27	B	847	CHL	C1D-CHD-C4C	-2.23	121.24	126.06
27	3	313	CHL	CHC-C1C-NC	-2.23	120.81	124.20
24	A	812	LHG	C18-C17-C16	-2.23	103.08	114.42
27	b	312	CHL	C1D-CHD-C4C	-2.23	121.24	126.06
27	7	320	CHL	CMB-C2B-C3B	2.23	128.86	124.68
27	B	820	CHL	CAC-C3C-C4C	2.23	127.71	124.81
27	5	322	CHL	CED-O2D-CGD	2.23	120.99	115.94
27	4	320	CHL	O2A-CGA-CBA	2.23	118.91	111.91
27	4	312	CHL	CED-O2D-CGD	2.23	120.98	115.94
27	K	204	CHL	CMB-C2B-C3B	2.23	128.85	124.68
27	B	847	CHL	CHC-C1C-NC	-2.23	120.82	124.20
27	6	307	CHL	O1D-CGD-CBD	-2.23	119.92	124.48
27	a	313	CHL	CMD-C2D-C1D	2.23	128.64	124.71
27	a	315	CHL	CMB-C2B-C3B	2.23	128.85	124.68
27	4	318	CHL	CMB-C2B-C3B	2.23	128.85	124.68
22	B	803	BCR	C15-C14-C13	-2.23	124.13	127.31
27	B	827	CHL	CAC-C3C-C4C	2.23	127.70	124.81
27	A	844	CHL	CHC-C1C-NC	-2.23	120.82	124.20
29	6	302	LUT	C36-C21-C26	2.23	112.92	109.55
27	A	859	CHL	CMD-C2D-C1D	2.23	128.64	124.71
23	5	306	LMT	C3'-C4'-C5'	-2.23	105.82	110.93
27	B	817	CHL	C11-C12-C13	-2.23	108.72	115.92
27	3	311	CHL	C3B-C4B-NB	2.23	112.09	109.21
27	A	821	CHL	CAC-C3C-C4C	2.23	127.70	124.81
27	7	316	CHL	CED-O2D-CGD	2.23	120.97	115.94
27	B	845	CHL	O2A-CGA-O1A	-2.23	117.97	123.59
27	A	843	CHL	C6-C5-C3	-2.23	107.62	113.45
27	B	833	CHL	CHC-C1C-NC	-2.23	120.83	124.20
27	L	303	CHL	C3D-C4D-CHA	-2.23	107.63	112.72
27	8	318	CHL	CMB-C2B-C3B	2.23	128.84	124.68
27	3	320	CHL	CMD-C2D-C1D	2.22	128.63	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	320	CHL	CAC-C3C-C4C	2.22	127.70	124.81
27	8	326	CHL	CMD-C2D-C1D	2.22	128.63	124.71
27	5	319	CHL	O1D-CGD-CBD	-2.22	119.93	124.48
27	B	828	CHL	CMD-C2D-C1D	2.22	128.63	124.71
27	a	313	CHL	C4-C3-C5	2.22	119.01	115.27
27	B	837	CHL	CMC-C2C-C1C	2.22	128.42	125.04
27	8	326	CHL	CHB-C4A-NA	2.22	127.58	124.51
22	A	806	BCR	C33-C5-C6	-2.22	122.03	124.53
27	K	206	CHL	CMB-C2B-C3B	2.22	128.84	124.68
27	8	322	CHL	C5-C3-C4	2.22	119.51	114.60
27	B	816	CHL	C3B-C4B-NB	2.22	112.08	109.21
27	B	824	CHL	CMD-C2D-C1D	2.22	128.63	124.71
27	6	305	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
27	5	307	CHL	C4-C3-C5	2.22	119.01	115.27
27	B	813	CHL	O2A-CGA-CBA	2.22	118.88	111.91
27	3	317	CHL	O2A-CGA-CBA	2.22	118.87	111.91
27	3	312	CHL	CMD-C2D-C1D	2.22	128.62	124.71
27	A	828	CHL	C1-C2-C3	-2.22	122.20	126.04
27	4	313	CHL	CAC-C3C-C4C	2.22	127.69	124.81
27	A	838	CHL	CHC-C1C-NC	-2.22	120.84	124.20
27	3	314	CHL	C6-C5-C3	-2.22	107.64	113.45
30	a	301	LMG	O2-C2-C1	-2.22	104.66	110.05
27	5	309	CHL	CMC-C2C-C1C	2.22	128.42	125.04
27	6	310	CHL	C3D-C4D-CHA	-2.22	107.65	112.72
27	7	320	CHL	C2D-C1D-ND	2.22	111.74	110.10
27	4	306	CHL	CED-O2D-CGD	2.22	120.95	115.94
27	8	319	CHL	C1-C2-C3	-2.22	122.21	126.04
27	7	321	CHL	C1D-CHD-C4C	-2.22	121.28	126.06
22	3	302	BCR	C15-C14-C13	-2.22	124.15	127.31
27	8	326	CHL	CHC-C1C-NC	-2.22	120.84	124.20
30	J	101	LMG	O3-C3-C2	-2.22	105.23	110.35
27	B	848	CHL	C1-C2-C3	-2.22	122.21	126.04
27	8	320	CHL	CAC-C3C-C4C	2.22	127.68	124.81
27	a	318	CHL	CED-O2D-CGD	2.22	120.95	115.94
27	B	831	CHL	CMD-C2D-C1D	2.21	128.62	124.71
27	A	859	CHL	C6-C5-C3	-2.21	107.65	113.45
27	B	847	CHL	C3D-C4D-CHA	-2.21	107.66	112.72
27	A	825	CHL	CAC-C3C-C4C	2.21	127.68	124.81
22	K	203	BCR	C11-C10-C9	-2.21	124.15	127.31
30	J	104	LMG	O3-C3-C2	-2.21	105.23	110.35
27	b	313	CHL	CMC-C2C-C1C	2.21	128.41	125.04
27	a	318	CHL	O1D-CGD-CBD	-2.21	119.96	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	320	CHL	CHA-C4D-ND	2.21	137.13	132.50
27	5	316	CHL	CMD-C2D-C3D	-2.21	122.53	127.61
27	8	321	CHL	C1-C2-C3	-2.21	122.22	126.04
27	6	319	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
27	B	830	CHL	CMC-C2C-C1C	2.21	128.40	125.04
27	A	855	CHL	O2A-CGA-O1A	-2.21	118.02	123.59
27	6	309	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
27	b	311	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
27	3	314	CHL	CMD-C2D-C1D	2.21	128.60	124.71
27	a	314	CHL	CHC-C1C-NC	-2.21	120.85	124.20
27	B	820	CHL	C3D-C4D-CHA	-2.21	107.67	112.72
27	A	831	CHL	C1-O2A-CGA	2.21	122.24	116.44
27	3	313	CHL	CMD-C2D-C1D	2.21	128.60	124.71
27	B	811	CHL	C1D-CHD-C4C	-2.21	121.30	126.06
27	6	316	CHL	C1D-CHD-C4C	-2.21	121.30	126.06
27	A	843	CHL	C4-C3-C2	-2.21	118.02	123.68
27	4	306	CHL	CMB-C2B-C3B	2.21	128.81	124.68
27	3	317	CHL	C1D-CHD-C4C	-2.21	121.30	126.06
24	b	302	LHG	C27-C26-C25	-2.21	103.22	114.42
27	B	815	CHL	C1D-CHD-C4C	-2.21	121.30	126.06
27	B	850	CHL	CMC-C2C-C1C	2.21	128.40	125.04
27	5	307	CHL	CMD-C2D-C1D	2.20	128.60	124.71
27	B	848	CHL	CMD-C2D-C1D	2.20	128.60	124.71
27	7	314	CHL	CAC-C3C-C4C	2.20	127.67	124.81
27	4	310	CHL	O1D-CGD-CBD	-2.20	119.98	124.48
27	B	848	CHL	C3B-C4B-NB	2.20	112.06	109.21
27	b	309	CHL	CED-O2D-CGD	2.20	120.92	115.94
27	B	848	CHL	C1-O2A-CGA	2.20	122.22	116.44
27	K	207	CHL	CMB-C2B-C3B	2.20	128.80	124.68
27	B	816	CHL	C1-C2-C3	-2.20	122.24	126.04
27	5	319	CHL	CMB-C2B-C3B	2.20	128.79	124.68
27	B	839	CHL	C3B-C4B-NB	2.20	112.05	109.21
27	A	841	CHL	C1-C2-C3	-2.20	122.24	126.04
27	A	851	CHL	CAC-C3C-C4C	2.20	127.66	124.81
27	5	315	CHL	C3D-C4D-CHA	-2.20	107.69	112.72
27	5	322	CHL	CMB-C2B-C3B	2.20	128.79	124.68
27	7	321	CHL	C2C-C3C-C4C	-2.20	104.92	106.49
27	5	319	CHL	C1D-CHD-C4C	-2.20	121.32	126.06
24	8	305	LHG	C18-C17-C16	-2.20	103.27	114.42
29	b	303	LUT	C28-C29-C30	2.20	122.31	118.94
27	6	310	CHL	CED-O2D-CGD	2.20	120.91	115.94
27	4	309	CHL	CMB-C2B-C3B	2.20	128.79	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	207	CHL	C4D-CHA-C1A	-2.20	118.58	121.25
27	B	823	CHL	CMC-C2C-C1C	2.20	128.38	125.04
27	B	849	CHL	O1D-CGD-CBD	-2.20	119.99	124.48
27	F	308	CHL	CMB-C2B-C3B	2.20	128.79	124.68
27	b	311	CHL	CMB-C2B-C3B	2.20	128.79	124.68
27	7	311	CHL	CMD-C2D-C1D	2.20	128.58	124.71
27	B	834	CHL	CHC-C1C-NC	-2.20	120.87	124.20
27	B	850	CHL	O2A-CGA-CBA	2.20	118.80	111.91
27	B	839	CHL	CHC-C1C-NC	-2.20	120.87	124.20
27	8	320	CHL	O2A-CGA-CBA	2.20	118.80	111.91
27	B	828	CHL	C3D-C4D-CHA	-2.20	107.70	112.72
27	A	847	CHL	C3D-C4D-CHA	-2.19	107.70	112.72
27	a	318	CHL	C2D-C1D-ND	2.19	111.72	110.10
27	B	841	CHL	CMD-C2D-C1D	2.19	128.58	124.71
27	b	304	CHL	CMD-C2D-C1D	2.19	128.58	124.71
27	8	319	CHL	CMC-C2C-C1C	2.19	128.38	125.04
27	8	323	CHL	C3B-C4B-NB	2.19	112.04	109.21
23	5	306	LMT	C3B-C4B-C5B	-2.19	106.33	110.24
27	F	308	CHL	CAC-C3C-C4C	2.19	127.65	124.81
27	3	320	CHL	CED-O2D-CGD	2.19	120.89	115.94
27	6	306	CHL	C1D-CHD-C4C	-2.19	121.33	126.06
27	4	320	CHL	CMB-C2B-C3B	2.19	128.78	124.68
27	4	306	CHL	C3D-C4D-CHA	-2.19	107.71	112.72
27	5	323	CHL	CMD-C2D-C1D	2.19	128.57	124.71
27	A	840	CHL	O2A-CGA-CBA	2.19	118.78	111.91
27	a	312	CHL	O2A-CGA-CBA	2.19	118.77	111.91
30	a	301	LMG	O1-C1-C2	-2.19	104.89	108.30
27	B	811	CHL	CAC-C3C-C4C	2.19	127.65	124.81
23	B	810	LMT	C1'-O5'-C5'	-2.19	109.39	113.69
27	6	316	CHL	C2A-C1A-CHA	-2.19	120.04	123.86
27	A	833	CHL	C2D-C1D-ND	2.19	111.72	110.10
28	7	307	DGD	C3G-C2G-C1G	-2.19	106.62	111.79
27	b	312	CHL	O1D-CGD-CBD	-2.19	120.01	124.48
27	B	827	CHL	C3D-C4D-CHA	-2.19	107.72	112.72
27	5	308	CHL	CED-O2D-CGD	2.18	120.88	115.94
27	B	845	CHL	C3B-C4B-NB	2.18	112.03	109.21
27	A	827	CHL	CAC-C3C-C4C	2.18	127.64	124.81
22	F	301	BCR	C27-C26-C25	2.18	125.90	122.73
27	8	318	CHL	CMD-C2D-C1D	2.18	128.56	124.71
27	4	305	CHL	CMB-C2B-C3B	2.18	128.76	124.68
27	3	312	CHL	CED-O2D-CGD	2.18	120.88	115.94
27	B	847	CHL	CAC-C3C-C4C	2.18	127.64	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	305	LHG	C27-C26-C25	-2.18	103.35	114.42
28	7	307	DGD	O5D-C6D-C5D	-2.18	105.01	109.05
27	3	316	CHL	CHA-C4D-ND	2.18	137.06	132.50
22	K	202	BCR	C11-C10-C9	-2.18	124.20	127.31
27	K	204	CHL	CAC-C3C-C4C	2.18	127.64	124.81
27	5	322	CHL	CHA-C4D-ND	2.18	137.06	132.50
22	I	801	BCR	C15-C16-C17	-2.18	119.01	123.47
27	6	316	CHL	CMB-C2B-C3B	2.18	128.75	124.68
27	4	320	CHL	C5-C3-C4	2.18	119.41	114.60
27	5	321	CHL	CMB-C2B-C3B	2.18	128.75	124.68
22	A	806	BCR	C15-C16-C17	-2.18	119.02	123.47
22	B	807	BCR	C16-C15-C14	-2.18	119.02	123.47
27	7	315	CHL	C3D-C4D-CHA	-2.18	107.74	112.72
27	b	310	CHL	CMB-C2B-C3B	2.18	128.75	124.68
27	b	312	CHL	C3D-C4D-CHA	-2.18	107.75	112.72
27	A	823	CHL	C11-C10-C8	-2.17	108.89	115.92
27	A	831	CHL	CMD-C2D-C3D	-2.17	122.61	127.61
27	B	828	CHL	O2A-CGA-CBA	2.17	118.73	111.91
24	7	302	LHG	C18-C17-C16	-2.17	103.39	114.42
27	4	312	CHL	C2D-C1D-ND	2.17	111.70	110.10
27	B	844	CHL	CHC-C1C-NC	-2.17	120.91	124.20
27	K	206	CHL	CAC-C3C-C4C	2.17	127.63	124.81
27	b	317	CHL	CMB-C2B-C3B	2.17	128.74	124.68
27	a	316	CHL	C1D-CHD-C4C	-2.17	121.37	126.06
27	B	816	CHL	C2A-C1A-CHA	-2.17	120.06	123.86
22	3	301	BCR	C31-C1-C6	2.17	113.82	110.30
27	A	856	CHL	CED-O2D-CGD	2.17	120.85	115.94
27	B	846	CHL	C3D-C4D-CHA	-2.17	107.76	112.72
27	3	308	CHL	C3D-C4D-CHA	-2.17	107.76	112.72
27	a	307	CHL	C1D-CHD-C4C	-2.17	121.38	126.06
27	A	837	CHL	CED-O2D-CGD	2.17	120.84	115.94
27	A	858	CHL	CMD-C2D-C1D	2.17	128.54	124.71
27	B	829	CHL	CAC-C3C-C4C	2.17	127.62	124.81
27	6	310	CHL	CMB-C2B-C3B	2.17	128.74	124.68
27	B	816	CHL	C3D-C4D-CHA	-2.17	107.76	112.72
27	8	322	CHL	C3B-C4B-NB	2.17	112.01	109.21
27	B	828	CHL	CHC-C1C-NC	-2.17	120.91	124.20
27	A	822	CHL	O2A-CGA-O1A	-2.17	118.12	123.59
27	a	311	CHL	C3D-C4D-CHA	-2.17	107.76	112.72
27	7	312	CHL	CMD-C2D-C1D	2.17	128.53	124.71
27	a	319	CHL	C3D-C4D-CHA	-2.17	107.77	112.72
28	B	809	DGD	O3G-C3G-C2G	-2.17	105.67	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	856	CHL	O1D-CGD-CBD	-2.17	120.05	124.48
27	3	320	CHL	C4-C3-C5	2.17	118.91	115.27
27	6	309	CHL	CMB-C2B-C3B	2.16	128.73	124.68
27	B	827	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
27	A	854	CHL	C3D-C4D-CHA	-2.16	107.77	112.72
27	3	312	CHL	C3D-C4D-CHA	-2.16	107.77	112.72
29	5	303	LUT	C10-C11-C12	-2.16	116.47	123.22
27	K	205	CHL	C3D-C4D-CHA	-2.16	107.77	112.72
27	6	306	CHL	C3D-C4D-CHA	-2.16	107.77	112.72
27	A	839	CHL	O2A-CGA-CBA	2.16	118.69	111.91
27	J	106	CHL	CMB-C2B-C3B	2.16	128.72	124.68
27	5	307	CHL	CAC-C3C-C4C	2.16	127.61	124.81
27	7	322	CHL	CMB-C2B-C3B	2.16	128.72	124.68
29	b	301	LUT	C17-C1-C6	-2.16	106.79	110.30
24	7	302	LHG	C27-C26-C25	-2.16	103.45	114.42
27	7	319	CHL	C2C-C3C-C4C	-2.16	104.95	106.49
27	A	823	CHL	CHB-C4A-NA	2.16	127.50	124.51
27	A	829	CHL	C3B-C4B-NB	2.16	112.00	109.21
27	3	308	CHL	C3B-C4B-NB	2.16	112.00	109.21
27	6	305	CHL	C1D-CHD-C4C	-2.16	121.40	126.06
22	B	802	BCR	C15-C14-C13	-2.16	124.23	127.31
27	B	851	CHL	O2A-CGA-CBA	2.16	118.68	111.91
27	6	316	CHL	CHC-C1C-NC	-2.16	120.93	124.20
27	A	857	CHL	CMD-C2D-C1D	2.16	128.52	124.71
24	5	324	LHG	C27-C26-C25	-2.16	103.47	114.42
22	J	102	BCR	C28-C27-C26	-2.16	110.23	114.08
27	a	314	CHL	C3D-C4D-CHA	-2.16	107.79	112.72
27	A	847	CHL	C3B-C4B-NB	2.16	112.00	109.21
27	A	853	CHL	C3B-C4B-NB	2.16	112.00	109.21
27	7	315	CHL	C3B-C4B-NB	2.16	112.00	109.21
27	B	827	CHL	C3B-C4B-NB	2.16	112.00	109.21
27	4	308	CHL	C3D-C4D-CHA	-2.16	107.79	112.72
27	A	836	CHL	C4C-C3C-C2C	-2.16	103.76	106.90
27	5	312	CHL	CMB-C2B-C3B	2.16	128.71	124.68
27	6	314	CHL	CMD-C2D-C1D	2.16	128.51	124.71
27	a	313	CHL	C1B-CHB-C4A	-2.15	125.85	130.12
27	8	323	CHL	CHD-C4C-C3C	-2.15	121.67	124.84
27	7	312	CHL	CED-O2D-CGD	2.15	120.81	115.94
22	A	804	BCR	C15-C16-C17	-2.15	119.06	123.47
27	B	832	CHL	CHB-C4A-NA	2.15	127.49	124.51
27	8	316	CHL	C3B-C4B-NB	2.15	111.99	109.21
27	6	312	CHL	O2A-CGA-CBA	2.15	120.74	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	321	CHL	CMD-C2D-C1D	2.15	128.51	124.71
27	3	319	CHL	CAC-C3C-C4C	2.15	127.60	124.81
28	7	307	DGD	CBB-CAB-C9B	-2.15	103.50	114.42
27	A	858	CHL	CED-O2D-CGD	2.15	120.81	115.94
22	B	807	BCR	C10-C11-C12	-2.15	116.50	123.22
22	A	806	BCR	C15-C14-C13	-2.15	124.24	127.31
22	A	807	BCR	C15-C16-C17	-2.15	119.07	123.47
27	3	321	CHL	C3D-C4D-CHA	-2.15	107.80	112.72
27	8	316	CHL	CAC-C3C-C4C	2.15	127.60	124.81
27	7	319	CHL	C4-C3-C2	-2.15	118.16	123.68
27	7	322	CHL	C2D-C1D-ND	2.15	111.69	110.10
27	A	836	CHL	C3D-C4D-CHA	-2.15	107.80	112.72
27	B	843	CHL	C3D-C4D-CHA	-2.15	107.80	112.72
27	A	832	CHL	C1-C2-C3	-2.15	122.33	126.04
27	4	306	CHL	C1-C2-C3	-2.15	122.33	126.04
28	7	307	DGD	C5B-C4B-C3B	-2.15	103.51	114.42
27	B	851	CHL	C3D-C4D-CHA	-2.15	107.81	112.72
27	A	844	CHL	O2A-CGA-CBA	2.15	118.65	111.91
27	B	829	CHL	C1D-CHD-C4C	-2.15	121.42	126.06
27	3	309	CHL	CED-O2D-CGD	2.15	120.80	115.94
27	F	308	CHL	C3D-C4D-CHA	-2.15	107.81	112.72
27	6	311	CHL	C6-C5-C3	-2.15	107.83	113.45
27	3	314	CHL	O2A-CGA-CBA	2.15	118.64	111.91
22	7	303	BCR	C15-C14-C13	-2.15	124.25	127.31
27	a	308	CHL	CMD-C2D-C1D	2.15	128.50	124.71
27	B	848	CHL	O2A-CGA-CBA	2.15	118.64	111.91
27	a	320	CHL	O2A-CGA-CBA	2.15	120.71	112.23
27	A	836	CHL	C1D-CHD-C4C	-2.15	121.43	126.06
27	A	834	CHL	CAC-C3C-C4C	2.15	127.59	124.81
27	4	320	CHL	C3D-C4D-CHA	-2.15	107.81	112.72
27	A	822	CHL	C1-C2-C3	-2.15	122.33	126.04
27	3	320	CHL	CHC-C1C-NC	-2.14	120.95	124.20
27	4	310	CHL	CED-O2D-CGD	2.14	120.79	115.94
27	b	307	CHL	CED-O2D-CGD	2.14	120.79	115.94
27	a	319	CHL	C1D-CHD-C4C	-2.14	121.43	126.06
27	a	316	CHL	CMB-C2B-C3B	2.14	128.69	124.68
27	B	824	CHL	CHC-C1C-NC	-2.14	120.95	124.20
27	8	317	CHL	C3D-C4D-CHA	-2.14	107.82	112.72
27	8	312	CHL	C1-O2A-CGA	2.14	122.07	116.44
27	7	322	CHL	CHA-C4D-ND	2.14	136.98	132.50
27	B	835	CHL	O2A-CGA-CBA	2.14	118.63	111.91
27	A	831	CHL	C4D-C3D-CAD	2.14	110.62	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	316	CHL	C1D-CHD-C4C	-2.14	121.44	126.06
23	F	302	LMT	O5B-C5B-C4B	2.14	113.58	109.69
27	K	205	CHL	CHC-C1C-NC	-2.14	120.95	124.20
27	8	323	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
27	7	312	CHL	CMB-C2B-C3B	2.14	128.68	124.68
27	7	313	CHL	C1-C2-C3	-2.14	122.34	126.04
27	4	313	CHL	O1D-CGD-CBD	-2.14	120.10	124.48
27	b	315	CHL	CMD-C2D-C1D	2.14	128.49	124.71
27	7	317	CHL	O2A-CGA-CBA	2.14	118.62	111.91
27	5	319	CHL	CHA-C4D-ND	2.14	136.97	132.50
27	A	817	CHL	C3B-C4B-NB	2.14	111.98	109.21
27	A	842	CHL	OBD-CAD-C3D	2.14	133.67	128.52
22	J	102	BCR	C15-C16-C17	-2.14	119.09	123.47
27	6	306	CHL	CED-O2D-CGD	2.14	120.77	115.94
27	A	845	CHL	C1D-CHD-C4C	-2.14	121.44	126.06
27	a	317	CHL	CMC-C2C-C1C	2.14	128.29	125.04
27	6	309	CHL	CMD-C2D-C1D	2.14	128.48	124.71
27	A	838	CHL	C3D-C4D-CHA	-2.14	107.83	112.72
27	b	314	CHL	C1B-CHB-C4A	-2.14	125.88	130.12
27	b	313	CHL	CED-O2D-CGD	2.14	120.77	115.94
27	B	850	CHL	C4C-C3C-C2C	-2.14	103.78	106.90
27	B	843	CHL	C3B-C4B-NB	2.14	111.97	109.21
27	7	312	CHL	C3D-C4D-CHA	-2.14	107.83	112.72
27	8	312	CHL	C4C-C3C-C2C	-2.14	103.78	106.90
29	5	303	LUT	C8-C7-C6	-2.14	121.20	127.20
27	3	310	CHL	C1-C2-C3	-2.14	122.35	126.04
27	7	318	CHL	C3B-C4B-NB	2.14	111.97	109.21
27	A	852	CHL	CBA-CAA-C2A	-2.14	107.56	113.86
27	3	311	CHL	CHC-C1C-NC	-2.13	120.96	124.20
27	L	303	CHL	CMD-C2D-C3D	-2.13	122.70	127.61
27	b	310	CHL	O2A-CGA-CBA	2.13	120.67	112.23
27	6	313	CHL	CMB-C2B-C3B	2.13	128.67	124.68
27	5	309	CHL	O2A-CGA-CBA	2.13	118.60	111.91
27	A	849	CHL	C3B-C4B-NB	2.13	111.97	109.21
27	5	325	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
27	b	311	CHL	O2A-CGA-CBA	2.13	120.66	112.23
27	4	304	CHL	C3B-C4B-NB	2.13	111.97	109.21
27	4	310	CHL	CMD-C2D-C1D	2.13	128.47	124.71
27	8	324	CHL	CHA-C4D-ND	2.13	136.96	132.50
27	b	315	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
27	B	828	CHL	CED-O2D-CGD	2.13	120.76	115.94
27	8	311	CHL	C3D-C4D-CHA	-2.13	107.85	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	836	CHL	C3D-C4D-CHA	-2.13	107.85	112.72
27	K	206	CHL	C3B-C4B-NB	2.13	111.96	109.21
22	L	301	BCR	C15-C14-C13	-2.13	124.27	127.31
27	4	318	CHL	CHC-C1C-NC	-2.13	120.97	124.20
27	A	850	CHL	C3B-C4B-NB	2.13	111.96	109.21
29	5	303	LUT	C4-C5-C6	-2.13	116.10	120.85
27	A	841	CHL	C1D-CHD-C4C	-2.13	121.46	126.06
27	b	304	CHL	C3D-C4D-CHA	-2.13	107.85	112.72
27	A	845	CHL	CMD-C2D-C1D	2.13	128.46	124.71
27	A	830	CHL	CMC-C2C-C1C	2.13	128.28	125.04
27	B	837	CHL	C3D-C2D-C1D	-2.13	102.93	105.83
27	A	834	CHL	CED-O2D-CGD	2.13	120.75	115.94
27	K	204	CHL	C5-C3-C4	2.13	119.30	114.60
27	5	323	CHL	CMB-C2B-C3B	2.13	128.66	124.68
27	4	317	CHL	CMC-C2C-C1C	2.13	128.28	125.04
22	3	303	BCR	C15-C16-C17	-2.13	119.12	123.47
27	A	854	CHL	CAC-C3C-C4C	2.13	127.57	124.81
27	A	824	CHL	C1D-CHD-C4C	-2.13	121.47	126.06
27	3	313	CHL	C4-C3-C5	2.13	118.85	115.27
27	a	318	CHL	CHA-C4D-ND	2.13	136.95	132.50
27	3	310	CHL	C1D-CHD-C4C	-2.13	121.47	126.06
27	J	106	CHL	CMD-C2D-C1D	2.13	128.46	124.71
27	8	323	CHL	C3C-C4C-NC	2.12	112.95	110.57
27	A	850	CHL	C3D-C4D-CHA	-2.12	107.86	112.72
27	L	304	CHL	C1D-CHD-C4C	-2.12	121.47	126.06
27	B	819	CHL	C1-C2-C3	-2.12	122.37	126.04
27	A	844	CHL	C3D-C4D-CHA	-2.12	107.86	112.72
27	5	318	CHL	C3D-C4D-CHA	-2.12	107.86	112.72
27	b	311	CHL	C2C-C3C-C4C	-2.12	104.97	106.49
27	7	323	CHL	CHB-C4A-NA	2.12	127.45	124.51
22	M	102	BCR	C33-C5-C6	-2.12	122.14	124.53
27	B	832	CHL	O2A-CGA-O1A	-2.12	118.23	123.59
27	B	814	CHL	CMC-C2C-C1C	2.12	128.27	125.04
27	8	320	CHL	C3D-C4D-CHA	-2.12	107.87	112.72
27	b	307	CHL	C1D-CHD-C4C	-2.12	121.48	126.06
27	8	326	CHL	C1D-CHD-C4C	-2.12	121.48	126.06
27	A	819	CHL	CAC-C3C-C4C	2.12	127.56	124.81
27	6	315	CHL	C3D-C4D-CHA	-2.12	107.87	112.72
27	B	848	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
27	a	316	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
22	A	807	BCR	C2-C1-C6	2.12	113.75	110.48
27	8	314	CHL	C4D-CHA-C1A	-2.12	118.67	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	317	CHL	C1D-CHD-C4C	-2.12	121.48	126.06
27	6	313	CHL	CED-O2D-CGD	2.12	120.73	115.94
22	L	301	BCR	C27-C26-C25	2.12	125.81	122.73
27	b	316	CHL	CED-O2D-CGD	2.12	120.73	115.94
27	4	313	CHL	C3D-C2D-C1D	-2.12	102.94	105.83
27	A	824	CHL	C1-C2-C3	-2.12	122.38	126.04
27	6	312	CHL	C3B-C4B-NB	2.12	111.95	109.21
27	b	307	CHL	CAC-C3C-C4C	2.12	127.56	124.81
27	A	836	CHL	CED-O2D-CGD	2.12	120.73	115.94
27	b	315	CHL	C1D-CHD-C4C	-2.12	121.49	126.06
27	F	308	CHL	O2A-CGA-CBA	2.12	120.60	112.23
27	B	832	CHL	C3B-C4B-NB	2.12	111.95	109.21
27	7	317	CHL	CMD-C2D-C1D	2.12	128.44	124.71
27	A	835	CHL	CMC-C2C-C1C	2.12	128.26	125.04
27	8	312	CHL	C1D-CHD-C4C	-2.12	121.49	126.06
27	5	310	CHL	C1-O2A-CGA	2.12	121.99	116.44
27	A	852	CHL	CHB-C4A-NA	2.12	127.44	124.51
27	L	303	CHL	O1D-CGD-CBD	-2.12	120.16	124.48
27	3	320	CHL	C1D-CHD-C4C	-2.11	121.50	126.06
27	8	317	CHL	CAC-C3C-C4C	2.11	127.55	124.81
27	b	317	CHL	C2A-C1A-CHA	-2.11	120.16	123.86
27	a	319	CHL	CED-O2D-CGD	2.11	120.72	115.94
27	5	310	CHL	C1-C2-C3	-2.11	122.39	126.04
27	a	314	CHL	C2A-C1A-CHA	-2.11	120.16	123.86
27	a	320	CHL	C3D-C4D-CHA	-2.11	107.89	112.72
27	5	309	CHL	CMB-C2B-C3B	2.11	128.63	124.68
27	A	833	CHL	CHA-C4D-ND	2.11	136.92	132.50
27	A	834	CHL	CMC-C2C-C1C	2.11	128.26	125.04
27	a	319	CHL	O2A-CGA-O1A	-2.11	118.26	123.59
27	A	859	CHL	C3D-C4D-CHA	-2.11	107.89	112.72
27	B	819	CHL	C1-O2A-CGA	2.11	121.98	116.44
27	A	844	CHL	CMC-C2C-C1C	2.11	128.25	125.04
27	B	829	CHL	CMD-C2D-C1D	2.11	128.43	124.71
27	B	839	CHL	CMC-C2C-C1C	2.11	128.25	125.04
27	A	837	CHL	C3B-C4B-NB	2.11	111.94	109.21
27	B	816	CHL	CMD-C2D-C1D	2.11	128.43	124.71
27	7	324	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
27	4	306	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
27	b	312	CHL	O2A-CGA-CBA	2.11	120.57	112.23
27	4	316	CHL	CMB-C2B-C3B	2.11	128.62	124.68
27	A	831	CHL	C3D-C4D-CHA	-2.11	107.90	112.72
27	a	313	CHL	C3D-C4D-CHA	-2.11	107.90	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	316	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
27	4	309	CHL	C1B-CHB-C4A	-2.11	125.94	130.12
29	8	304	LUT	C1-C6-C7	-2.11	109.81	115.78
27	A	849	CHL	C1B-CHB-C4A	-2.11	125.94	130.12
27	B	814	CHL	C1-C2-C3	-2.11	122.40	126.04
27	A	848	CHL	CHB-C4A-NA	2.11	127.43	124.51
27	a	309	CHL	CHB-C4A-NA	2.11	127.43	124.51
27	8	322	CHL	CHB-C4A-NA	2.11	127.43	124.51
27	3	313	CHL	C3D-C4D-CHA	-2.11	107.90	112.72
27	4	308	CHL	C3B-C4B-NB	2.11	111.93	109.21
27	K	204	CHL	C3D-C4D-CHA	-2.11	107.91	112.72
27	5	319	CHL	O2A-CGA-CBA	2.11	120.55	112.23
27	B	851	CHL	C4C-C3C-C2C	-2.10	103.83	106.90
27	5	307	CHL	O2A-CGA-O1A	-2.10	118.28	123.59
27	A	851	CHL	C3D-C4D-CHA	-2.10	107.91	112.72
27	B	831	CHL	C3D-C4D-CHA	-2.10	107.91	112.72
27	8	317	CHL	CMC-C2C-C1C	2.10	128.24	125.04
27	6	320	CHL	O2A-CGA-CBA	2.10	120.54	112.23
27	3	319	CHL	C3D-C4D-CHA	-2.10	107.92	112.72
27	6	317	CHL	C2D-C1D-ND	2.10	111.65	110.10
27	B	821	CHL	O1D-CGD-CBD	-2.10	120.19	124.48
22	L	301	BCR	C11-C10-C9	-2.10	124.31	127.31
27	4	307	CHL	CAC-C3C-C4C	2.10	127.53	124.81
27	A	825	CHL	CMD-C2D-C1D	2.10	128.41	124.71
27	3	315	CHL	C1-O2A-CGA	2.10	121.95	116.44
27	B	834	CHL	CMC-C2C-C1C	2.10	128.24	125.04
27	A	826	CHL	C1D-CHD-C4C	-2.10	121.53	126.06
27	7	315	CHL	C1D-CHD-C4C	-2.10	121.53	126.06
27	a	311	CHL	CED-O2D-CGD	2.10	120.68	115.94
27	7	322	CHL	C2C-C3C-C4C	-2.10	104.99	106.49
27	3	313	CHL	CMC-C2C-C1C	2.10	128.24	125.04
27	5	318	CHL	C3B-C4B-NB	2.10	111.92	109.21
27	B	846	CHL	CMB-C2B-C3B	2.10	128.60	124.68
27	F	309	CHL	C3D-C4D-CHA	-2.10	107.92	112.72
27	A	854	CHL	CED-O2D-CGD	2.10	120.68	115.94
27	B	839	CHL	CED-O2D-CGD	2.10	120.68	115.94
27	A	857	CHL	CHB-C4A-NA	2.10	127.41	124.51
27	B	850	CHL	CAC-C3C-C4C	2.10	127.53	124.81
27	b	309	CHL	CAC-C3C-C4C	2.10	127.53	124.81
23	5	326	LMT	C1'-O5'-C5'	-2.10	109.57	113.69
27	4	305	CHL	CMC-C2C-C1C	2.10	128.23	125.04
27	b	314	CHL	C3D-C4D-CHA	-2.10	107.93	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	316	CHL	CHA-C4D-ND	2.10	136.88	132.50
27	A	838	CHL	C3B-C4B-NB	2.10	111.92	109.21
27	A	854	CHL	C1-C2-C3	-2.10	122.42	126.04
27	B	831	CHL	O2A-CGA-CBA	2.10	120.51	112.23
27	K	207	CHL	O1D-CGD-CBD	-2.10	120.20	124.48
27	8	311	CHL	CAC-C3C-C4C	2.10	127.53	124.81
27	B	834	CHL	C3C-C4C-NC	2.10	112.92	110.57
27	A	830	CHL	C3B-C4B-NB	2.10	111.92	109.21
27	7	312	CHL	CAC-C3C-C4C	2.10	128.23	125.04
27	4	307	CHL	CMD-C2D-C1D	2.09	128.41	124.71
27	b	307	CHL	C4-C3-C5	2.09	118.80	115.27
27	B	837	CHL	C3B-C4B-NB	2.09	111.92	109.21
27	b	314	CHL	O2A-CGA-CBA	2.09	120.51	112.23
27	4	314	CHL	C2A-C1A-CHA	-2.09	120.20	123.86
24	A	810	LHG	C27-C26-C25	-2.09	103.79	114.42
27	4	316	CHL	CHA-C4D-ND	2.09	136.88	132.50
27	A	859	CHL	C3B-C4B-NB	2.09	111.92	109.21
28	7	307	DGD	CAB-C9B-C8B	-2.09	103.80	114.42
27	3	310	CHL	C3D-C4D-CHA	-2.09	107.93	112.72
27	B	818	CHL	CMB-C2B-C3B	2.09	128.59	124.68
27	6	320	CHL	C3D-C4D-CHA	-2.09	107.94	112.72
27	5	322	CHL	C2D-C1D-ND	2.09	111.65	110.10
27	7	313	CHL	O2A-CGA-CBA	2.09	118.47	111.91
27	a	317	CHL	C1-C2-C3	-2.09	122.42	126.04
27	A	818	CHL	C1-O2A-CGA	2.09	121.93	116.44
27	7	324	CHL	O2A-CGA-CBA	2.09	120.50	112.23
27	6	309	CHL	CMC-C2C-C1C	2.09	128.22	125.04
23	A	809	LMT	C3'-C4'-C5'	-2.09	106.13	110.93
27	5	319	CHL	C2D-C1D-ND	2.09	111.64	110.10
27	B	838	CHL	C1-C2-C3	-2.09	122.43	126.04
27	A	834	CHL	CMD-C2D-C1D	2.09	128.39	124.71
23	5	306	LMT	C1'-O5'-C5'	-2.09	109.59	113.69
29	F	303	LUT	C22-C23-C24	2.09	114.12	111.74
27	B	815	CHL	CED-O2D-CGD	2.09	120.66	115.94
27	A	858	CHL	C3D-C4D-CHA	-2.09	107.95	112.72
27	A	856	CHL	C3B-C4B-NB	2.09	111.91	109.21
27	5	321	CHL	C3D-C4D-CHA	-2.09	107.95	112.72
27	7	318	CHL	O2A-CGA-CBA	2.09	118.45	111.91
27	B	832	CHL	C6-C5-C3	-2.09	107.99	113.45
27	6	307	CHL	C1-O2A-CGA	2.09	121.92	116.44
27	A	821	CHL	C3D-C4D-CHA	-2.09	107.95	112.72
27	8	317	CHL	CED-O2D-CGD	2.09	120.65	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	318	CHL	CMB-C2B-C3B	2.09	128.58	124.68
27	5	314	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
27	7	323	CHL	CMC-C2C-C1C	2.08	128.21	125.04
27	5	325	CHL	C1D-CHD-C4C	-2.08	121.56	126.06
22	K	203	BCR	C15-C16-C17	-2.08	119.20	123.47
27	5	311	CHL	C3D-C4D-CHA	-2.08	107.95	112.72
27	4	318	CHL	CED-O2D-CGD	2.08	120.65	115.94
27	5	312	CHL	C3D-C4D-CHA	-2.08	107.95	112.72
27	B	845	CHL	CAC-C3C-C4C	2.08	127.51	124.81
24	7	306	LHG	C27-C26-C25	-2.08	103.85	114.42
27	5	325	CHL	O2A-CGA-CBA	2.08	120.47	112.23
27	5	307	CHL	C3D-C4D-CHA	-2.08	107.96	112.72
27	7	324	CHL	C4C-C3C-C2C	-2.08	103.86	106.90
27	A	836	CHL	CHC-C1C-NC	-2.08	121.04	124.20
27	5	320	CHL	CED-O2D-CGD	2.08	120.65	115.94
27	B	819	CHL	C3D-C4D-CHA	-2.08	107.96	112.72
28	B	809	DGD	O3E-C3E-C2E	-2.08	105.53	110.35
27	B	833	CHL	O2A-CGA-CBA	2.08	118.44	111.91
27	B	825	CHL	C1-C2-C3	-2.08	122.44	126.04
27	5	320	CHL	C3D-C4D-CHA	-2.08	107.96	112.72
27	B	848	CHL	C3D-C4D-CHA	-2.08	107.96	112.72
27	b	310	CHL	C3D-C4D-CHA	-2.08	107.96	112.72
23	5	326	LMT	C3'-C4'-C5'	-2.08	106.16	110.93
27	a	312	CHL	C3D-C4D-CHA	-2.08	107.96	112.72
27	6	317	CHL	CHA-C4D-ND	2.08	136.85	132.50
23	F	302	LMT	C1'-O5'-C5'	-2.08	109.61	113.69
27	A	854	CHL	CMD-C2D-C1D	2.08	128.38	124.71
27	8	326	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
27	3	310	CHL	CMC-C2C-C1C	2.08	128.21	125.04
27	A	839	CHL	CHC-C1C-NC	-2.08	121.05	124.20
27	B	842	CHL	C3D-C4D-CHA	-2.08	107.97	112.72
27	A	845	CHL	C4C-C3C-C2C	-2.08	103.87	106.90
27	A	850	CHL	CED-O2D-CGD	2.08	120.64	115.94
27	B	847	CHL	C1-C2-C3	-2.08	122.45	126.04
27	5	311	CHL	O2A-CGA-CBA	2.08	120.44	112.23
27	A	836	CHL	C3B-C4B-NB	2.08	111.89	109.21
32	5	305	PTY	C6-O7-C8	2.08	122.90	117.79
22	8	302	BCR	C7-C8-C9	-2.08	123.10	126.23
27	5	309	CHL	C3D-C4D-CHA	-2.08	107.97	112.72
27	A	827	CHL	CMD-C2D-C1D	2.08	128.37	124.71
27	4	315	CHL	C3D-C4D-CHA	-2.08	107.97	112.72
27	J	106	CHL	O1D-CGD-CBD	-2.08	120.24	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	847	CHL	O2A-CGA-CBA	2.07	118.42	111.91
27	A	841	CHL	CHB-C4A-NA	2.07	127.38	124.51
27	B	835	CHL	C1-C2-C3	-2.07	122.45	126.04
27	A	853	CHL	CMD-C2D-C1D	2.07	128.37	124.71
27	5	309	CHL	C3B-C4B-NB	2.07	111.89	109.21
27	b	304	CHL	CED-O2D-CGD	2.07	120.63	115.94
22	I	801	BCR	C27-C26-C25	2.07	125.74	122.73
27	8	318	CHL	CMC-C2C-C1C	2.07	128.20	125.04
27	5	318	CHL	O2A-CGA-CBA	2.07	118.41	111.91
27	7	311	CHL	C3B-C4B-NB	2.07	111.89	109.21
27	8	313	CHL	CMB-C2B-C3B	2.07	128.55	124.68
27	B	842	CHL	C3B-C4B-NB	2.07	111.89	109.21
27	7	319	CHL	C3B-C4B-NB	2.07	111.89	109.21
27	A	833	CHL	C1D-CHD-C4C	-2.07	121.59	126.06
22	F	301	BCR	C16-C15-C14	-2.07	119.23	123.47
22	A	805	BCR	C15-C14-C13	-2.07	124.35	127.31
27	A	822	CHL	C3D-C4D-CHA	-2.07	107.98	112.72
27	J	106	CHL	C3D-C4D-CHA	-2.07	107.99	112.72
27	3	311	CHL	C3D-C4D-CHA	-2.07	107.99	112.72
27	7	311	CHL	C3D-C4D-CHA	-2.07	107.99	112.72
27	b	307	CHL	C3D-C4D-CHA	-2.07	107.99	112.72
27	a	317	CHL	CED-O2D-CGD	2.07	120.62	115.94
27	A	843	CHL	CED-O2D-CGD	2.07	120.62	115.94
27	3	321	CHL	CED-O2D-CGD	2.07	120.62	115.94
30	J	104	LMG	O7-C10-O9	-2.07	118.70	123.70
27	B	828	CHL	C1D-CHD-C4C	-2.07	121.59	126.06
27	4	310	CHL	C1D-CHD-C4C	-2.07	121.59	126.06
27	4	311	CHL	CED-O2D-CGD	2.07	120.61	115.94
27	5	316	CHL	C1-O2A-CGA	2.07	121.87	116.44
27	A	820	CHL	C4C-C3C-C2C	-2.07	103.88	106.90
27	4	310	CHL	CMC-C2C-C1C	2.07	128.19	125.04
27	3	311	CHL	C1D-CHD-C4C	-2.07	121.60	126.06
27	5	307	CHL	C3B-C4B-NB	2.07	111.88	109.21
23	A	808	LMT	O5B-C5B-C4B	2.07	113.45	109.69
27	8	319	CHL	CED-O2D-CGD	2.07	120.61	115.94
27	A	818	CHL	CHB-C4A-NA	2.07	127.37	124.51
27	3	320	CHL	C3D-C4D-CHA	-2.07	108.00	112.72
27	A	825	CHL	CED-O2D-CGD	2.07	120.61	115.94
27	B	832	CHL	O2A-CGA-CBA	2.07	118.39	111.91
27	3	316	CHL	CAC-C3C-C4C	2.07	127.49	124.81
27	3	315	CHL	C1D-CHD-C4C	-2.07	121.60	126.06
27	K	207	CHL	CHA-C4D-ND	2.07	136.82	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	836	CHL	C1D-CHD-C4C	-2.07	121.60	126.06
27	7	311	CHL	C1D-CHD-C4C	-2.06	121.60	126.06
27	8	326	CHL	CED-O2D-CGD	2.06	120.61	115.94
27	A	847	CHL	C1-O2A-CGA	2.06	121.86	116.44
27	5	318	CHL	C1-O2A-CGA	2.06	121.86	116.44
27	B	822	CHL	C3D-C4D-CHA	-2.06	108.00	112.72
27	7	322	CHL	CED-O2D-CGD	2.06	120.60	115.94
22	B	806	BCR	C27-C26-C25	2.06	125.73	122.73
27	B	834	CHL	C16-C15-C13	-2.06	109.25	115.92
27	3	317	CHL	C3D-C4D-CHA	-2.06	108.00	112.72
27	A	821	CHL	C11-C10-C8	-2.06	109.26	115.92
27	5	308	CHL	C4C-C3C-C2C	-2.06	103.89	106.90
27	5	317	CHL	CHA-C4D-ND	2.06	136.81	132.50
27	A	832	CHL	C6-C7-C8	-2.06	109.26	115.92
27	8	314	CHL	CED-O2D-CGD	2.06	120.60	115.94
27	7	313	CHL	C1-O2A-CGA	2.06	121.85	116.44
27	K	206	CHL	C3D-C4D-CHA	-2.06	108.01	112.72
27	a	313	CHL	CAC-C3C-C4C	2.06	127.48	124.81
27	7	322	CHL	C3B-C4B-NB	2.06	111.87	109.21
27	5	318	CHL	CHC-C1C-NC	-2.06	121.08	124.20
27	a	311	CHL	C3B-C4B-NB	2.06	111.87	109.21
27	6	317	CHL	C3B-C4B-NB	2.06	111.87	109.21
27	4	312	CHL	CHA-C4D-ND	2.06	136.80	132.50
27	5	308	CHL	CAC-C3C-C4C	2.06	127.48	124.81
27	3	309	CHL	O2A-CGA-CBA	2.06	120.36	112.23
27	b	312	CHL	CED-O2D-CGD	2.06	120.59	115.94
27	4	314	CHL	C1D-CHD-C4C	-2.06	121.62	126.06
27	4	311	CHL	CMB-C2B-C3B	2.06	128.53	124.68
26	A	815	CL0	O1D-CGD-CBD	-2.06	120.28	124.48
27	B	830	CHL	C3B-C4B-NB	2.06	111.87	109.21
27	6	312	CHL	CED-O2D-CGD	2.06	120.59	115.94
27	7	311	CHL	CHC-C1C-NC	-2.06	121.08	124.20
27	4	307	CHL	C1D-CHD-C4C	-2.06	121.62	126.06
27	3	318	CHL	O1D-CGD-CBD	-2.06	120.28	124.48
27	a	315	CHL	O2A-CGA-O1A	-2.06	118.41	123.59
27	B	812	CHL	CHB-C4A-NA	2.06	127.35	124.51
27	4	319	CHL	CHC-C1C-NC	-2.06	121.08	124.20
27	3	312	CHL	CMC-C2C-C1C	2.05	128.17	125.04
28	B	809	DGD	O2D-C2D-C1D	-2.05	105.06	110.05
27	A	816	CHL	CED-O2D-CGD	2.05	120.58	115.94
22	B	802	BCR	C16-C15-C14	-2.05	119.27	123.47
29	3	305	LUT	C35-C15-C14	-2.05	119.27	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	307	CHL	C6-C5-C3	-2.05	108.07	113.45
27	B	832	CHL	C3D-C4D-CHA	-2.05	108.03	112.72
27	4	316	CHL	C2C-C3C-C4C	-2.05	105.03	106.49
27	A	834	CHL	C3D-C4D-CHA	-2.05	108.03	112.72
27	A	824	CHL	C4C-C3C-C2C	-2.05	103.91	106.90
27	4	310	CHL	C3D-C4D-CHA	-2.05	108.03	112.72
27	7	316	CHL	C3D-C4D-CHA	-2.05	108.03	112.72
27	8	321	CHL	CHA-C4D-ND	2.05	136.79	132.50
27	4	316	CHL	C1D-CHD-C4C	-2.05	121.64	126.06
27	a	307	CHL	C3D-C4D-CHA	-2.05	108.03	112.72
27	B	815	CHL	C3D-C4D-CHA	-2.05	108.03	112.72
27	7	317	CHL	C3B-C4B-NB	2.05	111.86	109.21
27	b	313	CHL	O2A-CGA-CBA	2.05	120.33	112.23
27	b	305	CHL	CMB-C2B-C3B	2.05	128.51	124.68
27	A	855	CHL	CMD-C2D-C1D	2.05	128.32	124.71
27	B	838	CHL	CED-O2D-CGD	2.05	120.57	115.94
27	A	832	CHL	C3B-C4B-NB	2.05	111.86	109.21
28	7	307	DGD	O3E-C3E-C2E	-2.05	105.62	110.35
27	B	840	CHL	C3D-C4D-CHA	-2.05	108.04	112.72
27	B	831	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
27	7	318	CHL	C1-O2A-CGA	2.05	121.81	116.44
27	K	207	CHL	C2D-C1D-ND	2.05	111.61	110.10
27	4	310	CHL	O2A-CGA-CBA	2.05	120.32	112.23
27	B	825	CHL	C1-O2A-CGA	2.05	121.81	116.44
27	B	850	CHL	C1-O2A-CGA	2.05	121.81	116.44
27	B	851	CHL	CED-O2D-CGD	2.05	120.56	115.94
28	B	809	DGD	C5B-C4B-C3B	-2.05	104.04	114.42
27	6	313	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
27	B	824	CHL	CED-O2D-CGD	2.04	120.56	115.94
27	A	830	CHL	CHB-C4A-NA	2.04	127.34	124.51
27	B	836	CHL	O1D-CGD-CBD	-2.04	120.30	124.48
22	3	302	BCR	C27-C26-C25	2.04	125.70	122.73
27	B	823	CHL	CAC-C3C-C4C	2.04	127.46	124.81
27	6	312	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
27	7	313	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
27	8	316	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
27	A	826	CHL	CAA-C2A-C3A	-2.04	107.18	112.78
30	7	301	LMG	O7-C10-O9	-2.04	118.77	123.70
27	7	319	CHL	CHA-C4D-ND	2.04	136.77	132.50
27	L	304	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
22	J	102	BCR	C3-C4-C5	-2.04	110.43	114.08
27	a	315	CHL	C2A-C1A-CHA	-2.04	120.29	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	821	CHL	CED-O2D-CGD	2.04	120.56	115.94
27	B	833	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
27	8	318	CHL	C3D-C4D-CHA	-2.04	108.05	112.72
27	a	315	CHL	CAA-CBA-CGA	-2.04	107.29	113.25
27	B	826	CHL	CMD-C2D-C1D	2.04	128.31	124.71
27	b	309	CHL	CMC-C2C-C1C	2.04	128.15	125.04
27	b	309	CHL	O2A-CGA-CBA	2.04	120.30	112.23
27	B	821	CHL	C3D-C4D-CHA	-2.04	108.06	112.72
27	B	840	CHL	C6-C7-C8	-2.04	109.32	115.92
27	A	853	CHL	CHC-C1C-NC	-2.04	121.11	124.20
27	3	315	CHL	C3D-C4D-CHA	-2.04	108.06	112.72
27	8	326	CHL	CMC-C2C-C1C	2.04	128.15	125.04
27	5	315	CHL	CED-O2D-CGD	2.04	120.55	115.94
27	7	317	CHL	CED-O2D-CGD	2.04	120.55	115.94
27	5	311	CHL	C1D-CHD-C4C	-2.04	121.66	126.06
22	F	301	BCR	C7-C8-C9	-2.04	123.15	126.23
23	F	302	LMT	O5B-C5B-C6B	2.04	111.50	106.44
27	4	312	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
22	K	202	BCR	C33-C5-C6	-2.04	122.24	124.53
27	8	314	CHL	O1D-CGD-CBD	-2.04	120.32	124.48
27	A	818	CHL	C3D-C4D-CHA	-2.04	108.06	112.72
27	6	311	CHL	C3D-C4D-CHA	-2.04	108.06	112.72
27	8	312	CHL	C4-C3-C5	2.04	118.70	115.27
27	3	318	CHL	C3D-C4D-CHA	-2.04	108.07	112.72
27	7	324	CHL	C3D-C4D-CHA	-2.04	108.07	112.72
27	b	310	CHL	CHC-C1C-NC	-2.03	121.12	124.20
27	a	311	CHL	CAC-C3C-C4C	2.03	127.45	124.81
27	a	310	CHL	C3D-C4D-CHA	-2.03	108.07	112.72
27	4	317	CHL	CAC-C3C-C4C	2.03	127.45	124.81
27	A	816	CHL	C4C-C3C-C2C	-2.03	103.93	106.90
27	7	311	CHL	CED-O2D-CGD	2.03	120.53	115.94
27	A	858	CHL	C4C-C3C-C2C	-2.03	103.93	106.90
27	4	313	CHL	O2A-CGA-CBA	2.03	120.56	114.03
27	K	205	CHL	C2A-C1A-CHA	-2.03	120.31	123.86
27	A	856	CHL	C3D-C4D-CHA	-2.03	108.07	112.72
27	7	314	CHL	CED-O2D-CGD	2.03	120.53	115.94
27	B	811	CHL	C4C-C3C-C2C	-2.03	103.94	106.90
27	b	317	CHL	C2C-C3C-C4C	-2.03	105.04	106.49
27	a	315	CHL	CHA-C4D-ND	2.03	136.75	132.50
27	8	323	CHL	CHD-C1D-C2D	2.03	129.74	125.48
27	6	318	CHL	CHA-C4D-ND	2.03	136.75	132.50
27	4	304	CHL	C3D-C4D-CHA	-2.03	108.08	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	817	CHL	CED-O2D-CGD	2.03	120.53	115.94
27	b	305	CHL	CED-O2D-CGD	2.03	120.53	115.94
27	B	842	CHL	CAC-C3C-C4C	2.03	127.44	124.81
29	b	301	LUT	C1-C6-C7	-2.03	110.03	115.78
27	8	325	CHL	CMB-C2B-C3B	2.03	128.48	124.68
27	6	314	CHL	C3D-C4D-CHA	-2.03	108.08	112.72
27	A	841	CHL	CHA-C4D-ND	2.03	136.75	132.50
27	7	321	CHL	CHA-C4D-ND	2.03	136.74	132.50
27	3	315	CHL	CAC-C3C-C4C	2.03	127.44	124.81
27	7	319	CHL	CAC-C3C-C4C	2.03	127.44	124.81
22	B	805	BCR	C11-C10-C9	-2.03	124.41	127.31
27	b	305	CHL	C3D-C4D-CHA	-2.03	108.08	112.72
27	A	838	CHL	C4C-C3C-C2C	-2.03	103.94	106.90
27	B	835	CHL	C3D-C4D-CHA	-2.03	108.08	112.72
27	B	838	CHL	C3D-C4D-CHA	-2.03	108.08	112.72
27	4	318	CHL	C3D-C4D-CHA	-2.03	108.08	112.72
27	B	814	CHL	C4C-C3C-C2C	-2.03	103.94	106.90
27	B	845	CHL	C3D-C4D-CHA	-2.03	108.08	112.72
30	a	301	LMG	O7-C10-O9	-2.03	118.80	123.70
27	B	825	CHL	CED-O2D-CGD	2.03	120.52	115.94
27	B	825	CHL	C1D-CHD-C4C	-2.03	121.69	126.06
27	8	313	CHL	C3D-C4D-CHA	-2.03	108.09	112.72
27	4	319	CHL	C1D-CHD-C4C	-2.03	121.69	126.06
27	a	309	CHL	C3B-C4B-NB	2.03	111.83	109.21
27	7	318	CHL	C1D-CHD-C4C	-2.03	121.69	126.06
27	B	834	CHL	C3D-C4D-CHA	-2.03	108.09	112.72
24	A	812	LHG	C27-C26-C25	-2.02	104.14	114.42
27	B	815	CHL	CAC-C3C-C4C	2.02	127.44	124.81
27	6	305	CHL	O2A-CGA-CBA	2.02	120.23	112.23
27	5	325	CHL	C3B-C4B-NB	2.02	111.83	109.21
27	6	317	CHL	O2A-CGA-CBA	2.02	120.23	112.23
27	A	832	CHL	C3D-C4D-CHA	-2.02	108.09	112.72
27	b	306	CHL	O2A-CGA-CBA	2.02	120.22	112.23
27	B	821	CHL	CMD-C2D-C1D	2.02	128.28	124.71
27	A	827	CHL	C3D-C4D-CHA	-2.02	108.10	112.72
27	5	308	CHL	C3D-C4D-CHA	-2.02	108.10	112.72
27	B	820	CHL	C3B-C4B-NB	2.02	111.82	109.21
27	A	833	CHL	O2A-CGA-CBA	2.02	118.25	111.91
27	a	319	CHL	C3B-C4B-NB	2.02	111.82	109.21
27	A	825	CHL	C3D-C4D-CHA	-2.02	108.10	112.72
27	6	318	CHL	C2C-C3C-C4C	-2.02	105.05	106.49
27	3	308	CHL	C1D-CHD-C4C	-2.02	121.70	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	828	CHL	CMC-C2C-C1C	2.02	128.12	125.04
27	5	322	CHL	O2A-CGA-CBA	2.02	120.21	112.23
27	8	319	CHL	C3D-C4D-CHA	-2.02	108.10	112.72
22	I	801	BCR	C16-C15-C14	-2.02	119.34	123.47
27	K	204	CHL	C1D-CHD-C4C	-2.02	121.70	126.06
27	B	811	CHL	C3D-C4D-CHA	-2.02	108.11	112.72
27	A	816	CHL	C1-C2-C3	-2.02	122.55	126.04
27	b	306	CHL	C4C-C3C-C2C	-2.02	103.96	106.90
27	a	308	CHL	CAC-C3C-C4C	2.02	127.43	124.81
27	A	839	CHL	C3D-C4D-CHA	-2.02	108.11	112.72
27	b	306	CHL	C3D-C4D-CHA	-2.02	108.11	112.72
27	a	309	CHL	CED-O2D-CGD	2.02	120.50	115.94
27	7	318	CHL	C3D-C4D-CHA	-2.02	108.11	112.72
27	K	206	CHL	O2A-CGA-CBA	2.02	120.20	112.23
27	5	321	CHL	O2A-CGA-CBA	2.02	120.20	112.23
27	B	825	CHL	C2A-C1A-CHA	-2.02	120.33	123.86
27	b	304	CHL	C1D-CHD-C4C	-2.02	121.71	126.06
27	A	825	CHL	C1D-CHD-C4C	-2.02	121.71	126.06
27	4	305	CHL	O2A-CGA-CBA	2.02	120.51	114.03
22	7	303	BCR	C29-C30-C25	2.02	113.58	110.48
27	4	312	CHL	CMB-C2B-C3B	2.01	128.45	124.68
24	A	811	LHG	C27-C26-C25	-2.01	104.20	114.42
27	B	823	CHL	C3D-C4D-CHA	-2.01	108.11	112.72
27	A	851	CHL	O2A-CGA-CBA	2.01	120.19	112.23
29	a	304	LUT	C8-C7-C6	-2.01	121.55	127.20
27	A	835	CHL	CHB-C4A-NA	2.01	127.30	124.51
27	8	316	CHL	CED-O2D-CGD	2.01	120.49	115.94
29	F	303	LUT	C16-C1-C6	-2.01	107.03	110.30
27	3	318	CHL	C3B-C4B-NB	2.01	111.81	109.21
29	8	304	LUT	C21-C26-C25	2.01	115.02	111.42
27	7	314	CHL	C4C-C3C-C2C	-2.01	103.96	106.90
27	A	845	CHL	O2A-CGA-CBA	2.01	118.22	111.91
27	A	844	CHL	C3B-C4B-NB	2.01	111.81	109.21
27	3	308	CHL	O2A-CGA-O1A	-2.01	118.52	123.59
27	B	824	CHL	C4C-C3C-C2C	-2.01	103.97	106.90
27	8	316	CHL	C1D-CHD-C4C	-2.01	121.72	126.06
27	8	326	CHL	C3D-C4D-CHA	-2.01	108.12	112.72
27	7	316	CHL	CMD-C2D-C1D	2.01	128.26	124.71
27	8	324	CHL	C2C-C3C-C4C	-2.01	105.06	106.49
27	A	857	CHL	O2A-CGA-CBA	2.01	120.17	112.23
27	A	835	CHL	C3B-C4B-NB	2.01	111.81	109.21
27	8	314	CHL	O2A-CGA-O1A	-2.01	118.52	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	317	CHL	C3D-C4D-CHA	-2.01	108.13	112.72
27	B	818	CHL	CMD-C2D-C1D	2.01	128.25	124.71
27	a	309	CHL	C3D-C4D-CHA	-2.01	108.13	112.72
27	4	318	CHL	CAC-C3C-C4C	2.01	127.41	124.81
27	4	305	CHL	C4C-C3C-C2C	-2.01	103.97	106.90
27	5	321	CHL	C1B-CHB-C4A	-2.01	126.14	130.12
27	B	815	CHL	C1-O2A-CGA	2.01	121.71	116.44
27	6	319	CHL	C3D-C4D-ND	2.01	113.48	110.24
27	B	846	CHL	C2A-C1A-CHA	-2.01	120.35	123.86
27	B	826	CHL	C3D-C4D-CHA	-2.01	108.14	112.72
27	6	320	CHL	C1D-CHD-C4C	-2.01	121.73	126.06
27	B	838	CHL	O2A-CGA-CBA	2.00	118.20	111.91
27	B	839	CHL	C3D-C4D-CHA	-2.00	108.14	112.72
27	4	309	CHL	CHA-C4D-ND	2.00	136.69	132.50
30	J	101	LMG	O2-C2-C1	-2.00	105.18	110.05
27	B	829	CHL	CED-O2D-CGD	2.00	120.47	115.94
27	b	313	CHL	C3D-C4D-CHA	-2.00	108.14	112.72
27	A	852	CHL	C1D-CHD-C4C	-2.00	121.74	126.06
27	6	314	CHL	O2A-CGA-CBA	2.00	120.14	112.23
27	a	314	CHL	CED-O2D-CGD	2.00	120.46	115.94
27	a	308	CHL	C3D-C4D-CHA	-2.00	108.15	112.72
27	b	309	CHL	C3D-C4D-CHA	-2.00	108.15	112.72
27	8	324	CHL	CMB-C2B-C3B	2.00	128.42	124.68

All (530) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	815	CL0	NC
27	A	816	CHL	ND
27	A	816	CHL	NA
27	A	816	CHL	NC
27	A	817	CHL	NC
27	A	818	CHL	NC
27	A	818	CHL	ND
27	A	818	CHL	NA
27	A	819	CHL	ND
27	A	819	CHL	NC
27	A	820	CHL	NA
27	A	820	CHL	NC
27	A	820	CHL	ND
27	A	821	CHL	NC
27	A	821	CHL	ND

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Mol	Chain	Res	Type	Atom
27	A	821	CHL	NA
27	A	822	CHL	NC
27	A	823	CHL	NC
27	A	823	CHL	ND
27	A	823	CHL	NA
27	A	824	CHL	NC
27	A	824	CHL	NA
27	A	825	CHL	NC
27	A	826	CHL	NC
27	A	827	CHL	NC
27	A	827	CHL	NA
27	A	828	CHL	ND
27	A	828	CHL	NA
27	A	829	CHL	NC
27	A	829	CHL	ND
27	A	830	CHL	NC
27	A	830	CHL	NA
27	A	831	CHL	NC
27	A	831	CHL	NA
27	A	832	CHL	NA
27	A	832	CHL	NC
27	A	833	CHL	NC
27	A	833	CHL	NA
27	A	834	CHL	NC
27	A	834	CHL	NA
27	A	835	CHL	NC
27	A	835	CHL	ND
27	A	835	CHL	NA
27	A	836	CHL	NC
27	A	836	CHL	ND
27	A	836	CHL	NA
27	A	837	CHL	NC
27	A	837	CHL	NA
27	A	838	CHL	NC
27	A	839	CHL	NA
27	A	839	CHL	NC
27	A	840	CHL	NC
27	A	840	CHL	ND
27	A	840	CHL	NA
27	A	841	CHL	ND
27	A	841	CHL	NA
27	A	841	CHL	NC

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Mol	Chain	Res	Type	Atom
27	A	842	CHL	ND
27	A	842	CHL	NA
27	A	843	CHL	NC
27	A	843	CHL	NA
27	A	844	CHL	NC
27	A	845	CHL	NC
27	A	846	CHL	NC
27	A	846	CHL	NA
27	A	847	CHL	NC
27	A	847	CHL	NA
27	A	848	CHL	ND
27	A	848	CHL	NC
27	A	849	CHL	NA
27	A	849	CHL	NC
27	A	850	CHL	NC
27	A	851	CHL	ND
27	A	851	CHL	NA
27	A	851	CHL	NC
27	A	852	CHL	NC
27	A	852	CHL	ND
27	A	852	CHL	NA
27	A	853	CHL	NC
27	A	853	CHL	ND
27	A	853	CHL	NA
27	A	854	CHL	NC
27	A	855	CHL	NC
27	A	856	CHL	NC
27	A	856	CHL	ND
27	A	857	CHL	NC
27	A	857	CHL	ND
27	A	857	CHL	NA
27	A	858	CHL	NC
27	A	858	CHL	ND
27	A	859	CHL	ND
27	A	859	CHL	NA
27	A	859	CHL	NC
27	B	811	CHL	ND
27	B	811	CHL	NC
27	B	812	CHL	ND
27	B	812	CHL	NC
27	B	813	CHL	NC
27	B	813	CHL	ND

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Mol	Chain	Res	Type	Atom
27	B	813	CHL	NA
27	B	814	CHL	NA
27	B	814	CHL	NC
27	B	814	CHL	ND
27	B	815	CHL	NC
27	B	815	CHL	ND
27	B	815	CHL	NA
27	B	816	CHL	ND
27	B	816	CHL	NA
27	B	816	CHL	NC
27	B	817	CHL	NA
27	B	817	CHL	ND
27	B	817	CHL	NC
27	B	818	CHL	NC
27	B	818	CHL	ND
27	B	819	CHL	NC
27	B	819	CHL	ND
27	B	819	CHL	NA
27	B	820	CHL	NC
27	B	821	CHL	NC
27	B	821	CHL	NA
27	B	822	CHL	ND
27	B	822	CHL	NA
27	B	823	CHL	NC
27	B	823	CHL	ND
27	B	823	CHL	NA
27	B	824	CHL	NC
27	B	824	CHL	NA
27	B	825	CHL	NC
27	B	825	CHL	NA
27	B	826	CHL	NC
27	B	827	CHL	NC
27	B	827	CHL	ND
27	B	827	CHL	NA
27	B	828	CHL	NC
27	B	828	CHL	ND
27	B	828	CHL	NA
27	B	829	CHL	NC
27	B	829	CHL	NA
27	B	830	CHL	NC
27	B	830	CHL	NA
27	B	831	CHL	NC

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Mol	Chain	Res	Type	Atom
27	B	831	CHL	NA
27	B	832	CHL	NC
27	B	832	CHL	ND
27	B	832	CHL	NA
27	B	833	CHL	NC
27	B	833	CHL	ND
27	B	833	CHL	NA
27	B	834	CHL	NC
27	B	834	CHL	ND
27	B	834	CHL	NA
27	B	835	CHL	ND
27	B	835	CHL	NC
27	B	836	CHL	NA
27	B	836	CHL	NC
27	B	837	CHL	NC
27	B	838	CHL	NC
27	B	839	CHL	NC
27	B	839	CHL	NA
27	B	840	CHL	NC
27	B	840	CHL	ND
27	B	840	CHL	NA
27	B	841	CHL	NC
27	B	841	CHL	NA
27	B	842	CHL	NC
27	B	842	CHL	ND
27	B	843	CHL	NC
27	B	843	CHL	ND
27	B	843	CHL	NA
27	B	844	CHL	ND
27	B	844	CHL	NA
27	B	844	CHL	NC
27	B	845	CHL	NC
27	B	845	CHL	NA
27	B	846	CHL	NC
27	B	846	CHL	ND
27	B	846	CHL	NA
27	B	847	CHL	NC
27	B	847	CHL	NA
27	B	848	CHL	NC
27	B	849	CHL	NC
27	B	849	CHL	ND
27	B	849	CHL	NA

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Mol	Chain	Res	Type	Atom
27	B	850	CHL	ND
27	B	850	CHL	NA
27	B	851	CHL	NC
27	B	851	CHL	NA
27	F	308	CHL	NC
27	F	308	CHL	ND
27	F	308	CHL	NA
27	F	309	CHL	NC
27	F	309	CHL	ND
27	F	309	CHL	NA
27	J	106	CHL	NC
27	J	106	CHL	ND
27	J	106	CHL	NA
27	K	204	CHL	NC
27	K	204	CHL	ND
27	K	204	CHL	NA
27	K	205	CHL	NC
27	K	205	CHL	ND
27	K	205	CHL	NA
27	K	206	CHL	NC
27	K	206	CHL	NA
27	K	207	CHL	NC
27	K	207	CHL	ND
27	K	207	CHL	NA
27	a	307	CHL	NC
27	a	307	CHL	ND
27	a	307	CHL	NA
27	a	308	CHL	NC
27	a	308	CHL	ND
27	a	308	CHL	NA
27	a	309	CHL	NA
27	a	309	CHL	NC
27	a	309	CHL	ND
27	a	310	CHL	NC
27	a	310	CHL	ND
27	a	311	CHL	NA
27	a	311	CHL	ND
27	a	312	CHL	NC
27	a	312	CHL	ND
27	a	312	CHL	NA
27	a	313	CHL	NC
27	a	313	CHL	ND

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Mol	Chain	Res	Type	Atom
27	a	313	CHL	NA
27	a	314	CHL	NC
27	a	314	CHL	NA
27	a	315	CHL	NA
27	a	315	CHL	NC
27	a	316	CHL	NC
27	a	316	CHL	ND
27	a	316	CHL	NA
27	a	317	CHL	NC
27	a	317	CHL	ND
27	a	317	CHL	NA
27	a	318	CHL	NC
27	a	318	CHL	ND
27	a	318	CHL	NA
27	a	319	CHL	ND
27	a	319	CHL	NA
27	a	320	CHL	ND
27	a	320	CHL	NA
27	a	320	CHL	NC
27	3	308	CHL	NC
27	3	308	CHL	ND
27	3	308	CHL	NA
27	3	309	CHL	NC
27	3	309	CHL	ND
27	3	309	CHL	NA
27	3	310	CHL	NC
27	3	310	CHL	ND
27	3	310	CHL	NA
27	3	311	CHL	NC
27	3	311	CHL	ND
27	3	311	CHL	NA
27	3	312	CHL	ND
27	3	312	CHL	NA
27	3	313	CHL	NC
27	3	313	CHL	ND
27	3	313	CHL	NA
27	3	314	CHL	NC
27	3	314	CHL	ND
27	3	314	CHL	NA
27	3	315	CHL	NC
27	3	315	CHL	NA
27	3	316	CHL	NC

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Mol	Chain	Res	Type	Atom
27	3	316	CHL	NA
27	3	317	CHL	NC
27	3	317	CHL	ND
27	3	318	CHL	NC
27	3	318	CHL	ND
27	3	318	CHL	NA
27	3	319	CHL	NC
27	3	319	CHL	NA
27	3	320	CHL	NC
27	3	320	CHL	ND
27	3	320	CHL	NA
27	3	321	CHL	NC
27	3	321	CHL	NA
27	4	304	CHL	NC
27	4	304	CHL	ND
27	4	304	CHL	NA
27	4	305	CHL	NC
27	4	305	CHL	ND
27	4	305	CHL	NA
27	4	306	CHL	NC
27	4	306	CHL	ND
27	4	306	CHL	NA
27	4	307	CHL	NC
27	4	307	CHL	NA
27	4	308	CHL	NC
27	4	308	CHL	ND
27	4	308	CHL	NA
27	4	309	CHL	NC
27	4	309	CHL	ND
27	4	309	CHL	NA
27	4	310	CHL	NC
27	4	310	CHL	ND
27	4	310	CHL	NA
27	4	311	CHL	NC
27	4	311	CHL	ND
27	4	311	CHL	NA
27	4	312	CHL	NA
27	4	312	CHL	NC
27	4	313	CHL	NC
27	4	314	CHL	NC
27	4	314	CHL	ND
27	4	314	CHL	NA

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Mol	Chain	Res	Type	Atom
27	4	315	CHL	NC
27	4	315	CHL	ND
27	4	315	CHL	NA
27	4	316	CHL	NC
27	4	316	CHL	ND
27	4	316	CHL	NA
27	4	317	CHL	NA
27	4	317	CHL	NC
27	4	318	CHL	NA
27	4	318	CHL	NC
27	4	318	CHL	ND
27	4	319	CHL	NA
27	4	319	CHL	NC
27	4	320	CHL	NC
27	4	320	CHL	ND
27	4	320	CHL	NA
27	5	307	CHL	NC
27	5	307	CHL	ND
27	5	307	CHL	NA
27	5	308	CHL	NC
27	5	308	CHL	ND
27	5	308	CHL	NA
27	5	309	CHL	NC
27	5	309	CHL	NA
27	5	310	CHL	NC
27	5	310	CHL	ND
27	5	310	CHL	NA
27	5	311	CHL	NA
27	5	311	CHL	NC
27	5	311	CHL	ND
27	5	312	CHL	NC
27	5	312	CHL	ND
27	5	312	CHL	NA
27	5	313	CHL	NC
27	5	313	CHL	NA
27	5	314	CHL	NC
27	5	314	CHL	NA
27	5	315	CHL	NC
27	5	315	CHL	ND
27	5	315	CHL	NA
27	5	316	CHL	NC
27	5	316	CHL	ND

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Mol	Chain	Res	Type	Atom
27	5	316	CHL	NA
27	5	317	CHL	NC
27	5	317	CHL	NA
27	5	318	CHL	ND
27	5	318	CHL	NA
27	5	318	CHL	NC
27	5	319	CHL	NA
27	5	319	CHL	NC
27	5	320	CHL	NA
27	5	320	CHL	NC
27	5	320	CHL	ND
27	5	321	CHL	NC
27	5	321	CHL	NA
27	5	322	CHL	NC
27	5	322	CHL	ND
27	5	322	CHL	NA
27	5	323	CHL	NC
27	5	323	CHL	ND
27	5	325	CHL	NA
27	5	325	CHL	NC
27	6	305	CHL	NC
27	6	305	CHL	ND
27	6	305	CHL	NA
27	6	306	CHL	NC
27	6	306	CHL	ND
27	6	306	CHL	NA
27	6	307	CHL	NC
27	6	307	CHL	NA
27	6	308	CHL	NC
27	6	308	CHL	ND
27	6	308	CHL	NA
27	6	309	CHL	NC
27	6	309	CHL	ND
27	6	309	CHL	NA
27	6	310	CHL	NC
27	6	310	CHL	ND
27	6	310	CHL	NA
27	6	311	CHL	NC
27	6	311	CHL	ND
27	6	311	CHL	NA
27	6	312	CHL	NC
27	6	312	CHL	ND

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Mol	Chain	Res	Type	Atom
27	6	312	CHL	NA
27	6	313	CHL	NC
27	6	313	CHL	NA
27	6	314	CHL	NC
27	6	314	CHL	ND
27	6	314	CHL	NA
27	6	315	CHL	NC
27	6	315	CHL	NA
27	6	316	CHL	NC
27	6	316	CHL	ND
27	6	316	CHL	NA
27	6	317	CHL	NC
27	6	317	CHL	NA
27	6	318	CHL	ND
27	6	318	CHL	NA
27	6	318	CHL	NC
27	6	319	CHL	NC
27	6	319	CHL	ND
27	6	319	CHL	NA
27	6	320	CHL	NC
27	6	320	CHL	ND
27	6	320	CHL	NA
27	7	311	CHL	NC
27	7	311	CHL	ND
27	7	311	CHL	NA
27	7	312	CHL	NC
27	7	312	CHL	ND
27	7	312	CHL	NA
27	7	313	CHL	NC
27	7	313	CHL	NA
27	7	314	CHL	NC
27	7	314	CHL	ND
27	7	314	CHL	NA
27	7	315	CHL	NA
27	7	315	CHL	ND
27	7	316	CHL	NC
27	7	316	CHL	ND
27	7	316	CHL	NA
27	7	317	CHL	NC
27	7	317	CHL	ND
27	7	317	CHL	NA
27	7	318	CHL	NC

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Mol	Chain	Res	Type	Atom
27	7	318	CHL	NA
27	7	319	CHL	NC
27	7	319	CHL	ND
27	7	319	CHL	NA
27	7	320	CHL	NC
27	7	320	CHL	ND
27	7	321	CHL	NC
27	7	321	CHL	ND
27	7	321	CHL	NA
27	7	322	CHL	NA
27	7	322	CHL	NC
27	7	323	CHL	NC
27	7	323	CHL	NA
27	7	324	CHL	NC
27	7	324	CHL	NA
27	8	311	CHL	NC
27	8	311	CHL	ND
27	8	311	CHL	NA
27	8	312	CHL	NC
27	8	312	CHL	ND
27	8	312	CHL	NA
27	8	313	CHL	NC
27	8	313	CHL	ND
27	8	313	CHL	NA
27	8	314	CHL	NC
27	8	314	CHL	ND
27	8	314	CHL	NA
27	8	315	CHL	NC
27	8	315	CHL	ND
27	8	316	CHL	ND
27	8	316	CHL	NA
27	8	317	CHL	NC
27	8	317	CHL	ND
27	8	317	CHL	NA
27	8	318	CHL	NC
27	8	318	CHL	ND
27	8	318	CHL	NA
27	8	319	CHL	NC
27	8	319	CHL	ND
27	8	319	CHL	NA
27	8	320	CHL	NA
27	8	320	CHL	NC

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Mol	Chain	Res	Type	Atom
27	8	321	CHL	NC
27	8	321	CHL	ND
27	8	321	CHL	NA
27	8	322	CHL	NC
27	8	322	CHL	NA
27	8	323	CHL	NA
27	8	323	CHL	NC
27	8	324	CHL	NC
27	8	324	CHL	ND
27	8	324	CHL	NA
27	8	325	CHL	NC
27	8	325	CHL	NA
27	8	326	CHL	NC
27	8	326	CHL	ND
27	8	326	CHL	NA
27	L	303	CHL	NC
27	L	303	CHL	NA
27	L	304	CHL	NC
27	L	304	CHL	NA
27	b	304	CHL	ND
27	b	304	CHL	NA
27	b	305	CHL	NA
27	b	305	CHL	NC
27	b	305	CHL	ND
27	b	306	CHL	NC
27	b	306	CHL	NA
27	b	307	CHL	ND
27	b	307	CHL	NA
27	b	308	CHL	NC
27	b	308	CHL	NA
27	b	309	CHL	NA
27	b	309	CHL	NC
27	b	309	CHL	ND
27	b	310	CHL	NA
27	b	310	CHL	NC
27	b	311	CHL	NC
27	b	311	CHL	ND
27	b	311	CHL	NA
27	b	312	CHL	NA
27	b	313	CHL	NC
27	b	313	CHL	ND
27	b	313	CHL	NA

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Mol	Chain	Res	Type	Atom
27	b	314	CHL	ND
27	b	314	CHL	NA
27	b	314	CHL	NC
27	b	315	CHL	NC
27	b	315	CHL	ND
27	b	315	CHL	NA
27	b	316	CHL	NC
27	b	316	CHL	ND
27	b	316	CHL	NA
27	b	317	CHL	NA
27	b	317	CHL	NC

All (2594) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	804	BCR	C7-C8-C9-C10
22	A	804	BCR	C7-C8-C9-C34
22	A	805	BCR	C1-C6-C7-C8
22	A	806	BCR	C1-C6-C7-C8
22	A	806	BCR	C7-C8-C9-C34
22	A	806	BCR	C20-C21-C22-C37
22	A	806	BCR	C23-C24-C25-C30
22	A	807	BCR	C7-C8-C9-C34
22	A	807	BCR	C21-C22-C23-C24
22	A	807	BCR	C37-C22-C23-C24
22	B	802	BCR	C1-C6-C7-C8
22	B	802	BCR	C7-C8-C9-C10
22	B	802	BCR	C7-C8-C9-C34
22	B	802	BCR	C21-C22-C23-C24
22	B	802	BCR	C37-C22-C23-C24
22	B	803	BCR	C37-C22-C23-C24
22	B	804	BCR	C1-C6-C7-C8
22	B	804	BCR	C7-C8-C9-C34
22	B	806	BCR	C7-C8-C9-C10
22	B	806	BCR	C7-C8-C9-C34
22	B	807	BCR	C1-C6-C7-C8
22	F	301	BCR	C7-C8-C9-C34
22	F	301	BCR	C37-C22-C23-C24
22	I	801	BCR	C7-C8-C9-C34
22	I	801	BCR	C11-C12-C13-C35
22	I	801	BCR	C20-C21-C22-C37
22	I	801	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	J	102	BCR	C7-C8-C9-C34
22	J	102	BCR	C23-C24-C25-C30
22	K	202	BCR	C7-C8-C9-C10
22	K	202	BCR	C7-C8-C9-C34
22	K	202	BCR	C23-C24-C25-C26
22	K	203	BCR	C23-C24-C25-C30
22	M	102	BCR	C1-C6-C7-C8
22	M	102	BCR	C7-C8-C9-C34
22	M	102	BCR	C22-C23-C24-C25
22	M	102	BCR	C23-C24-C25-C30
22	3	301	BCR	C7-C8-C9-C10
22	3	301	BCR	C7-C8-C9-C34
22	3	301	BCR	C23-C24-C25-C30
22	3	302	BCR	C1-C6-C7-C8
22	3	302	BCR	C7-C8-C9-C34
22	3	302	BCR	C11-C12-C13-C35
22	3	303	BCR	C23-C24-C25-C30
22	5	301	BCR	C6-C7-C8-C9
22	5	301	BCR	C7-C8-C9-C10
22	5	301	BCR	C7-C8-C9-C34
22	5	301	BCR	C17-C18-C19-C20
22	5	301	BCR	C36-C18-C19-C20
22	5	301	BCR	C18-C19-C20-C21
22	5	301	BCR	C20-C21-C22-C37
22	5	301	BCR	C23-C24-C25-C30
22	6	301	BCR	C6-C7-C8-C9
22	6	301	BCR	C11-C10-C9-C8
22	6	301	BCR	C11-C10-C9-C34
22	6	301	BCR	C10-C11-C12-C13
22	6	301	BCR	C11-C12-C13-C14
22	6	301	BCR	C11-C12-C13-C35
22	6	301	BCR	C18-C19-C20-C21
22	6	301	BCR	C21-C22-C23-C24
22	6	301	BCR	C37-C22-C23-C24
22	6	301	BCR	C22-C23-C24-C25
22	6	301	BCR	C23-C24-C25-C30
22	7	303	BCR	C20-C21-C22-C23
22	7	303	BCR	C20-C21-C22-C37
22	L	301	BCR	C1-C6-C7-C8
22	L	302	BCR	C37-C22-C23-C24
23	F	302	LMT	C2-C1-O1'-C1'
24	A	810	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	A	810	LHG	C3-O3-P-O4
24	A	811	LHG	O1-C1-C2-C3
24	A	811	LHG	C3-O3-P-O5
24	A	811	LHG	C4-O6-P-O4
24	A	811	LHG	C4-O6-P-O5
24	A	811	LHG	O9-C7-O7-C5
24	A	811	LHG	C8-C7-O7-C5
24	A	812	LHG	C3-O3-P-O6
24	4	303	LHG	C3-O3-P-O4
24	4	303	LHG	C3-O3-P-O5
24	4	303	LHG	C3-O3-P-O6
24	5	304	LHG	C3-O3-P-O4
24	5	324	LHG	C1-C2-C3-O3
24	5	324	LHG	C2-C3-O3-P
24	5	324	LHG	C3-O3-P-O4
24	7	302	LHG	O2-C2-C3-O3
24	7	302	LHG	O9-C7-O7-C5
24	7	302	LHG	C8-C7-O7-C5
24	7	306	LHG	C3-O3-P-O4
24	7	306	LHG	C4-O6-P-O4
24	b	302	LHG	O1-C1-C2-C3
24	b	302	LHG	C4-O6-P-O5
27	A	816	CHL	CHA-CBD-CGD-O2D
27	A	816	CHL	CBD-CGD-O2D-CED
27	A	817	CHL	CBD-CGD-O2D-CED
27	A	817	CHL	O1D-CGD-O2D-CED
27	A	818	CHL	CHA-CBD-CGD-O2D
27	A	821	CHL	C1A-C2A-CAA-CBA
27	A	821	CHL	CBD-CGD-O2D-CED
27	A	823	CHL	CHA-CBD-CGD-O1D
27	A	824	CHL	C1A-C2A-CAA-CBA
27	A	824	CHL	CBD-CGD-O2D-CED
27	A	825	CHL	CBD-CGD-O2D-CED
27	A	826	CHL	C1A-C2A-CAA-CBA
27	A	826	CHL	CBD-CGD-O2D-CED
27	A	828	CHL	CBD-CGD-O2D-CED
27	A	828	CHL	O1D-CGD-O2D-CED
27	A	830	CHL	CHA-CBD-CGD-O2D
27	A	830	CHL	CBD-CGD-O2D-CED
27	A	830	CHL	C2-C3-C5-C6
27	A	830	CHL	C4-C3-C5-C6
27	A	833	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	A	833	CHL	C3A-C2A-CAA-CBA
27	A	833	CHL	C1C-C2C-CMC-OMC
27	A	833	CHL	C3C-C2C-CMC-OMC
27	A	833	CHL	CAD-CBD-CGD-O2D
27	A	833	CHL	CBD-CGD-O2D-CED
27	A	834	CHL	CHA-CBD-CGD-O2D
27	A	835	CHL	C1A-C2A-CAA-CBA
27	A	835	CHL	C3A-C2A-CAA-CBA
27	A	836	CHL	CBD-CGD-O2D-CED
27	A	837	CHL	CHA-CBD-CGD-O2D
27	A	837	CHL	CBD-CGD-O2D-CED
27	A	837	CHL	O1D-CGD-O2D-CED
27	A	838	CHL	CBD-CGD-O2D-CED
27	A	839	CHL	CBD-CGD-O2D-CED
27	A	841	CHL	C1C-C2C-CMC-OMC
27	A	841	CHL	C3C-C2C-CMC-OMC
27	A	841	CHL	CAD-CBD-CGD-O2D
27	A	842	CHL	CHA-CBD-CGD-O1D
27	A	842	CHL	CBD-CGD-O2D-CED
27	A	844	CHL	CBD-CGD-O2D-CED
27	A	844	CHL	O1D-CGD-O2D-CED
27	A	845	CHL	CHA-CBD-CGD-O1D
27	A	847	CHL	CBD-CGD-O2D-CED
27	A	847	CHL	C4-C3-C5-C6
27	A	848	CHL	C1A-C2A-CAA-CBA
27	A	848	CHL	CBD-CGD-O2D-CED
27	A	849	CHL	CBD-CGD-O2D-CED
27	A	850	CHL	CBD-CGD-O2D-CED
27	A	851	CHL	CHA-CBD-CGD-O1D
27	A	852	CHL	CBD-CGD-O2D-CED
27	A	852	CHL	C2-C3-C5-C6
27	A	853	CHL	CHA-CBD-CGD-O2D
27	A	853	CHL	CBD-CGD-O2D-CED
27	A	854	CHL	CHA-CBD-CGD-O1D
27	A	854	CHL	CBD-CGD-O2D-CED
27	A	855	CHL	CHA-CBD-CGD-O2D
27	A	856	CHL	CBD-CGD-O2D-CED
27	A	856	CHL	O1D-CGD-O2D-CED
27	A	857	CHL	CHA-CBD-CGD-O1D
27	A	858	CHL	CBD-CGD-O2D-CED
27	A	858	CHL	O1D-CGD-O2D-CED
27	A	859	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	811	CHL	CBD-CGD-O2D-CED
27	B	811	CHL	O1D-CGD-O2D-CED
27	B	812	CHL	CBD-CGD-O2D-CED
27	B	812	CHL	O1D-CGD-O2D-CED
27	B	814	CHL	CHA-CBD-CGD-O2D
27	B	814	CHL	CBD-CGD-O2D-CED
27	B	814	CHL	O1D-CGD-O2D-CED
27	B	815	CHL	CBD-CGD-O2D-CED
27	B	816	CHL	CHA-CBD-CGD-O2D
27	B	816	CHL	CBD-CGD-O2D-CED
27	B	817	CHL	CHA-CBD-CGD-O1D
27	B	818	CHL	CBD-CGD-O2D-CED
27	B	818	CHL	O1D-CGD-O2D-CED
27	B	819	CHL	O1D-CGD-O2D-CED
27	B	820	CHL	CBD-CGD-O2D-CED
27	B	821	CHL	CBD-CGD-O2D-CED
27	B	821	CHL	O1D-CGD-O2D-CED
27	B	822	CHL	O1D-CGD-O2D-CED
27	B	823	CHL	CHA-CBD-CGD-O2D
27	B	825	CHL	CBD-CGD-O2D-CED
27	B	826	CHL	C1A-C2A-CAA-CBA
27	B	828	CHL	CBD-CGD-O2D-CED
27	B	829	CHL	CBD-CGD-O2D-CED
27	B	830	CHL	CBD-CGD-O2D-CED
27	B	830	CHL	O1D-CGD-O2D-CED
27	B	831	CHL	CBD-CGD-O2D-CED
27	B	833	CHL	CHA-CBD-CGD-O1D
27	B	835	CHL	C1A-C2A-CAA-CBA
27	B	835	CHL	CBD-CGD-O2D-CED
27	B	835	CHL	O1D-CGD-O2D-CED
27	B	836	CHL	CBD-CGD-O2D-CED
27	B	836	CHL	O1D-CGD-O2D-CED
27	B	837	CHL	C2-C3-C5-C6
27	B	837	CHL	C4-C3-C5-C6
27	B	838	CHL	CBD-CGD-O2D-CED
27	B	839	CHL	CBD-CGD-O2D-CED
27	B	839	CHL	O1D-CGD-O2D-CED
27	B	841	CHL	CHA-CBD-CGD-O1D
27	B	841	CHL	C2-C3-C5-C6
27	B	841	CHL	C4-C3-C5-C6
27	B	842	CHL	CBD-CGD-O2D-CED
27	B	843	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	843	CHL	O1D-CGD-O2D-CED
27	B	844	CHL	CBD-CGD-O2D-CED
27	B	845	CHL	CBD-CGD-O2D-CED
27	B	846	CHL	CHA-CBD-CGD-O2D
27	B	846	CHL	CBD-CGD-O2D-CED
27	B	847	CHL	CBD-CGD-O2D-CED
27	B	848	CHL	CBD-CGD-O2D-CED
27	B	850	CHL	CBD-CGD-O2D-CED
27	B	851	CHL	CBD-CGD-O2D-CED
27	F	308	CHL	CHA-CBD-CGD-O1D
27	F	308	CHL	CBD-CGD-O2D-CED
27	F	309	CHL	CBD-CGD-O2D-CED
27	F	309	CHL	O1D-CGD-O2D-CED
27	J	106	CHL	CBD-CGD-O2D-CED
27	J	106	CHL	O1D-CGD-O2D-CED
27	K	205	CHL	CHA-CBD-CGD-O2D
27	K	205	CHL	CBD-CGD-O2D-CED
27	K	206	CHL	CBD-CGD-O2D-CED
27	K	207	CHL	CHA-CBD-CGD-O1D
27	K	207	CHL	CBD-CGD-O2D-CED
27	K	207	CHL	O1D-CGD-O2D-CED
27	a	307	CHL	CBD-CGD-O2D-CED
27	a	307	CHL	O1D-CGD-O2D-CED
27	a	308	CHL	CBD-CGD-O2D-CED
27	a	309	CHL	CHA-CBD-CGD-O1D
27	a	309	CHL	CBD-CGD-O2D-CED
27	a	311	CHL	CBD-CGD-O2D-CED
27	a	312	CHL	CBD-CGD-O2D-CED
27	a	313	CHL	CBD-CGD-O2D-CED
27	a	313	CHL	O1D-CGD-O2D-CED
27	a	314	CHL	C1A-C2A-CAA-CBA
27	a	314	CHL	C3A-C2A-CAA-CBA
27	a	314	CHL	C2A-CAA-CBA-CGA
27	a	314	CHL	CBD-CGD-O2D-CED
27	a	314	CHL	O1D-CGD-O2D-CED
27	a	315	CHL	CHA-CBD-CGD-O1D
27	a	315	CHL	CBD-CGD-O2D-CED
27	a	315	CHL	O1D-CGD-O2D-CED
27	a	316	CHL	C1C-C2C-CMC-OMC
27	a	316	CHL	C3C-C2C-CMC-OMC
27	a	316	CHL	CBD-CGD-O2D-CED
27	a	316	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	a	317	CHL	C1A-C2A-CAA-CBA
27	a	317	CHL	C3A-C2A-CAA-CBA
27	a	317	CHL	CBD-CGD-O2D-CED
27	a	317	CHL	O1D-CGD-O2D-CED
27	a	318	CHL	C1C-C2C-CMC-OMC
27	a	318	CHL	C3C-C2C-CMC-OMC
27	a	318	CHL	CBD-CGD-O2D-CED
27	a	319	CHL	CBD-CGD-O2D-CED
27	a	319	CHL	O1D-CGD-O2D-CED
27	a	320	CHL	CBD-CGD-O2D-CED
27	a	320	CHL	O1D-CGD-O2D-CED
27	3	308	CHL	CBD-CGD-O2D-CED
27	3	309	CHL	CBD-CGD-O2D-CED
27	3	310	CHL	CBD-CGD-O2D-CED
27	3	310	CHL	O1D-CGD-O2D-CED
27	3	311	CHL	C1A-C2A-CAA-CBA
27	3	311	CHL	C3A-C2A-CAA-CBA
27	3	312	CHL	CBD-CGD-O2D-CED
27	3	313	CHL	CHA-CBD-CGD-O2D
27	3	313	CHL	CBD-CGD-O2D-CED
27	3	314	CHL	CHA-CBD-CGD-O1D
27	3	314	CHL	CBD-CGD-O2D-CED
27	3	316	CHL	C1A-C2A-CAA-CBA
27	3	316	CHL	CHA-CBD-CGD-O2D
27	3	316	CHL	CBD-CGD-O2D-CED
27	3	316	CHL	O1D-CGD-O2D-CED
27	3	317	CHL	CBD-CGD-O2D-CED
27	3	317	CHL	C4-C3-C5-C6
27	3	318	CHL	CBD-CGD-O2D-CED
27	3	318	CHL	O1D-CGD-O2D-CED
27	3	318	CHL	C2-C3-C5-C6
27	3	318	CHL	C4-C3-C5-C6
27	3	319	CHL	CBD-CGD-O2D-CED
27	3	319	CHL	O1D-CGD-O2D-CED
27	3	319	CHL	C2-C3-C5-C6
27	3	319	CHL	C4-C3-C5-C6
27	3	321	CHL	CHA-CBD-CGD-O1D
27	3	321	CHL	CBD-CGD-O2D-CED
27	4	304	CHL	CBD-CGD-O2D-CED
27	4	304	CHL	O1D-CGD-O2D-CED
27	4	305	CHL	CBD-CGD-O2D-CED
27	4	306	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	4	306	CHL	O1D-CGD-O2D-CED
27	4	307	CHL	CBD-CGD-O2D-CED
27	4	308	CHL	CBD-CGD-O2D-CED
27	4	309	CHL	C3C-C2C-CMC-OMC
27	4	309	CHL	CBD-CGD-O2D-CED
27	4	309	CHL	O1D-CGD-O2D-CED
27	4	310	CHL	CHA-CBD-CGD-O1D
27	4	310	CHL	CBD-CGD-O2D-CED
27	4	310	CHL	O1D-CGD-O2D-CED
27	4	311	CHL	CBD-CGD-O2D-CED
27	4	311	CHL	O1D-CGD-O2D-CED
27	4	312	CHL	C1C-C2C-CMC-OMC
27	4	312	CHL	C3C-C2C-CMC-OMC
27	4	312	CHL	CHA-CBD-CGD-O1D
27	4	312	CHL	CHA-CBD-CGD-O2D
27	4	312	CHL	CBD-CGD-O2D-CED
27	4	313	CHL	C1A-C2A-CAA-CBA
27	4	314	CHL	CBD-CGD-O2D-CED
27	4	314	CHL	O1D-CGD-O2D-CED
27	4	315	CHL	O1D-CGD-O2D-CED
27	4	316	CHL	C1C-C2C-CMC-OMC
27	4	316	CHL	C3C-C2C-CMC-OMC
27	4	316	CHL	CHA-CBD-CGD-O2D
27	4	316	CHL	CBD-CGD-O2D-CED
27	4	316	CHL	O1D-CGD-O2D-CED
27	4	317	CHL	CHA-CBD-CGD-O1D
27	4	317	CHL	CHA-CBD-CGD-O2D
27	4	317	CHL	CBD-CGD-O2D-CED
27	4	318	CHL	CBD-CGD-O2D-CED
27	4	318	CHL	O1D-CGD-O2D-CED
27	4	320	CHL	CBD-CGD-O2D-CED
27	5	307	CHL	CBD-CGD-O2D-CED
27	5	308	CHL	CBD-CGD-O2D-CED
27	5	309	CHL	CBD-CGD-O2D-CED
27	5	309	CHL	C2-C3-C5-C6
27	5	309	CHL	C4-C3-C5-C6
27	5	310	CHL	CHA-CBD-CGD-O2D
27	5	310	CHL	CBD-CGD-O2D-CED
27	5	311	CHL	CHA-CBD-CGD-O2D
27	5	311	CHL	CBD-CGD-O2D-CED
27	5	313	CHL	C2-C3-C5-C6
27	5	313	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	5	314	CHL	CBD-CGD-O2D-CED
27	5	314	CHL	O1D-CGD-O2D-CED
27	5	315	CHL	CBD-CGD-O2D-CED
27	5	315	CHL	O1D-CGD-O2D-CED
27	5	316	CHL	C3C-C2C-CMC-OMC
27	5	317	CHL	CBD-CGD-O2D-CED
27	5	318	CHL	CHA-CBD-CGD-O2D
27	5	318	CHL	CBD-CGD-O2D-CED
27	5	319	CHL	C1C-C2C-CMC-OMC
27	5	319	CHL	C3C-C2C-CMC-OMC
27	5	319	CHL	CBD-CGD-O2D-CED
27	5	319	CHL	O1D-CGD-O2D-CED
27	5	320	CHL	CBD-CGD-O2D-CED
27	5	320	CHL	O1D-CGD-O2D-CED
27	5	321	CHL	CBD-CGD-O2D-CED
27	5	322	CHL	CBD-CGD-O2D-CED
27	5	322	CHL	O1D-CGD-O2D-CED
27	5	323	CHL	C1A-C2A-CAA-CBA
27	5	323	CHL	CHA-CBD-CGD-O2D
27	5	323	CHL	CBD-CGD-O2D-CED
27	5	325	CHL	C1C-C2C-CMC-OMC
27	5	325	CHL	C3C-C2C-CMC-OMC
27	5	325	CHL	CHA-CBD-CGD-O1D
27	5	325	CHL	CBD-CGD-O2D-CED
27	5	325	CHL	O1D-CGD-O2D-CED
27	6	305	CHL	C1A-C2A-CAA-CBA
27	6	305	CHL	C3A-C2A-CAA-CBA
27	6	305	CHL	CBD-CGD-O2D-CED
27	6	305	CHL	O1D-CGD-O2D-CED
27	6	306	CHL	C1A-C2A-CAA-CBA
27	6	306	CHL	CBD-CGD-O2D-CED
27	6	306	CHL	O1D-CGD-O2D-CED
27	6	308	CHL	C1A-C2A-CAA-CBA
27	6	308	CHL	C3A-C2A-CAA-CBA
27	6	308	CHL	C1C-C2C-CMC-OMC
27	6	308	CHL	C3C-C2C-CMC-OMC
27	6	308	CHL	CHA-CBD-CGD-O1D
27	6	308	CHL	CHA-CBD-CGD-O2D
27	6	308	CHL	C2-C3-C5-C6
27	6	308	CHL	C4-C3-C5-C6
27	6	309	CHL	CHA-CBD-CGD-O2D
27	6	309	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	6	310	CHL	CHA-CBD-CGD-O1D
27	6	310	CHL	CBD-CGD-O2D-CED
27	6	311	CHL	CHA-CBD-CGD-O2D
27	6	311	CHL	CBD-CGD-O2D-CED
27	6	311	CHL	O1D-CGD-O2D-CED
27	6	312	CHL	CBD-CGD-O2D-CED
27	6	312	CHL	O1D-CGD-O2D-CED
27	6	313	CHL	CBD-CGD-O2D-CED
27	6	314	CHL	CBD-CGD-O2D-CED
27	6	315	CHL	CBD-CGD-O2D-CED
27	6	315	CHL	O1D-CGD-O2D-CED
27	6	316	CHL	C1A-C2A-CAA-CBA
27	6	316	CHL	C3A-C2A-CAA-CBA
27	6	316	CHL	C3C-C2C-CMC-OMC
27	6	317	CHL	C1A-C2A-CAA-CBA
27	6	317	CHL	C3A-C2A-CAA-CBA
27	6	317	CHL	C3C-C2C-CMC-OMC
27	6	317	CHL	CBD-CGD-O2D-CED
27	6	318	CHL	C1C-C2C-CMC-OMC
27	6	318	CHL	C3C-C2C-CMC-OMC
27	6	318	CHL	CHA-CBD-CGD-O1D
27	6	318	CHL	CHA-CBD-CGD-O2D
27	6	318	CHL	CBD-CGD-O2D-CED
27	6	318	CHL	O1D-CGD-O2D-CED
27	6	319	CHL	C1A-C2A-CAA-CBA
27	6	319	CHL	C3A-C2A-CAA-CBA
27	6	319	CHL	C1C-C2C-CMC-OMC
27	6	319	CHL	C3C-C2C-CMC-OMC
27	6	319	CHL	CBD-CGD-O2D-CED
27	6	320	CHL	CHA-CBD-CGD-O2D
27	6	320	CHL	CBD-CGD-O2D-CED
27	6	320	CHL	O1D-CGD-O2D-CED
27	7	311	CHL	CHA-CBD-CGD-O2D
27	7	311	CHL	CBD-CGD-O2D-CED
27	7	312	CHL	CBD-CGD-O2D-CED
27	7	313	CHL	CBD-CGD-O2D-CED
27	7	316	CHL	CHA-CBD-CGD-O2D
27	7	316	CHL	CBD-CGD-O2D-CED
27	7	316	CHL	O1D-CGD-O2D-CED
27	7	317	CHL	CBD-CGD-O2D-CED
27	7	318	CHL	CBD-CGD-O2D-CED
27	7	319	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	7	319	CHL	C1C-C2C-CMC-OMC
27	7	319	CHL	C3C-C2C-CMC-OMC
27	7	319	CHL	CBD-CGD-O2D-CED
27	7	319	CHL	O1D-CGD-O2D-CED
27	7	320	CHL	C3C-C2C-CMC-OMC
27	7	320	CHL	CBD-CGD-O2D-CED
27	7	322	CHL	C1C-C2C-CMC-OMC
27	7	322	CHL	C3C-C2C-CMC-OMC
27	7	322	CHL	CBD-CGD-O2D-CED
27	7	323	CHL	C1A-C2A-CAA-CBA
27	7	323	CHL	C3A-C2A-CAA-CBA
27	7	323	CHL	C3-C5-C6-C7
27	7	324	CHL	C1A-C2A-CAA-CBA
27	7	324	CHL	CBD-CGD-O2D-CED
27	7	324	CHL	O1D-CGD-O2D-CED
27	8	311	CHL	CBD-CGD-O2D-CED
27	8	311	CHL	O1D-CGD-O2D-CED
27	8	312	CHL	CBD-CGD-O2D-CED
27	8	313	CHL	CBD-CGD-O2D-CED
27	8	314	CHL	C3C-C2C-CMC-OMC
27	8	314	CHL	CHA-CBD-CGD-O1D
27	8	314	CHL	CBD-CGD-O2D-CED
27	8	314	CHL	O1D-CGD-O2D-CED
27	8	316	CHL	CBD-CGD-O2D-CED
27	8	316	CHL	O1D-CGD-O2D-CED
27	8	317	CHL	C1A-C2A-CAA-CBA
27	8	317	CHL	CBD-CGD-O2D-CED
27	8	319	CHL	O1D-CGD-O2D-CED
27	8	320	CHL	CHA-CBD-CGD-O1D
27	8	321	CHL	C1A-C2A-CAA-CBA
27	8	321	CHL	C3A-C2A-CAA-CBA
27	8	321	CHL	C3C-C2C-CMC-OMC
27	8	321	CHL	CBD-CGD-O2D-CED
27	8	321	CHL	C2-C3-C5-C6
27	8	321	CHL	C4-C3-C5-C6
27	8	322	CHL	CBD-CGD-O2D-CED
27	8	322	CHL	O1D-CGD-O2D-CED
27	8	323	CHL	C1A-C2A-CAA-CBA
27	8	323	CHL	C3A-C2A-CAA-CBA
27	8	323	CHL	CBA-CGA-O2A-C1
27	8	323	CHL	O1A-CGA-O2A-C1
27	8	324	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	8	324	CHL	O1D-CGD-O2D-CED
27	8	325	CHL	CHA-CBD-CGD-O1D
27	8	325	CHL	CBD-CGD-O2D-CED
27	8	326	CHL	CBD-CGD-O2D-CED
27	L	304	CHL	CBD-CGD-O2D-CED
27	b	304	CHL	CBD-CGD-O2D-CED
27	b	304	CHL	O1D-CGD-O2D-CED
27	b	305	CHL	CHA-CBD-CGD-O1D
27	b	305	CHL	CBD-CGD-O2D-CED
27	b	306	CHL	C1A-C2A-CAA-CBA
27	b	306	CHL	CBD-CGD-O2D-CED
27	b	306	CHL	O1D-CGD-O2D-CED
27	b	307	CHL	CBD-CGD-O2D-CED
27	b	307	CHL	O1D-CGD-O2D-CED
27	b	308	CHL	CBD-CGD-O2D-CED
27	b	309	CHL	CBD-CGD-O2D-CED
27	b	309	CHL	O1D-CGD-O2D-CED
27	b	310	CHL	CHA-CBD-CGD-O2D
27	b	310	CHL	CBD-CGD-O2D-CED
27	b	310	CHL	O1D-CGD-O2D-CED
27	b	311	CHL	C1C-C2C-CMC-OMC
27	b	311	CHL	C3C-C2C-CMC-OMC
27	b	311	CHL	CHA-CBD-CGD-O2D
27	b	311	CHL	CBD-CGD-O2D-CED
27	b	311	CHL	O1D-CGD-O2D-CED
27	b	312	CHL	CBD-CGD-O2D-CED
27	b	312	CHL	O1D-CGD-O2D-CED
27	b	313	CHL	C3A-C2A-CAA-CBA
27	b	313	CHL	CBD-CGD-O2D-CED
27	b	313	CHL	O1D-CGD-O2D-CED
27	b	314	CHL	CBD-CGD-O2D-CED
27	b	314	CHL	O1D-CGD-O2D-CED
27	b	315	CHL	C3A-C2A-CAA-CBA
27	b	315	CHL	CBD-CGD-O2D-CED
27	b	315	CHL	O1D-CGD-O2D-CED
27	b	316	CHL	C1C-C2C-CMC-OMC
27	b	316	CHL	C3C-C2C-CMC-OMC
27	b	316	CHL	CBD-CGD-O2D-CED
27	b	316	CHL	O1D-CGD-O2D-CED
27	b	317	CHL	CBD-CGD-O2D-CED
27	b	317	CHL	O1D-CGD-O2D-CED
28	B	809	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
28	B	809	DGD	O2G-C2G-C3G-O3G
29	F	303	LUT	C5-C6-C7-C8
29	F	303	LUT	C7-C8-C9-C19
29	F	303	LUT	C11-C10-C9-C8
29	F	303	LUT	C20-C13-C14-C15
29	F	303	LUT	C27-C28-C29-C30
29	F	303	LUT	C39-C29-C30-C31
29	F	303	LUT	C31-C32-C33-C34
29	F	303	LUT	C40-C33-C34-C35
29	J	103	LUT	C5-C6-C7-C8
29	J	103	LUT	C11-C10-C9-C19
29	J	103	LUT	C11-C12-C13-C20
29	J	103	LUT	C20-C13-C14-C15
29	J	103	LUT	C28-C29-C30-C31
29	J	103	LUT	C39-C29-C30-C31
29	J	103	LUT	C40-C33-C34-C35
29	a	302	LUT	C5-C6-C7-C8
29	a	302	LUT	C7-C8-C9-C19
29	a	302	LUT	C11-C10-C9-C19
29	a	302	LUT	C11-C12-C13-C14
29	a	302	LUT	C20-C13-C14-C15
29	a	302	LUT	C40-C33-C34-C35
29	a	304	LUT	C5-C6-C7-C8
29	a	304	LUT	C7-C8-C9-C19
29	a	304	LUT	C11-C10-C9-C8
29	a	304	LUT	C11-C10-C9-C19
29	a	304	LUT	C11-C12-C13-C20
29	a	304	LUT	C12-C13-C14-C15
29	a	304	LUT	C20-C13-C14-C15
29	a	304	LUT	C39-C29-C30-C31
29	a	304	LUT	C29-C30-C31-C32
29	a	304	LUT	C40-C33-C34-C35
29	3	304	LUT	C5-C6-C7-C8
29	3	304	LUT	C7-C8-C9-C10
29	3	304	LUT	C11-C10-C9-C19
29	3	304	LUT	C11-C12-C13-C14
29	3	304	LUT	C20-C13-C14-C15
29	3	304	LUT	C28-C29-C30-C31
29	3	304	LUT	C40-C33-C34-C35
29	3	305	LUT	C5-C6-C7-C8
29	3	305	LUT	C11-C10-C9-C19
29	3	305	LUT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
29	3	305	LUT	C20-C13-C14-C15
29	3	305	LUT	C27-C28-C29-C30
29	3	305	LUT	C39-C29-C30-C31
29	3	305	LUT	C40-C33-C34-C35
29	4	301	LUT	C7-C8-C9-C19
29	4	301	LUT	C11-C10-C9-C19
29	4	301	LUT	C11-C12-C13-C20
29	4	301	LUT	C20-C13-C14-C15
29	4	301	LUT	C27-C28-C29-C39
29	4	301	LUT	C39-C29-C30-C31
29	4	301	LUT	C40-C33-C34-C35
29	4	302	LUT	C11-C10-C9-C8
29	4	302	LUT	C11-C10-C9-C19
29	4	302	LUT	C11-C12-C13-C20
29	4	302	LUT	C20-C13-C14-C15
29	4	302	LUT	C28-C29-C30-C31
29	4	302	LUT	C31-C32-C33-C34
29	4	302	LUT	C31-C32-C33-C40
29	4	302	LUT	C40-C33-C34-C35
29	5	302	LUT	C5-C6-C7-C8
29	5	302	LUT	C7-C8-C9-C19
29	5	302	LUT	C11-C10-C9-C19
29	5	302	LUT	C11-C12-C13-C14
29	5	302	LUT	C20-C13-C14-C15
29	5	302	LUT	C28-C29-C30-C31
29	5	302	LUT	C29-C30-C31-C32
29	5	302	LUT	C31-C32-C33-C34
29	5	302	LUT	C31-C32-C33-C40
29	5	302	LUT	C40-C33-C34-C35
29	5	303	LUT	C5-C6-C7-C8
29	5	303	LUT	C11-C10-C9-C8
29	5	303	LUT	C11-C10-C9-C19
29	5	303	LUT	C12-C13-C14-C15
29	5	303	LUT	C20-C13-C14-C15
29	5	303	LUT	C13-C14-C15-C35
29	5	303	LUT	C27-C28-C29-C30
29	5	303	LUT	C39-C29-C30-C31
29	5	303	LUT	C40-C33-C34-C35
29	6	302	LUT	C5-C6-C7-C8
29	6	302	LUT	C11-C10-C9-C19
29	6	302	LUT	C11-C12-C13-C14
29	6	302	LUT	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	6	302	LUT	C27-C28-C29-C30
29	6	302	LUT	C28-C29-C30-C31
29	6	302	LUT	C39-C29-C30-C31
29	6	302	LUT	C31-C32-C33-C34
29	6	302	LUT	C31-C32-C33-C40
29	6	302	LUT	C32-C33-C34-C35
29	6	302	LUT	C40-C33-C34-C35
29	6	303	LUT	C11-C10-C9-C8
29	6	303	LUT	C11-C10-C9-C19
29	6	303	LUT	C11-C12-C13-C14
29	6	303	LUT	C11-C12-C13-C20
29	6	303	LUT	C27-C28-C29-C30
29	6	303	LUT	C27-C28-C29-C39
29	6	303	LUT	C39-C29-C30-C31
29	6	303	LUT	C40-C33-C34-C35
29	7	304	LUT	C5-C6-C7-C8
29	7	304	LUT	C7-C8-C9-C10
29	7	304	LUT	C7-C8-C9-C19
29	7	304	LUT	C11-C10-C9-C19
29	7	304	LUT	C20-C13-C14-C15
29	7	304	LUT	C39-C29-C30-C31
29	7	304	LUT	C40-C33-C34-C35
29	8	303	LUT	C5-C6-C7-C8
29	8	303	LUT	C11-C10-C9-C19
29	8	303	LUT	C20-C13-C14-C15
29	8	303	LUT	C28-C29-C30-C31
29	8	303	LUT	C40-C33-C34-C35
29	8	304	LUT	C11-C10-C9-C8
29	8	304	LUT	C20-C13-C14-C15
29	8	304	LUT	C39-C29-C30-C31
29	8	304	LUT	C40-C33-C34-C35
29	8	304	LUT	C33-C34-C35-C15
29	b	301	LUT	C5-C6-C7-C8
29	b	301	LUT	C7-C8-C9-C10
29	b	301	LUT	C7-C8-C9-C19
29	b	301	LUT	C11-C10-C9-C8
29	b	301	LUT	C11-C10-C9-C19
29	b	301	LUT	C11-C12-C13-C14
29	b	301	LUT	C11-C12-C13-C20
29	b	301	LUT	C12-C13-C14-C15
29	b	301	LUT	C39-C29-C30-C31
29	b	301	LUT	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	b	303	LUT	C1-C6-C7-C8
29	b	303	LUT	C10-C11-C12-C13
29	b	303	LUT	C11-C12-C13-C14
29	b	303	LUT	C11-C12-C13-C20
29	b	303	LUT	C14-C15-C35-C34
29	b	303	LUT	C26-C27-C28-C29
29	b	303	LUT	C28-C29-C30-C31
29	b	303	LUT	C39-C29-C30-C31
29	b	303	LUT	C30-C31-C32-C33
29	b	303	LUT	C31-C32-C33-C34
29	b	303	LUT	C31-C32-C33-C40
30	J	104	LMG	C2-C1-O1-C7
30	J	104	LMG	O6-C1-O1-C7
30	J	104	LMG	O9-C10-O7-C8
30	8	307	LMG	C2-C1-O1-C7
30	8	307	LMG	O6-C1-O1-C7
30	8	307	LMG	O9-C10-O7-C8
30	8	307	LMG	C11-C10-O7-C8
32	5	305	PTY	C5-O14-P1-O11
32	5	305	PTY	C5-O14-P1-O12
32	5	305	PTY	C5-O14-P1-O13
33	7	305	XAT	C11-C10-C9-C8
33	7	305	XAT	C11-C10-C9-C19
33	7	305	XAT	C10-C11-C12-C13
34	8	301	SQD	O5-C5-C6-S
35	8	306	DGA	CG1-CG2-CG3-OXT
35	8	306	DGA	OG2-CG2-CG3-OXT
27	A	816	CHL	O1D-CGD-O2D-CED
27	A	820	CHL	O1D-CGD-O2D-CED
27	A	821	CHL	O1D-CGD-O2D-CED
27	A	823	CHL	O1D-CGD-O2D-CED
27	A	826	CHL	O1D-CGD-O2D-CED
27	A	832	CHL	O1D-CGD-O2D-CED
27	A	835	CHL	O1D-CGD-O2D-CED
27	A	836	CHL	O1D-CGD-O2D-CED
27	A	848	CHL	O1D-CGD-O2D-CED
27	A	849	CHL	O1D-CGD-O2D-CED
27	A	854	CHL	O1D-CGD-O2D-CED
27	A	859	CHL	O1D-CGD-O2D-CED
27	B	824	CHL	O1D-CGD-O2D-CED
27	B	827	CHL	O1D-CGD-O2D-CED
27	B	828	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	829	CHL	O1D-CGD-O2D-CED
27	B	831	CHL	O1D-CGD-O2D-CED
27	B	834	CHL	O1D-CGD-O2D-CED
27	B	838	CHL	O1D-CGD-O2D-CED
27	B	841	CHL	O1D-CGD-O2D-CED
27	B	842	CHL	O1D-CGD-O2D-CED
27	B	845	CHL	O1D-CGD-O2D-CED
27	B	847	CHL	O1D-CGD-O2D-CED
27	B	850	CHL	O1D-CGD-O2D-CED
27	K	205	CHL	O1D-CGD-O2D-CED
27	K	206	CHL	O1D-CGD-O2D-CED
27	a	308	CHL	O1D-CGD-O2D-CED
27	a	309	CHL	O1D-CGD-O2D-CED
27	a	311	CHL	O1D-CGD-O2D-CED
27	3	315	CHL	O1D-CGD-O2D-CED
27	3	320	CHL	O1D-CGD-O2D-CED
27	4	307	CHL	O1D-CGD-O2D-CED
27	4	317	CHL	O1D-CGD-O2D-CED
27	5	307	CHL	O1D-CGD-O2D-CED
27	5	310	CHL	O1D-CGD-O2D-CED
27	5	312	CHL	O1D-CGD-O2D-CED
27	5	318	CHL	O1D-CGD-O2D-CED
27	5	323	CHL	O1D-CGD-O2D-CED
27	6	313	CHL	O1D-CGD-O2D-CED
27	7	311	CHL	O1D-CGD-O2D-CED
27	8	318	CHL	O1D-CGD-O2D-CED
27	8	320	CHL	O1D-CGD-O2D-CED
27	L	304	CHL	O1D-CGD-O2D-CED
27	b	305	CHL	O1D-CGD-O2D-CED
27	A	819	CHL	O1D-CGD-O2D-CED
27	A	822	CHL	O1D-CGD-O2D-CED
27	A	824	CHL	O1D-CGD-O2D-CED
27	A	825	CHL	O1D-CGD-O2D-CED
27	A	830	CHL	O1D-CGD-O2D-CED
27	A	834	CHL	O1D-CGD-O2D-CED
27	A	838	CHL	O1D-CGD-O2D-CED
27	A	840	CHL	O1D-CGD-O2D-CED
27	A	845	CHL	O1D-CGD-O2D-CED
27	A	851	CHL	O1D-CGD-O2D-CED
27	A	857	CHL	O1D-CGD-O2D-CED
27	B	813	CHL	O1D-CGD-O2D-CED
27	B	816	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	817	CHL	O1D-CGD-O2D-CED
27	B	825	CHL	O1D-CGD-O2D-CED
27	B	826	CHL	O1D-CGD-O2D-CED
27	B	833	CHL	O1D-CGD-O2D-CED
27	B	837	CHL	O1D-CGD-O2D-CED
27	B	840	CHL	O1D-CGD-O2D-CED
27	K	204	CHL	O1D-CGD-O2D-CED
27	a	310	CHL	O1D-CGD-O2D-CED
27	a	312	CHL	O1D-CGD-O2D-CED
27	3	308	CHL	O1D-CGD-O2D-CED
27	3	309	CHL	O1D-CGD-O2D-CED
27	3	311	CHL	O1D-CGD-O2D-CED
27	3	314	CHL	O1D-CGD-O2D-CED
27	3	317	CHL	O1D-CGD-O2D-CED
27	3	321	CHL	O1D-CGD-O2D-CED
27	4	308	CHL	O1D-CGD-O2D-CED
27	4	320	CHL	O1D-CGD-O2D-CED
27	5	308	CHL	O1D-CGD-O2D-CED
27	5	311	CHL	O1D-CGD-O2D-CED
27	5	321	CHL	O1D-CGD-O2D-CED
27	6	310	CHL	O1D-CGD-O2D-CED
27	6	317	CHL	O1D-CGD-O2D-CED
27	6	319	CHL	O1D-CGD-O2D-CED
27	7	314	CHL	O1D-CGD-O2D-CED
27	7	318	CHL	O1D-CGD-O2D-CED
27	7	323	CHL	O1D-CGD-O2D-CED
27	8	315	CHL	O1D-CGD-O2D-CED
27	A	819	CHL	CBD-CGD-O2D-CED
27	A	820	CHL	CBD-CGD-O2D-CED
27	A	822	CHL	CBD-CGD-O2D-CED
27	A	823	CHL	CBD-CGD-O2D-CED
27	A	829	CHL	CBD-CGD-O2D-CED
27	A	831	CHL	CBD-CGD-O2D-CED
27	A	832	CHL	CBD-CGD-O2D-CED
27	A	834	CHL	CBD-CGD-O2D-CED
27	A	835	CHL	CBD-CGD-O2D-CED
27	A	840	CHL	CBD-CGD-O2D-CED
27	A	841	CHL	CBD-CGD-O2D-CED
27	A	845	CHL	CBD-CGD-O2D-CED
27	A	851	CHL	CBD-CGD-O2D-CED
27	A	857	CHL	CBD-CGD-O2D-CED
27	B	813	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	B	817	CHL	CBD-CGD-O2D-CED
27	B	819	CHL	CBD-CGD-O2D-CED
27	B	822	CHL	CBD-CGD-O2D-CED
27	B	824	CHL	CBD-CGD-O2D-CED
27	B	826	CHL	CBD-CGD-O2D-CED
27	B	827	CHL	CBD-CGD-O2D-CED
27	B	834	CHL	CBD-CGD-O2D-CED
27	B	837	CHL	CBD-CGD-O2D-CED
27	B	840	CHL	CBD-CGD-O2D-CED
27	B	841	CHL	CBD-CGD-O2D-CED
27	K	204	CHL	CBD-CGD-O2D-CED
27	a	310	CHL	CBD-CGD-O2D-CED
27	3	311	CHL	CBD-CGD-O2D-CED
27	3	315	CHL	CBD-CGD-O2D-CED
27	3	320	CHL	CBD-CGD-O2D-CED
27	4	315	CHL	CBD-CGD-O2D-CED
27	4	319	CHL	CBD-CGD-O2D-CED
27	5	312	CHL	CBD-CGD-O2D-CED
27	7	314	CHL	CBD-CGD-O2D-CED
27	7	323	CHL	CBD-CGD-O2D-CED
27	8	315	CHL	CBD-CGD-O2D-CED
27	8	318	CHL	CBD-CGD-O2D-CED
27	8	319	CHL	CBD-CGD-O2D-CED
27	8	320	CHL	CBD-CGD-O2D-CED
24	A	810	LHG	O10-C23-O8-C6
27	A	843	CHL	O1A-CGA-O2A-C1
27	B	846	CHL	O1A-CGA-O2A-C1
27	A	827	CHL	O1D-CGD-O2D-CED
27	A	829	CHL	O1D-CGD-O2D-CED
27	A	839	CHL	O1D-CGD-O2D-CED
27	A	842	CHL	O1D-CGD-O2D-CED
27	A	850	CHL	O1D-CGD-O2D-CED
27	A	853	CHL	O1D-CGD-O2D-CED
27	B	823	CHL	O1D-CGD-O2D-CED
27	B	848	CHL	O1D-CGD-O2D-CED
27	a	318	CHL	O1D-CGD-O2D-CED
27	4	305	CHL	O1D-CGD-O2D-CED
27	4	312	CHL	O1D-CGD-O2D-CED
27	4	319	CHL	O1D-CGD-O2D-CED
27	5	309	CHL	O1D-CGD-O2D-CED
27	6	309	CHL	O1D-CGD-O2D-CED
27	6	314	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	7	312	CHL	O1D-CGD-O2D-CED
27	7	317	CHL	O1D-CGD-O2D-CED
27	7	322	CHL	O1D-CGD-O2D-CED
27	8	313	CHL	O1D-CGD-O2D-CED
27	8	317	CHL	O1D-CGD-O2D-CED
27	8	321	CHL	O1D-CGD-O2D-CED
27	8	325	CHL	O1D-CGD-O2D-CED
27	5	316	CHL	C5-C6-C7-C8
27	A	818	CHL	O1D-CGD-O2D-CED
27	A	847	CHL	O1D-CGD-O2D-CED
27	A	852	CHL	O1D-CGD-O2D-CED
27	B	815	CHL	O1D-CGD-O2D-CED
27	B	820	CHL	O1D-CGD-O2D-CED
27	B	844	CHL	O1D-CGD-O2D-CED
27	B	846	CHL	O1D-CGD-O2D-CED
27	B	851	CHL	O1D-CGD-O2D-CED
27	F	308	CHL	O1D-CGD-O2D-CED
27	3	312	CHL	O1D-CGD-O2D-CED
27	3	313	CHL	O1D-CGD-O2D-CED
27	7	313	CHL	O1D-CGD-O2D-CED
27	8	312	CHL	O1D-CGD-O2D-CED
27	8	326	CHL	O1D-CGD-O2D-CED
27	b	308	CHL	O1D-CGD-O2D-CED
27	B	846	CHL	CBA-CGA-O2A-C1
27	A	827	CHL	CBD-CGD-O2D-CED
27	B	823	CHL	CBD-CGD-O2D-CED
27	B	833	CHL	CBD-CGD-O2D-CED
27	5	316	CHL	CBD-CGD-O2D-CED
24	4	303	LHG	O10-C23-O8-C6
30	J	101	LMG	O10-C28-O8-C9
30	a	301	LMG	O10-C28-O8-C9
32	5	305	PTY	O30-C30-O4-C1
35	8	306	DGA	OA1-CA1-OG1-CG1
27	5	317	CHL	O1D-CGD-O2D-CED
28	B	809	DGD	O1B-C1B-O2G-C2G
27	A	823	CHL	C3-C5-C6-C7
27	A	826	CHL	C3-C5-C6-C7
27	B	821	CHL	C3-C5-C6-C7
27	B	827	CHL	C3-C5-C6-C7
27	B	829	CHL	C3-C5-C6-C7
27	B	833	CHL	C3-C5-C6-C7
27	B	837	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	a	311	CHL	C3-C5-C6-C7
27	a	313	CHL	C3-C5-C6-C7
27	3	310	CHL	C3-C5-C6-C7
27	3	314	CHL	C3-C5-C6-C7
27	5	318	CHL	C3-C5-C6-C7
27	6	310	CHL	C3-C5-C6-C7
27	7	316	CHL	C3-C5-C6-C7
27	7	317	CHL	C3-C5-C6-C7
24	A	810	LHG	C24-C23-O8-C6
27	8	312	CHL	CBA-CGA-O2A-C1
30	J	101	LMG	C29-C28-O8-C9
30	a	301	LMG	C29-C28-O8-C9
32	5	305	PTY	C31-C30-O4-C1
35	8	306	DGA	CA2-CA1-OG1-CG1
30	7	301	LMG	O6-C5-C6-O5
27	7	320	CHL	C2C-C3C-CAC-CBC
27	4	316	CHL	C2C-C3C-CAC-CBC
27	6	316	CHL	C2C-C3C-CAC-CBC
27	a	316	CHL	C2C-C3C-CAC-CBC
27	A	826	CHL	C4-C3-C5-C6
27	3	317	CHL	C2-C3-C5-C6
27	A	844	CHL	C2A-CAA-CBA-CGA
27	B	846	CHL	C2A-CAA-CBA-CGA
27	a	315	CHL	C2A-CAA-CBA-CGA
27	6	305	CHL	C2A-CAA-CBA-CGA
27	6	318	CHL	C2A-CAA-CBA-CGA
27	b	313	CHL	C2A-CAA-CBA-CGA
24	a	305	LHG	C11-C12-C13-C14
27	A	831	CHL	C3-C5-C6-C7
27	B	823	CHL	C3-C5-C6-C7
27	6	307	CHL	C3-C5-C6-C7
24	4	303	LHG	C24-C23-O8-C6
27	B	851	CHL	CBA-CGA-O2A-C1
27	8	317	CHL	CBA-CGA-O2A-C1
30	8	307	LMG	C29-C28-O8-C9
23	5	306	LMT	C4B-C5B-C6B-O6B
24	4	303	LHG	C11-C10-C9-C8
27	A	831	CHL	O1D-CGD-O2D-CED
27	8	312	CHL	O1A-CGA-O2A-C1
27	8	317	CHL	O1A-CGA-O2A-C1
27	b	316	CHL	C2C-C3C-CAC-CBC
29	a	302	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
29	4	301	LUT	C29-C30-C31-C32
29	4	302	LUT	C13-C14-C15-C35
29	4	302	LUT	C29-C30-C31-C32
29	6	302	LUT	C29-C30-C31-C32
29	7	304	LUT	C9-C10-C11-C12
29	8	303	LUT	C33-C34-C35-C15
33	7	305	XAT	C29-C30-C31-C32
23	5	306	LMT	O5B-C5B-C6B-O6B
23	7	308	LMT	O5B-C5B-C6B-O6B
27	A	818	CHL	CBD-CGD-O2D-CED
27	B	849	CHL	CBD-CGD-O2D-CED
27	6	308	CHL	CBD-CGD-O2D-CED
24	A	811	LHG	O2-C2-C3-O3
27	A	832	CHL	C3-C5-C6-C7
27	3	310	CHL	CBA-CGA-O2A-C1
27	7	319	CHL	CBA-CGA-O2A-C1
27	B	851	CHL	O1A-CGA-O2A-C1
27	3	310	CHL	O1A-CGA-O2A-C1
27	7	319	CHL	O1A-CGA-O2A-C1
30	a	301	LMG	O6-C5-C6-O5
27	8	321	CHL	C2C-C3C-CAC-CBC
24	8	305	LHG	C23-C24-C25-C26
24	a	305	LHG	C9-C10-C11-C12
24	a	305	LHG	C17-C18-C19-C20
24	4	303	LHG	C32-C33-C34-C35
24	5	304	LHG	C10-C11-C12-C13
24	a	305	LHG	C15-C16-C17-C18
23	5	326	LMT	C4'-C5'-C6'-O6'
30	a	301	LMG	C4-C5-C6-O5
30	7	301	LMG	C4-C5-C6-O5
27	A	853	CHL	C3-C5-C6-C7
30	8	307	LMG	O10-C28-O8-C9
23	7	308	LMT	C3'-C4'-O1B-C1B
24	5	304	LHG	C25-C26-C27-C28
27	7	320	CHL	C4C-C3C-CAC-CBC
27	A	832	CHL	C4-C3-C5-C6
27	A	858	CHL	C4-C3-C5-C6
27	B	820	CHL	C4-C3-C5-C6
27	3	315	CHL	C4-C3-C5-C6
27	6	306	CHL	C4-C3-C5-C6
27	7	319	CHL	C4-C3-C5-C6
27	8	319	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	832	CHL	C2-C3-C5-C6
27	A	847	CHL	C2-C3-C5-C6
27	A	858	CHL	C2-C3-C5-C6
27	B	820	CHL	C2-C3-C5-C6
27	3	315	CHL	C2-C3-C5-C6
27	6	306	CHL	C2-C3-C5-C6
27	7	319	CHL	C2-C3-C5-C6
27	8	319	CHL	C2-C3-C5-C6
27	7	321	CHL	CBD-CGD-O2D-CED
27	4	310	CHL	C2A-CAA-CBA-CGA
27	4	320	CHL	C2A-CAA-CBA-CGA
28	B	809	DGD	O6E-C5E-C6E-O5E
23	B	810	LMT	O5'-C1'-O1'-C1
24	a	305	LHG	C13-C14-C15-C16
24	a	305	LHG	C32-C33-C34-C35
27	A	831	CHL	C2C-C3C-CAC-CBC
27	4	316	CHL	C4C-C3C-CAC-CBC
27	6	316	CHL	C4C-C3C-CAC-CBC
28	B	809	DGD	C4E-C5E-C6E-O5E
27	7	320	CHL	O1D-CGD-O2D-CED
23	7	308	LMT	C4B-C5B-C6B-O6B
27	a	311	CHL	O1A-CGA-O2A-C1
27	5	323	CHL	C3-C5-C6-C7
24	B	808	LHG	C24-C23-O8-C6
27	A	831	CHL	CBA-CGA-O2A-C1
27	A	836	CHL	CBA-CGA-O2A-C1
27	A	847	CHL	CBA-CGA-O2A-C1
27	B	820	CHL	CBA-CGA-O2A-C1
27	a	311	CHL	CBA-CGA-O2A-C1
27	5	313	CHL	CBA-CGA-O2A-C1
27	5	315	CHL	CBA-CGA-O2A-C1
27	b	315	CHL	CBA-CGA-O2A-C1
24	b	302	LHG	C28-C29-C30-C31
29	F	303	LUT	C29-C30-C31-C32
29	3	304	LUT	C29-C30-C31-C32
29	6	303	LUT	C33-C34-C35-C15
24	4	303	LHG	C10-C11-C12-C13
24	7	302	LHG	C28-C29-C30-C31
27	a	316	CHL	C4C-C3C-CAC-CBC
27	5	317	CHL	C2C-C3C-CAC-CBC
27	6	318	CHL	C2C-C3C-CAC-CBC
27	5	319	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	4	303	LHG	O2-C2-C3-O3
24	5	324	LHG	O2-C2-C3-O3
24	5	324	LHG	O7-C5-C6-O8
30	7	301	LMG	O7-C8-C9-O8
23	5	326	LMT	O5'-C5'-C6'-O6'
27	A	826	CHL	C2-C3-C5-C6
27	A	843	CHL	C14-C13-C15-C16
27	B	817	CHL	C6-C7-C8-C9
27	6	308	CHL	C14-C13-C15-C16
27	7	319	CHL	C6-C7-C8-C9
27	8	321	CHL	C14-C13-C15-C16
22	B	805	BCR	C7-C8-C9-C34
22	K	202	BCR	C37-C22-C23-C24
22	3	301	BCR	C37-C22-C23-C24
22	5	301	BCR	C37-C22-C23-C24
22	6	301	BCR	C36-C18-C19-C20
22	L	301	BCR	C7-C8-C9-C34
22	L	301	BCR	C37-C22-C23-C24
29	F	303	LUT	C31-C32-C33-C40
29	J	103	LUT	C7-C8-C9-C19
29	a	304	LUT	C27-C28-C29-C39
29	a	304	LUT	C31-C32-C33-C40
29	3	305	LUT	C7-C8-C9-C19
29	5	303	LUT	C7-C8-C9-C19
29	5	303	LUT	C11-C12-C13-C20
29	6	302	LUT	C7-C8-C9-C19
29	8	303	LUT	C7-C8-C9-C19
29	8	304	LUT	C7-C8-C9-C19
29	8	304	LUT	C11-C12-C13-C20
29	8	304	LUT	C27-C28-C29-C39
29	b	303	LUT	C27-C28-C29-C39
33	7	305	XAT	C11-C12-C13-C20
22	K	202	BCR	C21-C22-C23-C24
22	5	301	BCR	C21-C22-C23-C24
22	6	301	BCR	C17-C18-C19-C20
22	L	301	BCR	C7-C8-C9-C10
22	L	301	BCR	C21-C22-C23-C24
29	J	103	LUT	C11-C12-C13-C14
29	a	302	LUT	C27-C28-C29-C30
29	3	304	LUT	C27-C28-C29-C30
29	3	304	LUT	C31-C32-C33-C34
29	3	305	LUT	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	4	301	LUT	C31-C32-C33-C34
29	6	303	LUT	C31-C32-C33-C34
29	7	304	LUT	C11-C12-C13-C14
29	7	304	LUT	C27-C28-C29-C30
29	7	304	LUT	C31-C32-C33-C34
29	8	303	LUT	C11-C12-C13-C14
29	8	303	LUT	C27-C28-C29-C30
29	8	303	LUT	C31-C32-C33-C34
29	8	304	LUT	C31-C32-C33-C34
29	b	301	LUT	C31-C32-C33-C34
29	b	303	LUT	C27-C28-C29-C30
32	5	305	PTY	C11-C8-O7-C6
24	A	810	LHG	C23-C24-C25-C26
27	A	831	CHL	O1A-CGA-O2A-C1
27	A	836	CHL	O1A-CGA-O2A-C1
27	5	315	CHL	O1A-CGA-O2A-C1
20	A	801	PQN	C25-C26-C27-C28
27	A	838	CHL	C10-C11-C12-C13
27	B	815	CHL	C5-C6-C7-C8
27	5	316	CHL	C8-C10-C11-C12
27	8	315	CHL	C13-C15-C16-C17
27	8	316	CHL	C8-C10-C11-C12
27	L	303	CHL	C10-C11-C12-C13
23	A	809	LMT	O5'-C5'-C6'-O6'
27	b	316	CHL	C4C-C3C-CAC-CBC
27	3	317	CHL	C3-C5-C6-C7
27	B	840	CHL	C8-C10-C11-C12
27	3	308	CHL	C10-C11-C12-C13
27	6	308	CHL	C10-C11-C12-C13
24	5	304	LHG	C7-C8-C9-C10
24	5	304	LHG	C23-C24-C25-C26
30	J	101	LMG	C10-C11-C12-C13
27	A	825	CHL	C5-C6-C7-C8
27	A	843	CHL	C8-C10-C11-C12
27	A	843	CHL	C13-C15-C16-C17
27	A	843	CHL	C15-C16-C17-C18
27	B	832	CHL	C15-C16-C17-C18
27	B	846	CHL	C5-C6-C7-C8
27	3	311	CHL	C5-C6-C7-C8
27	L	303	CHL	C5-C6-C7-C8
27	5	313	CHL	O1A-CGA-O2A-C1
24	B	808	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	5	324	LHG	C23-C24-C25-C26
24	7	306	LHG	C7-C8-C9-C10
28	B	809	DGD	C1B-C2B-C3B-C4B
30	8	307	LMG	C28-C29-C30-C31
34	8	301	SQD	C7-C8-C9-C10
23	A	809	LMT	C4'-C5'-C6'-O6'
27	a	313	CHL	C5-C6-C7-C8
27	3	314	CHL	C8-C10-C11-C12
27	7	313	CHL	C8-C10-C11-C12
27	7	322	CHL	C10-C11-C12-C13
27	A	832	CHL	CBA-CGA-O2A-C1
27	B	821	CHL	CBA-CGA-O2A-C1
27	5	316	CHL	O1D-CGD-O2D-CED
23	A	808	LMT	O5B-C5B-C6B-O6B
27	8	317	CHL	C15-C16-C17-C18
24	a	305	LHG	C30-C31-C32-C33
27	8	321	CHL	C4C-C3C-CAC-CBC
27	A	833	CHL	C8-C10-C11-C12
27	B	842	CHL	C8-C10-C11-C12
27	5	316	CHL	C13-C15-C16-C17
27	A	843	CHL	C11-C10-C8-C7
27	B	835	CHL	C6-C7-C8-C10
27	a	310	CHL	C11-C10-C8-C7
27	5	309	CHL	C6-C7-C8-C10
27	8	314	CHL	C11-C12-C13-C15
27	A	821	CHL	C3-C5-C6-C7
27	B	817	CHL	C3-C5-C6-C7
27	8	316	CHL	C3-C5-C6-C7
27	A	847	CHL	O1A-CGA-O2A-C1
27	B	820	CHL	O1A-CGA-O2A-C1
29	J	103	LUT	C9-C10-C11-C12
29	4	302	LUT	C9-C10-C11-C12
29	5	303	LUT	C29-C30-C31-C32
29	6	303	LUT	C13-C14-C15-C35
29	7	304	LUT	C29-C30-C31-C32
29	8	303	LUT	C29-C30-C31-C32
29	8	304	LUT	C29-C30-C31-C32
29	b	303	LUT	C29-C30-C31-C32
29	b	303	LUT	C33-C34-C35-C15
32	5	305	PTY	C8-C11-C12-C13
27	A	838	CHL	C2A-CAA-CBA-CGA
27	8	317	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	B	833	CHL	C5-C6-C7-C8
27	3	308	CHL	C13-C15-C16-C17
27	8	312	CHL	C15-C16-C17-C18
24	5	304	LHG	C12-C13-C14-C15
27	b	315	CHL	O1A-CGA-O2A-C1
23	F	302	LMT	O5'-C1'-O1'-C1
27	A	828	CHL	C15-C16-C17-C18
27	3	308	CHL	C8-C10-C11-C12
27	3	312	CHL	C5-C6-C7-C8
27	B	848	CHL	C15-C16-C17-C18
27	5	315	CHL	C10-C11-C12-C13
27	A	832	CHL	O1A-CGA-O2A-C1
24	5	304	LHG	C8-C7-O7-C5
30	J	104	LMG	C11-C10-O7-C8
27	A	825	CHL	C8-C10-C11-C12
27	5	316	CHL	C10-C11-C12-C13
24	A	811	LHG	C4-O6-P-O3
24	5	304	LHG	C3-O3-P-O6
24	5	324	LHG	C3-O3-P-O6
24	7	302	LHG	C3-O3-P-O6
24	b	302	LHG	C4-O6-P-O3
32	5	305	PTY	C3-O11-P1-O14
28	7	307	DGD	C1B-C2B-C3B-C4B
27	B	811	CHL	CBA-CGA-O2A-C1
27	a	313	CHL	CBA-CGA-O2A-C1
27	B	821	CHL	O1A-CGA-O2A-C1
24	A	811	LHG	C1-C2-C3-O3
24	7	302	LHG	C1-C2-C3-O3
24	5	304	LHG	O9-C7-O7-C5
32	5	305	PTY	O10-C8-O7-C6
27	B	822	CHL	C10-C11-C12-C13
27	b	315	CHL	C13-C15-C16-C17
27	A	816	CHL	C2A-CAA-CBA-CGA
27	A	825	CHL	C2A-CAA-CBA-CGA
27	A	826	CHL	C2A-CAA-CBA-CGA
27	A	859	CHL	C2A-CAA-CBA-CGA
27	3	321	CHL	C2A-CAA-CBA-CGA
27	4	311	CHL	C2A-CAA-CBA-CGA
27	6	317	CHL	C2A-CAA-CBA-CGA
27	8	312	CHL	C3-C5-C6-C7
27	3	315	CHL	CBA-CGA-O2A-C1
27	7	317	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	7	302	LHG	C32-C33-C34-C35
29	J	103	LUT	C33-C34-C35-C15
29	3	305	LUT	C29-C30-C31-C32
29	5	302	LUT	C33-C34-C35-C15
29	5	303	LUT	C33-C34-C35-C15
29	6	303	LUT	C29-C30-C31-C32
29	b	301	LUT	C29-C30-C31-C32
23	A	809	LMT	C2-C3-C4-C5
24	8	305	LHG	C27-C28-C29-C30
30	J	101	LMG	C11-C12-C13-C14
22	A	803	BCR	C16-C17-C18-C36
22	B	803	BCR	C20-C21-C22-C37
22	B	806	BCR	C20-C21-C22-C37
22	B	807	BCR	C20-C21-C22-C37
22	F	301	BCR	C35-C13-C14-C15
22	3	301	BCR	C20-C21-C22-C37
22	3	302	BCR	C20-C21-C22-C37
22	3	303	BCR	C20-C21-C22-C37
22	6	301	BCR	C35-C13-C14-C15
22	8	302	BCR	C20-C21-C22-C37
29	a	302	LUT	C39-C29-C30-C31
29	3	304	LUT	C39-C29-C30-C31
29	5	302	LUT	C39-C29-C30-C31
29	6	303	LUT	C20-C13-C14-C15
29	8	303	LUT	C39-C29-C30-C31
29	8	304	LUT	C11-C10-C9-C19
29	b	301	LUT	C20-C13-C14-C15
29	b	303	LUT	C20-C13-C14-C15
29	b	303	LUT	C40-C33-C34-C35
27	8	321	CHL	C3-C5-C6-C7
24	A	811	LHG	C28-C29-C30-C31
24	A	812	LHG	C12-C13-C14-C15
24	a	305	LHG	C24-C25-C26-C27
24	A	810	LHG	C7-C8-C9-C10
28	7	307	DGD	C9A-CAA-CBA-CCA
30	7	301	LMG	C11-C12-C13-C14
30	7	301	LMG	C32-C33-C34-C35
24	7	302	LHG	C29-C30-C31-C32
28	7	307	DGD	C5A-C6A-C7A-C8A
28	7	307	DGD	C5B-C6B-C7B-C8B
24	A	810	LHG	O2-C2-C3-O3
24	7	306	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	b	302	LHG	O2-C2-C3-O3
23	B	810	LMT	C6-C7-C8-C9
23	F	302	LMT	O1'-C1-C2-C3
23	5	326	LMT	C4-C5-C6-C7
24	a	305	LHG	C28-C29-C30-C31
24	7	306	LHG	C28-C29-C30-C31
27	A	831	CHL	C4C-C3C-CAC-CBC
27	A	855	CHL	O1D-CGD-O2D-CED
22	A	806	BCR	C20-C21-C22-C23
22	A	807	BCR	C11-C10-C9-C8
22	B	804	BCR	C11-C10-C9-C8
22	I	801	BCR	C16-C17-C18-C19
22	I	801	BCR	C20-C21-C22-C23
22	M	102	BCR	C11-C10-C9-C8
22	5	301	BCR	C20-C21-C22-C23
22	6	301	BCR	C12-C13-C14-C15
22	8	302	BCR	C20-C21-C22-C23
22	L	302	BCR	C11-C10-C9-C8
23	F	302	LMT	C2'-C1'-O1'-C1
29	F	303	LUT	C12-C13-C14-C15
29	F	303	LUT	C28-C29-C30-C31
29	J	103	LUT	C11-C10-C9-C8
29	a	302	LUT	C28-C29-C30-C31
29	3	304	LUT	C12-C13-C14-C15
29	3	305	LUT	C28-C29-C30-C31
29	4	301	LUT	C12-C13-C14-C15
29	4	301	LUT	C28-C29-C30-C31
29	6	303	LUT	C12-C13-C14-C15
29	6	303	LUT	C28-C29-C30-C31
29	7	304	LUT	C11-C10-C9-C8
29	7	304	LUT	C28-C29-C30-C31
29	8	303	LUT	C12-C13-C14-C15
29	b	303	LUT	C12-C13-C14-C15
29	b	303	LUT	C32-C33-C34-C35
27	A	839	CHL	CBA-CGA-O2A-C1
27	4	308	CHL	CBA-CGA-O2A-C1
30	J	101	LMG	C32-C33-C34-C35
32	5	305	PTY	C31-C32-C33-C34
27	5	316	CHL	C16-C17-C18-C20
27	6	307	CHL	C16-C17-C18-C20
27	7	316	CHL	C6-C7-C8-C9
27	A	820	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	A	840	CHL	C4-C3-C5-C6
27	a	313	CHL	C4-C3-C5-C6
24	4	303	LHG	C11-C12-C13-C14
24	7	302	LHG	C27-C28-C29-C30
27	A	816	CHL	C11-C10-C8-C9
27	A	843	CHL	C11-C12-C13-C14
27	a	310	CHL	C6-C7-C8-C9
27	5	318	CHL	C11-C10-C8-C9
27	6	307	CHL	C6-C7-C8-C9
30	8	307	LMG	C10-C11-C12-C13
24	7	306	LHG	C29-C30-C31-C32
28	7	307	DGD	C4A-C5A-C6A-C7A
30	J	101	LMG	C18-C19-C20-C21
27	B	814	CHL	C8-C10-C11-C12
27	A	823	CHL	C2A-CAA-CBA-CGA
27	B	832	CHL	C2A-CAA-CBA-CGA
27	B	851	CHL	C2A-CAA-CBA-CGA
29	F	303	LUT	C11-C12-C13-C20
29	J	103	LUT	C31-C32-C33-C40
29	4	302	LUT	C7-C8-C9-C19
29	4	302	LUT	C27-C28-C29-C39
29	6	303	LUT	C7-C8-C9-C19
29	b	301	LUT	C27-C28-C29-C39
24	b	302	LHG	C27-C28-C29-C30
30	J	101	LMG	C33-C34-C35-C36
24	a	305	LHG	O1-C1-C2-C3
24	5	324	LHG	O1-C1-C2-C3
24	7	302	LHG	O1-C1-C2-C3
24	8	305	LHG	O1-C1-C2-C3
22	F	301	BCR	C21-C22-C23-C24
22	M	102	BCR	C7-C8-C9-C10
22	3	302	BCR	C7-C8-C9-C10
29	J	103	LUT	C27-C28-C29-C30
29	a	302	LUT	C31-C32-C33-C34
29	4	301	LUT	C11-C12-C13-C14
29	4	302	LUT	C7-C8-C9-C10
29	4	302	LUT	C11-C12-C13-C14
29	5	302	LUT	C27-C28-C29-C30
29	5	303	LUT	C31-C32-C33-C34
27	B	813	CHL	C3-C5-C6-C7
27	a	310	CHL	C3-C5-C6-C7
27	L	303	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	A	823	CHL	C5-C6-C7-C8
27	A	839	CHL	C8-C10-C11-C12
23	5	326	LMT	C6-C7-C8-C9
24	7	306	LHG	C32-C33-C34-C35
28	B	809	DGD	C2B-C3B-C4B-C5B
28	7	307	DGD	CAB-CBB-CCB-CDB
23	7	308	LMT	O1'-C1-C2-C3
24	A	810	LHG	C27-C28-C29-C30
24	A	812	LHG	C16-C17-C18-C19
24	4	303	LHG	C9-C10-C11-C12
27	7	319	CHL	C5-C6-C7-C8
23	B	810	LMT	O1'-C1-C2-C3
24	A	811	LHG	C32-C33-C34-C35
24	4	303	LHG	C30-C31-C32-C33
24	4	303	LHG	C34-C35-C36-C37
28	B	809	DGD	C7A-C8A-C9A-CAA
30	J	101	LMG	C30-C31-C32-C33
27	8	318	CHL	CBA-CGA-O2A-C1
27	5	313	CHL	CBD-CGD-O2D-CED
24	5	304	LHG	C26-C27-C28-C29
24	7	306	LHG	C12-C13-C14-C15
24	7	306	LHG	C13-C14-C15-C16
28	B	809	DGD	C7B-C8B-C9B-CAB
30	J	101	LMG	C35-C36-C37-C38
30	a	301	LMG	C33-C34-C35-C36
24	b	302	LHG	C23-C24-C25-C26
24	a	305	LHG	C14-C15-C16-C17
24	7	302	LHG	C26-C27-C28-C29
27	3	313	CHL	CBA-CGA-O2A-C1
24	A	811	LHG	C27-C28-C29-C30
24	7	302	LHG	C17-C18-C19-C20
24	7	302	LHG	C25-C26-C27-C28
27	A	821	CHL	C3A-C2A-CAA-CBA
27	A	826	CHL	C3A-C2A-CAA-CBA
27	A	846	CHL	C3A-C2A-CAA-CBA
27	A	848	CHL	C3A-C2A-CAA-CBA
27	a	308	CHL	C3A-C2A-CAA-CBA
27	3	310	CHL	C3A-C2A-CAA-CBA
27	4	313	CHL	C3A-C2A-CAA-CBA
27	6	306	CHL	C3A-C2A-CAA-CBA
27	7	324	CHL	C3A-C2A-CAA-CBA
27	b	304	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	b	306	CHL	C3A-C2A-CAA-CBA
22	6	301	BCR	C19-C20-C21-C22
23	5	306	LMT	C2-C1-O1'-C1'
27	B	811	CHL	O1A-CGA-O2A-C1
28	B	809	DGD	C9A-CAA-CBA-CCA
28	7	307	DGD	C3A-C4A-C5A-C6A
28	7	307	DGD	C7B-C8B-C9B-CAB
27	6	316	CHL	CBD-CGD-O2D-CED
27	A	858	CHL	C3-C5-C6-C7
27	B	839	CHL	C3-C5-C6-C7
24	A	811	LHG	C23-C24-C25-C26
24	a	305	LHG	C10-C11-C12-C13
28	7	307	DGD	C3B-C4B-C5B-C6B
27	a	313	CHL	O1A-CGA-O2A-C1
27	B	812	CHL	C13-C15-C16-C17
27	A	834	CHL	C4-C3-C5-C6
27	4	306	CHL	C4-C3-C5-C6
27	L	303	CHL	C4-C3-C5-C6
27	B	840	CHL	C2-C3-C5-C6
27	a	313	CHL	C2-C3-C5-C6
27	4	306	CHL	C2-C3-C5-C6
27	L	303	CHL	C2-C3-C5-C6
24	A	812	LHG	C8-C7-O7-C5
30	a	301	LMG	C11-C10-O7-C8
30	7	301	LMG	C31-C32-C33-C34
27	4	312	CHL	C2A-CAA-CBA-CGA
24	A	810	LHG	O1-C1-C2-O2
24	A	811	LHG	O1-C1-C2-O2
24	b	302	LHG	O1-C1-C2-O2
23	7	308	LMT	C6-C7-C8-C9
27	5	316	CHL	C16-C17-C18-C19
27	L	303	CHL	C11-C12-C13-C14
23	B	810	LMT	C2-C3-C4-C5
27	B	820	CHL	C3-C5-C6-C7
27	3	312	CHL	C3-C5-C6-C7
27	5	313	CHL	C3-C5-C6-C7
24	7	306	LHG	C11-C10-C9-C8
27	B	822	CHL	C2C-C3C-CAC-CBC
27	5	319	CHL	C4C-C3C-CAC-CBC
27	3	315	CHL	O1A-CGA-O2A-C1
27	7	317	CHL	O1A-CGA-O2A-C1
24	A	810	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	b	302	LHG	C1-C2-C3-O3
24	8	305	LHG	C28-C29-C30-C31
27	5	317	CHL	C4C-C3C-CAC-CBC
27	6	318	CHL	C4C-C3C-CAC-CBC
28	B	809	DGD	C5A-C6A-C7A-C8A
30	J	101	LMG	C22-C23-C24-C25
27	B	846	CHL	C2-C1-O2A-CGA
27	3	310	CHL	C2-C1-O2A-CGA
30	J	101	LMG	C19-C20-C21-C22
27	A	858	CHL	C8-C10-C11-C12
27	b	315	CHL	C8-C10-C11-C12
27	A	839	CHL	O1A-CGA-O2A-C1
24	a	305	LHG	C19-C20-C21-C22
24	4	303	LHG	C12-C13-C14-C15
27	6	307	CHL	C16-C17-C18-C19
22	A	805	BCR	C5-C6-C7-C8
22	A	806	BCR	C5-C6-C7-C8
22	A	806	BCR	C23-C24-C25-C26
22	B	802	BCR	C5-C6-C7-C8
22	B	802	BCR	C23-C24-C25-C26
22	B	802	BCR	C23-C24-C25-C30
22	B	803	BCR	C1-C6-C7-C8
22	B	803	BCR	C5-C6-C7-C8
22	B	804	BCR	C5-C6-C7-C8
22	B	806	BCR	C23-C24-C25-C30
22	B	807	BCR	C5-C6-C7-C8
22	I	801	BCR	C1-C6-C7-C8
22	I	801	BCR	C5-C6-C7-C8
22	J	102	BCR	C23-C24-C25-C26
22	K	202	BCR	C1-C6-C7-C8
22	K	202	BCR	C5-C6-C7-C8
22	K	202	BCR	C23-C24-C25-C30
22	K	203	BCR	C23-C24-C25-C26
22	M	102	BCR	C5-C6-C7-C8
22	M	102	BCR	C23-C24-C25-C26
22	3	301	BCR	C23-C24-C25-C26
22	3	302	BCR	C5-C6-C7-C8
22	3	302	BCR	C23-C24-C25-C26
22	3	303	BCR	C23-C24-C25-C26
22	5	301	BCR	C23-C24-C25-C26
22	6	301	BCR	C1-C6-C7-C8
22	6	301	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	6	301	BCR	C23-C24-C25-C26
22	7	303	BCR	C23-C24-C25-C26
22	7	303	BCR	C23-C24-C25-C30
22	8	302	BCR	C23-C24-C25-C30
22	L	301	BCR	C5-C6-C7-C8
22	L	301	BCR	C23-C24-C25-C26
22	L	301	BCR	C23-C24-C25-C30
22	L	302	BCR	C1-C6-C7-C8
22	L	302	BCR	C5-C6-C7-C8
27	a	317	CHL	C3-C5-C6-C7
29	4	301	LUT	C5-C6-C7-C8
29	4	302	LUT	C1-C6-C7-C8
29	6	303	LUT	C5-C6-C7-C8
29	7	304	LUT	C1-C6-C7-C8
29	8	304	LUT	C5-C6-C7-C8
29	b	303	LUT	C5-C6-C7-C8
31	a	303	AXT	C25-C26-C27-C28
28	7	307	DGD	CCB-CDB-CEB-CFB
27	B	829	CHL	C5-C6-C7-C8
24	4	303	LHG	C8-C7-O7-C5
23	A	808	LMT	C4-C5-C6-C7
24	A	812	LHG	C28-C29-C30-C31
24	A	812	LHG	C29-C30-C31-C32
24	8	305	LHG	C32-C33-C34-C35
30	J	101	LMG	C31-C32-C33-C34
27	3	313	CHL	O1A-CGA-O2A-C1
27	4	308	CHL	O1A-CGA-O2A-C1
23	A	809	LMT	C3-C4-C5-C6
27	A	829	CHL	C4-C3-C5-C6
27	A	839	CHL	C4-C3-C5-C6
27	B	825	CHL	C4-C3-C5-C6
27	B	840	CHL	C4-C3-C5-C6
27	A	816	CHL	C11-C10-C8-C7
27	A	834	CHL	C2-C3-C5-C6
27	A	836	CHL	C2-C3-C5-C6
27	A	839	CHL	C2-C3-C5-C6
27	A	840	CHL	C2-C3-C5-C6
27	A	840	CHL	C12-C13-C15-C16
27	A	843	CHL	C11-C12-C13-C15
27	A	855	CHL	C11-C10-C8-C7
27	B	825	CHL	C2-C3-C5-C6
27	a	310	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
27	5	309	CHL	C11-C10-C8-C7
27	5	318	CHL	C11-C10-C8-C7
27	6	307	CHL	C6-C7-C8-C10
27	8	321	CHL	C12-C13-C15-C16
23	7	308	LMT	C5'-C4'-O1B-C1B
24	7	306	LHG	C24-C25-C26-C27
24	8	305	LHG	C15-C16-C17-C18
27	A	831	CHL	C5-C6-C7-C8
29	b	301	LUT	C13-C14-C15-C35
27	7	316	CHL	C6-C7-C8-C10
24	4	303	LHG	O9-C7-O7-C5
30	7	301	LMG	C28-C29-C30-C31
27	3	319	CHL	CBA-CGA-O2A-C1
28	B	809	DGD	C3B-C4B-C5B-C6B
27	B	839	CHL	C2A-CAA-CBA-CGA
27	6	306	CHL	C2A-CAA-CBA-CGA
27	A	855	CHL	C15-C16-C17-C18
27	B	838	CHL	C8-C10-C11-C12
28	7	307	DGD	CBB-CCB-CDB-CEB
23	B	810	LMT	O5'-C5'-C6'-O6'
27	6	308	CHL	O1D-CGD-O2D-CED
23	5	306	LMT	C2-C3-C4-C5
24	a	305	LHG	C27-C28-C29-C30
27	5	316	CHL	C2C-C3C-CAC-CBC
32	5	305	PTY	C32-C33-C34-C35
23	F	302	LMT	O5B-C5B-C6B-O6B
27	B	819	CHL	CBA-CGA-O2A-C1
24	A	811	LHG	C7-C8-C9-C10
24	b	302	LHG	C8-C7-O7-C5
27	B	841	CHL	C3-C5-C6-C7
30	7	301	LMG	C2-C1-O1-C7
24	a	305	LHG	C29-C30-C31-C32
24	5	304	LHG	C9-C10-C11-C12
27	A	836	CHL	C4-C3-C5-C6
27	b	315	CHL	C4-C3-C5-C6
27	A	820	CHL	C2-C3-C5-C6
27	A	829	CHL	C2-C3-C5-C6
24	a	305	LHG	C34-C35-C36-C37
27	A	828	CHL	C11-C10-C8-C9
27	A	840	CHL	C14-C13-C15-C16
27	A	843	CHL	C11-C10-C8-C9
27	A	855	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
27	B	849	CHL	C14-C13-C15-C16
27	a	310	CHL	C11-C10-C8-C9
27	5	309	CHL	C11-C10-C8-C9
27	5	316	CHL	C11-C12-C13-C14
27	7	313	CHL	C6-C7-C8-C9
27	8	314	CHL	C11-C12-C13-C14
27	B	822	CHL	C3-C5-C6-C7
27	b	315	CHL	C2A-CAA-CBA-CGA
24	b	302	LHG	C9-C10-C11-C12
22	B	804	BCR	C7-C8-C9-C10
22	F	301	BCR	C7-C8-C9-C10
22	M	102	BCR	C17-C18-C19-C20
27	3	319	CHL	O1A-CGA-O2A-C1
27	A	846	CHL	C1A-C2A-CAA-CBA
27	A	850	CHL	C1A-C2A-CAA-CBA
27	B	836	CHL	C1A-C2A-CAA-CBA
27	a	307	CHL	C1A-C2A-CAA-CBA
27	a	308	CHL	C1A-C2A-CAA-CBA
27	a	310	CHL	C1A-C2A-CAA-CBA
27	3	308	CHL	C1A-C2A-CAA-CBA
27	3	310	CHL	C1A-C2A-CAA-CBA
27	3	315	CHL	C1A-C2A-CAA-CBA
27	4	304	CHL	C1A-C2A-CAA-CBA
27	4	307	CHL	C1A-C2A-CAA-CBA
27	5	307	CHL	C1A-C2A-CAA-CBA
27	5	313	CHL	C1A-C2A-CAA-CBA
27	7	311	CHL	C1A-C2A-CAA-CBA
27	7	319	CHL	C1A-C2A-CAA-CBA
27	8	315	CHL	C1A-C2A-CAA-CBA
27	8	318	CHL	C1A-C2A-CAA-CBA
27	8	319	CHL	C1A-C2A-CAA-CBA
27	b	304	CHL	C1A-C2A-CAA-CBA
27	b	313	CHL	C1A-C2A-CAA-CBA
27	b	315	CHL	C1A-C2A-CAA-CBA
24	A	812	LHG	O9-C7-O7-C5
24	A	812	LHG	C33-C34-C35-C36
24	4	303	LHG	C28-C29-C30-C31
29	J	103	LUT	C29-C30-C31-C32
29	3	305	LUT	C33-C34-C35-C15
24	A	811	LHG	C9-C10-C11-C12
27	a	318	CHL	C2C-C3C-CAC-CBC
27	A	829	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	8	316	CHL	C5-C6-C7-C8
27	5	316	CHL	CBA-CGA-O2A-C1
24	4	303	LHG	O6-C4-C5-C6
32	5	305	PTY	O14-C5-C6-C1
23	B	810	LMT	C1-C2-C3-C4
27	a	317	CHL	C8-C10-C11-C12
23	5	306	LMT	C3-C4-C5-C6
24	a	305	LHG	C18-C19-C20-C21
27	A	850	CHL	CBA-CGA-O2A-C1
27	B	824	CHL	CBA-CGA-O2A-C1
24	b	302	LHG	O9-C7-O7-C5
24	A	812	LHG	C17-C18-C19-C20
24	A	811	LHG	C4-C5-C6-O8
24	7	302	LHG	C4-C5-C6-O8
28	B	809	DGD	C1G-C2G-C3G-O3G
30	J	101	LMG	C23-C24-C25-C26
30	7	301	LMG	O1-C7-C8-C9
27	A	856	CHL	C8-C10-C11-C12
24	8	305	LHG	C11-C12-C13-C14
30	a	301	LMG	C8-C7-O1-C1
24	7	302	LHG	C33-C34-C35-C36
30	7	301	LMG	C30-C31-C32-C33
27	B	819	CHL	O1A-CGA-O2A-C1
27	b	308	CHL	CBA-CGA-O2A-C1
30	J	101	LMG	C36-C37-C38-C39
24	7	302	LHG	O1-C1-C2-O2
30	a	301	LMG	C35-C36-C37-C38
27	7	313	CHL	C5-C6-C7-C8
28	B	809	DGD	C4A-C5A-C6A-C7A
22	B	806	BCR	C16-C17-C18-C36
22	K	202	BCR	C20-C21-C22-C37
27	A	824	CHL	C4-C3-C5-C6
27	A	849	CHL	C4-C3-C5-C6
27	A	855	CHL	C4-C3-C5-C6
27	B	829	CHL	C4-C3-C5-C6
27	a	315	CHL	C4-C3-C5-C6
27	4	308	CHL	C4-C3-C5-C6
27	5	316	CHL	C4-C3-C5-C6
27	5	318	CHL	C4-C3-C5-C6
24	7	302	LHG	C9-C10-C11-C12
28	7	307	DGD	CFB-CGB-CHB-CIB
30	J	101	LMG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	a	301	LMG	C18-C19-C20-C21
34	8	301	SQD	C25-C26-C27-C28
27	A	855	CHL	C2-C3-C5-C6
27	4	308	CHL	C2-C3-C5-C6
34	8	301	SQD	C23-C24-C25-C26
27	A	853	CHL	C13-C15-C16-C17
27	B	840	CHL	C10-C11-C12-C13
24	A	811	LHG	C24-C25-C26-C27
28	B	809	DGD	C9B-CAB-CBB-CCB
24	A	811	LHG	C24-C23-O8-C6
27	A	853	CHL	CBA-CGA-O2A-C1
27	4	320	CHL	CBA-CGA-O2A-C1
27	8	325	CHL	CBA-CGA-O2A-C1
34	8	301	SQD	C24-C23-O48-C46
27	B	827	CHL	C11-C12-C13-C15
24	4	303	LHG	C7-C8-C9-C10
24	B	808	LHG	O10-C23-O8-C6
27	B	824	CHL	O1A-CGA-O2A-C1
27	5	316	CHL	O1A-CGA-O2A-C1
22	A	807	BCR	C20-C21-C22-C23
22	J	102	BCR	C20-C21-C22-C23
27	A	827	CHL	C6-C7-C8-C9
30	J	101	LMG	O7-C8-C9-O8
30	8	307	LMG	C32-C33-C34-C35
27	A	850	CHL	O1A-CGA-O2A-C1
27	5	313	CHL	O1D-CGD-O2D-CED
27	B	816	CHL	C4-C3-C5-C6
27	B	833	CHL	C4-C3-C5-C6
27	B	838	CHL	C4-C3-C5-C6
27	6	310	CHL	C4-C3-C5-C6
27	7	322	CHL	C4-C3-C5-C6
27	A	824	CHL	C2-C3-C5-C6
27	A	828	CHL	C11-C10-C8-C7
27	A	849	CHL	C2-C3-C5-C6
27	B	814	CHL	C11-C12-C13-C15
27	B	816	CHL	C2-C3-C5-C6
27	B	829	CHL	C2-C3-C5-C6
27	B	833	CHL	C2-C3-C5-C6
27	B	838	CHL	C2-C3-C5-C6
27	B	849	CHL	C12-C13-C15-C16
27	a	315	CHL	C2-C3-C5-C6
27	5	316	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	5	316	CHL	C6-C7-C8-C10
27	5	316	CHL	C11-C12-C13-C15
27	5	318	CHL	C2-C3-C5-C6
27	6	308	CHL	C11-C12-C13-C15
27	7	313	CHL	C6-C7-C8-C10
27	7	317	CHL	C11-C10-C8-C7
27	7	319	CHL	C11-C10-C8-C7
27	7	322	CHL	C2-C3-C5-C6
27	8	312	CHL	C11-C10-C8-C7
27	8	316	CHL	C11-C12-C13-C15
27	A	850	CHL	C6-C7-C8-C9
27	B	814	CHL	C11-C12-C13-C14
27	B	835	CHL	C6-C7-C8-C9
27	B	844	CHL	C11-C12-C13-C14
27	B	844	CHL	C14-C13-C15-C16
27	5	316	CHL	C6-C7-C8-C9
27	6	308	CHL	C11-C12-C13-C14
27	7	317	CHL	C11-C10-C8-C9
27	7	319	CHL	C11-C10-C8-C9
27	8	312	CHL	C11-C10-C8-C9
27	B	813	CHL	C5-C6-C7-C8
27	6	307	CHL	C13-C15-C16-C17
27	A	835	CHL	C2A-CAA-CBA-CGA
29	J	103	LUT	C7-C8-C9-C10
29	J	103	LUT	C31-C32-C33-C34
33	7	305	XAT	C11-C12-C13-C14
24	4	303	LHG	C35-C36-C37-C38
24	5	324	LHG	C24-C25-C26-C27
27	B	827	CHL	C10-C11-C12-C13
24	A	810	LHG	C10-C11-C12-C13
27	A	821	CHL	CBA-CGA-O2A-C1
27	3	314	CHL	CBA-CGA-O2A-C1
27	5	323	CHL	CBA-CGA-O2A-C1
27	B	848	CHL	C5-C6-C7-C8
23	5	326	LMT	O1'-C1-C2-C3
27	B	822	CHL	C4C-C3C-CAC-CBC
30	7	301	LMG	C12-C13-C14-C15
23	A	809	LMT	C4B-C5B-C6B-O6B
24	7	302	LHG	O6-C4-C5-C6
27	A	855	CHL	C8-C10-C11-C12
27	B	821	CHL	C4-C3-C5-C6
27	3	314	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	6	310	CHL	C2-C3-C5-C6
30	J	101	LMG	C28-C29-C30-C31
27	7	316	CHL	C5-C6-C7-C8
27	A	853	CHL	O1A-CGA-O2A-C1
24	A	810	LHG	C11-C10-C9-C8
23	A	808	LMT	C7-C8-C9-C10
27	A	825	CHL	CBA-CGA-O2A-C1
27	a	312	CHL	CBA-CGA-O2A-C1
30	J	104	LMG	C29-C28-O8-C9
27	B	814	CHL	C3A-C2A-CAA-CBA
27	5	323	CHL	C3A-C2A-CAA-CBA
27	8	317	CHL	C3A-C2A-CAA-CBA
27	A	833	CHL	C2C-C3C-CAC-CBC
30	J	101	LMG	C15-C16-C17-C18
29	a	304	LUT	C13-C14-C15-C35
23	A	808	LMT	C2-C1-O1'-C1'
27	B	842	CHL	C3-C5-C6-C7
28	7	307	DGD	CBA-CCA-CDA-CEA
27	A	843	CHL	CBA-CGA-O2A-C1
27	L	303	CHL	CBA-CGA-O2A-C1
27	B	817	CHL	C8-C10-C11-C12
27	6	307	CHL	C8-C10-C11-C12
24	5	324	LHG	C4-C5-C6-O8
30	J	101	LMG	C7-C8-C9-O8
30	7	301	LMG	C7-C8-C9-O8
32	5	305	PTY	O4-C1-C6-C5
23	5	326	LMT	C3-C4-C5-C6
24	A	812	LHG	C11-C10-C9-C8
24	7	302	LHG	C14-C15-C16-C17
27	A	825	CHL	C3-C5-C6-C7
27	A	843	CHL	C3-C5-C6-C7
27	B	813	CHL	C4-C3-C5-C6
27	B	814	CHL	C4-C3-C5-C6
27	B	821	CHL	C2-C3-C5-C6
27	b	315	CHL	C2-C3-C5-C6
24	A	810	LHG	C3-O3-P-O6
24	7	302	LHG	C4-O6-P-O3
27	a	315	CHL	C3C-C2C-CMC-OMC
34	8	301	SQD	C9-C10-C11-C12
24	5	324	LHG	O6-C4-C5-O7
32	5	305	PTY	O14-C5-C6-O7
27	4	320	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	8	325	CHL	O1A-CGA-O2A-C1
34	8	301	SQD	O10-C23-O48-C46
24	A	810	LHG	C12-C13-C14-C15
27	8	318	CHL	O1A-CGA-O2A-C1
24	A	810	LHG	O7-C5-C6-O8
24	A	812	LHG	O7-C5-C6-O8
30	7	301	LMG	O1-C7-C8-O7
27	a	315	CHL	CBA-CGA-O2A-C1
27	6	307	CHL	C5-C6-C7-C8
27	B	827	CHL	C11-C12-C13-C14
28	B	809	DGD	O6E-C1E-O5D-C6D
23	A	808	LMT	O5B-C1B-O1B-C4'
27	4	313	CHL	CBD-CGD-O2D-CED
27	3	314	CHL	C2-C3-C5-C6
27	6	311	CHL	C11-C12-C13-C14
27	7	314	CHL	C11-C10-C8-C9
27	8	316	CHL	C11-C12-C13-C14
24	4	303	LHG	C16-C17-C18-C19
27	A	828	CHL	C13-C15-C16-C17
27	A	852	CHL	C4-C3-C5-C6
30	a	301	LMG	C15-C16-C17-C18
27	A	833	CHL	C2A-CAA-CBA-CGA
22	A	803	BCR	C1-C6-C7-C8
22	A	803	BCR	C5-C6-C7-C8
22	A	803	BCR	C23-C24-C25-C26
22	A	804	BCR	C1-C6-C7-C8
22	A	804	BCR	C23-C24-C25-C26
22	A	804	BCR	C23-C24-C25-C30
22	A	805	BCR	C23-C24-C25-C26
22	B	803	BCR	C23-C24-C25-C26
22	B	803	BCR	C23-C24-C25-C30
22	B	804	BCR	C23-C24-C25-C26
22	B	805	BCR	C1-C6-C7-C8
22	B	805	BCR	C5-C6-C7-C8
22	B	805	BCR	C23-C24-C25-C26
22	B	805	BCR	C23-C24-C25-C30
22	B	806	BCR	C5-C6-C7-C8
22	B	806	BCR	C23-C24-C25-C26
22	B	807	BCR	C23-C24-C25-C26
22	F	301	BCR	C1-C6-C7-C8
22	F	301	BCR	C5-C6-C7-C8
22	K	203	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	K	203	BCR	C5-C6-C7-C8
22	3	301	BCR	C1-C6-C7-C8
22	3	301	BCR	C5-C6-C7-C8
22	3	302	BCR	C23-C24-C25-C30
22	3	303	BCR	C5-C6-C7-C8
22	8	302	BCR	C5-C6-C7-C8
22	8	302	BCR	C23-C24-C25-C26
26	A	815	CL0	C15-C16-C17-C18
27	A	844	CHL	C13-C15-C16-C17
27	B	818	CHL	C5-C6-C7-C8
27	5	316	CHL	C4C-C3C-CAC-CBC
22	3	303	BCR	C7-C8-C9-C34
30	J	101	LMG	C17-C18-C19-C20
22	A	806	BCR	C7-C8-C9-C10
22	A	806	BCR	C21-C22-C23-C24
22	B	803	BCR	C21-C22-C23-C24
22	B	805	BCR	C7-C8-C9-C10
27	J	106	CHL	C1A-C2A-CAA-CBA
29	F	303	LUT	C7-C8-C9-C10
24	b	302	LHG	C11-C10-C9-C8
30	J	101	LMG	C34-C35-C36-C37
24	4	303	LHG	C23-C24-C25-C26
27	8	315	CHL	C8-C10-C11-C12
27	A	821	CHL	O1A-CGA-O2A-C1
27	5	323	CHL	O1A-CGA-O2A-C1
28	7	307	DGD	C2B-C3B-C4B-C5B
30	7	301	LMG	C16-C17-C18-C19
27	A	832	CHL	C6-C7-C8-C10
27	A	839	CHL	C11-C10-C8-C7
27	A	850	CHL	C6-C7-C8-C10
27	B	812	CHL	C12-C13-C15-C16
27	B	813	CHL	C2-C3-C5-C6
27	B	814	CHL	C2-C3-C5-C6
27	B	840	CHL	C11-C12-C13-C15
27	B	844	CHL	C11-C12-C13-C15
27	B	844	CHL	C12-C13-C15-C16
27	6	308	CHL	C12-C13-C15-C16
27	6	311	CHL	C11-C12-C13-C15
27	7	314	CHL	C11-C10-C8-C7
27	7	319	CHL	C6-C7-C8-C10
28	B	809	DGD	CAB-CBB-CCB-CDB
27	5	309	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	7	317	CHL	C13-C15-C16-C17
29	a	302	LUT	C33-C34-C35-C15
27	L	303	CHL	C11-C12-C13-C15
27	3	314	CHL	O1A-CGA-O2A-C1
27	7	322	CHL	C2C-C3C-CAC-CBC
22	A	803	BCR	C20-C21-C22-C37
22	B	805	BCR	C20-C21-C22-C37
22	J	102	BCR	C20-C21-C22-C37
22	3	302	BCR	C35-C13-C14-C15
22	3	303	BCR	C16-C17-C18-C36
29	b	303	LUT	C11-C10-C9-C19
27	8	315	CHL	C10-C11-C12-C13
27	A	819	CHL	CBA-CGA-O2A-C1
27	B	836	CHL	CBA-CGA-O2A-C1
27	B	838	CHL	CBA-CGA-O2A-C1
27	3	318	CHL	CBA-CGA-O2A-C1
27	A	840	CHL	C10-C11-C12-C13
30	J	101	LMG	C14-C15-C16-C17
27	A	819	CHL	CAD-CBD-CGD-O2D
27	A	820	CHL	CAD-CBD-CGD-O2D
27	A	842	CHL	CAD-CBD-CGD-O2D
27	A	851	CHL	CAD-CBD-CGD-O2D
27	B	814	CHL	CAD-CBD-CGD-O2D
27	B	824	CHL	CAD-CBD-CGD-O2D
27	3	316	CHL	CAD-CBD-CGD-O2D
27	3	320	CHL	CAD-CBD-CGD-O2D
27	4	312	CHL	CAD-CBD-CGD-O2D
27	5	312	CHL	CAD-CBD-CGD-O2D
27	5	317	CHL	CAD-CBD-CGD-O2D
27	6	310	CHL	CAD-CBD-CGD-O2D
27	6	313	CHL	CAD-CBD-CGD-O2D
27	7	320	CHL	CAD-CBD-CGD-O2D
27	8	315	CHL	CAD-CBD-CGD-O2D
27	b	311	CHL	CAD-CBD-CGD-O2D
32	5	305	PTY	C1-C6-O7-C8
27	B	847	CHL	C13-C15-C16-C17
27	3	317	CHL	C8-C10-C11-C12
27	A	825	CHL	O1A-CGA-O2A-C1
24	5	304	LHG	C24-C23-O8-C6
27	B	835	CHL	C4-C3-C5-C6
27	3	311	CHL	C4-C3-C5-C6
27	a	318	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	5	306	LMT	O5'-C1'-O1'-C1
24	5	304	LHG	C4-C5-C6-O8
24	7	302	LHG	C2-C3-O3-P
24	A	812	LHG	O6-C4-C5-O7
24	4	303	LHG	O6-C4-C5-O7
24	5	304	LHG	O6-C4-C5-O7
24	7	302	LHG	O6-C4-C5-O7
27	3	316	CHL	C16-C17-C18-C19
27	A	819	CHL	CHA-CBD-CGD-O1D
27	A	820	CHL	CHA-CBD-CGD-O1D
27	A	832	CHL	CHA-CBD-CGD-O1D
27	A	836	CHL	CHA-CBD-CGD-O2D
27	A	839	CHL	CHA-CBD-CGD-O2D
27	A	842	CHL	CHA-CBD-CGD-O2D
27	A	849	CHL	CHA-CBD-CGD-O1D
27	A	849	CHL	CHA-CBD-CGD-O2D
27	B	813	CHL	CHA-CBD-CGD-O1D
27	B	819	CHL	CHA-CBD-CGD-O1D
27	B	824	CHL	CHA-CBD-CGD-O1D
27	B	825	CHL	CHA-CBD-CGD-O2D
27	B	832	CHL	CHA-CBD-CGD-O1D
27	B	838	CHL	CHA-CBD-CGD-O2D
27	B	849	CHL	CHA-CBD-CGD-O1D
27	F	308	CHL	CHA-CBD-CGD-O2D
27	K	204	CHL	CHA-CBD-CGD-O1D
27	a	310	CHL	CHA-CBD-CGD-O1D
27	a	311	CHL	CHA-CBD-CGD-O2D
27	a	315	CHL	CHA-CBD-CGD-O2D
27	3	314	CHL	CHA-CBD-CGD-O2D
27	3	320	CHL	CHA-CBD-CGD-O1D
27	4	309	CHL	CHA-CBD-CGD-O1D
27	4	309	CHL	CHA-CBD-CGD-O2D
27	5	310	CHL	CHA-CBD-CGD-O1D
27	5	312	CHL	CHA-CBD-CGD-O1D
27	5	316	CHL	CHA-CBD-CGD-O1D
27	5	316	CHL	CHA-CBD-CGD-O2D
27	5	325	CHL	CHA-CBD-CGD-O2D
27	6	312	CHL	CHA-CBD-CGD-O1D
27	7	314	CHL	CHA-CBD-CGD-O1D
27	7	319	CHL	CHA-CBD-CGD-O1D
27	8	317	CHL	CHA-CBD-CGD-O2D
27	b	311	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	a	312	CHL	O1A-CGA-O2A-C1
27	L	303	CHL	O1A-CGA-O2A-C1
22	F	301	BCR	C12-C13-C14-C15
28	B	809	DGD	C2E-C1E-O5D-C6D
29	a	302	LUT	C12-C13-C14-C15
29	4	301	LUT	C11-C10-C9-C8
29	4	302	LUT	C12-C13-C14-C15
29	5	302	LUT	C12-C13-C14-C15
29	5	303	LUT	C28-C29-C30-C31
29	b	303	LUT	C11-C10-C9-C8
28	7	307	DGD	C9B-CAB-CBB-CCB
24	A	811	LHG	O7-C5-C6-O8
24	7	302	LHG	O7-C5-C6-O8
32	5	305	PTY	O4-C1-C6-O7
27	A	841	CHL	CBA-CGA-O2A-C1
27	6	308	CHL	C8-C10-C11-C12
27	a	315	CHL	O1A-CGA-O2A-C1
24	a	305	LHG	O1-C1-C2-O2
24	a	305	LHG	C35-C36-C37-C38
27	5	309	CHL	C3-C5-C6-C7
27	A	841	CHL	C4-C3-C5-C6
27	B	848	CHL	C4-C3-C5-C6
27	3	310	CHL	C4-C3-C5-C6
27	7	313	CHL	C4-C3-C5-C6
27	7	317	CHL	C4-C3-C5-C6
27	3	318	CHL	O1A-CGA-O2A-C1
27	A	841	CHL	C2-C3-C5-C6
27	B	848	CHL	C2-C3-C5-C6
27	7	317	CHL	C2-C3-C5-C6
27	A	832	CHL	C6-C7-C8-C9
28	B	809	DGD	C6B-C7B-C8B-C9B
24	5	304	LHG	O10-C23-O8-C6
27	A	822	CHL	O1A-CGA-O2A-C1
27	7	319	CHL	C2A-CAA-CBA-CGA
27	B	836	CHL	O1A-CGA-O2A-C1
27	B	838	CHL	O1A-CGA-O2A-C1
27	A	822	CHL	CBA-CGA-O2A-C1
29	3	304	LUT	C7-C8-C9-C19
27	A	849	CHL	C5-C6-C7-C8
22	A	803	BCR	C21-C22-C23-C24
22	J	102	BCR	C7-C8-C9-C10
22	3	303	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	A	824	CHL	C3-C5-C6-C7
27	A	830	CHL	C1A-C2A-CAA-CBA
27	A	839	CHL	C1A-C2A-CAA-CBA
27	A	845	CHL	C1A-C2A-CAA-CBA
27	B	822	CHL	C1A-C2A-CAA-CBA
27	F	308	CHL	C1A-C2A-CAA-CBA
27	4	320	CHL	C1A-C2A-CAA-CBA
27	7	314	CHL	C1A-C2A-CAA-CBA
27	7	317	CHL	C1A-C2A-CAA-CBA
26	A	815	CL0	C16-C17-C18-C19
27	6	308	CHL	C16-C17-C18-C19
24	b	302	LHG	C24-C23-O8-C6
27	A	845	CHL	CBA-CGA-O2A-C1
27	3	317	CHL	CBA-CGA-O2A-C1
29	4	301	LUT	C33-C34-C35-C15
29	b	303	LUT	C13-C14-C15-C35
24	5	304	LHG	C4-O6-P-O3
24	7	306	LHG	C3-O3-P-O6
24	8	305	LHG	O2-C2-C3-O3
34	8	301	SQD	C10-C11-C12-C13
27	A	819	CHL	C4-C3-C5-C6
27	A	837	CHL	C4-C3-C5-C6
27	A	850	CHL	C4-C3-C5-C6
27	B	819	CHL	C4-C3-C5-C6
24	7	302	LHG	C5-C4-O6-P
27	A	841	CHL	O1A-CGA-O2A-C1
27	A	845	CHL	O1A-CGA-O2A-C1
24	A	810	LHG	C3-O3-P-O5
24	A	812	LHG	C3-O3-P-O5
24	7	302	LHG	C3-O3-P-O5
24	7	302	LHG	C4-O6-P-O4
24	b	302	LHG	C4-O6-P-O4
32	5	305	PTY	C3-O11-P1-O13
30	a	301	LMG	O6-C1-O1-C7
24	5	304	LHG	O6-C4-C5-C6
27	5	313	CHL	C8-C10-C11-C12
27	B	812	CHL	C2A-CAA-CBA-CGA
24	7	306	LHG	C10-C11-C12-C13
27	A	820	CHL	CAD-CBD-CGD-O1D
27	A	846	CHL	CAD-CBD-CGD-O1D
27	A	857	CHL	CAD-CBD-CGD-O1D
27	B	819	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	B	849	CHL	CAD-CBD-CGD-O1D
27	3	316	CHL	CAD-CBD-CGD-O1D
27	5	316	CHL	CAD-CBD-CGD-O1D
27	6	312	CHL	CAD-CBD-CGD-O1D
34	8	301	SQD	C5-C6-S-O7
28	7	307	DGD	CEB-CFB-CGB-CHB
27	A	819	CHL	O1A-CGA-O2A-C1
27	A	843	CHL	C10-C11-C12-C13
24	7	306	LHG	C24-C23-O8-C6
34	8	301	SQD	C11-C10-C9-C8
27	A	831	CHL	C6-C7-C8-C10
23	7	308	LMT	C4'-C5'-C6'-O6'
27	A	836	CHL	C6-C7-C8-C10
27	B	815	CHL	C12-C13-C15-C16
27	B	817	CHL	C6-C7-C8-C10
27	B	825	CHL	C6-C7-C8-C10
27	8	315	CHL	C6-C7-C8-C10
29	a	302	LUT	C25-C26-C27-C28
27	B	820	CHL	C15-C16-C17-C18
27	3	317	CHL	O1A-CGA-O2A-C1
27	3	310	CHL	C2A-CAA-CBA-CGA
27	8	312	CHL	C2A-CAA-CBA-CGA
23	A	808	LMT	C2B-C1B-O1B-C4'
27	a	315	CHL	C1C-C2C-CMC-OMC
27	4	309	CHL	C1C-C2C-CMC-OMC
27	5	316	CHL	C1C-C2C-CMC-OMC
27	6	316	CHL	C1C-C2C-CMC-OMC
27	6	317	CHL	C1C-C2C-CMC-OMC
27	7	320	CHL	C1C-C2C-CMC-OMC
27	8	314	CHL	C1C-C2C-CMC-OMC
27	8	321	CHL	C1C-C2C-CMC-OMC
30	J	101	LMG	O1-C7-C8-C9
24	5	304	LHG	O7-C5-C6-O8
34	8	301	SQD	O6-C44-C45-O47
24	4	303	LHG	C24-C25-C26-C27
23	B	810	LMT	C7-C8-C9-C10
27	5	309	CHL	C8-C10-C11-C12
23	5	326	LMT	C5-C6-C7-C8
27	8	320	CHL	C4-C3-C5-C6
27	7	318	CHL	CBA-CGA-O2A-C1
27	B	835	CHL	C2-C3-C5-C6
27	3	310	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	6	306	CHL	C5-C6-C7-C8
27	A	839	CHL	C11-C10-C8-C9
27	B	812	CHL	C14-C13-C15-C16
27	B	840	CHL	C11-C12-C13-C14
27	6	307	CHL	C11-C12-C13-C14
27	7	322	CHL	C11-C10-C8-C9
27	7	318	CHL	O1A-CGA-O2A-C1
27	8	317	CHL	C3-C5-C6-C7
23	7	308	LMT	O5'-C5'-C6'-O6'
29	F	303	LUT	C10-C11-C12-C13
29	a	304	LUT	C30-C31-C32-C33
29	5	303	LUT	C10-C11-C12-C13
29	6	302	LUT	C30-C31-C32-C33
29	6	303	LUT	C10-C11-C12-C13
27	8	325	CHL	C3-C5-C6-C7
24	7	302	LHG	C7-C8-C9-C10
27	a	317	CHL	C4-C3-C5-C6
24	4	303	LHG	O7-C7-C8-C9
34	8	301	SQD	C24-C25-C26-C27
27	B	822	CHL	C8-C10-C11-C12
27	7	317	CHL	C5-C6-C7-C8
27	8	312	CHL	C16-C17-C18-C19
23	7	308	LMT	C5-C6-C7-C8
27	A	823	CHL	C13-C15-C16-C17
28	7	307	DGD	O1G-C1A-C2A-C3A
24	a	305	LHG	C31-C32-C33-C34
24	5	324	LHG	O6-C4-C5-C6
27	B	816	CHL	C2A-CAA-CBA-CGA
27	3	320	CHL	C2A-CAA-CBA-CGA
27	4	307	CHL	C2A-CAA-CBA-CGA
27	A	831	CHL	C2-C1-O2A-CGA
27	A	853	CHL	C2-C1-O2A-CGA
27	B	821	CHL	C2-C1-O2A-CGA
27	B	841	CHL	C2-C1-O2A-CGA
27	B	851	CHL	C2-C1-O2A-CGA
27	3	312	CHL	C2-C1-O2A-CGA
28	7	307	DGD	C6B-C7B-C8B-C9B
27	A	833	CHL	CAA-CBA-CGA-O2A
24	8	305	LHG	C9-C10-C11-C12
24	a	305	LHG	C2-C3-O3-P
27	B	823	CHL	C4-C3-C5-C6
27	7	318	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	803	BCR	C23-C24-C25-C30
22	A	804	BCR	C5-C6-C7-C8
22	A	805	BCR	C23-C24-C25-C30
22	B	806	BCR	C1-C6-C7-C8
22	B	807	BCR	C23-C24-C25-C30
22	3	303	BCR	C1-C6-C7-C8
27	A	819	CHL	C2-C3-C5-C6
27	B	819	CHL	C2-C3-C5-C6
27	3	311	CHL	C2-C3-C5-C6
27	7	313	CHL	C2-C3-C5-C6
27	4	319	CHL	C2C-C3C-CAC-CBC
27	7	322	CHL	C4C-C3C-CAC-CBC
27	B	840	CHL	CAA-CBA-CGA-O2A
30	a	301	LMG	O7-C8-C9-O8
30	8	307	LMG	O1-C7-C8-O7
27	B	847	CHL	C5-C6-C7-C8
24	A	811	LHG	C3-O3-P-O6
27	B	837	CHL	C10-C11-C12-C13
24	b	302	LHG	C11-C12-C13-C14
24	7	306	LHG	C4-C5-C6-O8
34	8	301	SQD	O6-C44-C45-C46
20	B	801	PQN	C23-C25-C26-C27
27	5	316	CHL	C11-C10-C8-C7
27	6	307	CHL	C12-C13-C15-C16
27	8	321	CHL	O1A-CGA-O2A-C1
27	A	836	CHL	C6-C7-C8-C9
27	B	815	CHL	C14-C13-C15-C16
27	B	825	CHL	C6-C7-C8-C9
27	5	309	CHL	C6-C7-C8-C9
27	8	315	CHL	C6-C7-C8-C9
27	B	820	CHL	C5-C6-C7-C8
22	B	803	BCR	C19-C20-C21-C22
22	5	301	BCR	C19-C20-C21-C22
29	F	303	LUT	C9-C10-C11-C12
29	J	103	LUT	C13-C14-C15-C35
29	6	302	LUT	C33-C34-C35-C15
27	3	319	CHL	C2A-CAA-CBA-CGA
22	8	302	BCR	C7-C8-C9-C34
29	7	304	LUT	C11-C12-C13-C20
27	8	312	CHL	C16-C17-C18-C20
27	b	307	CHL	CBA-CGA-O2A-C1
24	5	324	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
26	A	815	CL0	C13-C15-C16-C17
22	B	807	BCR	C21-C22-C23-C24
28	B	809	DGD	C5B-C6B-C7B-C8B
24	7	306	LHG	C1-C2-C3-O3
24	8	305	LHG	C1-C2-C3-O3
27	A	825	CHL	C4-C3-C5-C6
27	A	842	CHL	C4-C3-C5-C6
24	B	808	LHG	C7-C8-C9-C10
24	5	324	LHG	O1-C1-C2-O2
27	6	310	CHL	CBA-CGA-O2A-C1
27	8	321	CHL	CBA-CGA-O2A-C1
27	b	308	CHL	O1A-CGA-O2A-C1
27	7	315	CHL	CAA-CBA-CGA-O2A
23	5	326	LMT	O5'-C1'-O1'-C1
22	B	806	BCR	C19-C20-C21-C22
29	3	304	LUT	C13-C14-C15-C35
28	B	809	DGD	C8A-C9A-CAA-CBA
27	6	310	CHL	O1A-CGA-O2A-C1
22	K	203	BCR	C18-C19-C20-C21
22	L	301	BCR	C18-C19-C20-C21
27	A	858	CHL	C16-C17-C18-C20
30	a	301	LMG	C37-C38-C39-C40
24	5	304	LHG	C24-C25-C26-C27
27	4	313	CHL	O1D-CGD-O2D-CED
27	3	319	CHL	C5-C6-C7-C8
28	7	307	DGD	CDB-CEB-CFB-CGB
27	4	314	CHL	CAA-CBA-CGA-O1A
27	B	838	CHL	C2-C1-O2A-CGA
27	B	842	CHL	C2-C1-O2A-CGA
27	3	311	CHL	C2-C1-O2A-CGA
27	7	319	CHL	C2-C1-O2A-CGA
27	a	311	CHL	C5-C6-C7-C8
27	b	315	CHL	C2C-C3C-CAC-CBC
23	A	809	LMT	C1-C2-C3-C4
27	B	822	CHL	C2A-CAA-CBA-CGA
27	4	306	CHL	C2A-CAA-CBA-CGA
27	6	311	CHL	C2A-CAA-CBA-CGA
27	7	314	CHL	C2A-CAA-CBA-CGA
27	8	315	CHL	C2A-CAA-CBA-CGA
27	b	305	CHL	C2A-CAA-CBA-CGA
28	7	307	DGD	O1A-C1A-C2A-C3A
27	A	858	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	B	822	CHL	C3A-C2A-CAA-CBA
27	a	314	CHL	CAA-CBA-CGA-O2A
27	7	312	CHL	CAA-CBA-CGA-O1A
22	L	301	BCR	C13-C14-C15-C16
29	8	304	LUT	C9-C10-C11-C12
27	5	314	CHL	CAA-CBA-CGA-O1A
27	B	832	CHL	O1D-CGD-O2D-CED
27	A	837	CHL	C2-C3-C5-C6
27	A	826	CHL	C11-C10-C8-C9
27	B	814	CHL	C14-C13-C15-C16
27	B	815	CHL	C6-C7-C8-C9
27	5	316	CHL	C14-C13-C15-C16
27	8	315	CHL	C11-C10-C8-C9
27	7	315	CHL	CAA-CBA-CGA-O1A
27	B	837	CHL	O1A-CGA-O2A-C1
22	A	807	BCR	C16-C17-C18-C36
22	B	804	BCR	C11-C10-C9-C34
22	B	804	BCR	C20-C21-C22-C37
22	L	302	BCR	C11-C10-C9-C34
22	L	302	BCR	C16-C17-C18-C36
27	A	855	CHL	C3-C5-C6-C7
27	B	849	CHL	CAA-CBA-CGA-O2A
27	a	314	CHL	CAA-CBA-CGA-O1A
27	6	316	CHL	CAA-CBA-CGA-O1A
27	b	315	CHL	C4C-C3C-CAC-CBC
27	4	314	CHL	CAA-CBA-CGA-O2A
27	B	840	CHL	C3-C5-C6-C7
29	a	302	LUT	C7-C8-C9-C10
24	A	811	LHG	C30-C31-C32-C33
27	A	858	CHL	C1A-C2A-CAA-CBA
27	A	859	CHL	C1A-C2A-CAA-CBA
27	B	814	CHL	C1A-C2A-CAA-CBA
27	B	821	CHL	C1A-C2A-CAA-CBA
27	B	838	CHL	C1A-C2A-CAA-CBA
27	a	313	CHL	C1A-C2A-CAA-CBA
27	5	315	CHL	C1A-C2A-CAA-CBA
27	6	313	CHL	C1A-C2A-CAA-CBA
27	8	312	CHL	C1A-C2A-CAA-CBA
27	8	325	CHL	C1A-C2A-CAA-CBA
27	B	844	CHL	CBA-CGA-O2A-C1
24	5	304	LHG	C13-C14-C15-C16
27	4	319	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
27	A	823	CHL	C12-C13-C15-C16
27	A	838	CHL	C6-C7-C8-C10
27	8	320	CHL	C2-C3-C5-C6
28	7	307	DGD	CCA-CDA-CEA-CFA
27	3	310	CHL	C5-C6-C7-C8
27	A	827	CHL	CBA-CGA-O2A-C1
27	A	828	CHL	CBA-CGA-O2A-C1
27	b	307	CHL	O1A-CGA-O2A-C1
24	8	305	LHG	C29-C30-C31-C32
27	a	310	CHL	C2A-CAA-CBA-CGA
27	a	319	CHL	C2A-CAA-CBA-CGA
27	3	315	CHL	C2A-CAA-CBA-CGA
27	5	310	CHL	C2A-CAA-CBA-CGA
27	6	308	CHL	C2A-CAA-CBA-CGA
27	B	851	CHL	C8-C10-C11-C12
27	3	317	CHL	CAA-CBA-CGA-O2A
27	7	312	CHL	CAA-CBA-CGA-O2A
27	7	313	CHL	CBA-CGA-O2A-C1
24	A	811	LHG	C11-C12-C13-C14
27	A	844	CHL	C4-C3-C5-C6
27	B	847	CHL	C4-C3-C5-C6
27	5	314	CHL	CAA-CBA-CGA-O2A
22	A	807	BCR	C16-C17-C18-C19
22	3	302	BCR	C20-C21-C22-C23
22	3	303	BCR	C11-C10-C9-C8
24	7	306	LHG	O7-C5-C6-O8
22	6	301	BCR	C13-C14-C15-C16
22	7	303	BCR	C19-C20-C21-C22
29	5	303	LUT	C9-C10-C11-C12
29	6	302	LUT	C13-C14-C15-C35
33	7	305	XAT	C9-C10-C11-C12
28	7	307	DGD	C6A-C7A-C8A-C9A
27	A	833	CHL	C10-C11-C12-C13
28	B	809	DGD	C3A-C4A-C5A-C6A
27	B	844	CHL	O1A-CGA-O2A-C1
24	5	304	LHG	C1-C2-C3-O3
24	B	808	LHG	C24-C25-C26-C27
24	7	302	LHG	C30-C31-C32-C33
27	B	839	CHL	C4-C3-C5-C6
27	A	826	CHL	C2-C1-O2A-CGA
27	A	829	CHL	C2-C1-O2A-CGA
27	A	832	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
27	A	855	CHL	C2-C1-O2A-CGA
27	B	832	CHL	C2-C1-O2A-CGA
27	B	834	CHL	C2-C1-O2A-CGA
27	6	306	CHL	C2-C1-O2A-CGA
27	A	825	CHL	C2-C3-C5-C6
27	A	842	CHL	C2-C3-C5-C6
27	3	311	CHL	C2C-C3C-CAC-CBC
27	A	827	CHL	O1A-CGA-O2A-C1
27	A	853	CHL	C11-C10-C8-C9
27	3	311	CHL	O1A-CGA-O2A-C1
27	7	313	CHL	O1A-CGA-O2A-C1
23	A	808	LMT	C9-C10-C11-C12
27	8	325	CHL	C8-C10-C11-C12
27	4	304	CHL	C2A-CAA-CBA-CGA
27	B	837	CHL	CBA-CGA-O2A-C1
22	A	807	BCR	C1-C6-C7-C8
22	B	804	BCR	C23-C24-C25-C30
22	F	301	BCR	C23-C24-C25-C30
22	I	801	BCR	C23-C24-C25-C30
22	J	102	BCR	C1-C6-C7-C8
22	J	102	BCR	C5-C6-C7-C8
22	7	303	BCR	C1-C6-C7-C8
22	7	303	BCR	C5-C6-C7-C8
22	8	302	BCR	C1-C6-C7-C8
22	L	302	BCR	C23-C24-C25-C26
22	L	302	BCR	C23-C24-C25-C30
29	3	304	LUT	C1-C6-C7-C8
29	5	303	LUT	C1-C6-C7-C8
30	J	104	LMG	O1-C7-C8-C9
30	8	307	LMG	O1-C7-C8-C9
22	6	301	BCR	C9-C10-C11-C12
29	F	303	LUT	C33-C34-C35-C15
29	4	302	LUT	C33-C34-C35-C15
27	A	829	CHL	CBA-CGA-O2A-C1
27	A	845	CHL	C4-C3-C5-C6
27	B	817	CHL	C4-C3-C5-C6
27	B	818	CHL	C4-C3-C5-C6
27	B	827	CHL	C4-C3-C5-C6
27	a	309	CHL	C4-C3-C5-C6
27	3	313	CHL	C4-C3-C5-C6
27	7	316	CHL	C4-C3-C5-C6
27	7	323	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	7	303	BCR	C21-C22-C23-C24
27	8	314	CHL	C8-C10-C11-C12
24	B	808	LHG	C11-C10-C9-C8
27	B	823	CHL	C2-C3-C5-C6
27	a	317	CHL	C2-C3-C5-C6
27	7	318	CHL	C2-C3-C5-C6
27	7	323	CHL	C2-C3-C5-C6
27	A	842	CHL	C3-C5-C6-C7
27	6	308	CHL	C3-C5-C6-C7
27	A	824	CHL	C8-C10-C11-C12
26	A	815	CL0	C3-C5-C6-C7
27	B	814	CHL	C15-C16-C17-C18
30	7	301	LMG	C13-C14-C15-C16
24	7	302	LHG	C16-C17-C18-C19
27	3	311	CHL	CBA-CGA-O2A-C1
27	A	841	CHL	O1D-CGD-O2D-CED
27	5	318	CHL	C8-C10-C11-C12
27	B	832	CHL	C4-C3-C5-C6
27	B	846	CHL	C4-C3-C5-C6
27	6	311	CHL	C4-C3-C5-C6
27	8	317	CHL	C4-C3-C5-C6
24	A	811	LHG	C35-C36-C37-C38
27	A	844	CHL	C2-C3-C5-C6
27	B	822	CHL	C11-C10-C8-C7
27	a	309	CHL	C2-C3-C5-C6
27	A	828	CHL	O1A-CGA-O2A-C1
24	b	302	LHG	C24-C25-C26-C27
27	3	311	CHL	C4C-C3C-CAC-CBC
30	J	101	LMG	O1-C7-C8-O7
24	4	303	LHG	C15-C16-C17-C18
27	b	317	CHL	CAA-CBA-CGA-O2A
24	7	302	LHG	C34-C35-C36-C37
27	4	313	CHL	CAA-CBA-CGA-O2A
27	4	317	CHL	CAA-CBA-CGA-O2A
22	A	807	BCR	C11-C10-C9-C34
22	B	802	BCR	C20-C21-C22-C37
22	6	301	BCR	C20-C21-C22-C37
27	A	827	CHL	C5-C6-C7-C8
29	F	303	LUT	C11-C10-C9-C19
29	4	302	LUT	C39-C29-C30-C31
27	B	815	CHL	CAA-CBA-CGA-O2A
27	4	308	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	b	307	CHL	CAA-CBA-CGA-O2A
27	a	319	CHL	C2C-C3C-CAC-CBC
27	A	818	CHL	C4-C3-C5-C6
27	A	821	CHL	C4-C3-C5-C6
27	A	823	CHL	C4-C3-C5-C6
27	A	827	CHL	C4-C3-C5-C6
27	A	838	CHL	C4-C3-C5-C6
27	A	856	CHL	C4-C3-C5-C6
27	B	830	CHL	C4-C3-C5-C6
27	B	844	CHL	C4-C3-C5-C6
27	A	838	CHL	C5-C6-C7-C8
24	7	306	LHG	C11-C12-C13-C14
27	A	850	CHL	C2-C3-C5-C6
24	A	812	LHG	C23-C24-C25-C26
27	B	811	CHL	CAA-CBA-CGA-O2A
27	4	310	CHL	CAA-CBA-CGA-O2A
27	A	858	CHL	C6-C7-C8-C9
27	B	822	CHL	C11-C10-C8-C9
27	7	319	CHL	C14-C13-C15-C16
27	A	829	CHL	O1A-CGA-O2A-C1
27	6	316	CHL	CAA-CBA-CGA-O2A
27	A	824	CHL	C3A-C2A-CAA-CBA
27	A	859	CHL	C3A-C2A-CAA-CBA
27	B	826	CHL	C3A-C2A-CAA-CBA
27	B	835	CHL	C3A-C2A-CAA-CBA
27	B	838	CHL	C3A-C2A-CAA-CBA
27	B	846	CHL	C3A-C2A-CAA-CBA
27	5	315	CHL	C3A-C2A-CAA-CBA
27	5	319	CHL	C3A-C2A-CAA-CBA
27	L	303	CHL	C3A-C2A-CAA-CBA
27	5	307	CHL	O1A-CGA-O2A-C1
24	7	302	LHG	O7-C7-C8-C9
26	A	815	CL0	CAA-CBA-CGA-O2A
27	A	821	CHL	CAA-CBA-CGA-O2A
27	B	835	CHL	CAA-CBA-CGA-O2A
27	A	829	CHL	CAD-CBD-CGD-O2D
27	A	832	CHL	CAD-CBD-CGD-O2D
27	A	857	CHL	CAD-CBD-CGD-O2D
27	B	813	CHL	CAD-CBD-CGD-O2D
27	B	819	CHL	CAD-CBD-CGD-O2D
27	B	827	CHL	CAD-CBD-CGD-O2D
27	B	832	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	F	309	CHL	CAD-CBD-CGD-O2D
27	a	309	CHL	CAD-CBD-CGD-O2D
27	a	310	CHL	CAD-CBD-CGD-O2D
27	a	315	CHL	CAD-CBD-CGD-O2D
27	3	321	CHL	CAD-CBD-CGD-O2D
27	4	309	CHL	CAD-CBD-CGD-O2D
27	5	307	CHL	CAD-CBD-CGD-O2D
27	5	319	CHL	CAD-CBD-CGD-O2D
27	5	322	CHL	CAD-CBD-CGD-O2D
27	5	325	CHL	CAD-CBD-CGD-O2D
27	6	312	CHL	CAD-CBD-CGD-O2D
27	7	314	CHL	CAD-CBD-CGD-O2D
27	7	318	CHL	CAD-CBD-CGD-O2D
27	7	323	CHL	CAD-CBD-CGD-O2D
27	8	320	CHL	CAD-CBD-CGD-O2D
27	b	305	CHL	CAD-CBD-CGD-O2D
27	b	317	CHL	CAD-CBD-CGD-O2D
27	A	858	CHL	C16-C17-C18-C19
24	A	812	LHG	C32-C33-C34-C35
30	a	301	LMG	O9-C10-O7-C8
27	A	825	CHL	C2-C1-O2A-CGA
27	B	829	CHL	C2-C1-O2A-CGA
27	6	312	CHL	CAA-CBA-CGA-O2A
27	A	859	CHL	C4-C3-C5-C6
27	B	815	CHL	C4-C3-C5-C6
27	6	307	CHL	C4-C3-C5-C6
27	8	314	CHL	C4-C3-C5-C6
27	B	817	CHL	C2-C3-C5-C6
27	B	846	CHL	C2-C3-C5-C6
27	B	847	CHL	C2-C3-C5-C6
27	3	313	CHL	C2-C3-C5-C6
27	3	320	CHL	CAA-CBA-CGA-O2A
27	8	313	CHL	CAA-CBA-CGA-O2A
24	4	303	LHG	C26-C27-C28-C29
22	A	807	BCR	C7-C8-C9-C10
27	A	818	CHL	CAA-CBA-CGA-O2A
27	8	312	CHL	CAA-CBA-CGA-O2A
30	J	101	LMG	O8-C28-C29-C30
27	4	305	CHL	CAA-CBA-CGA-O1A
27	4	305	CHL	CAA-CBA-CGA-O2A
27	4	317	CHL	CAA-CBA-CGA-O1A
27	K	207	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	3	312	CHL	CAA-CBA-CGA-O2A
27	4	313	CHL	CAA-CBA-CGA-O1A
27	A	845	CHL	C13-C15-C16-C17
24	A	812	LHG	C1-C2-C3-O3
27	A	821	CHL	CHA-CBD-CGD-O2D
27	A	823	CHL	CHA-CBD-CGD-O2D
27	A	830	CHL	CHA-CBD-CGD-O1D
27	A	835	CHL	CHA-CBD-CGD-O2D
27	A	839	CHL	CHA-CBD-CGD-O1D
27	A	840	CHL	CHA-CBD-CGD-O2D
27	A	845	CHL	CHA-CBD-CGD-O2D
27	A	859	CHL	CHA-CBD-CGD-O2D
27	B	811	CHL	CHA-CBD-CGD-O1D
27	B	814	CHL	CHA-CBD-CGD-O1D
27	B	818	CHL	CHA-CBD-CGD-O2D
27	B	820	CHL	CHA-CBD-CGD-O2D
27	B	822	CHL	CHA-CBD-CGD-O1D
27	B	831	CHL	CHA-CBD-CGD-O1D
27	B	834	CHL	CHA-CBD-CGD-O1D
27	B	835	CHL	CHA-CBD-CGD-O2D
27	B	844	CHL	CHA-CBD-CGD-O1D
27	B	850	CHL	CHA-CBD-CGD-O2D
27	J	106	CHL	CHA-CBD-CGD-O2D
27	K	204	CHL	CHA-CBD-CGD-O2D
27	K	207	CHL	CHA-CBD-CGD-O2D
27	a	308	CHL	CHA-CBD-CGD-O1D
27	a	309	CHL	CHA-CBD-CGD-O2D
27	a	313	CHL	CHA-CBD-CGD-O2D
27	a	314	CHL	CHA-CBD-CGD-O2D
27	a	316	CHL	CHA-CBD-CGD-O1D
27	a	316	CHL	CHA-CBD-CGD-O2D
27	a	319	CHL	CHA-CBD-CGD-O2D
27	a	320	CHL	CHA-CBD-CGD-O1D
27	3	311	CHL	CHA-CBD-CGD-O2D
27	3	319	CHL	CHA-CBD-CGD-O1D
27	4	306	CHL	CHA-CBD-CGD-O1D
27	4	306	CHL	CHA-CBD-CGD-O2D
27	4	314	CHL	CHA-CBD-CGD-O2D
27	4	316	CHL	CHA-CBD-CGD-O1D
27	4	318	CHL	CHA-CBD-CGD-O2D
27	4	319	CHL	CHA-CBD-CGD-O1D
27	4	320	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	5	308	CHL	CHA-CBD-CGD-O2D
27	5	309	CHL	CHA-CBD-CGD-O2D
27	5	315	CHL	CHA-CBD-CGD-O1D
27	5	319	CHL	CHA-CBD-CGD-O1D
27	5	321	CHL	CHA-CBD-CGD-O2D
27	6	306	CHL	CHA-CBD-CGD-O2D
27	6	307	CHL	CHA-CBD-CGD-O2D
27	6	311	CHL	CHA-CBD-CGD-O1D
27	6	313	CHL	CHA-CBD-CGD-O1D
27	6	314	CHL	CHA-CBD-CGD-O1D
27	8	315	CHL	CHA-CBD-CGD-O1D
27	8	315	CHL	CHA-CBD-CGD-O2D
27	8	318	CHL	CHA-CBD-CGD-O2D
27	8	321	CHL	CHA-CBD-CGD-O1D
27	8	326	CHL	CHA-CBD-CGD-O2D
27	b	305	CHL	CHA-CBD-CGD-O2D
27	b	306	CHL	CHA-CBD-CGD-O2D
27	b	309	CHL	CHA-CBD-CGD-O2D
27	b	310	CHL	CHA-CBD-CGD-O1D
27	b	314	CHL	CHA-CBD-CGD-O2D
27	A	845	CHL	C2-C3-C5-C6
27	4	308	CHL	C5-C6-C7-C8
24	A	812	LHG	O6-C4-C5-C6
22	B	804	BCR	C20-C21-C22-C23
22	6	301	BCR	C20-C21-C22-C23
29	8	304	LUT	C28-C29-C30-C31
24	A	810	LHG	C28-C29-C30-C31
27	5	311	CHL	CAA-CBA-CGA-O2A
27	6	305	CHL	CAA-CBA-CGA-O2A
27	6	309	CHL	CAA-CBA-CGA-O2A
27	A	850	CHL	C5-C6-C7-C8
27	b	315	CHL	C10-C11-C12-C13
27	A	836	CHL	CAA-CBA-CGA-O2A
27	4	311	CHL	CAA-CBA-CGA-O2A
27	5	309	CHL	CAA-CBA-CGA-O2A
30	8	307	LMG	O8-C28-C29-C30
27	F	309	CHL	C2A-CAA-CBA-CGA
27	b	311	CHL	C2C-C3C-CAC-CBC
24	8	305	LHG	C7-C8-C9-C10
24	A	812	LHG	O7-C7-C8-C9
27	4	307	CHL	CAA-CBA-CGA-O2A
27	b	312	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	7	301	LMG	C18-C19-C20-C21
27	A	823	CHL	C11-C10-C8-C7
27	A	853	CHL	C11-C10-C8-C7
27	B	815	CHL	C2-C3-C5-C6
27	B	844	CHL	C2-C3-C5-C6
27	8	314	CHL	C2-C3-C5-C6
27	A	828	CHL	CAA-CBA-CGA-O2A
27	A	823	CHL	C14-C13-C15-C16
27	A	838	CHL	C6-C7-C8-C9
27	6	307	CHL	C14-C13-C15-C16
29	7	304	LUT	C33-C34-C35-C15
27	5	309	CHL	C10-C11-C12-C13
27	B	847	CHL	CAA-CBA-CGA-O2A
27	a	320	CHL	CAA-CBA-CGA-O2A
27	5	325	CHL	CAA-CBA-CGA-O2A
34	8	301	SQD	O48-C23-C24-C25
24	A	811	LHG	C12-C13-C14-C15
27	A	832	CHL	C2A-CAA-CBA-CGA
27	6	310	CHL	C2A-CAA-CBA-CGA
27	8	325	CHL	C2A-CAA-CBA-CGA
27	6	312	CHL	CAA-CBA-CGA-O1A
27	A	817	CHL	C8-C10-C11-C12
27	A	831	CHL	C2-C3-C5-C6
27	5	307	CHL	CBA-CGA-O2A-C1
27	6	311	CHL	CBA-CGA-O2A-C1
27	8	316	CHL	C13-C15-C16-C17
24	a	305	LHG	C1-C2-C3-O3
27	A	828	CHL	C1A-C2A-CAA-CBA
27	A	841	CHL	C1A-C2A-CAA-CBA
27	B	827	CHL	C1A-C2A-CAA-CBA
27	B	834	CHL	C1A-C2A-CAA-CBA
27	B	839	CHL	C1A-C2A-CAA-CBA
27	B	846	CHL	C1A-C2A-CAA-CBA
27	4	309	CHL	C1A-C2A-CAA-CBA
27	4	312	CHL	C1A-C2A-CAA-CBA
27	5	319	CHL	C1A-C2A-CAA-CBA
27	6	307	CHL	C1A-C2A-CAA-CBA
27	7	315	CHL	CHA-CBD-CGD-O2D
27	4	310	CHL	CAA-CBA-CGA-O1A
27	b	307	CHL	CAA-CBA-CGA-O1A
27	a	319	CHL	C4C-C3C-CAC-CBC
27	A	822	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	4	303	LHG	C18-C19-C20-C21
24	A	810	LHG	O10-C23-C24-C25
24	A	812	LHG	O9-C7-C8-C9
27	A	818	CHL	CAA-CBA-CGA-O1A
27	K	207	CHL	CAA-CBA-CGA-O1A
27	4	308	CHL	CAA-CBA-CGA-O1A
27	8	313	CHL	CAA-CBA-CGA-O1A
27	b	317	CHL	CAA-CBA-CGA-O1A
24	8	305	LHG	C24-C25-C26-C27
24	A	810	LHG	C4-C5-C6-O8
24	8	305	LHG	C4-C5-C6-O8
23	A	808	LMT	C4'-C5'-C6'-O6'
27	A	858	CHL	C2A-CAA-CBA-CGA
27	B	827	CHL	C2A-CAA-CBA-CGA
27	3	318	CHL	C2A-CAA-CBA-CGA
27	b	308	CHL	C2A-CAA-CBA-CGA
27	B	848	CHL	C16-C17-C18-C19
27	A	821	CHL	CAA-CBA-CGA-O1A
30	8	307	LMG	O10-C28-C29-C30
34	8	301	SQD	O10-C23-C24-C25
27	b	313	CHL	CAA-CBA-CGA-O2A
27	B	815	CHL	C3-C5-C6-C7
24	7	306	LHG	O10-C23-C24-C25
27	B	815	CHL	CAA-CBA-CGA-O1A
23	5	326	LMT	C2'-C1'-O1'-C1
27	8	321	CHL	C10-C11-C12-C13
24	7	306	LHG	C3-O3-P-O5
20	B	801	PQN	C26-C27-C28-C29
27	A	828	CHL	CAA-CBA-CGA-O1A
27	B	835	CHL	CAA-CBA-CGA-O1A
27	3	312	CHL	CAA-CBA-CGA-O1A
27	5	311	CHL	CAA-CBA-CGA-O1A
27	6	305	CHL	CAA-CBA-CGA-O1A
27	6	309	CHL	CAA-CBA-CGA-O1A
27	8	312	CHL	CAA-CBA-CGA-O1A
22	A	807	BCR	C5-C6-C7-C8
22	F	301	BCR	C23-C24-C25-C26
22	I	801	BCR	C23-C24-C25-C26
27	5	309	CHL	CAA-CBA-CGA-O1A
27	a	317	CHL	CAA-CBA-CGA-O2A
27	8	316	CHL	CAA-CBA-CGA-O2A
27	B	819	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	B	803	BCR	C18-C19-C20-C21
22	B	805	BCR	C10-C11-C12-C13
27	8	319	CHL	C2A-CAA-CBA-CGA
24	7	302	LHG	O9-C7-C8-C9
27	7	324	CHL	C4C-C3C-CAC-CBC
27	8	317	CHL	CAA-CBA-CGA-O2A
24	4	303	LHG	C33-C34-C35-C36
30	7	301	LMG	C17-C18-C19-C20
27	B	847	CHL	CAA-CBA-CGA-O1A
30	a	301	LMG	C32-C33-C34-C35
27	A	823	CHL	CAD-CBD-CGD-O1D
27	B	811	CHL	CAD-CBD-CGD-O1D
27	B	814	CHL	CAD-CBD-CGD-O1D
27	B	822	CHL	CAD-CBD-CGD-O1D
27	B	825	CHL	CAD-CBD-CGD-O1D
27	B	826	CHL	CAD-CBD-CGD-O1D
27	B	831	CHL	CAD-CBD-CGD-O1D
27	B	834	CHL	CAD-CBD-CGD-O1D
27	4	307	CHL	CAD-CBD-CGD-O1D
27	6	313	CHL	CAD-CBD-CGD-O1D
27	6	320	CHL	CAD-CBD-CGD-O1D
27	7	316	CHL	CAD-CBD-CGD-O1D
27	7	317	CHL	CAD-CBD-CGD-O1D
27	b	314	CHL	CAD-CBD-CGD-O1D
24	A	812	LHG	O10-C23-C24-C25
27	b	312	CHL	CAA-CBA-CGA-O1A
24	8	305	LHG	C11-C10-C9-C8
24	a	305	LHG	O8-C23-C24-C25
27	F	309	CHL	CAA-CBA-CGA-O2A
27	3	311	CHL	CAA-CBA-CGA-O2A
27	5	313	CHL	C11-C10-C8-C9
27	B	819	CHL	C4C-C3C-CAC-CBC
20	A	801	PQN	C18-C20-C21-C22
27	A	839	CHL	C5-C6-C7-C8
27	B	815	CHL	C10-C11-C12-C13
27	3	310	CHL	C8-C10-C11-C12
27	A	836	CHL	CAA-CBA-CGA-O1A
24	4	303	LHG	C29-C30-C31-C32
27	A	834	CHL	C2A-CAA-CBA-CGA
27	a	307	CHL	C2A-CAA-CBA-CGA
24	A	811	LHG	C11-C10-C9-C8
24	A	810	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
27	B	823	CHL	C5-C6-C7-C8
27	B	837	CHL	C5-C6-C7-C8
24	A	810	LHG	C18-C19-C20-C21
30	a	301	LMG	C14-C15-C16-C17
24	8	305	LHG	C30-C31-C32-C33
35	8	306	DGA	CB4-CB5-CB6-CB7
27	7	314	CHL	C4-C3-C5-C6
27	A	818	CHL	C5-C6-C7-C8
29	5	303	LUT	C27-C28-C29-C39
30	7	301	LMG	C29-C30-C31-C32
20	A	801	PQN	C22-C23-C25-C26
20	B	801	PQN	C16-C17-C18-C20
26	A	815	CL0	C12-C13-C15-C16
27	A	826	CHL	C11-C10-C8-C7
27	B	818	CHL	C2-C3-C5-C6
27	B	846	CHL	C11-C10-C8-C7
27	3	316	CHL	C3A-C2A-CAA-CBA
27	4	309	CHL	C3A-C2A-CAA-CBA
27	8	325	CHL	C3A-C2A-CAA-CBA
27	A	858	CHL	CAA-CBA-CGA-O1A
27	a	320	CHL	CAA-CBA-CGA-O1A
27	4	307	CHL	CAA-CBA-CGA-O1A
27	4	311	CHL	CAA-CBA-CGA-O1A
27	A	858	CHL	CAA-CBA-CGA-O2A
27	B	826	CHL	CAA-CBA-CGA-O2A
27	8	315	CHL	CAA-CBA-CGA-O2A
22	I	801	BCR	C7-C8-C9-C10
22	3	302	BCR	C11-C12-C13-C14
27	B	826	CHL	CAA-CBA-CGA-O1A
27	8	316	CHL	CAA-CBA-CGA-O1A
27	b	313	CHL	CAA-CBA-CGA-O1A
22	3	303	BCR	C15-C16-C17-C18
24	A	812	LHG	O8-C23-C24-C25
27	a	310	CHL	CAA-CBA-CGA-O2A
27	7	320	CHL	CAA-CBA-CGA-O2A
27	3	311	CHL	C10-C11-C12-C13
30	J	104	LMG	O10-C28-O8-C9
27	7	324	CHL	C2C-C3C-CAC-CBC
30	J	101	LMG	O10-C28-C29-C30
27	A	828	CHL	C10-C11-C12-C13
24	a	305	LHG	O2-C2-C3-O3
27	B	813	CHL	C2A-CAA-CBA-CGA

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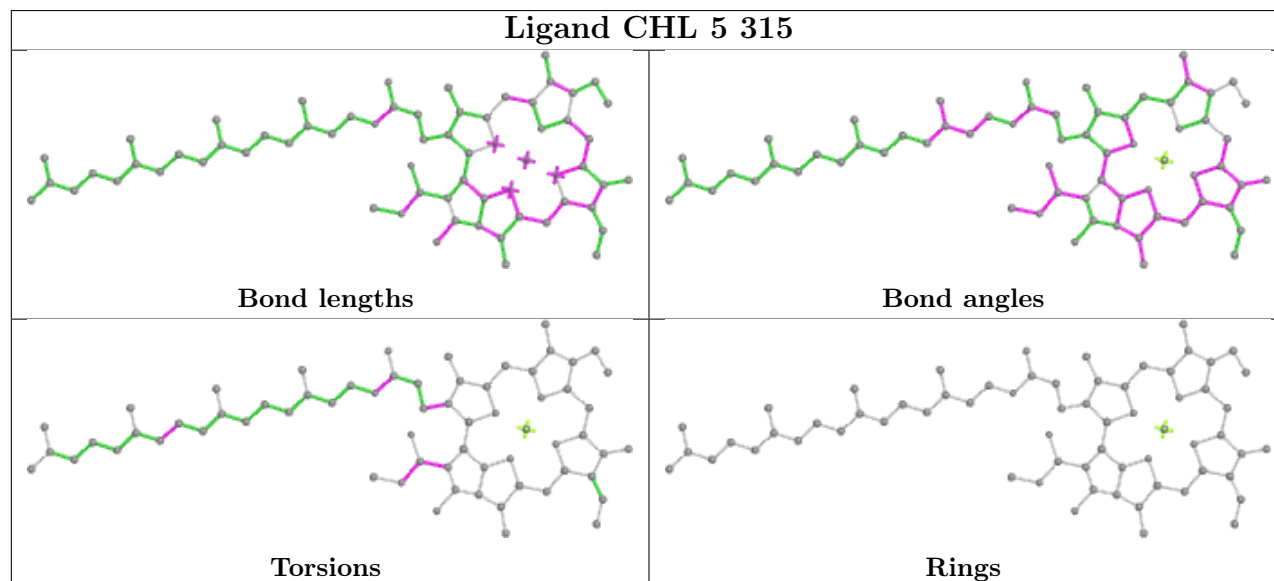
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Mol	Chain	Res	Type	Atoms
27	B	823	CHL	C2A-CAA-CBA-CGA
27	8	316	CHL	C10-C11-C12-C13
27	A	831	CHL	C4-C3-C5-C6
27	A	843	CHL	CAA-CBA-CGA-O2A
27	F	308	CHL	CAA-CBA-CGA-O2A

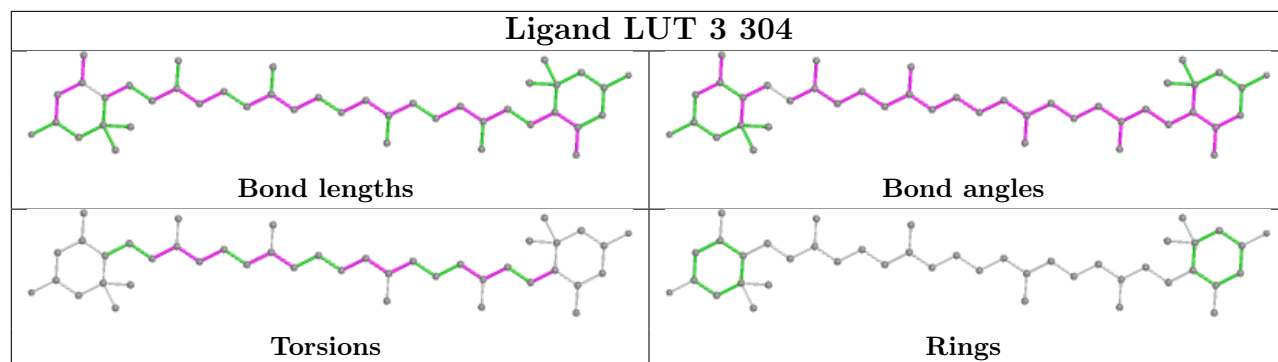
There are no ring outliers.

No monomer is involved in short contacts.

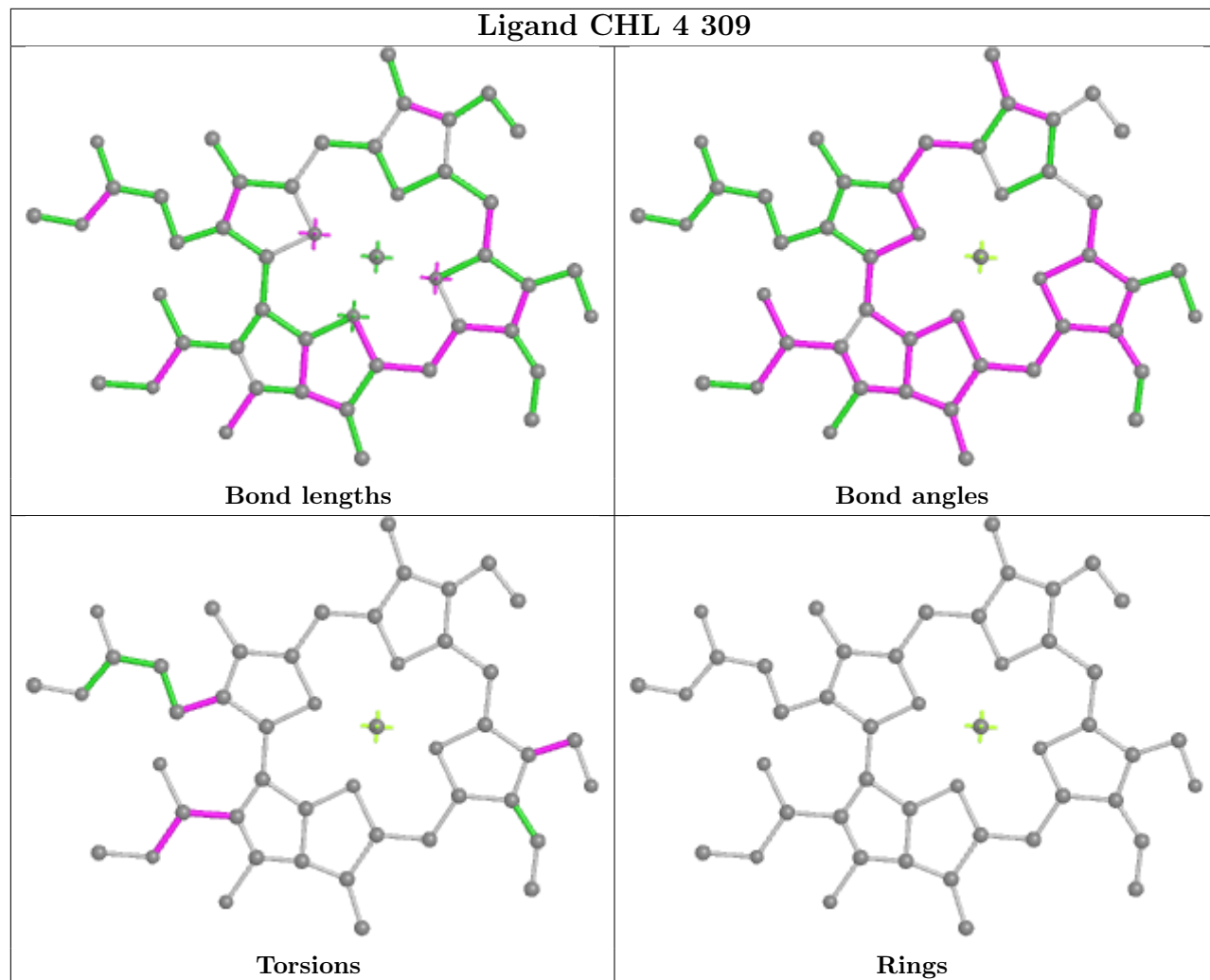
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



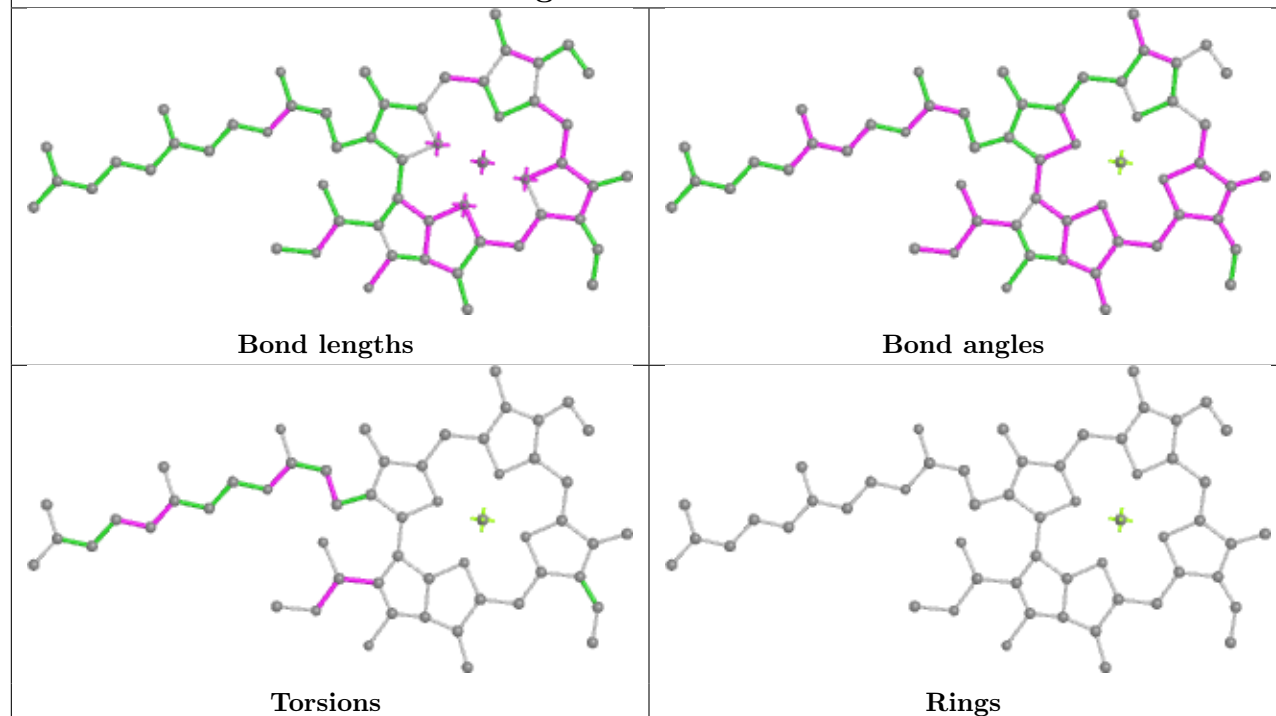
Ligand LUT 3 304



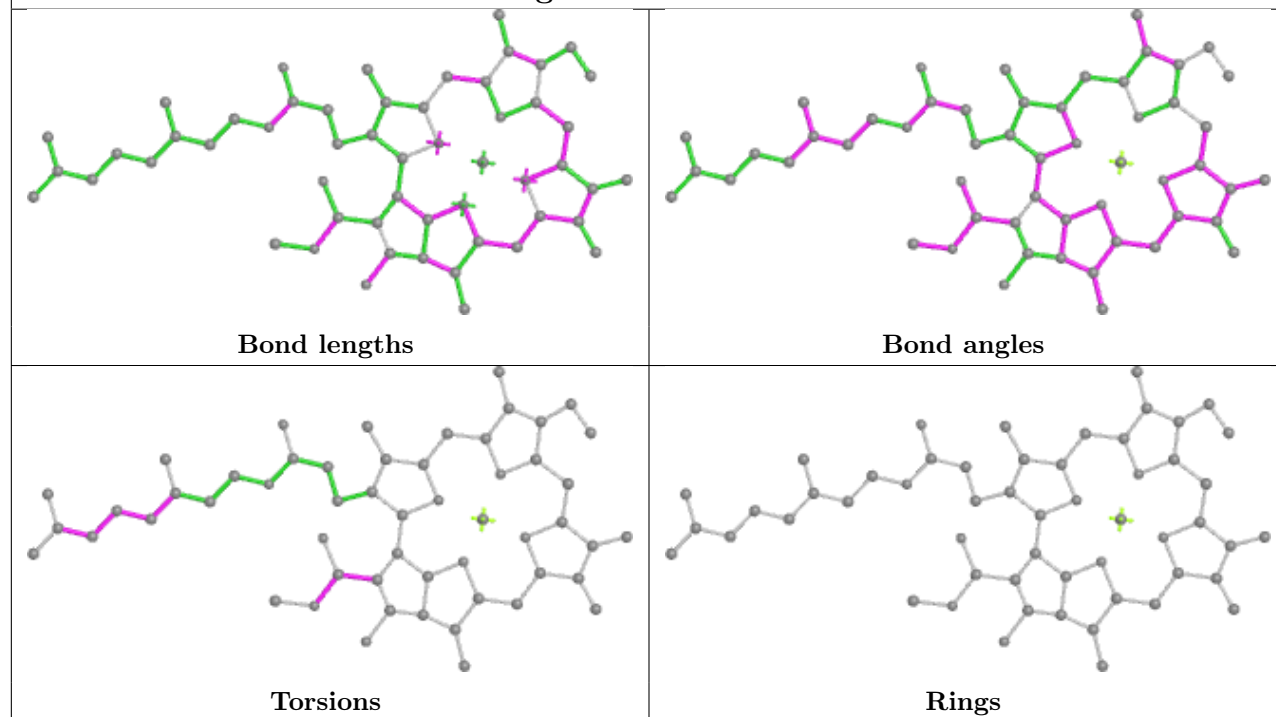
Ligand CHL 4 309



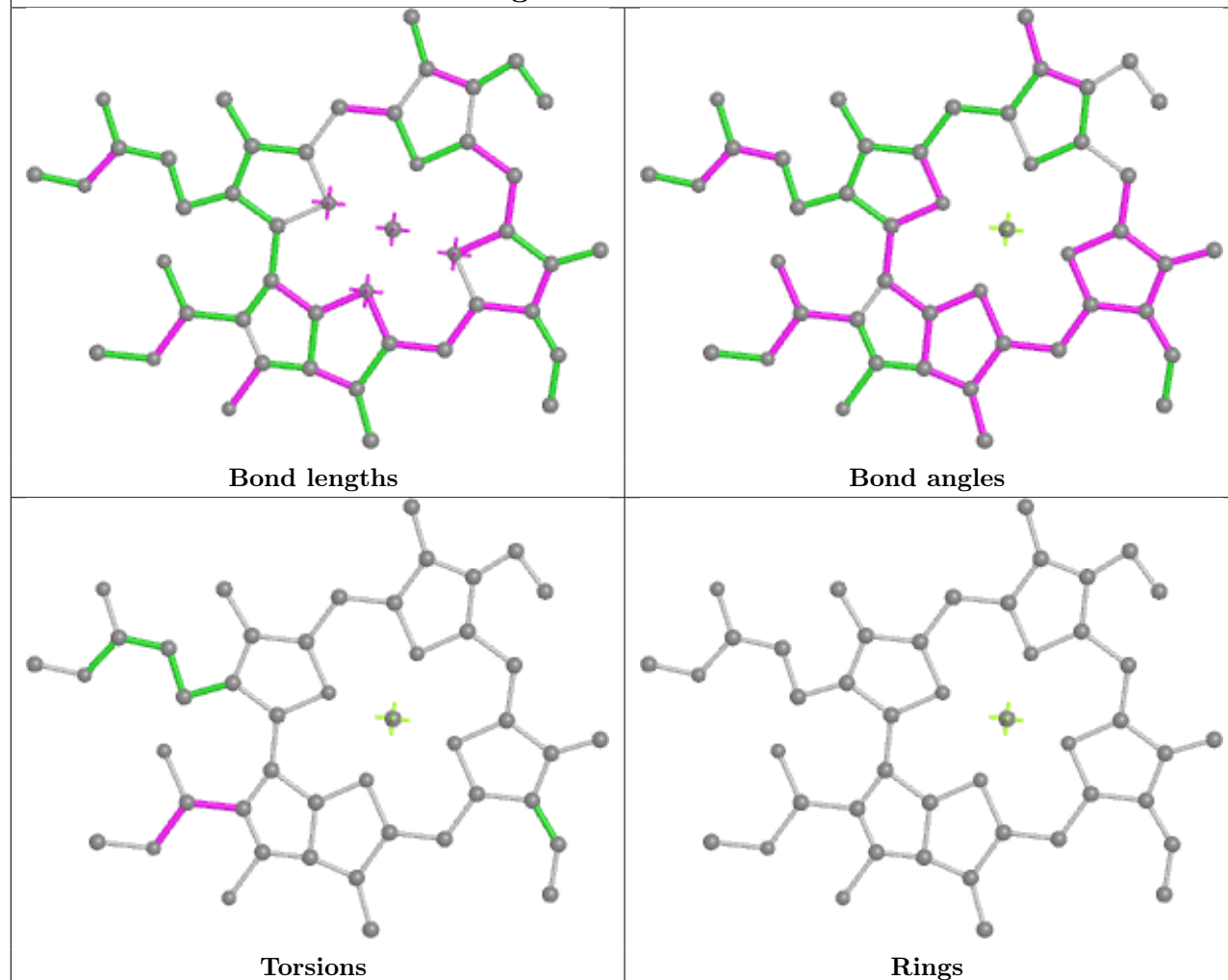
Ligand CHL 6 310



Ligand CHL 7 316



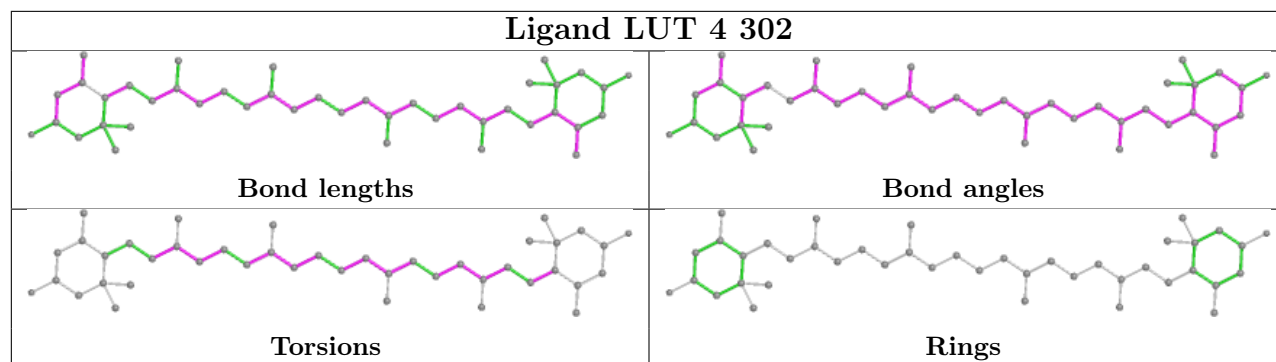
Ligand CHL A 851



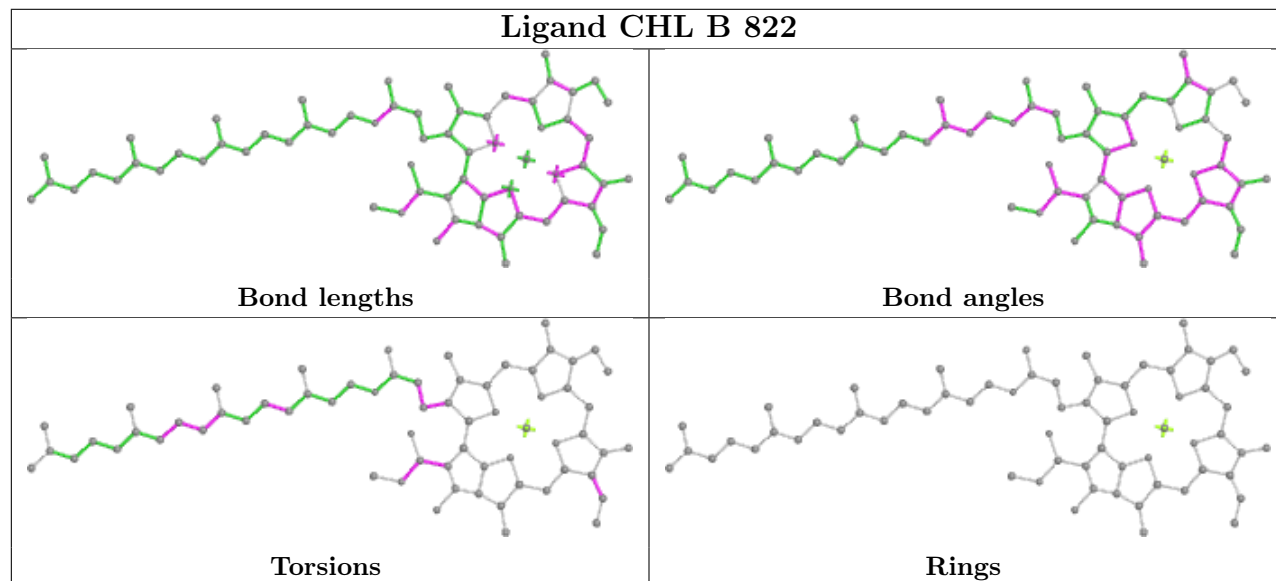
Ligand LUT 7 304



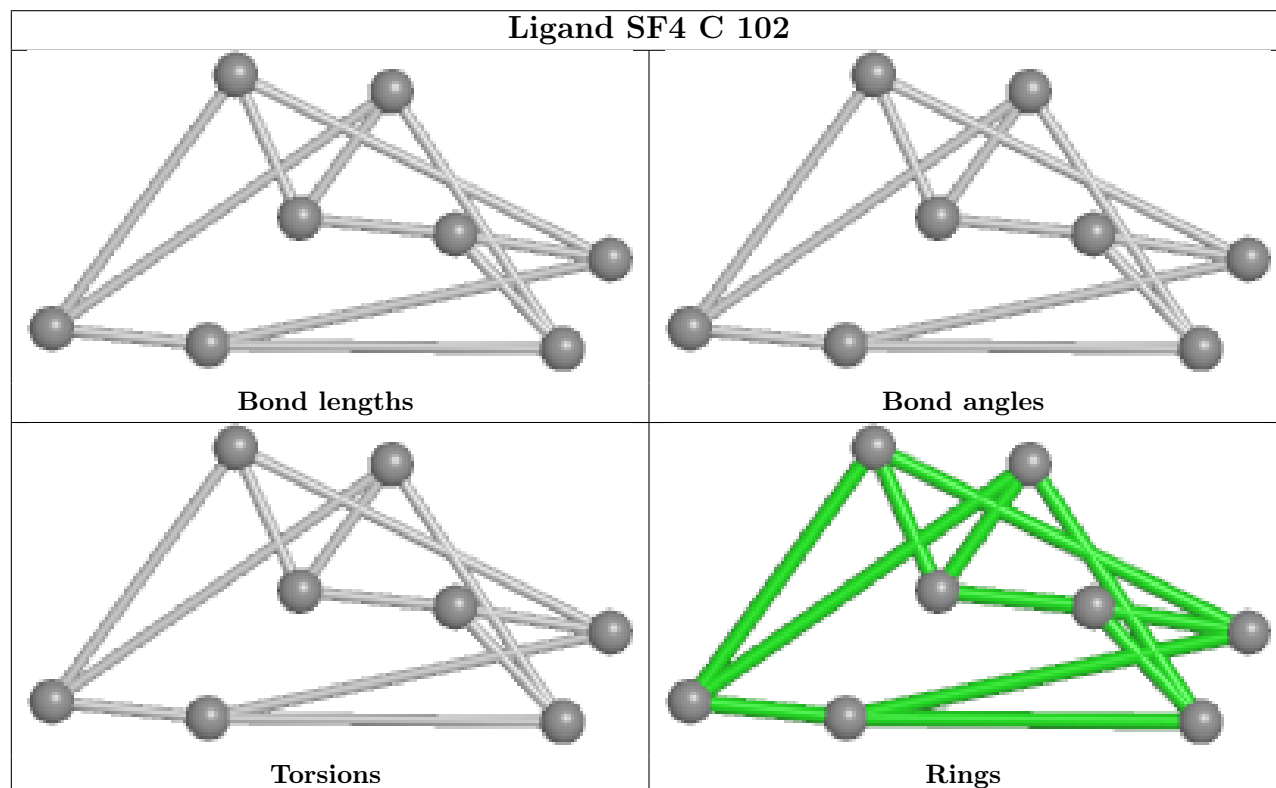
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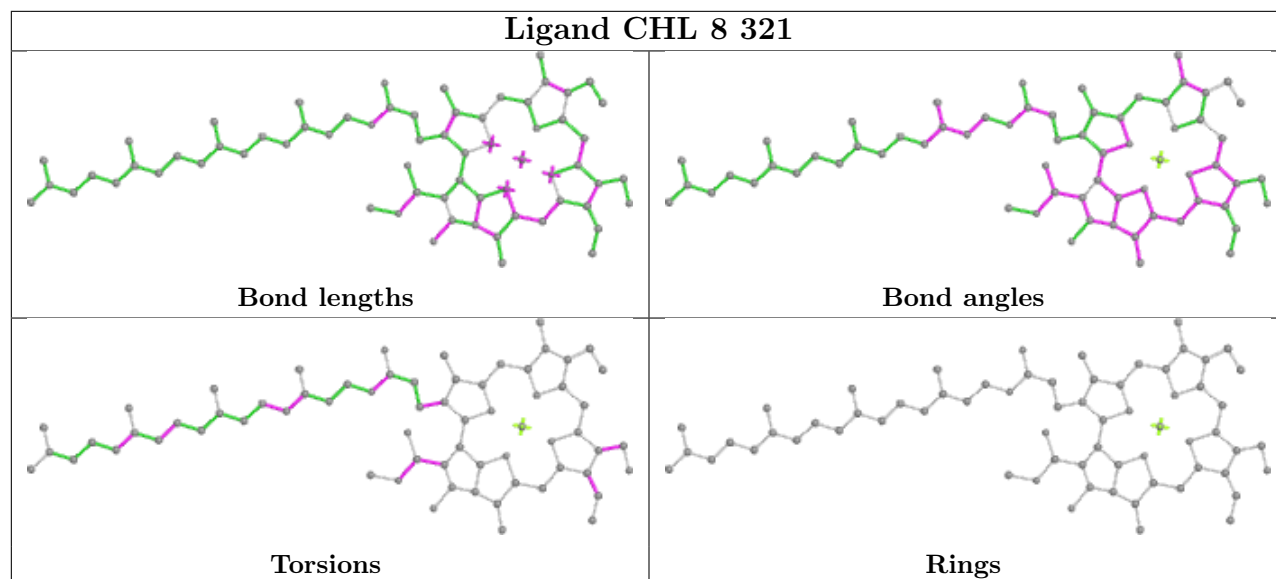
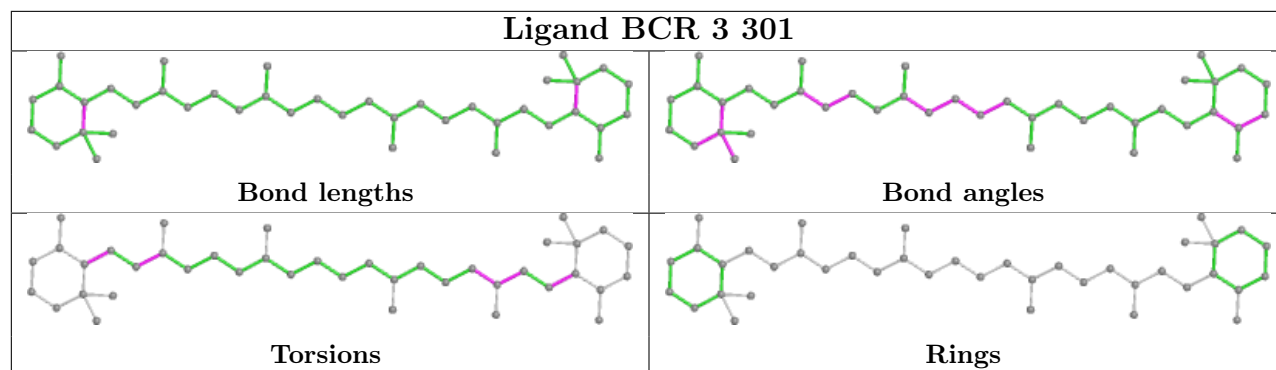


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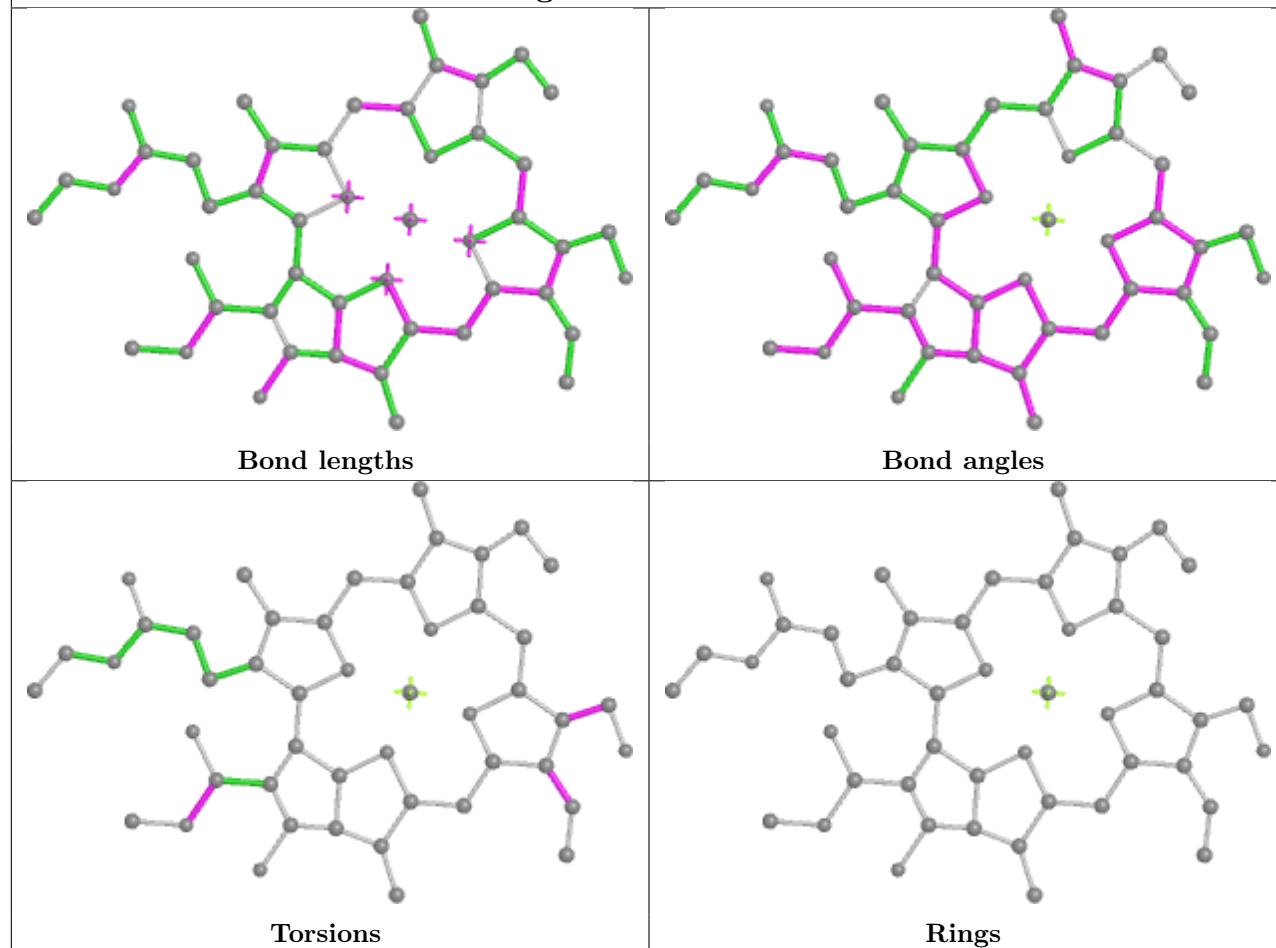


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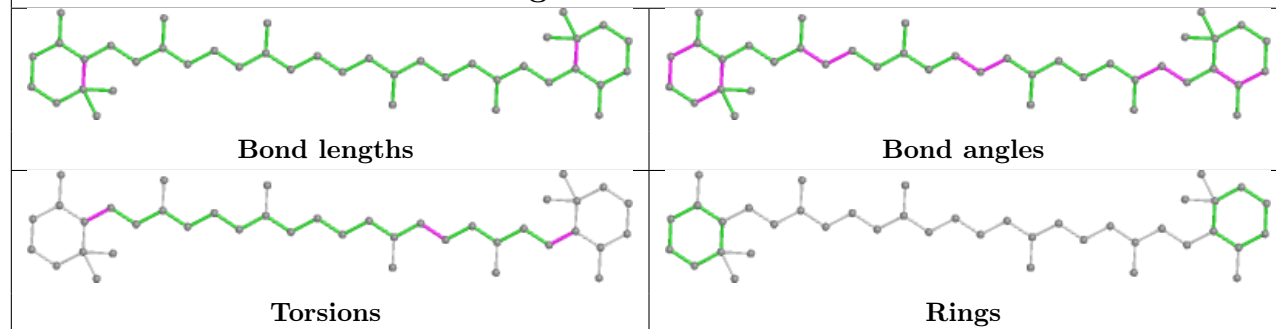


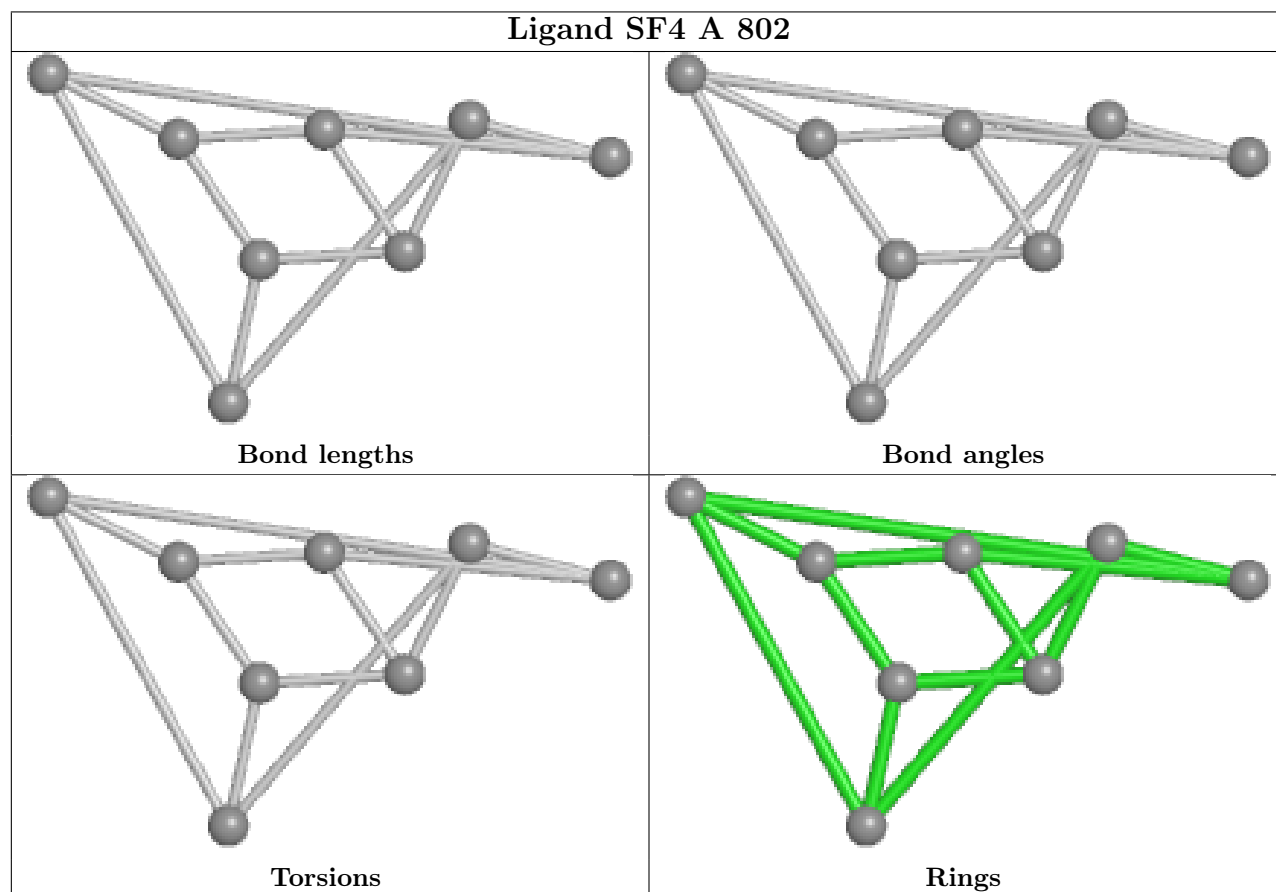
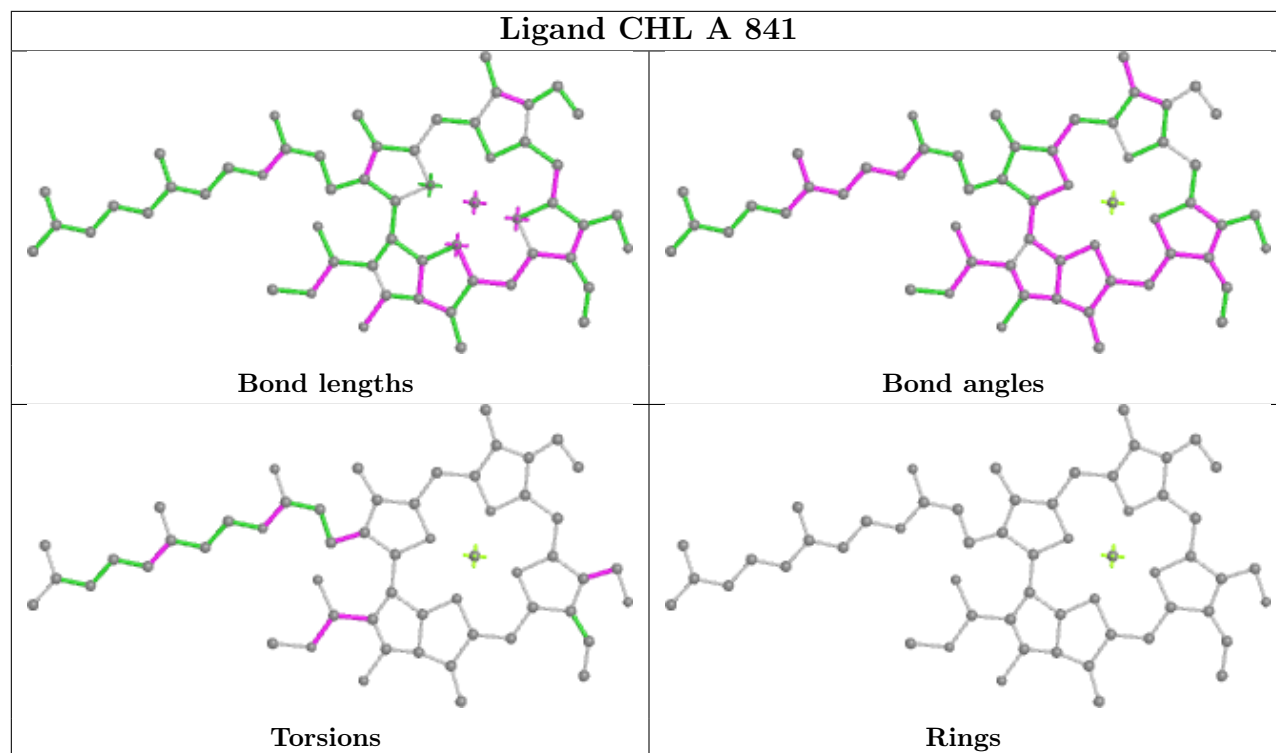


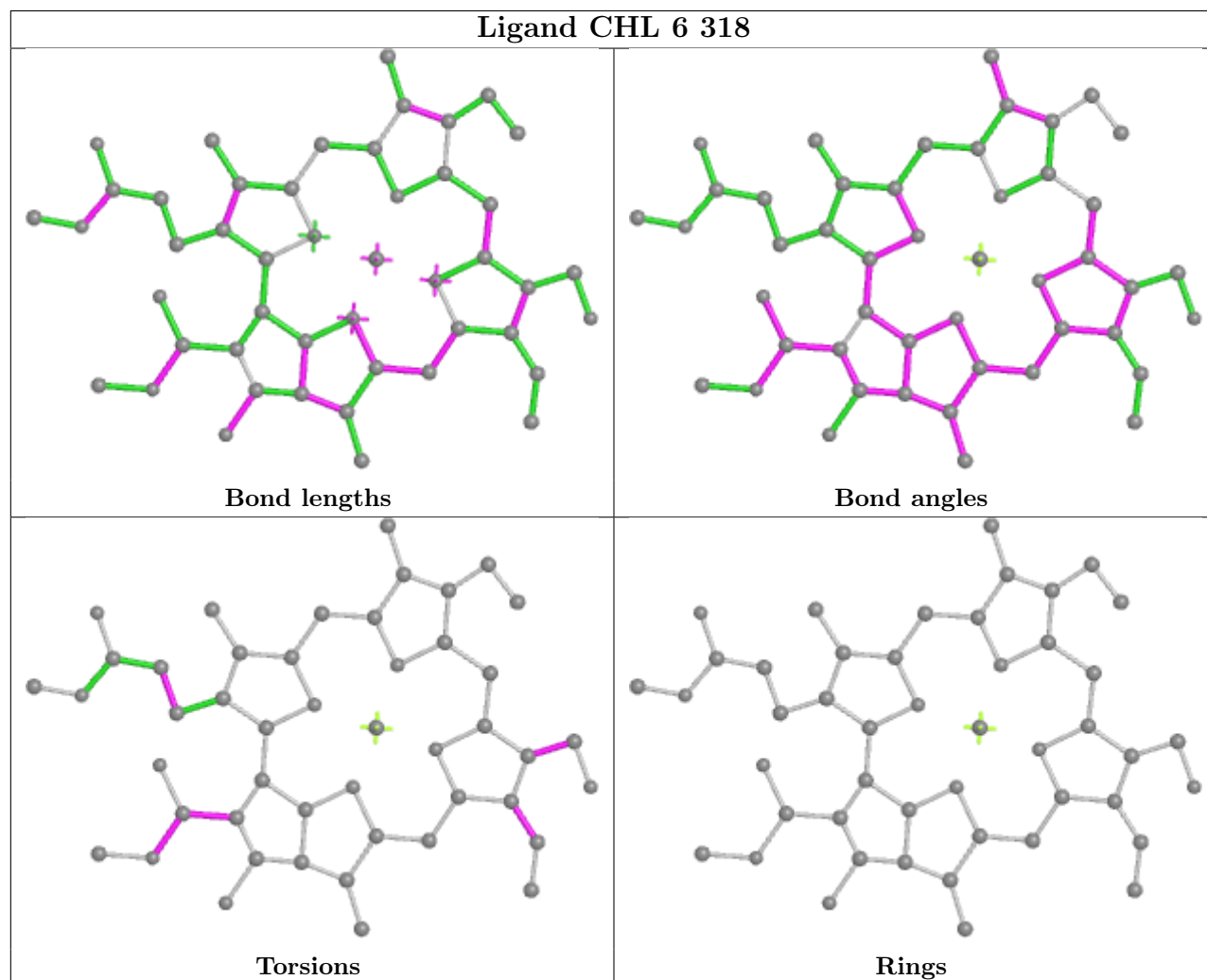
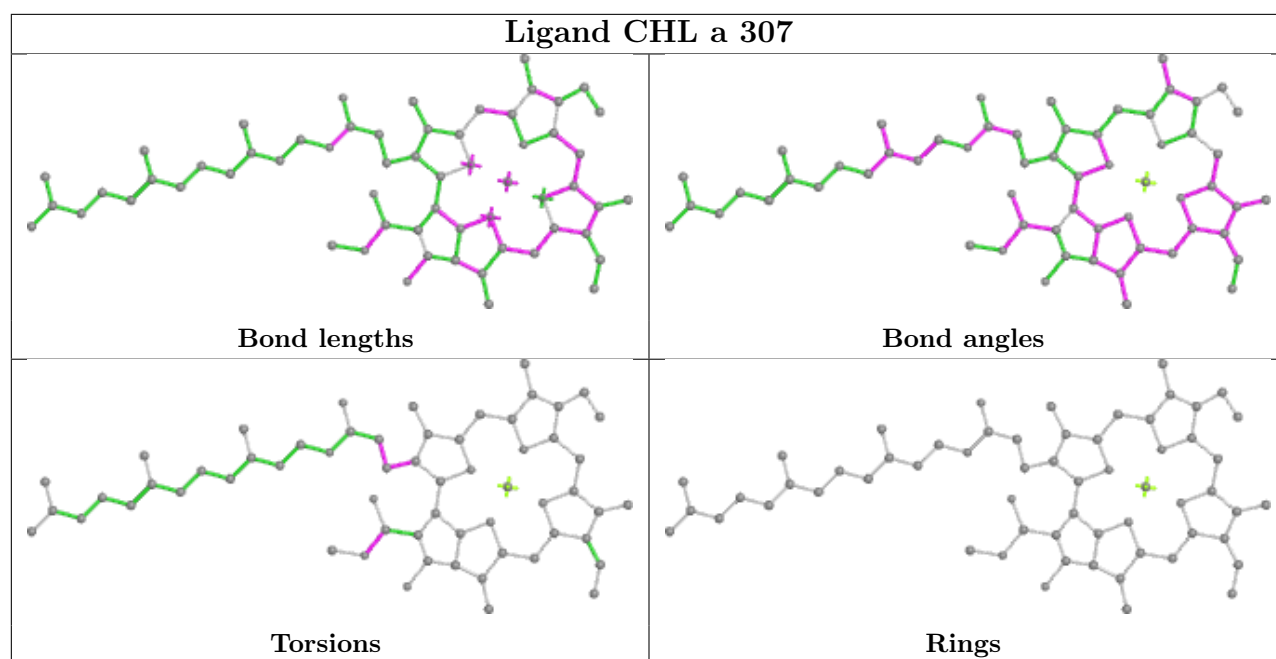
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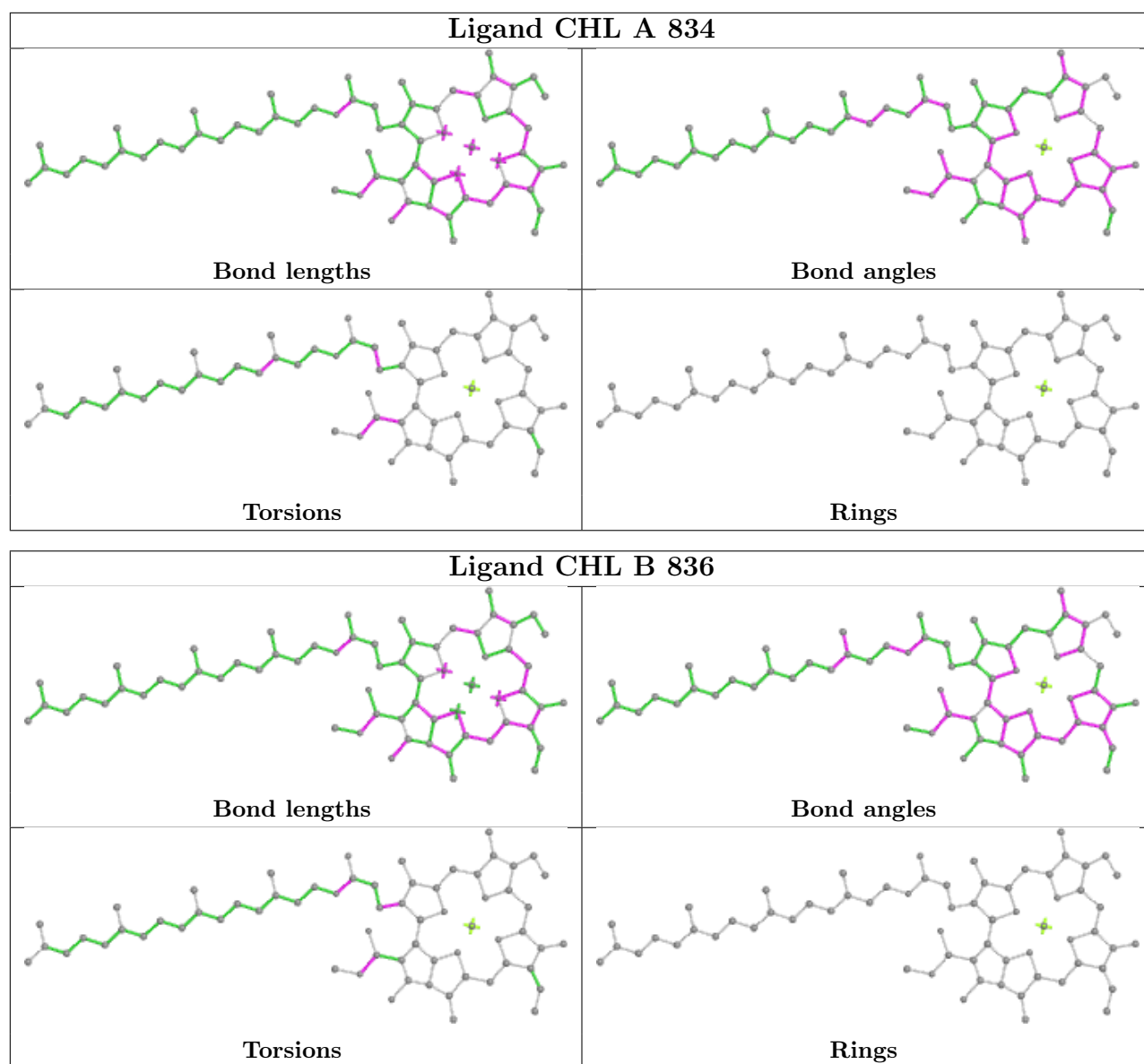


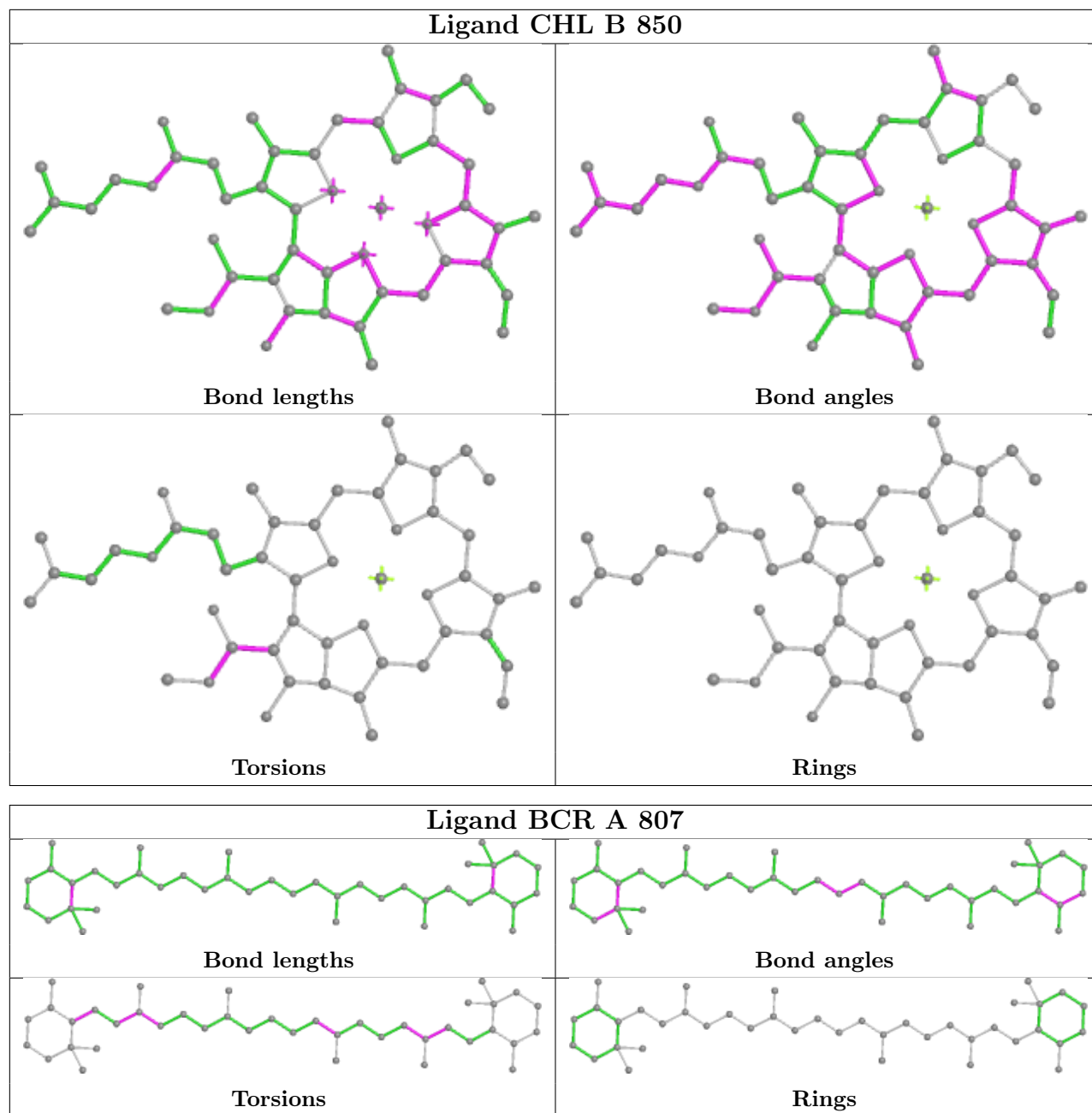
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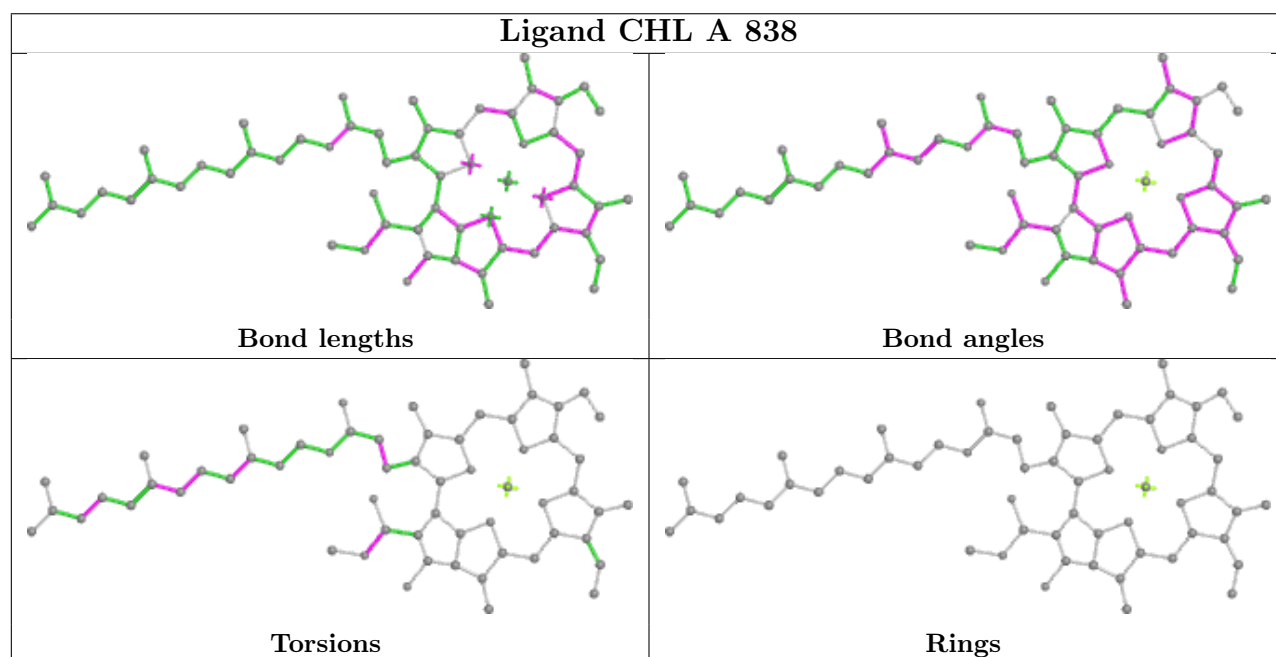
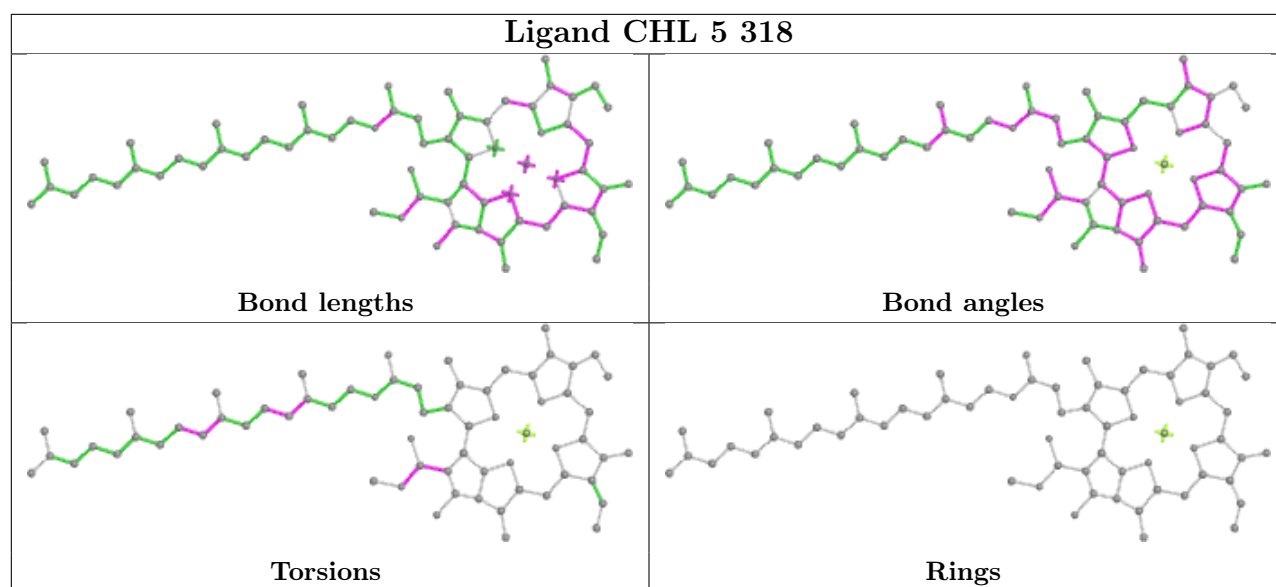




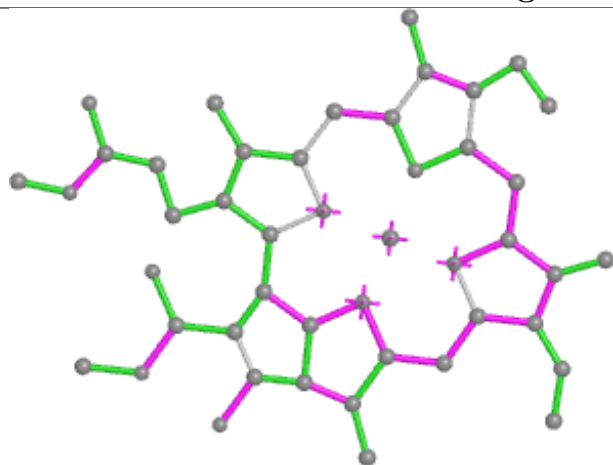




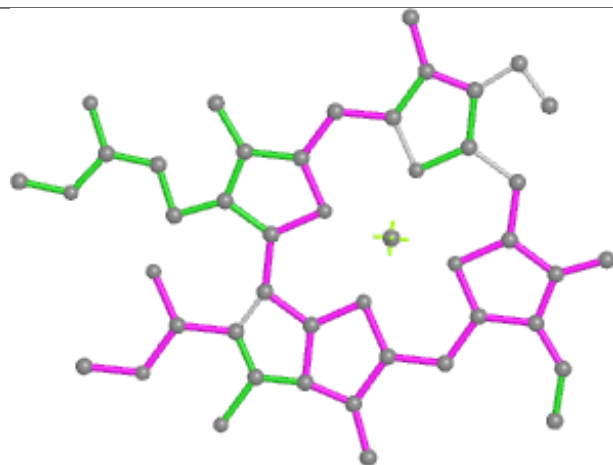




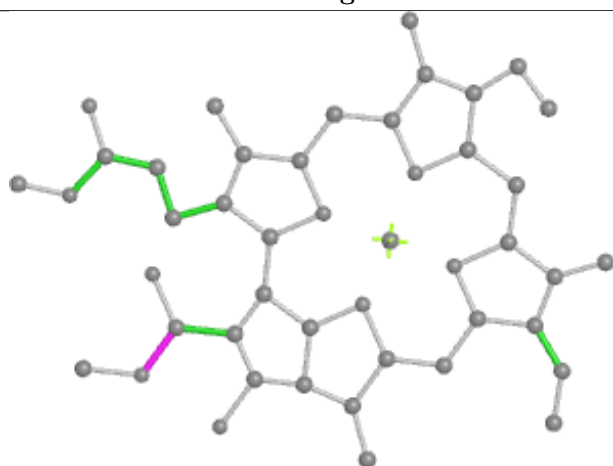
Ligand CHL 5 320



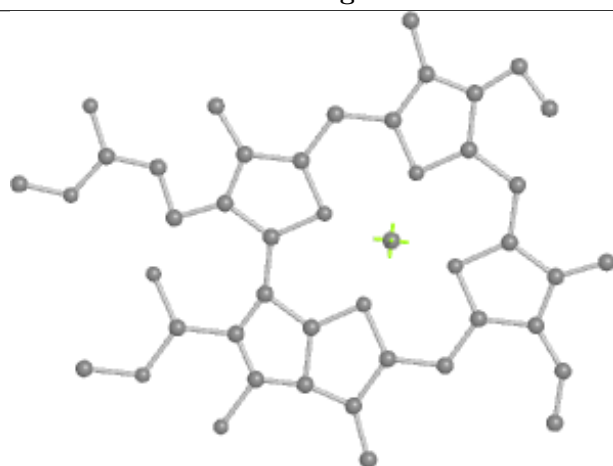
Bond lengths



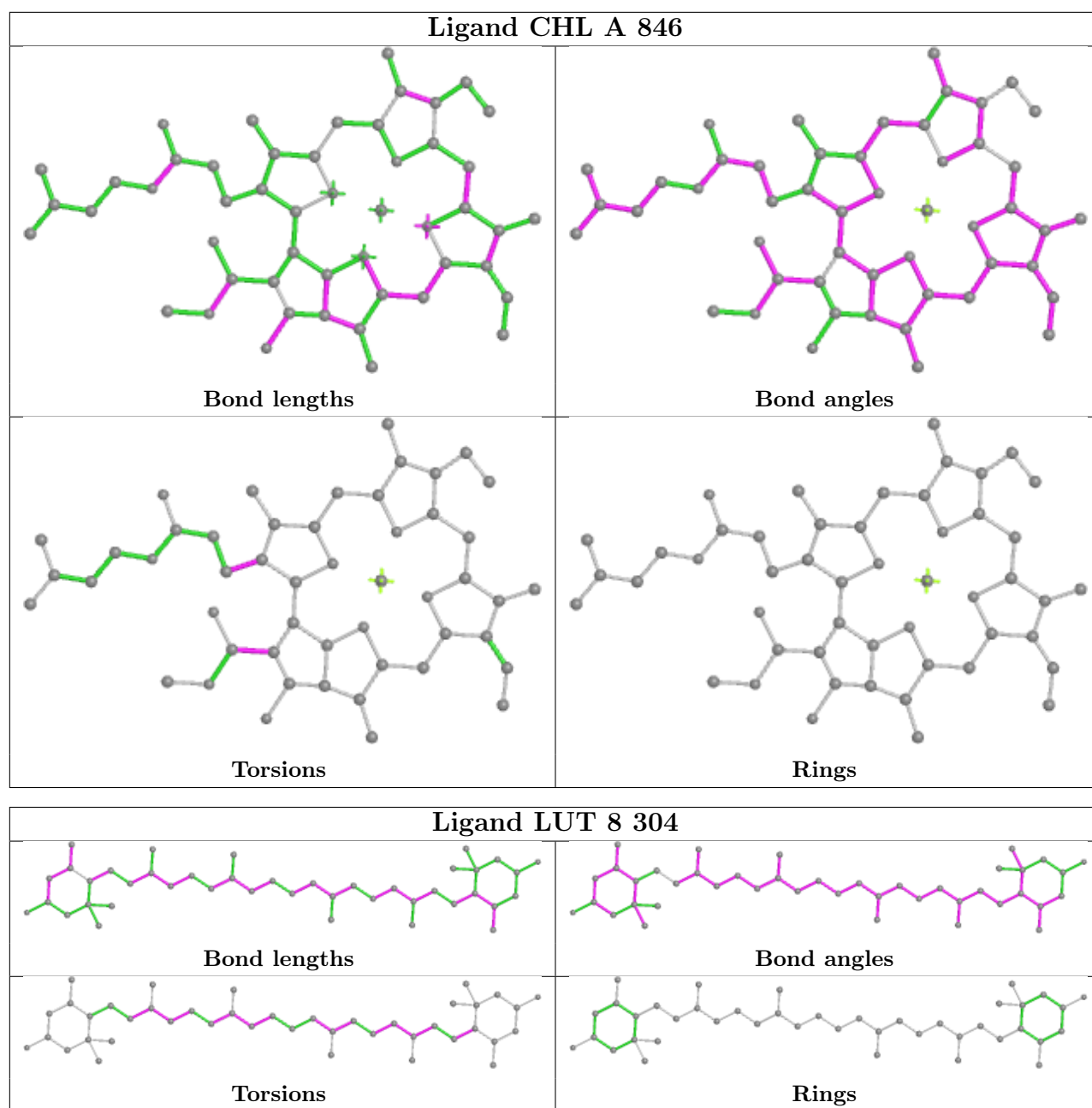
Bond angles

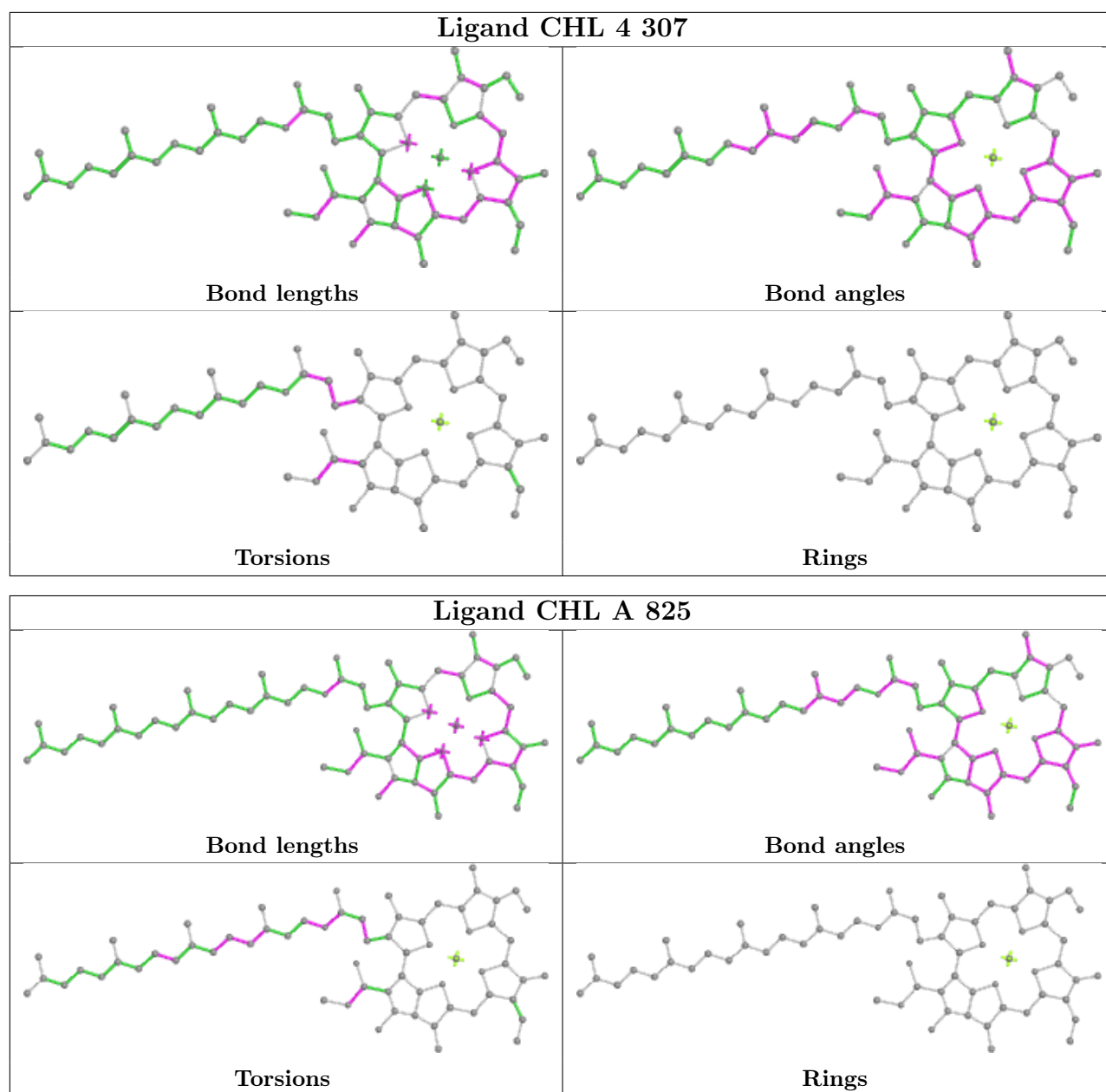


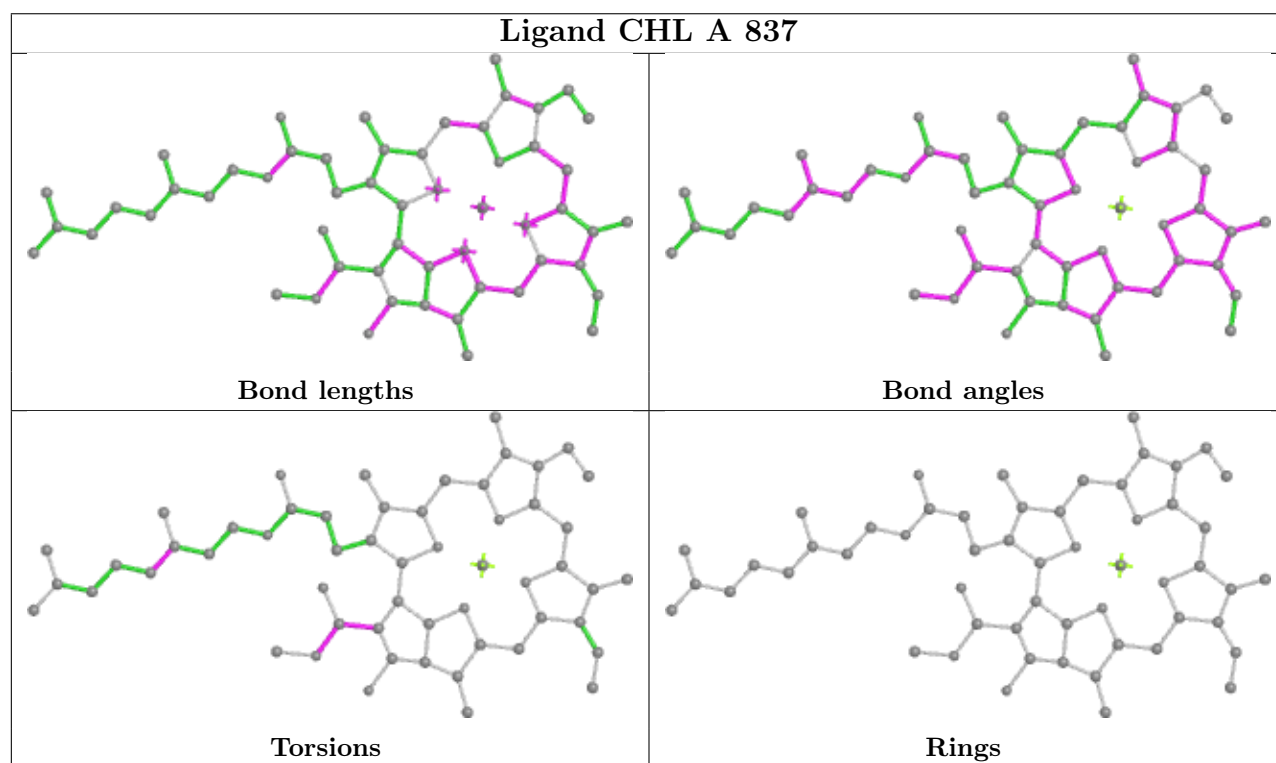
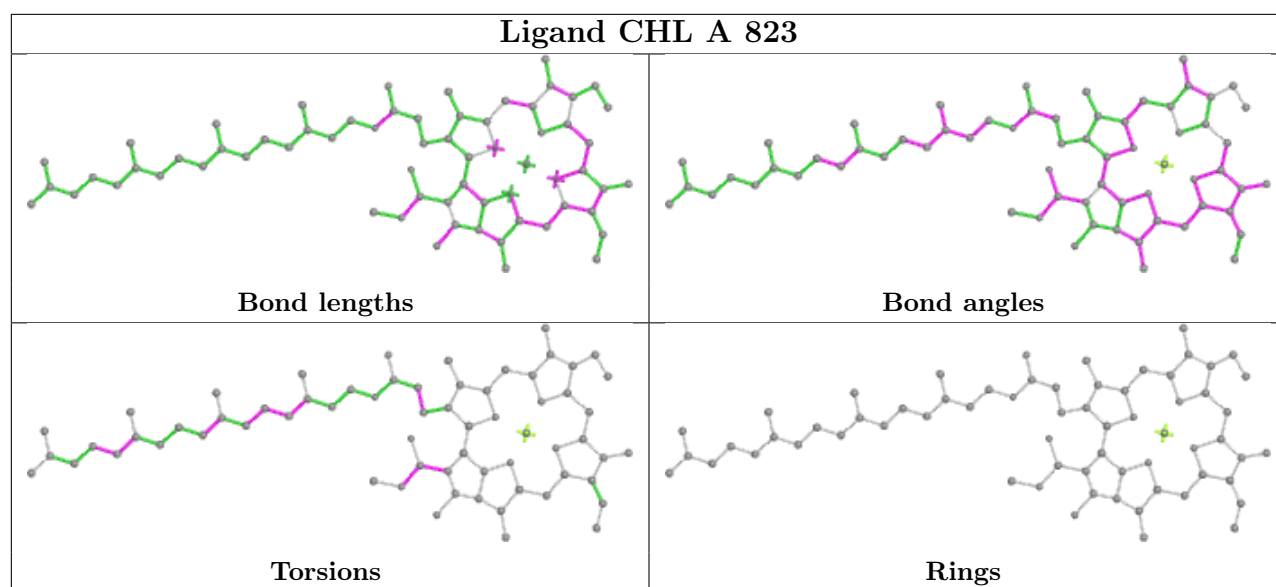
Torsions



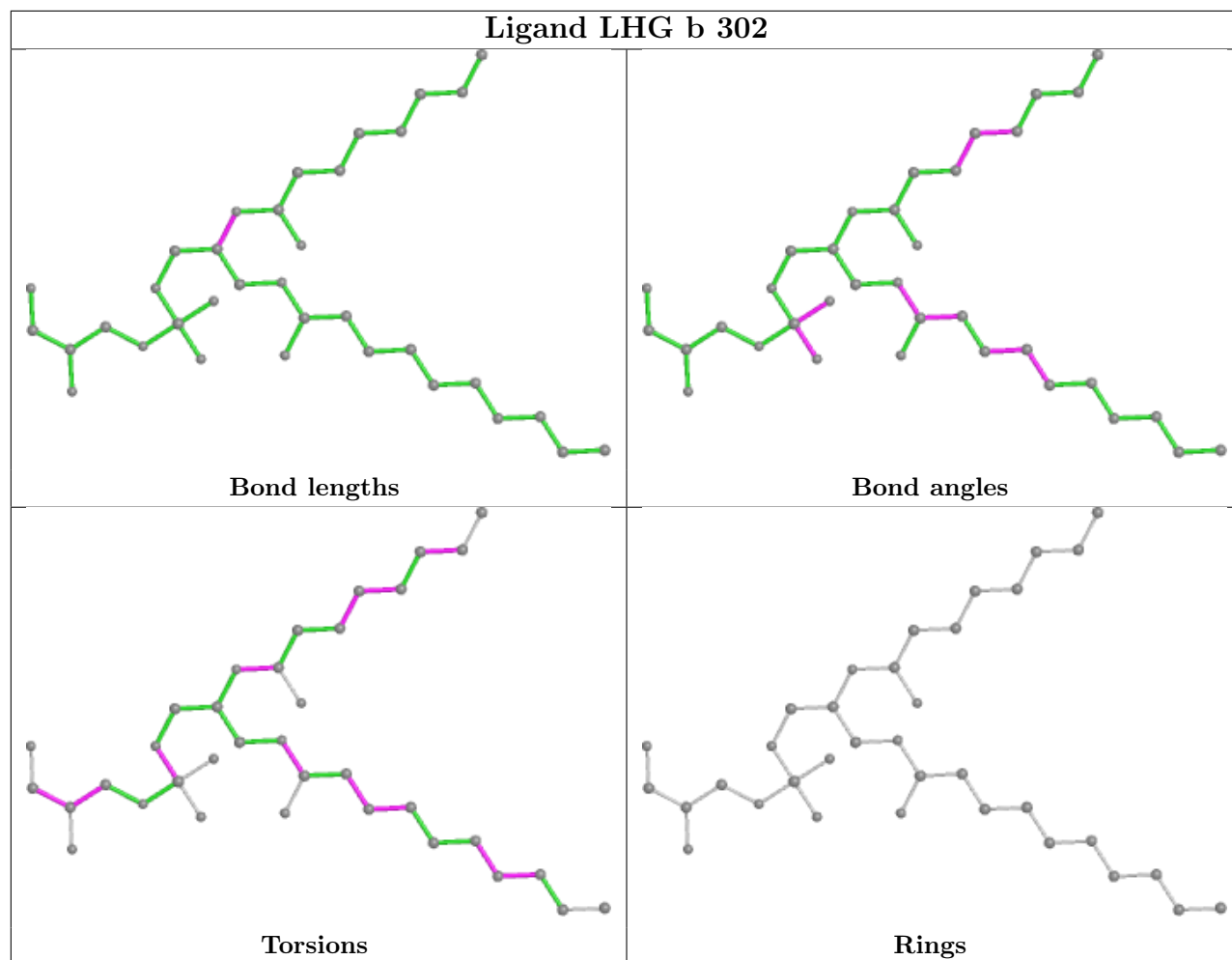
Rings



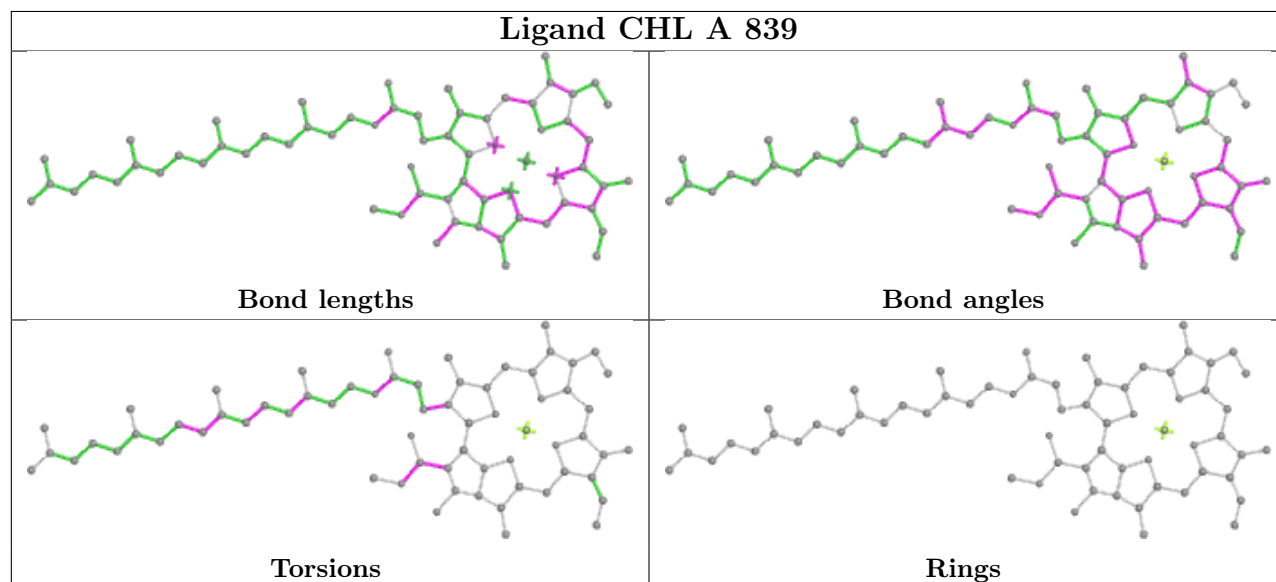


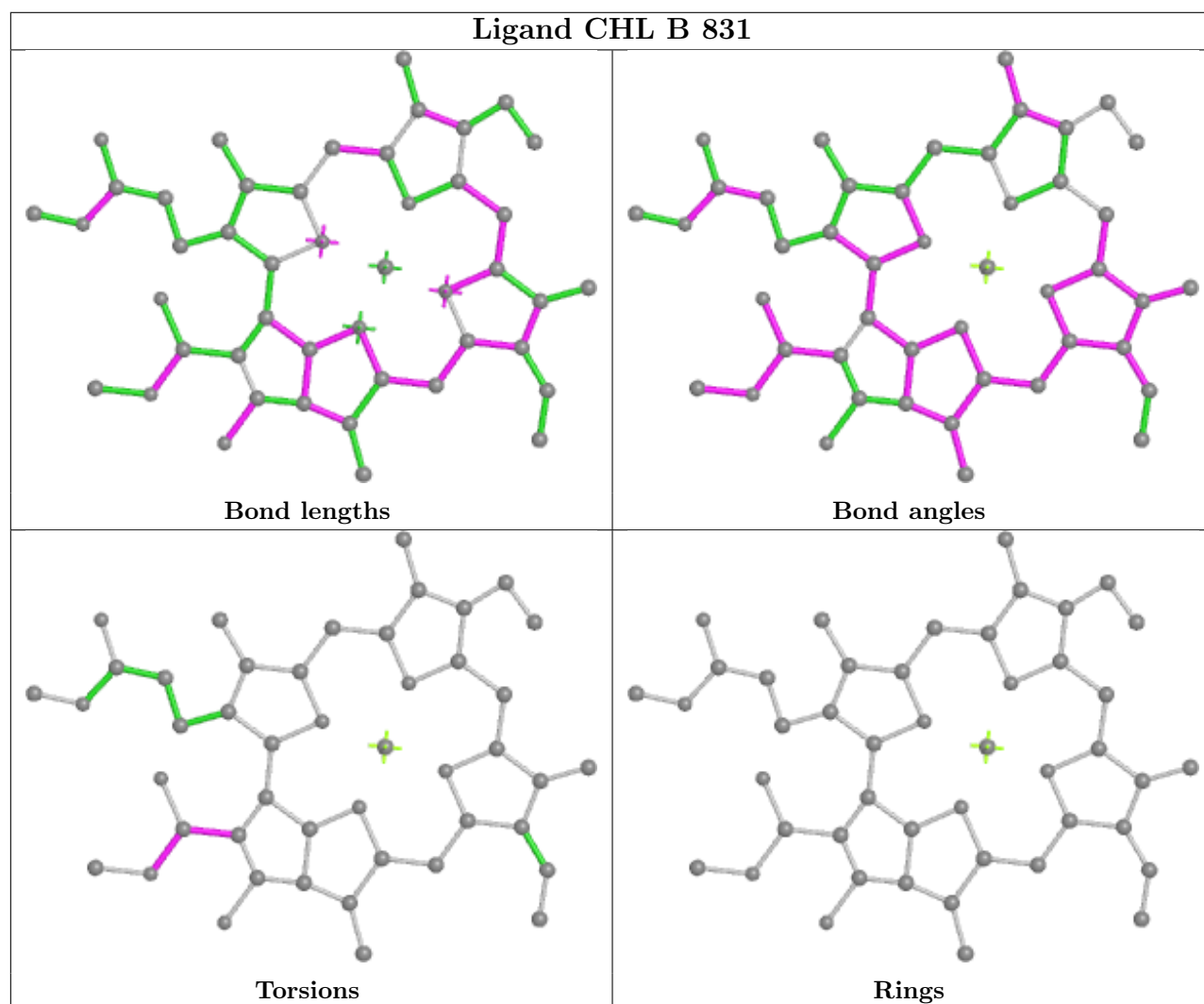
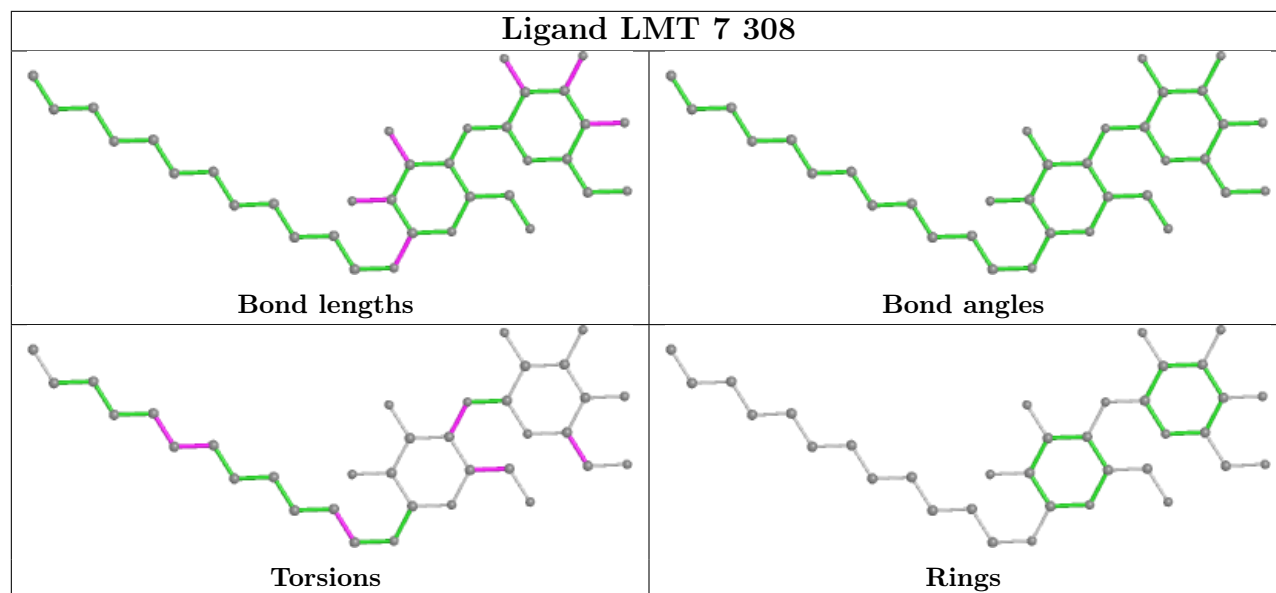


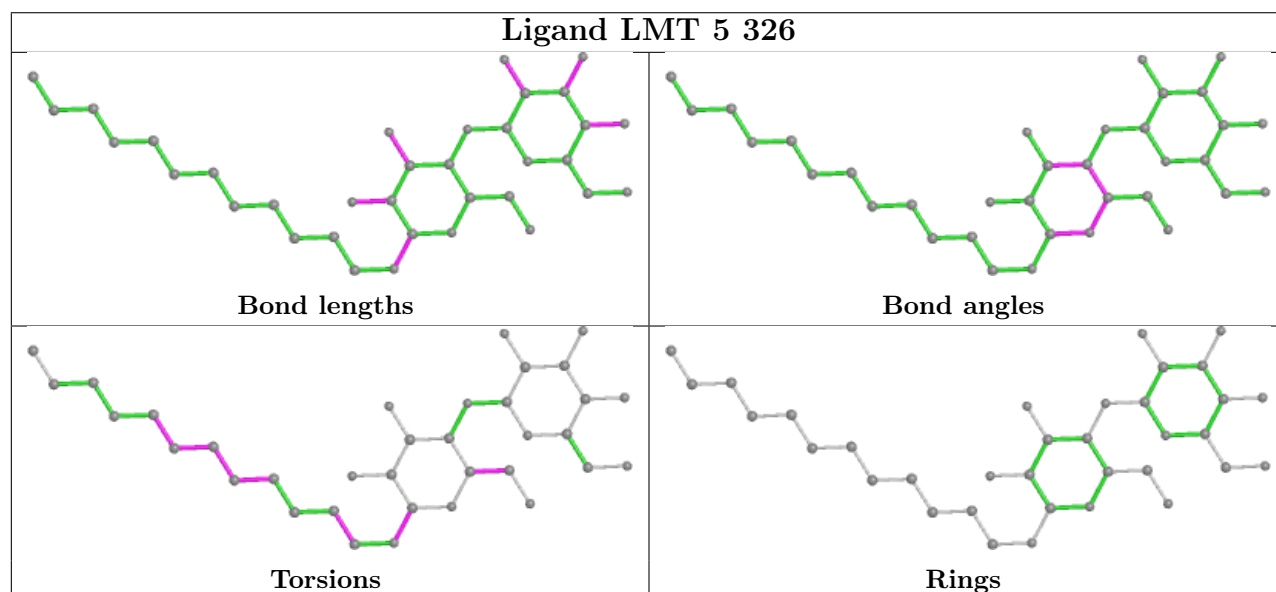
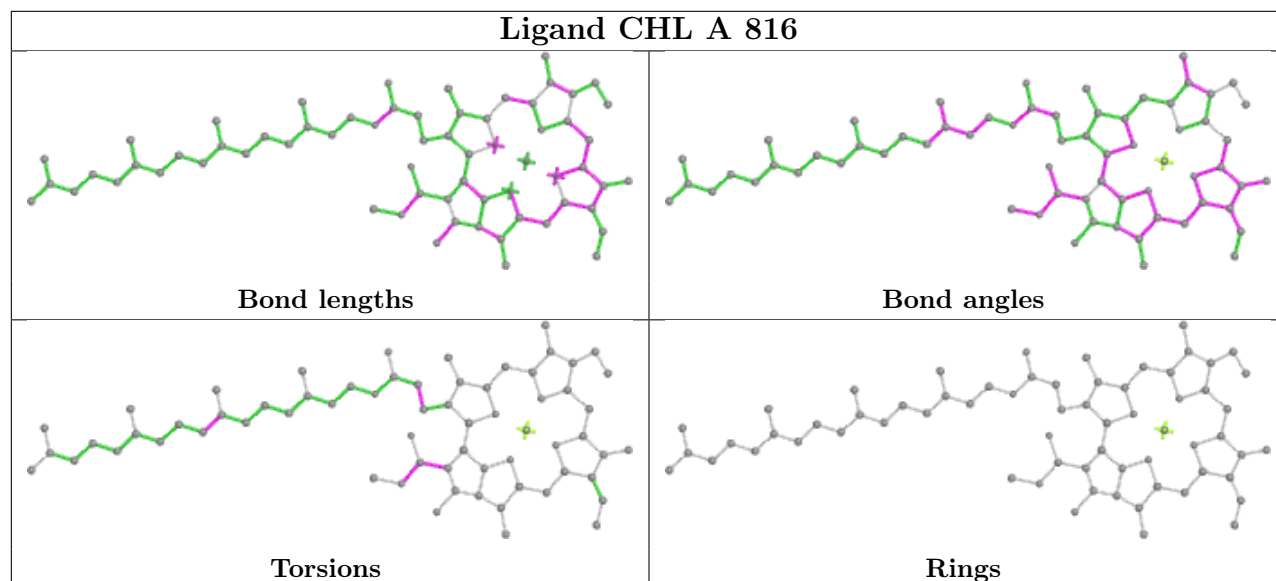
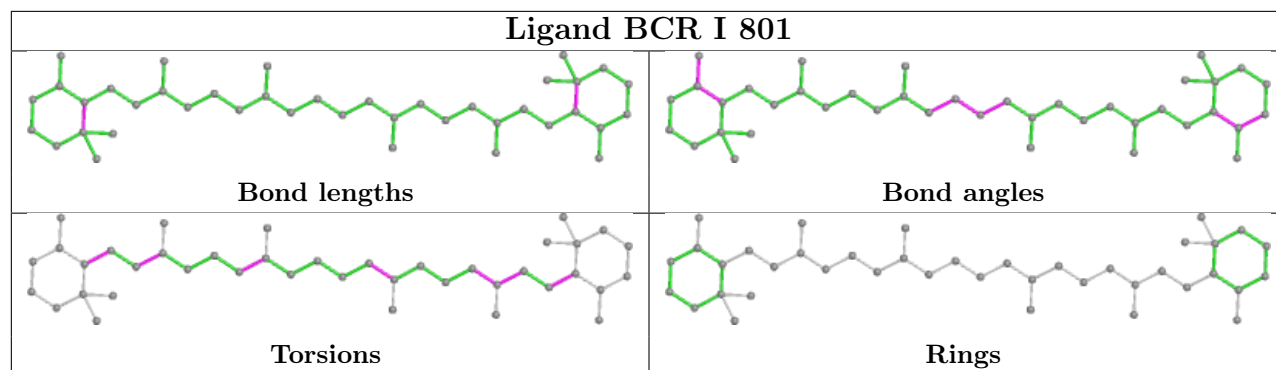
Ligand LHG b 302

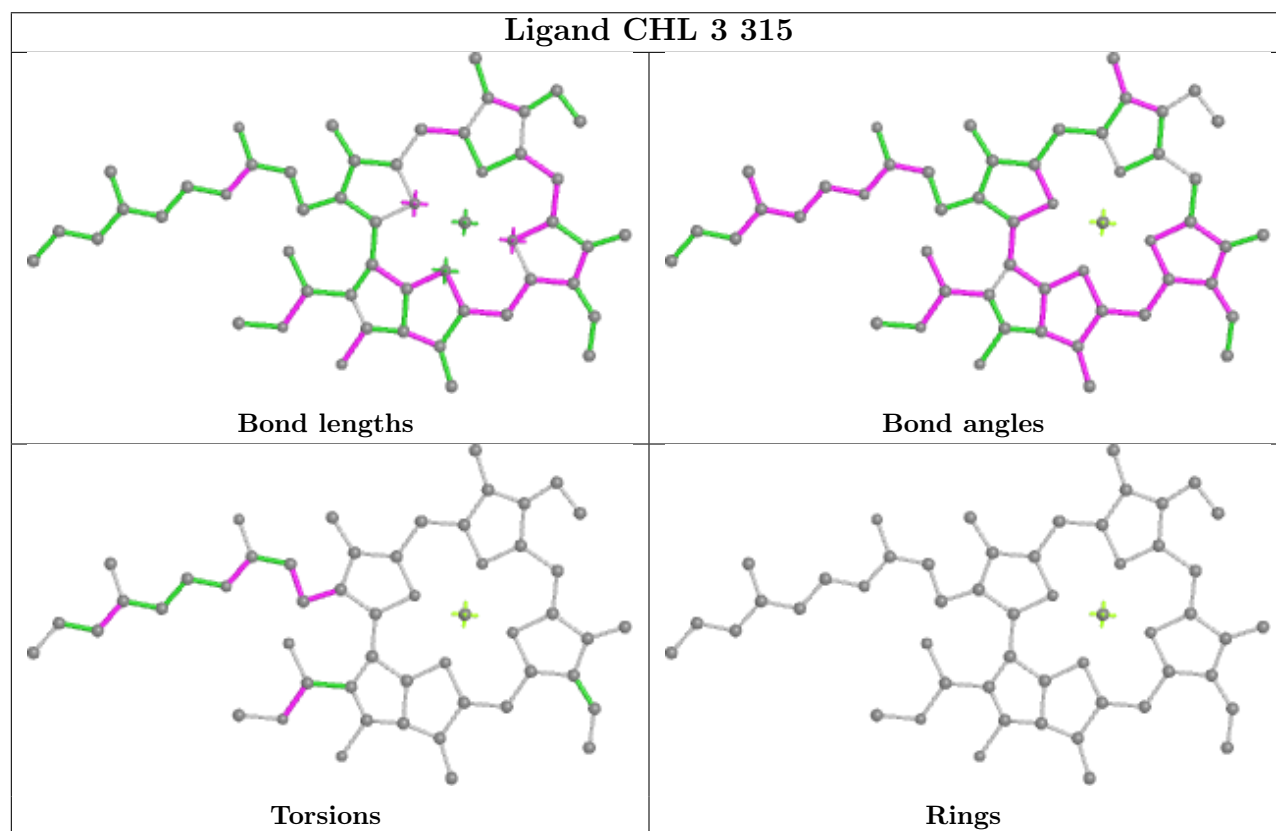
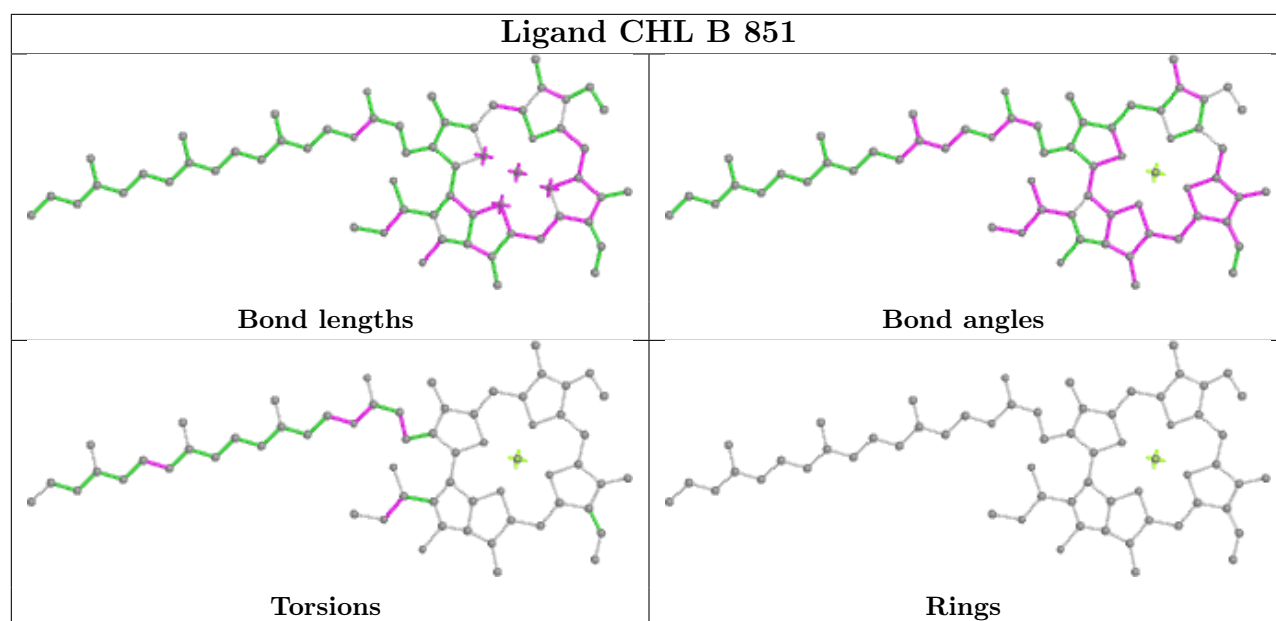


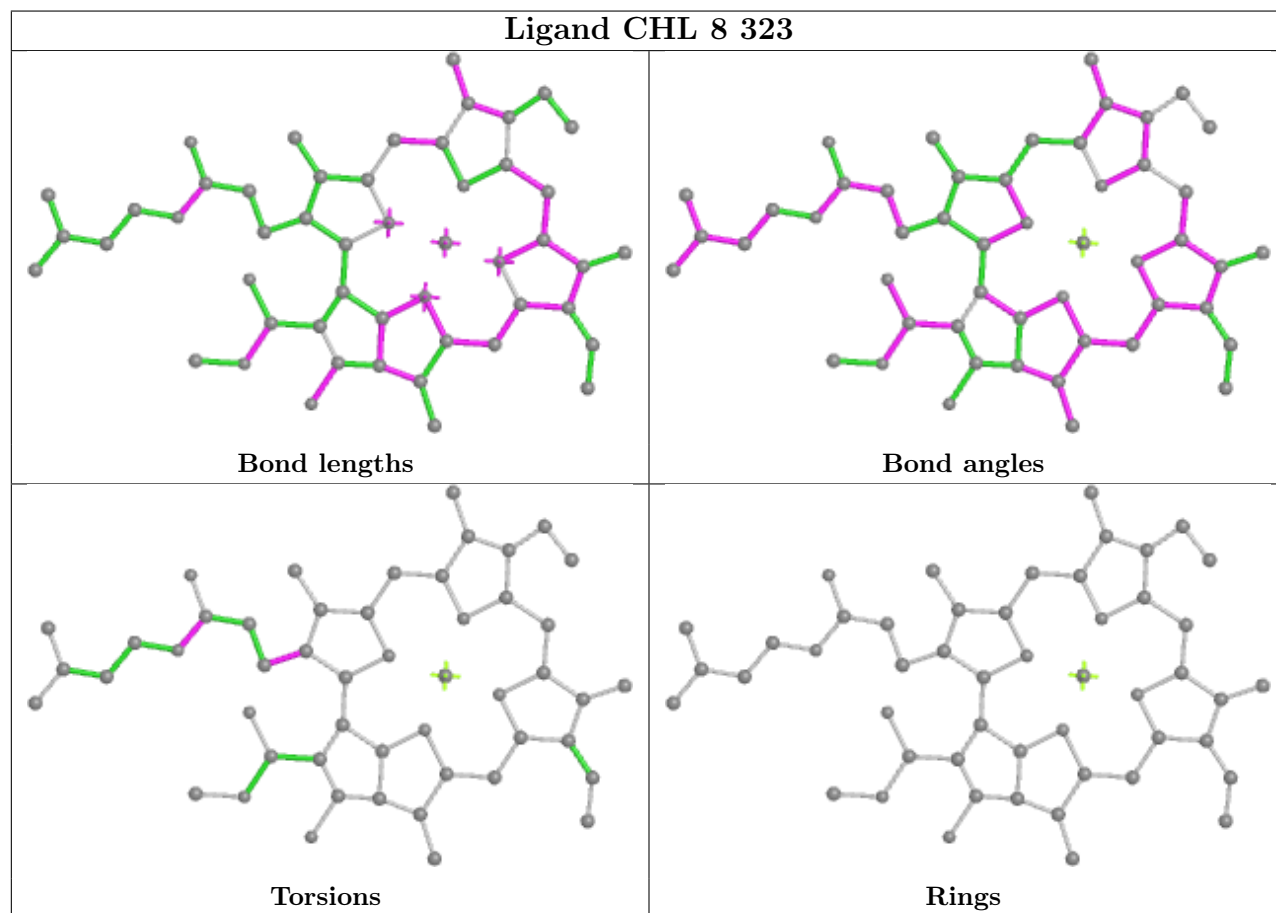
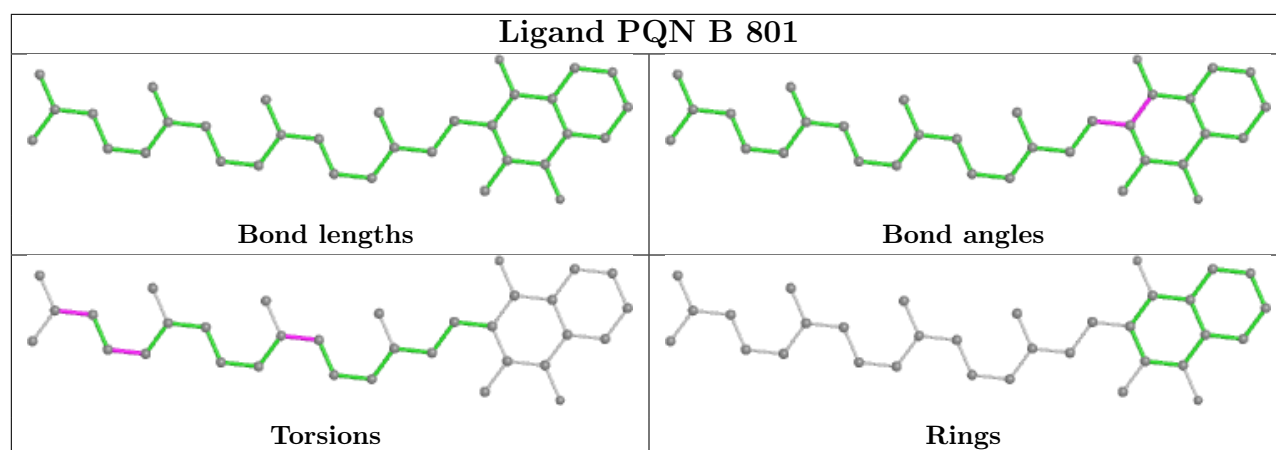
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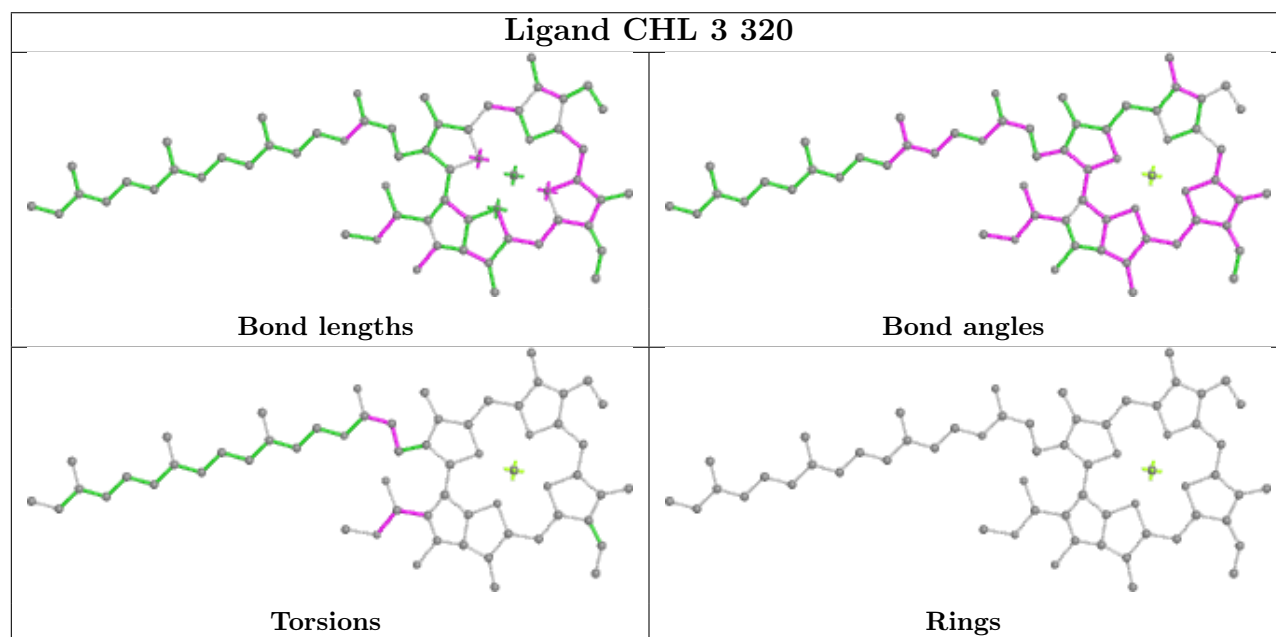
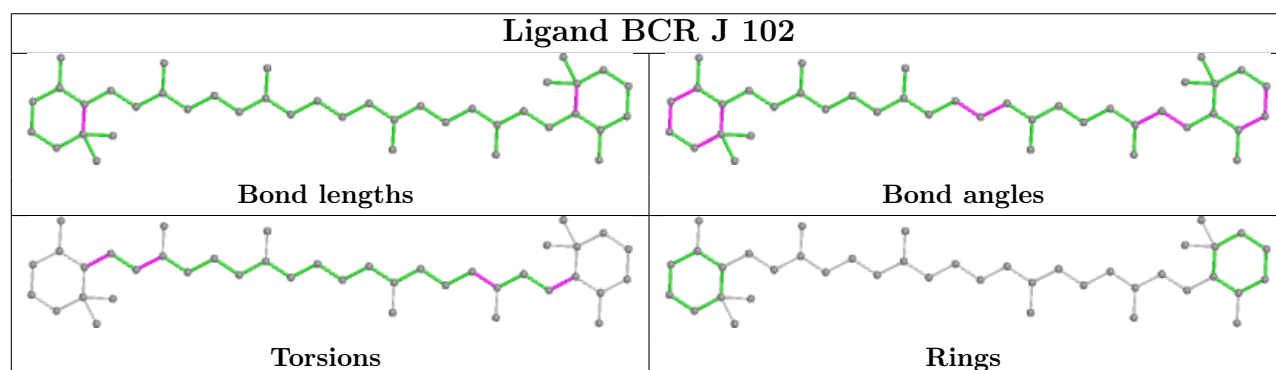
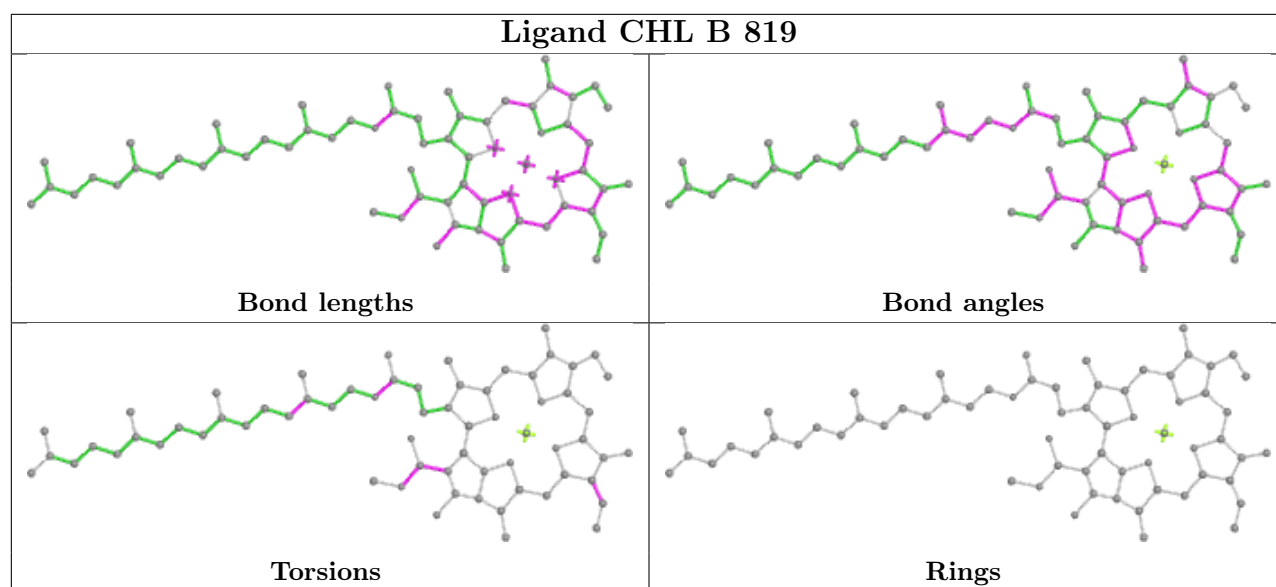




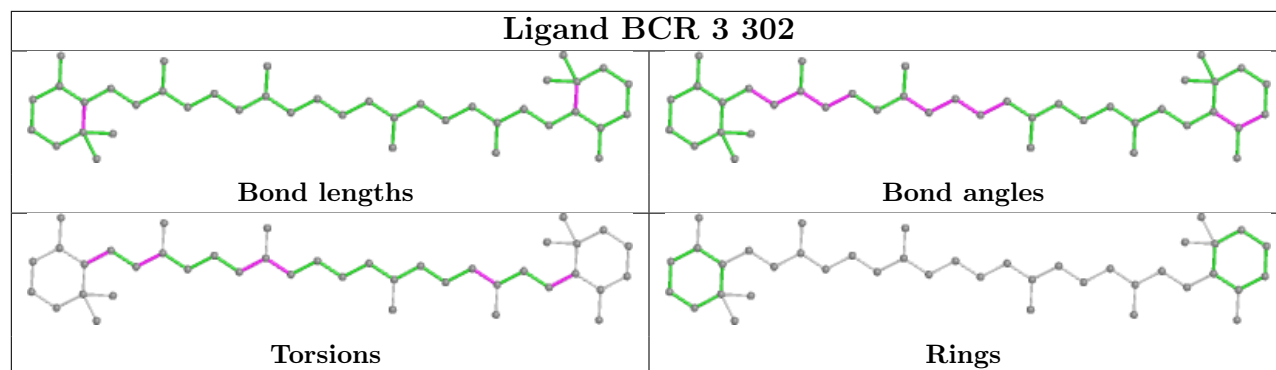




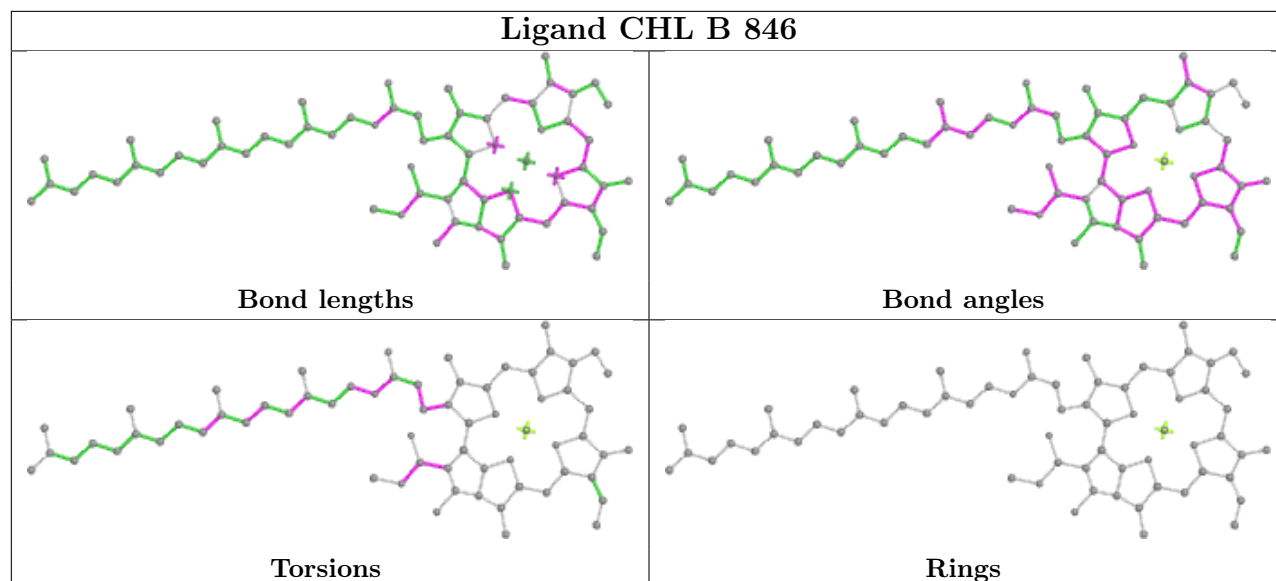




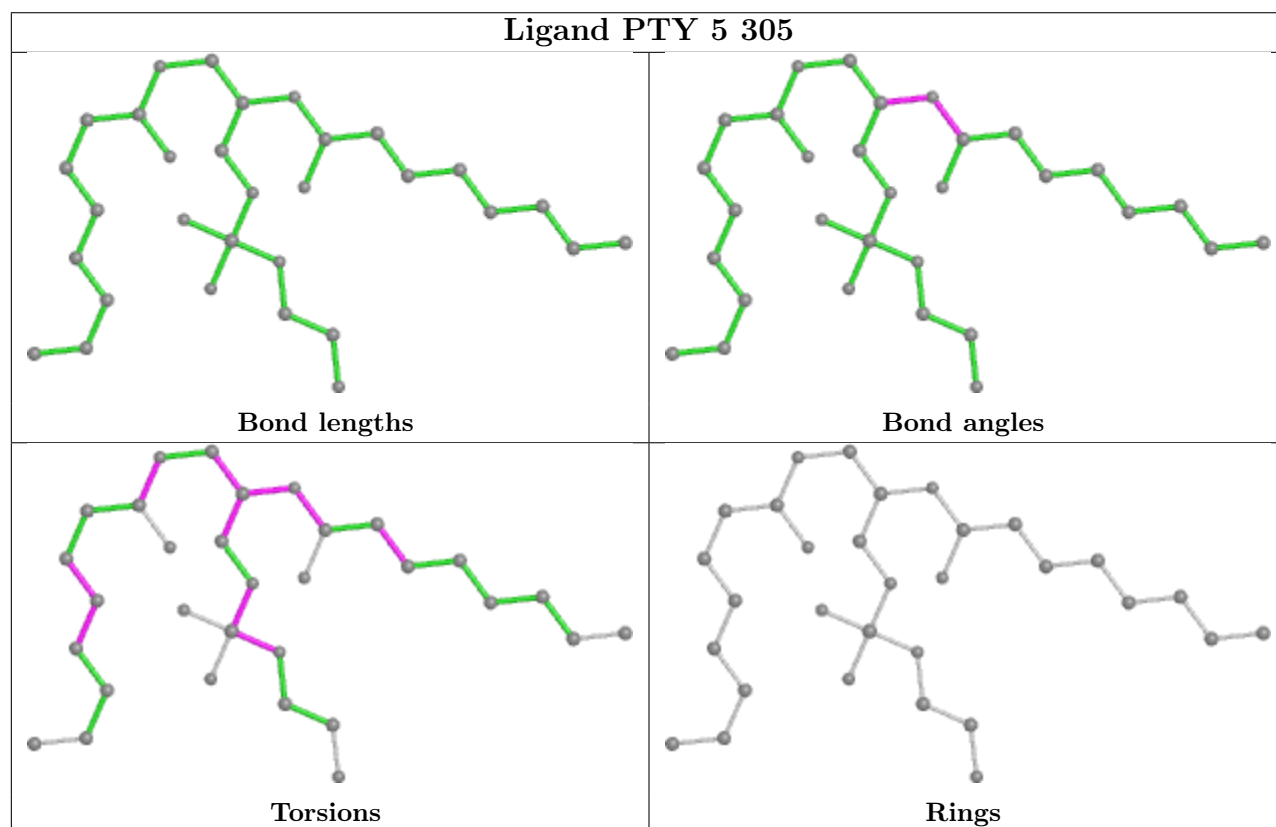
Ligand BCR 3 302

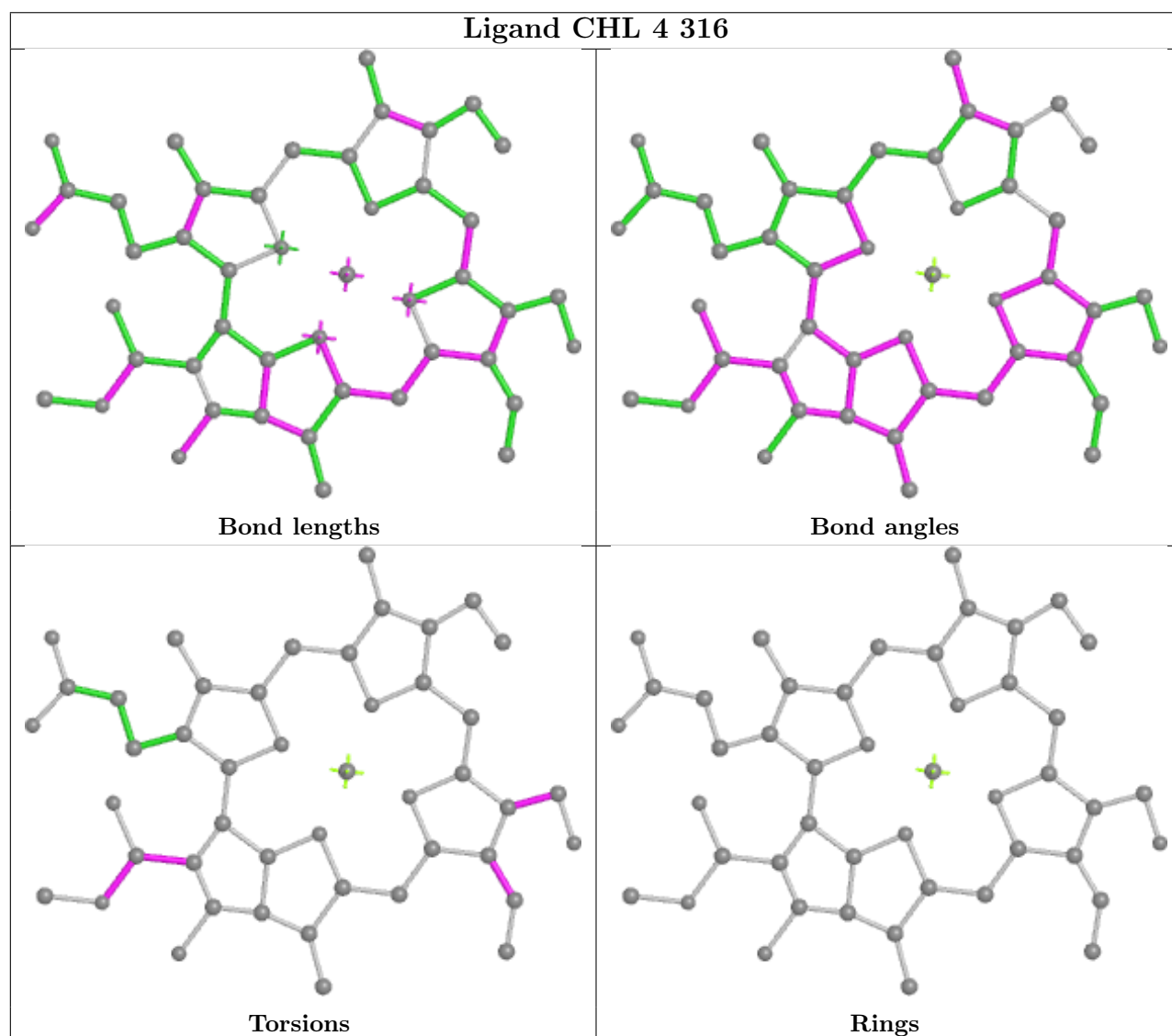
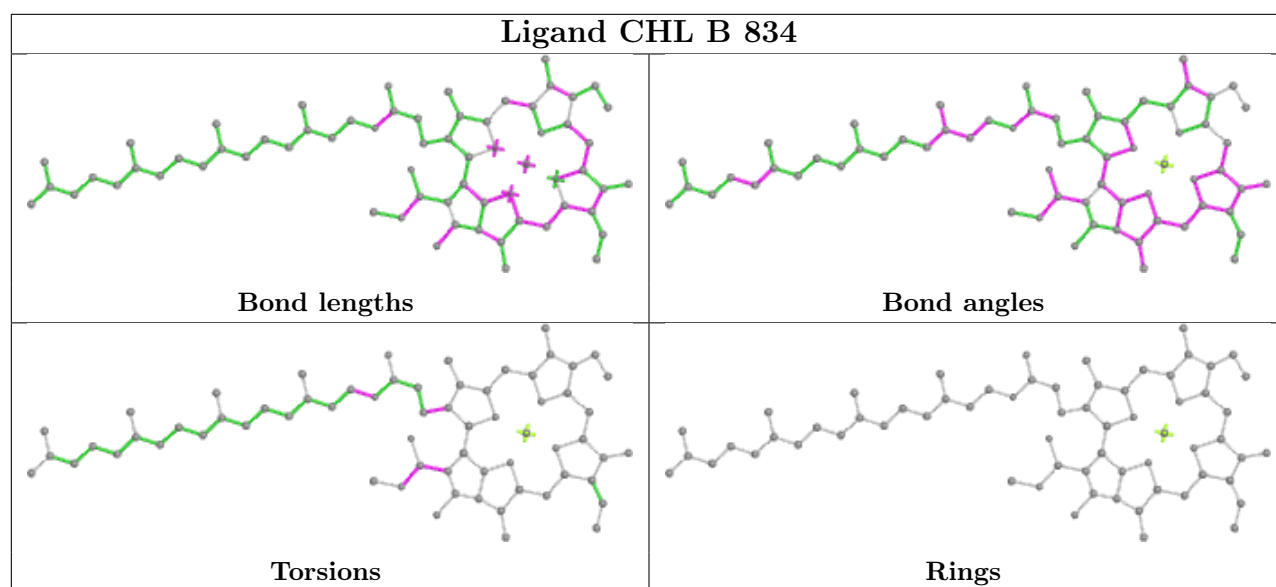


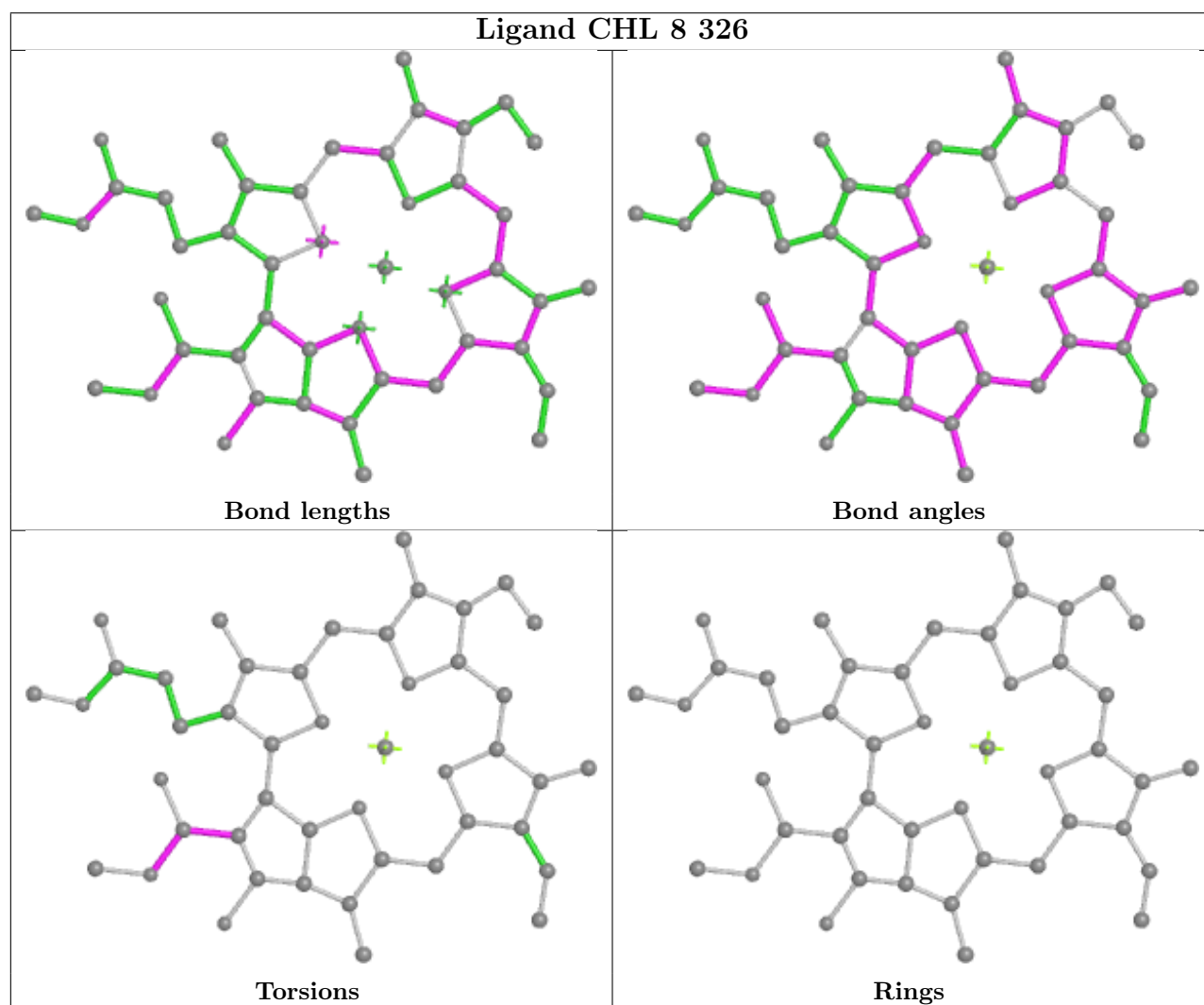
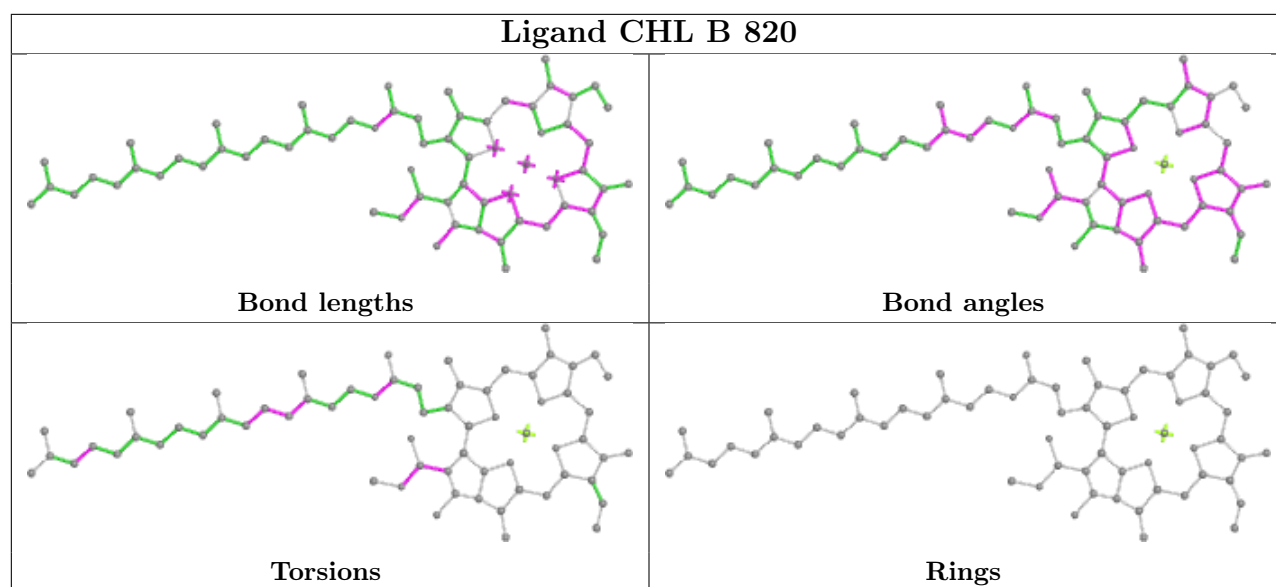
Ligand CHL B 846

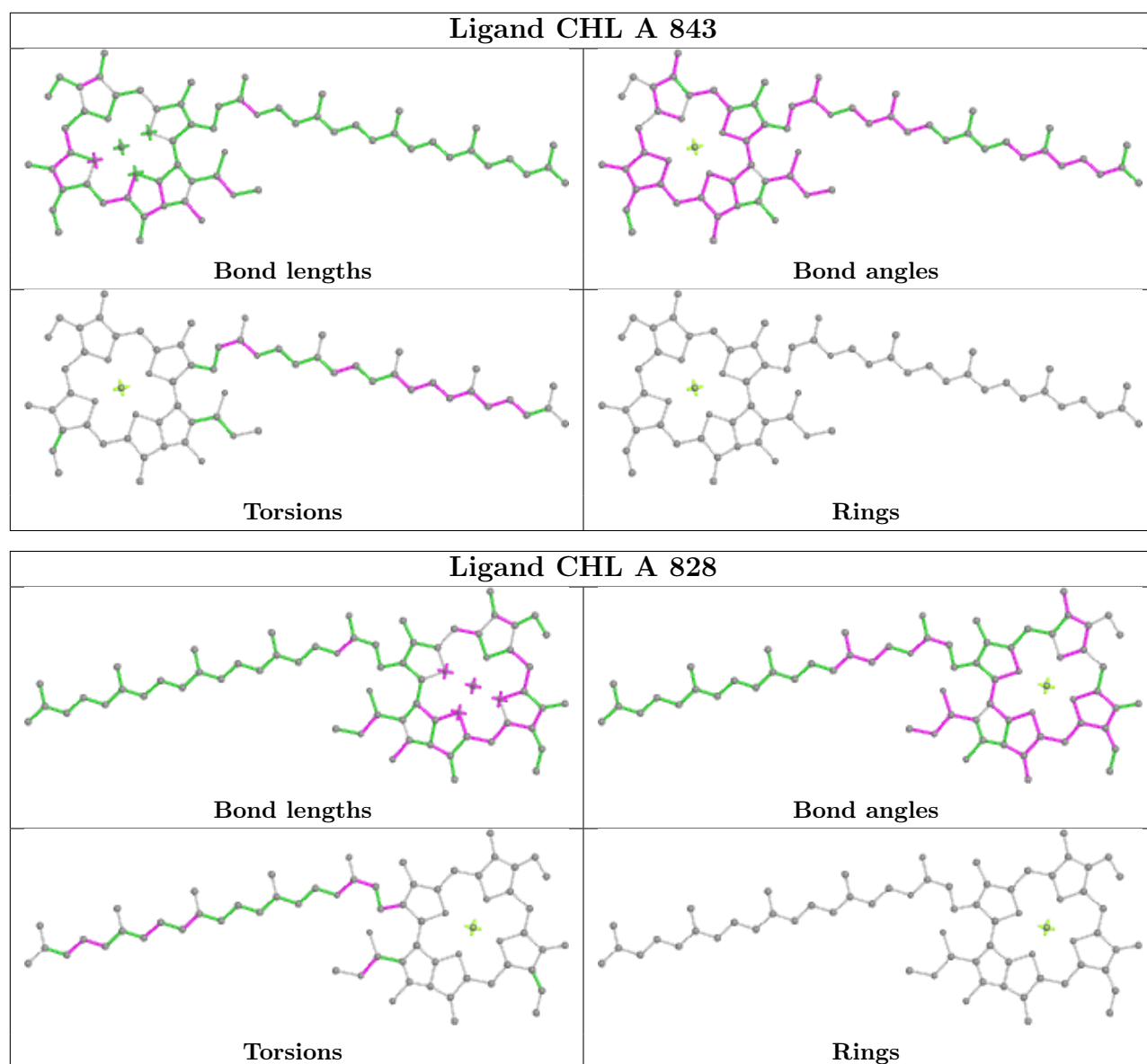


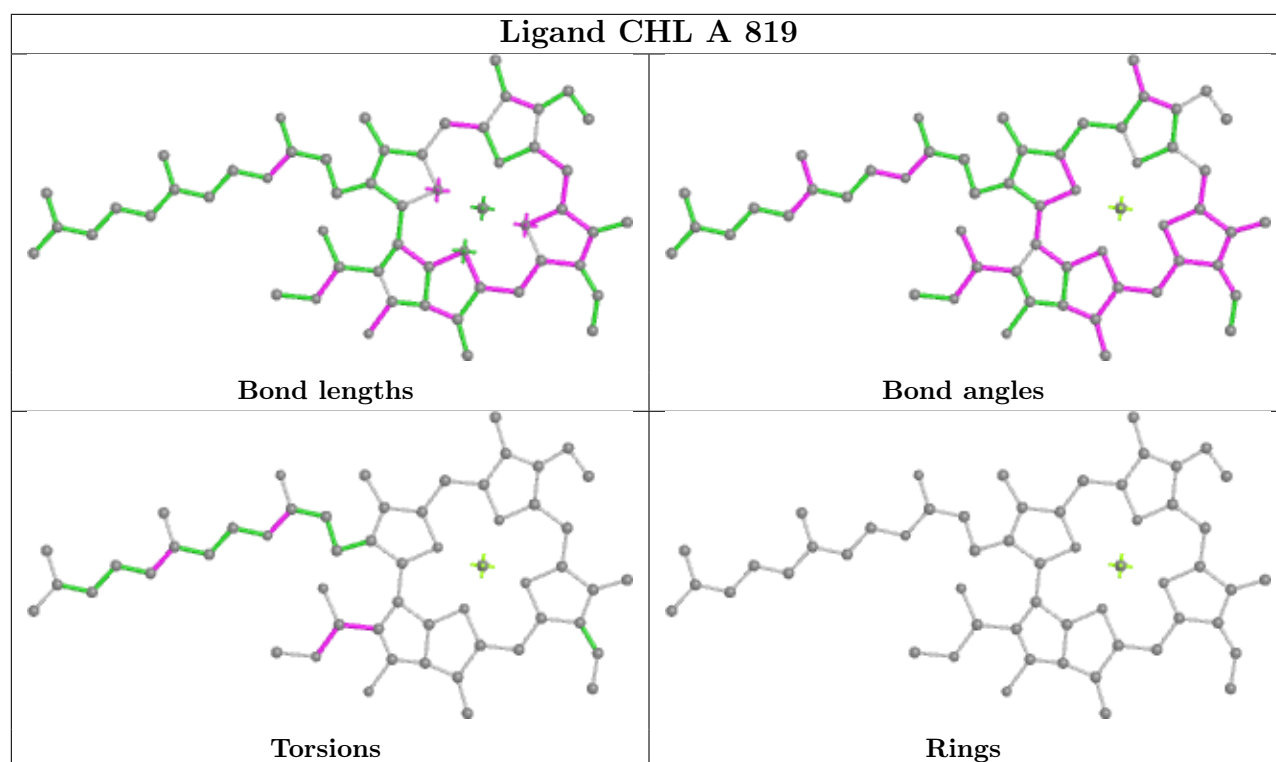
Ligand PTY 5 305



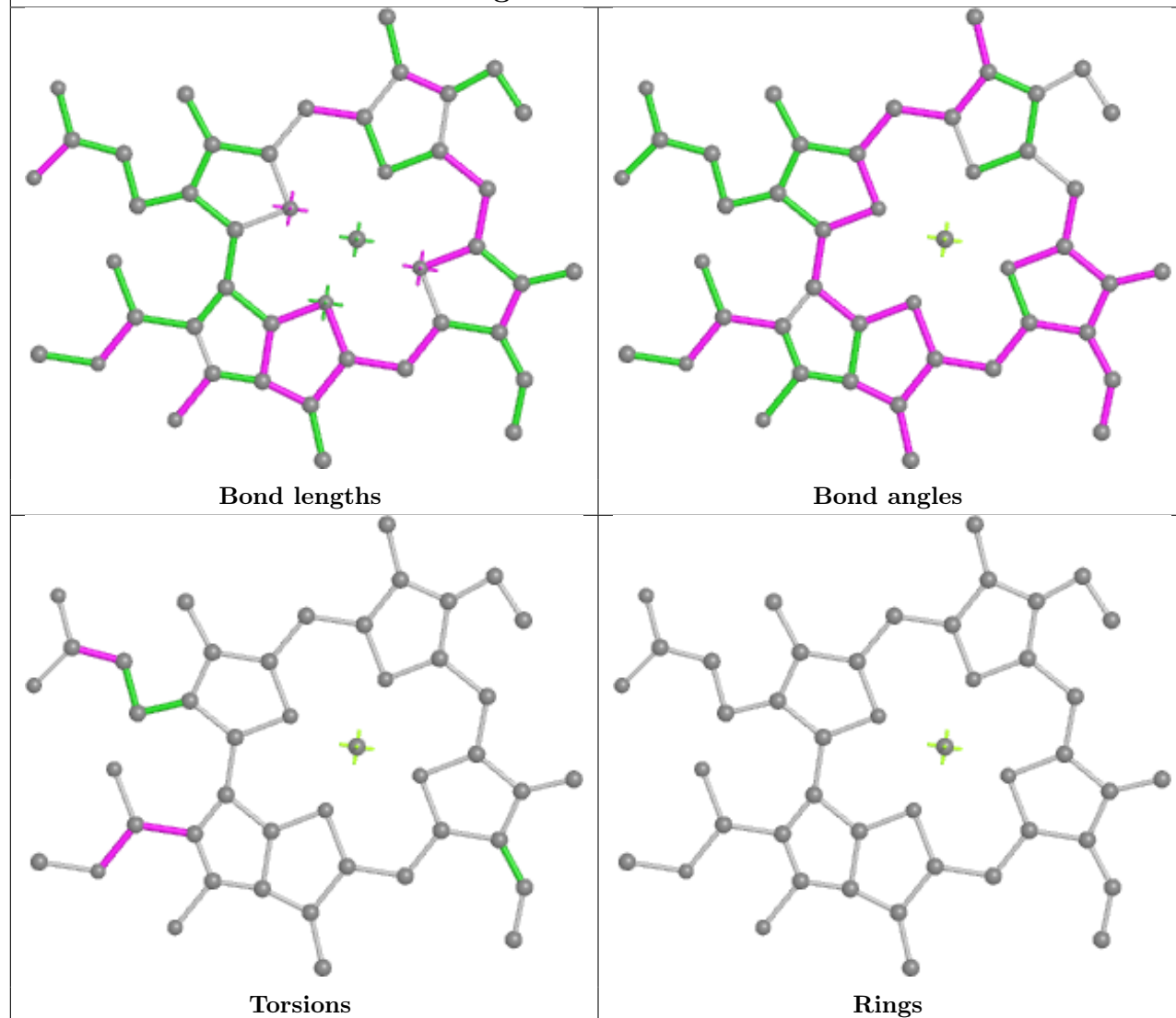




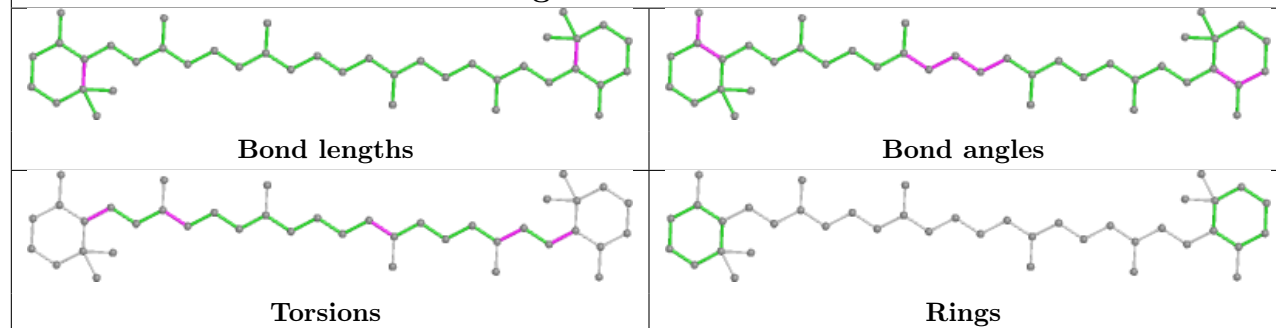


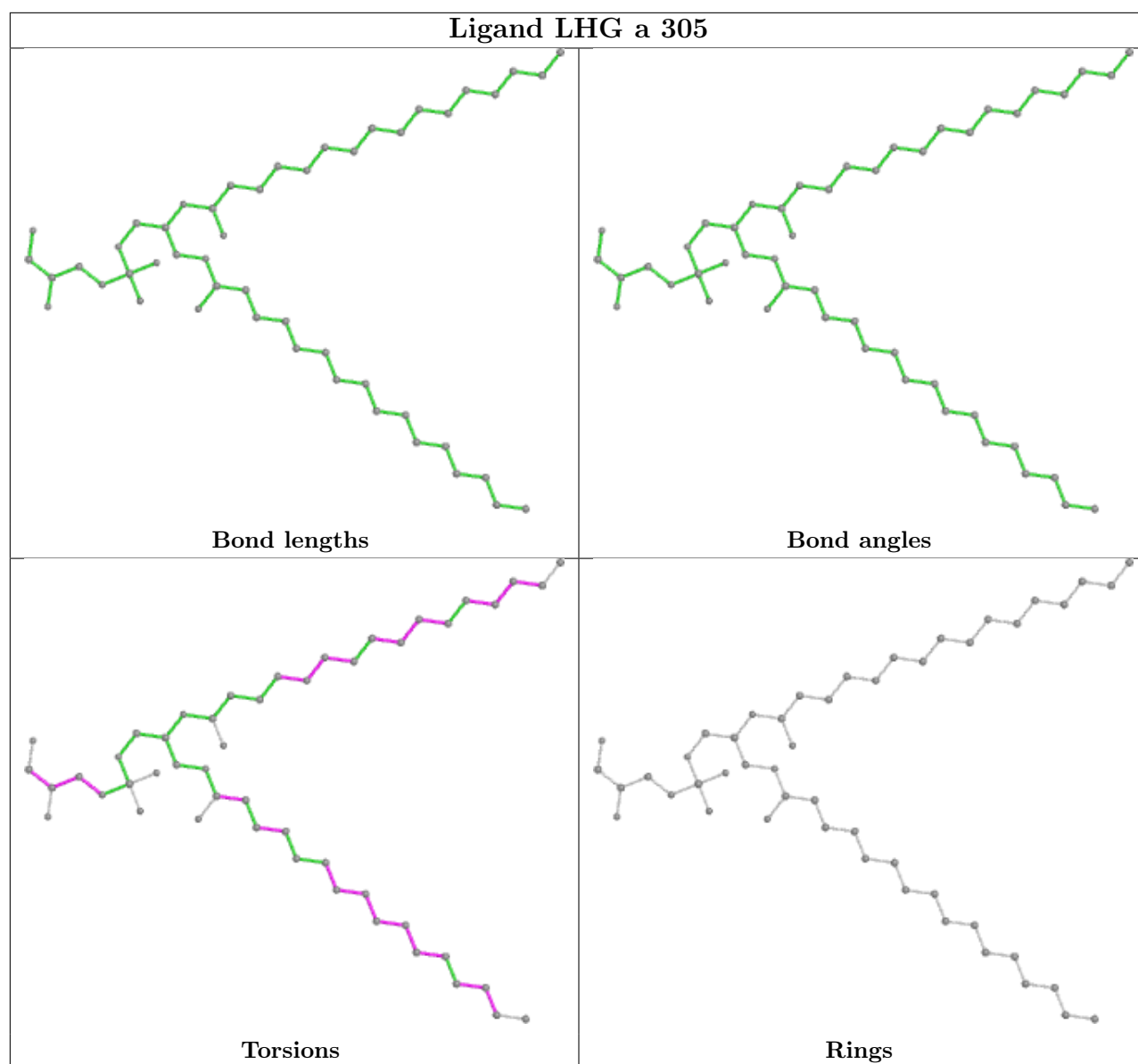


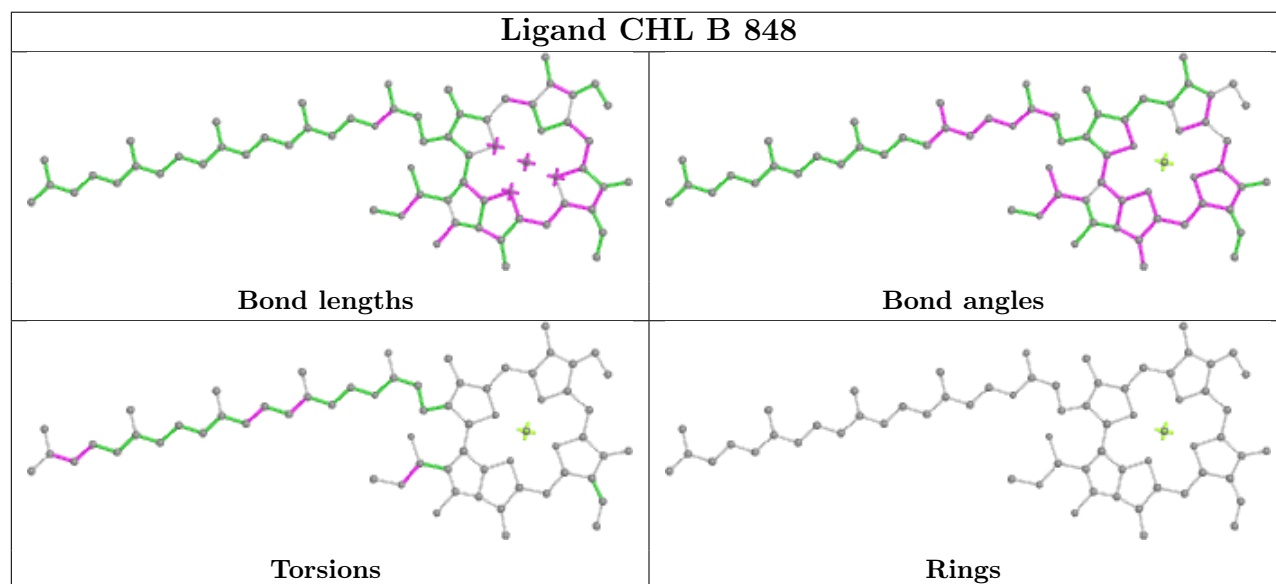
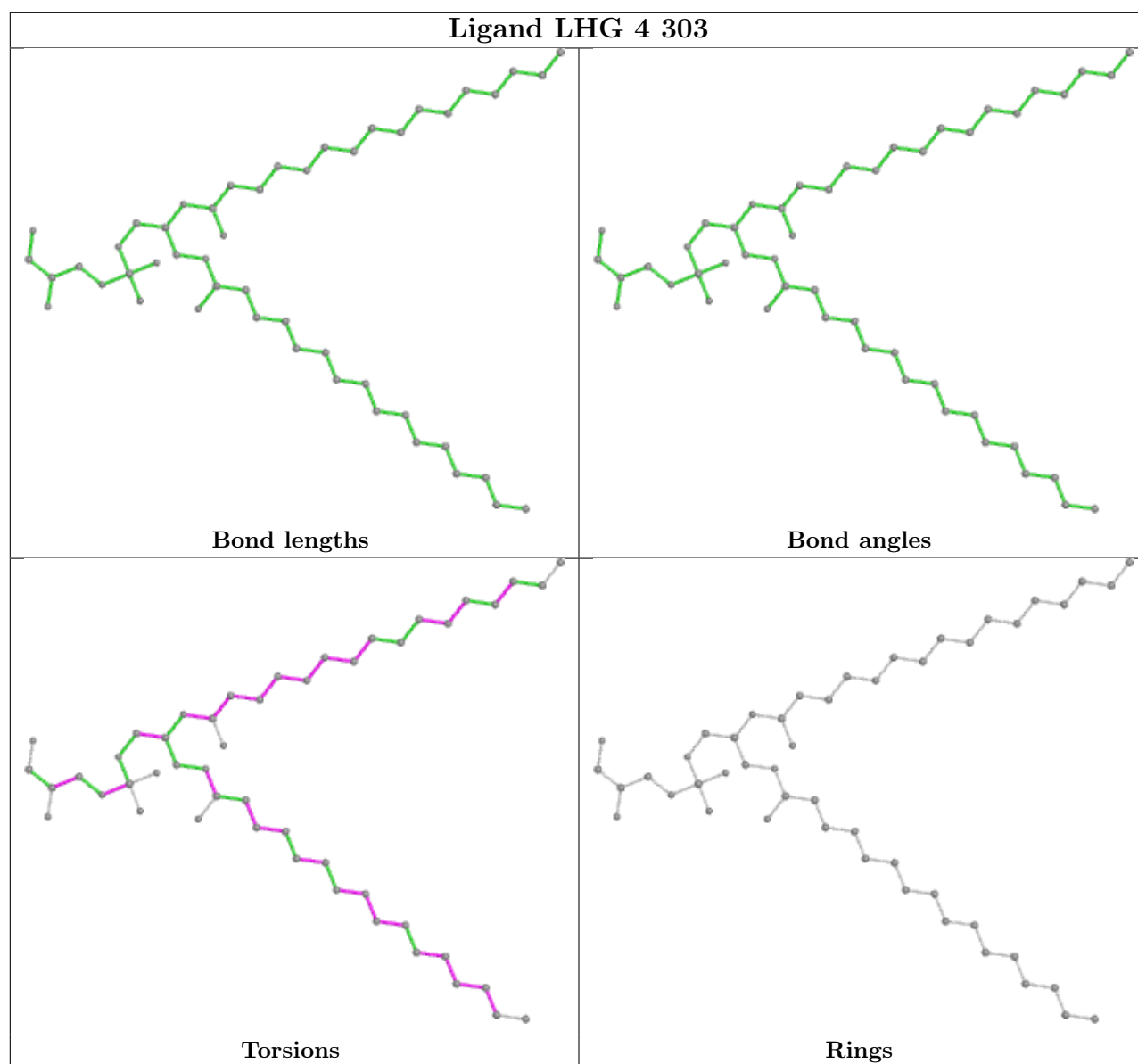
Ligand CHL 4 317

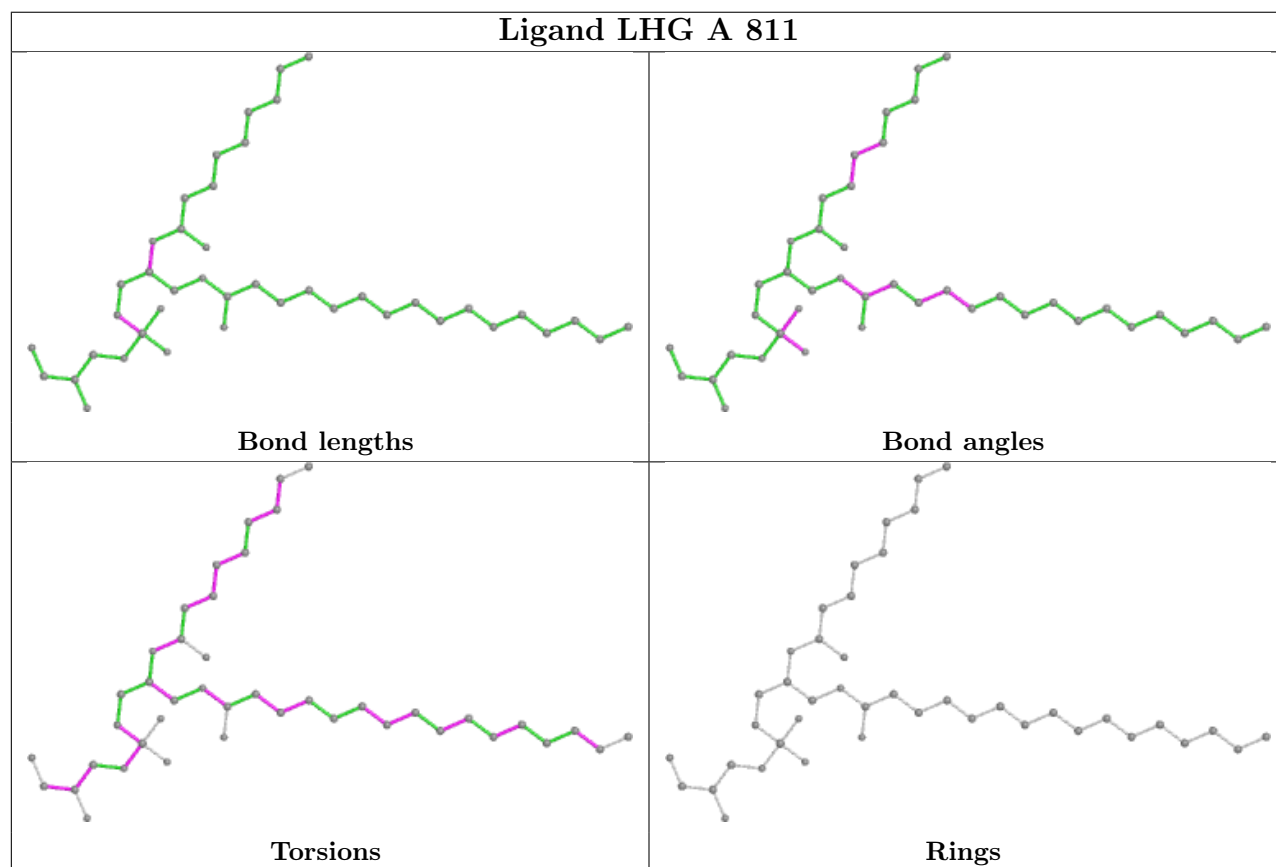
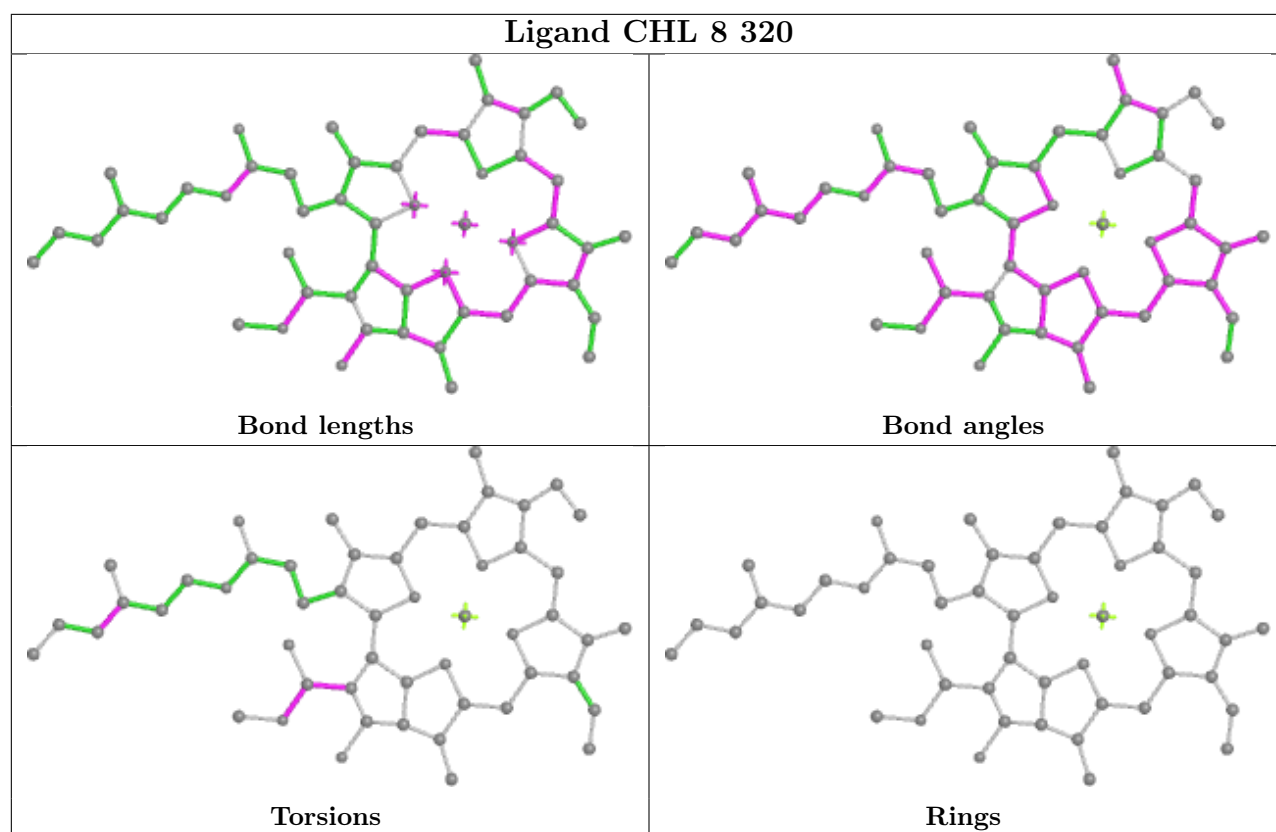


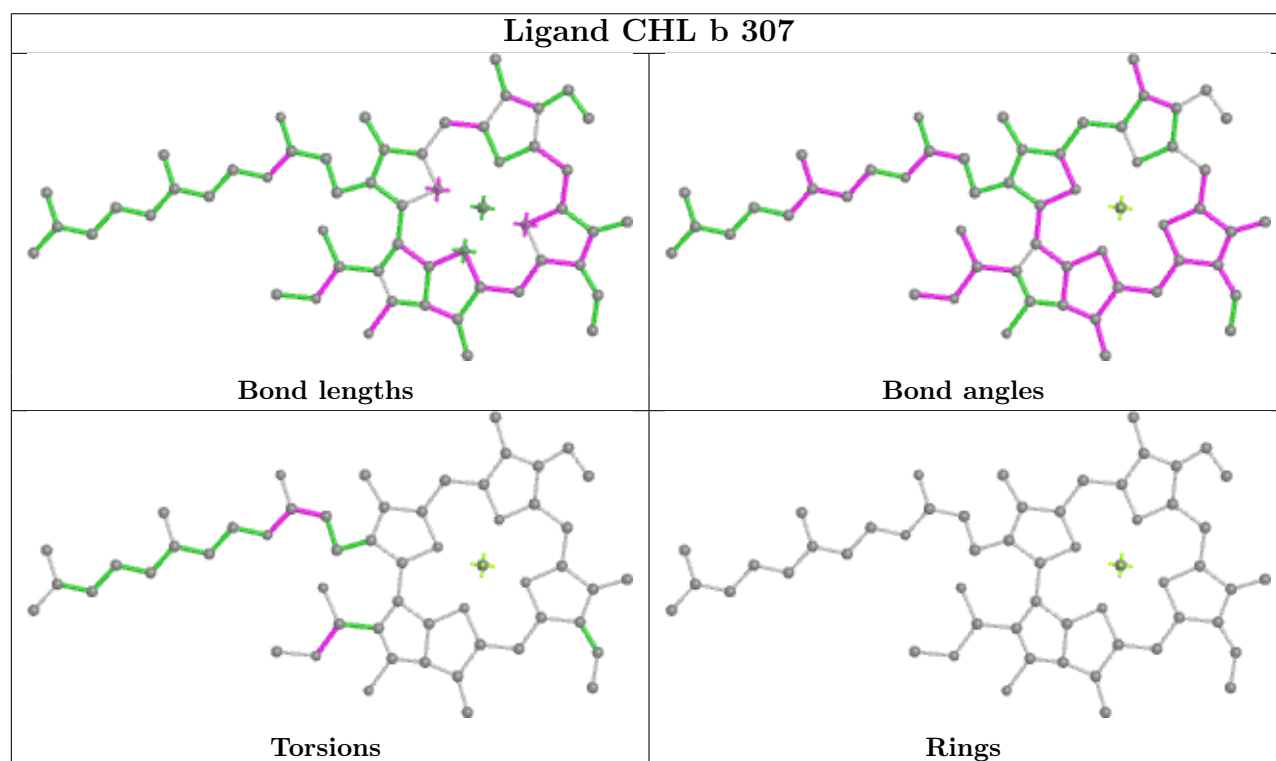
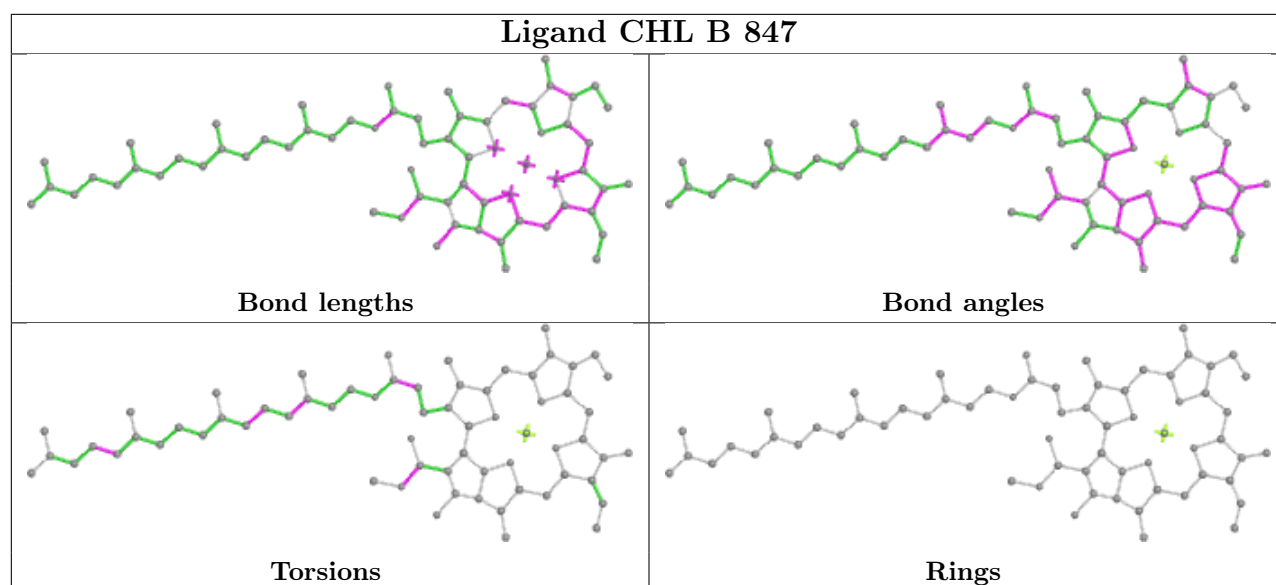
Ligand BCR L 302



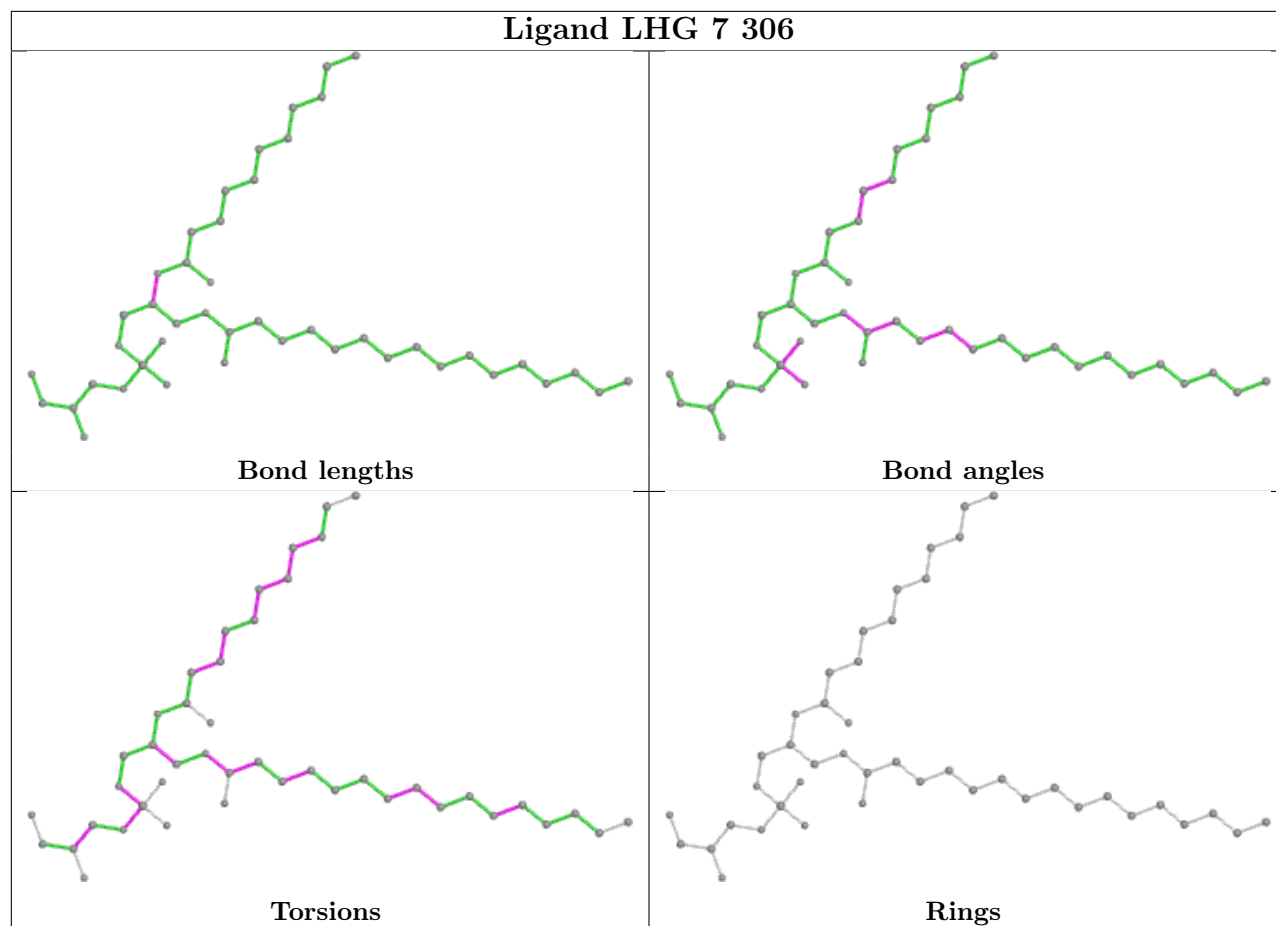




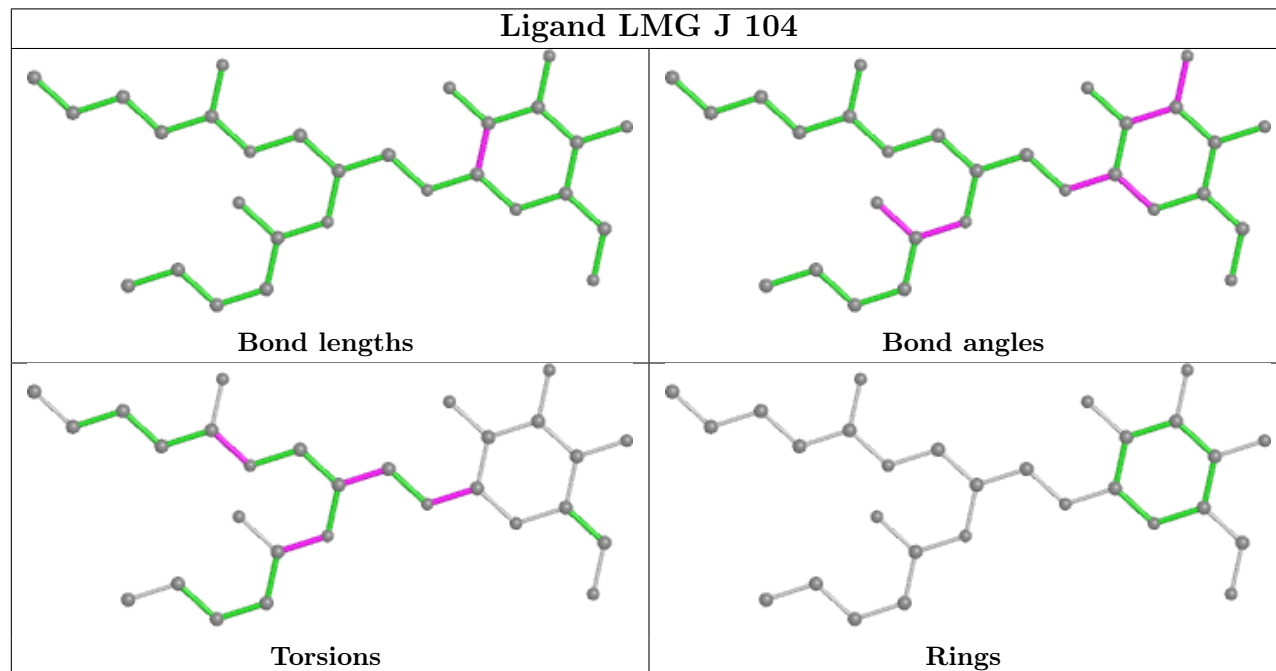


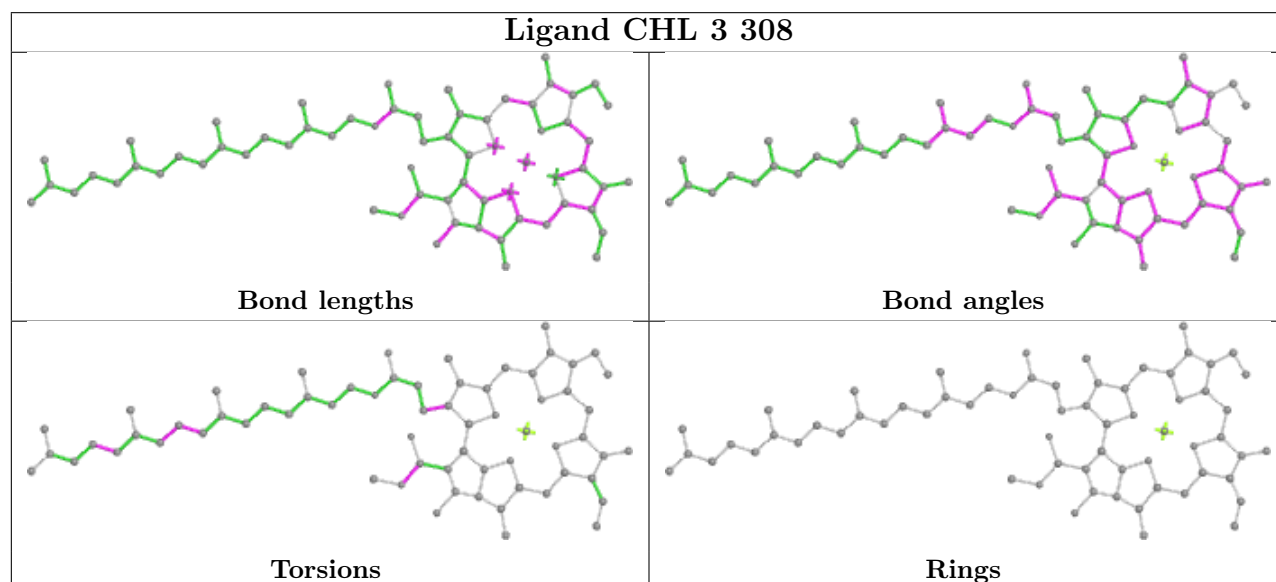
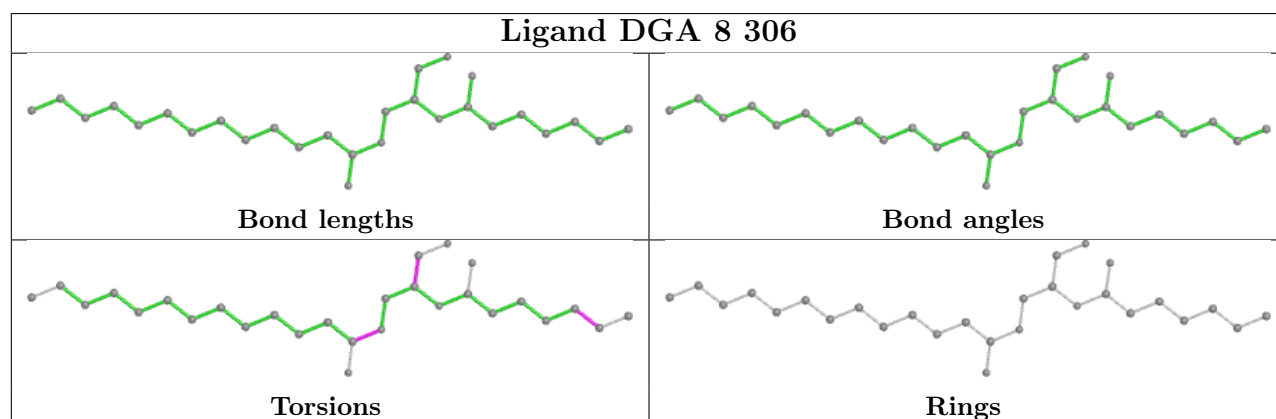
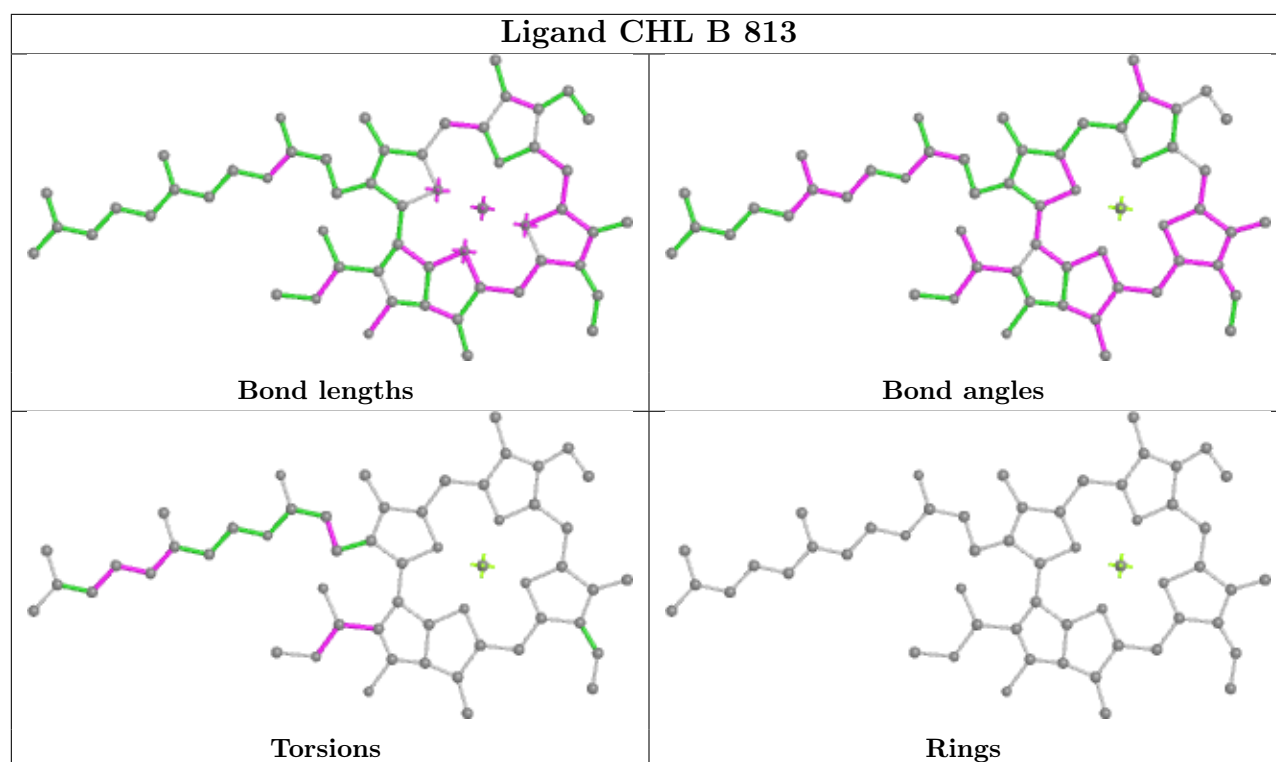


Ligand LHG 7 306

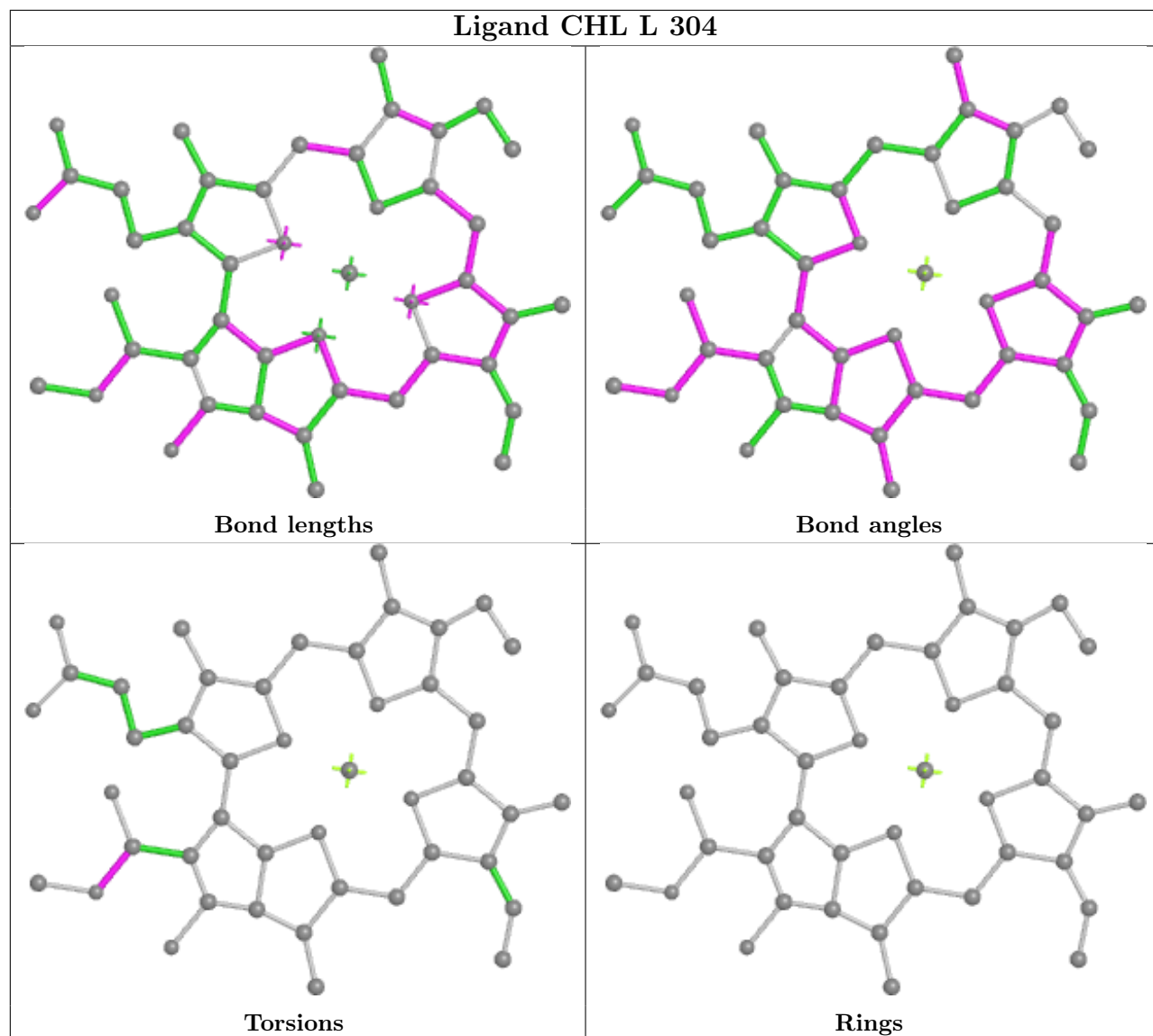


Ligand LMG J 104

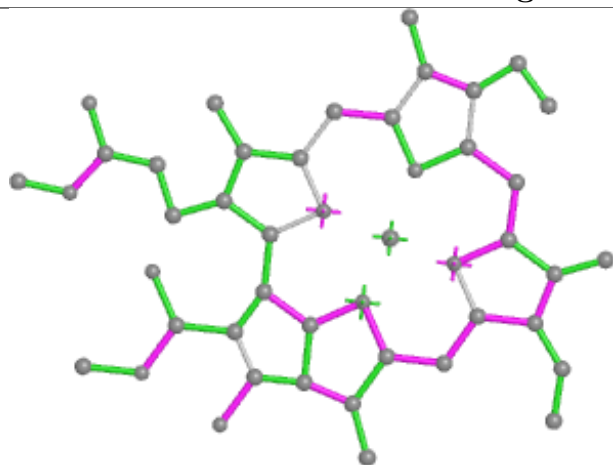




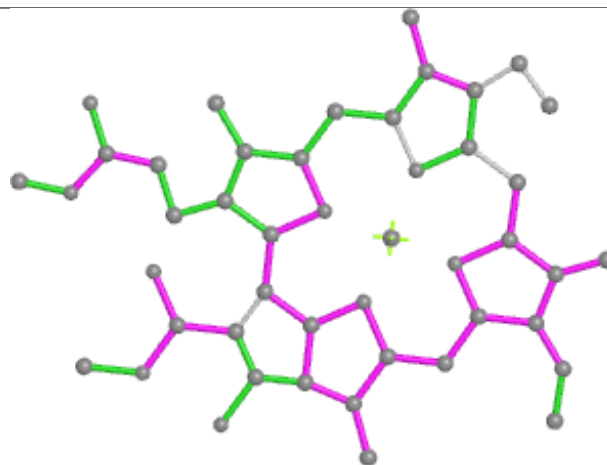
Ligand CHL L 304



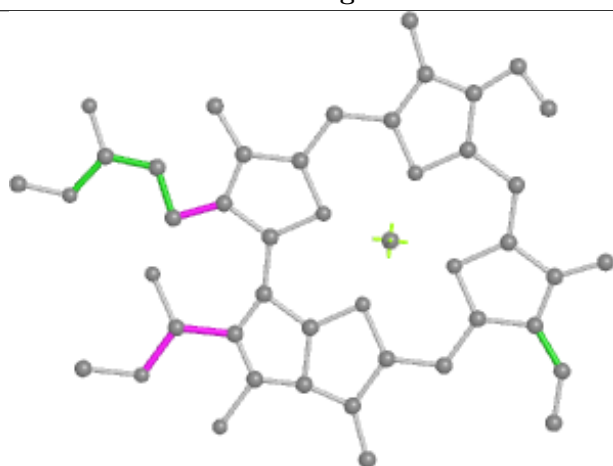
Ligand CHL b 306



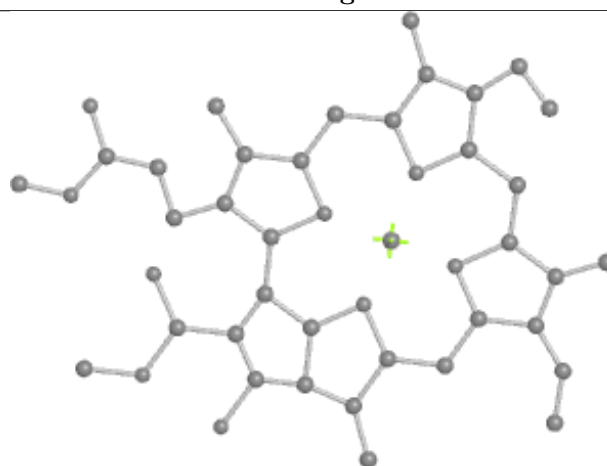
Bond lengths



Bond angles

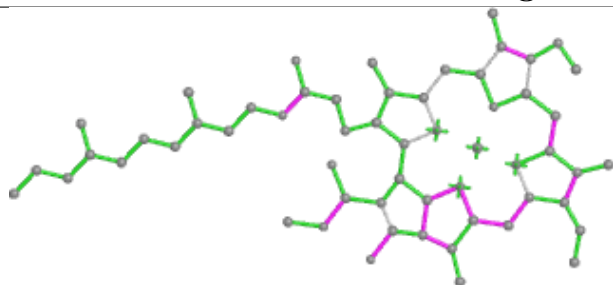


Torsions

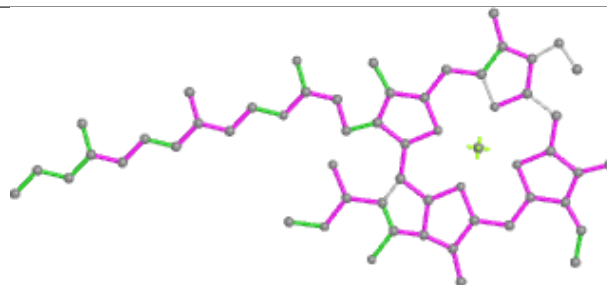


Rings

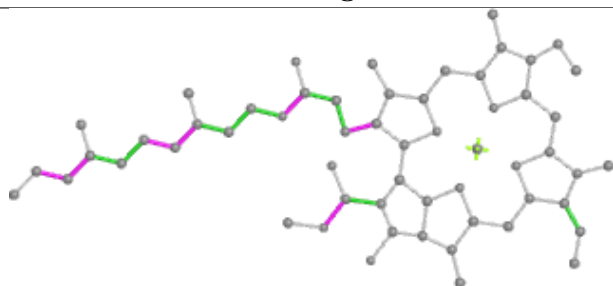
Ligand CHL 5 313



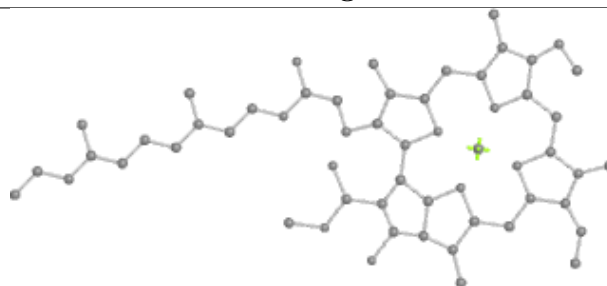
Bond lengths



Bond angles

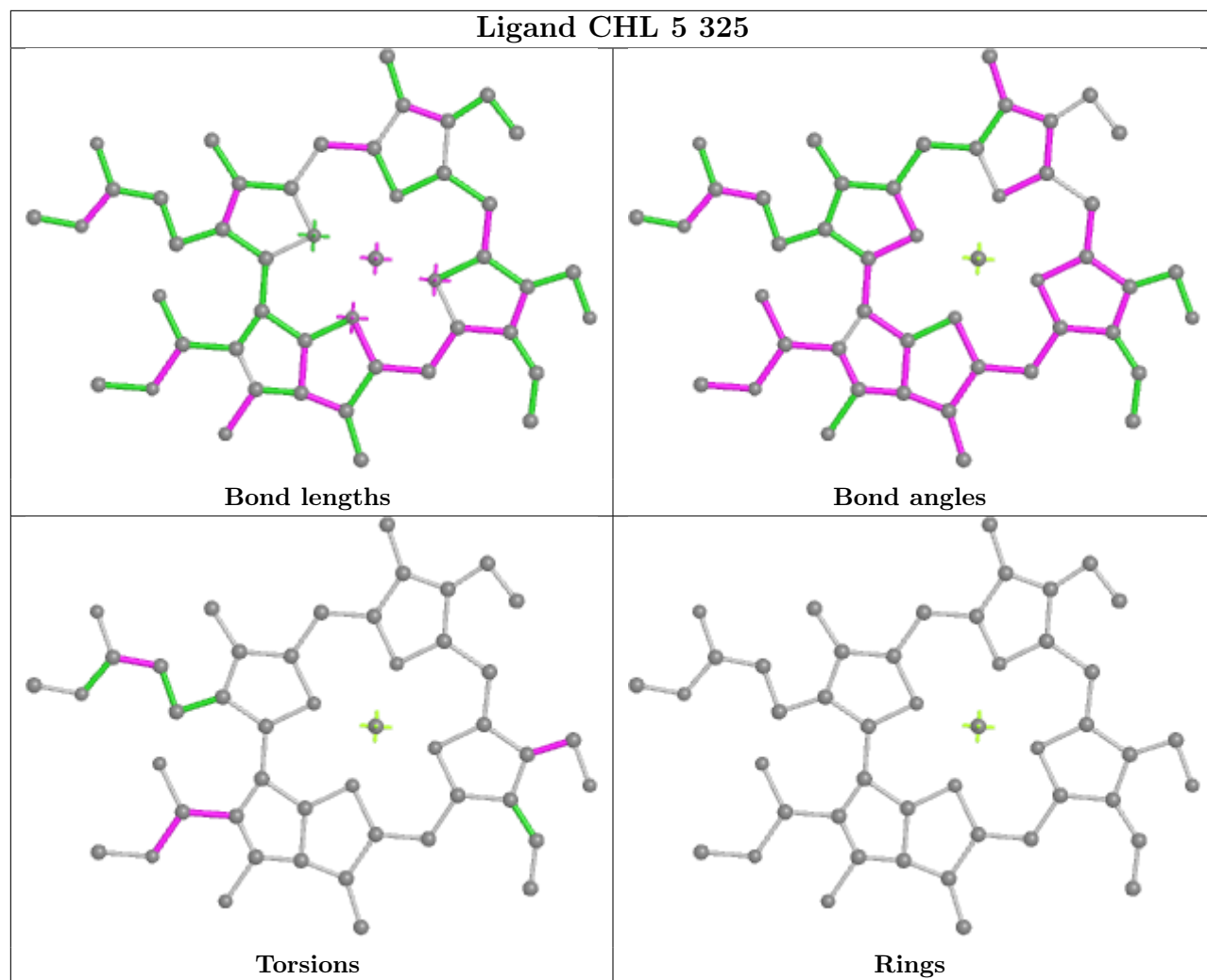


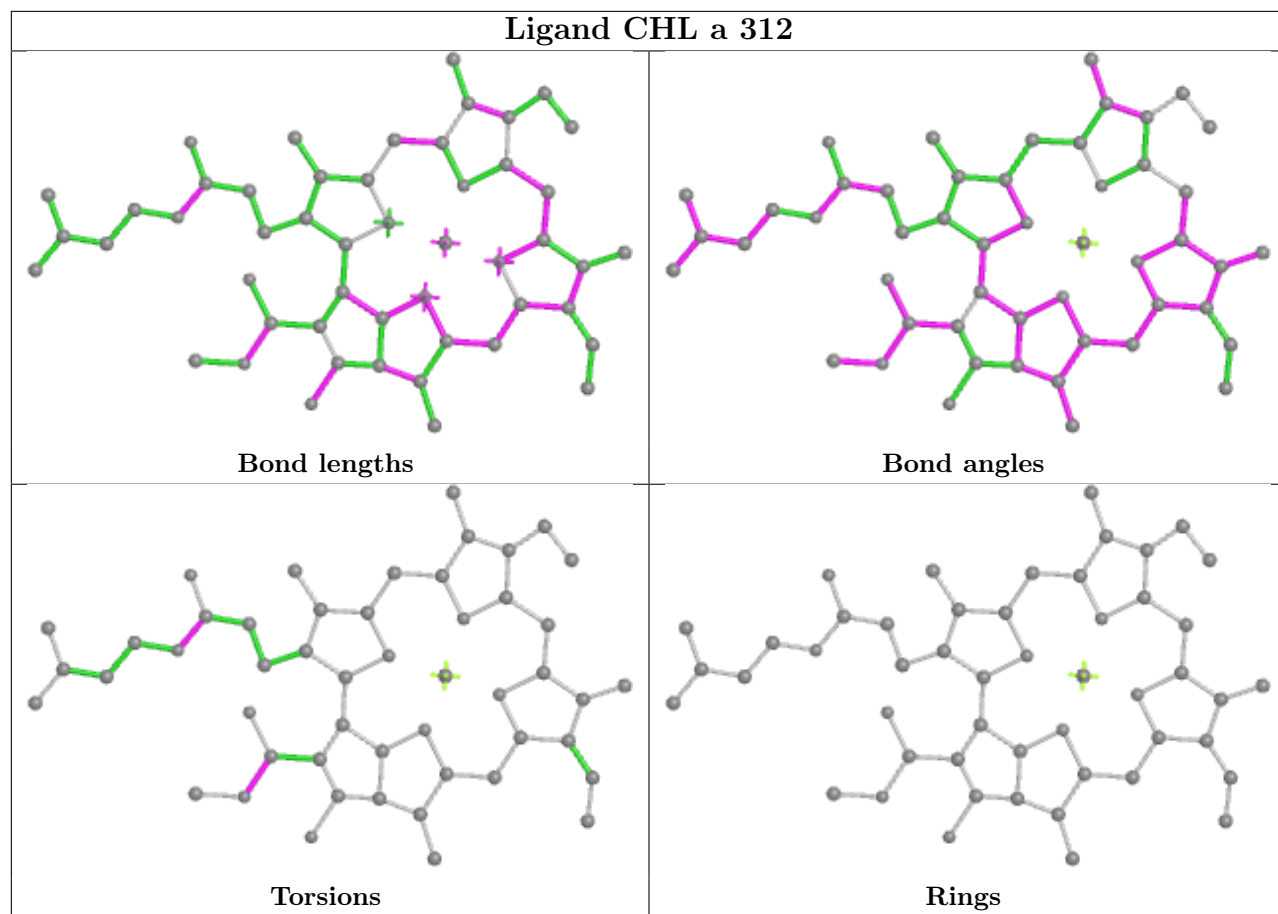
Torsions



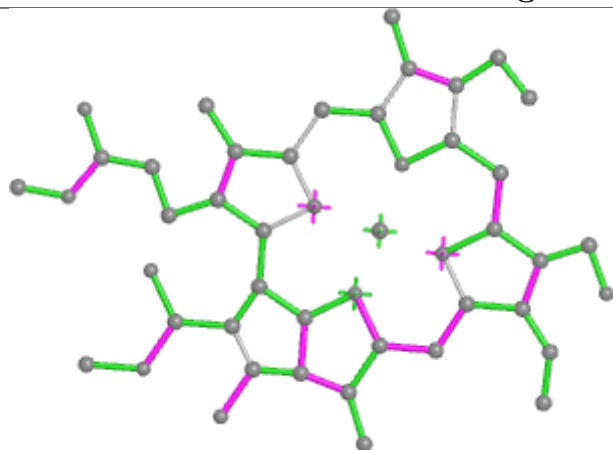
Rings

Ligand CHL 5 325

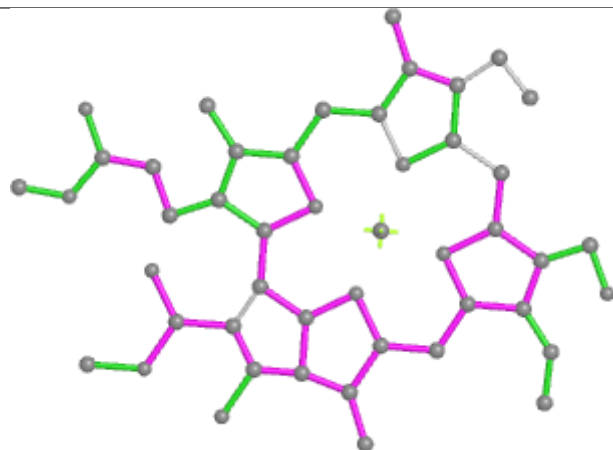




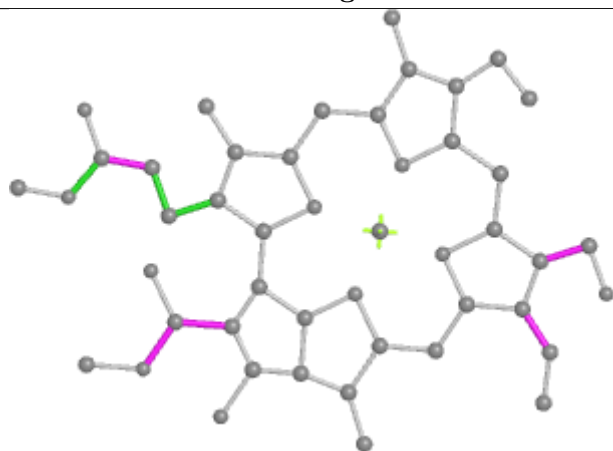
Ligand CHL 7 320



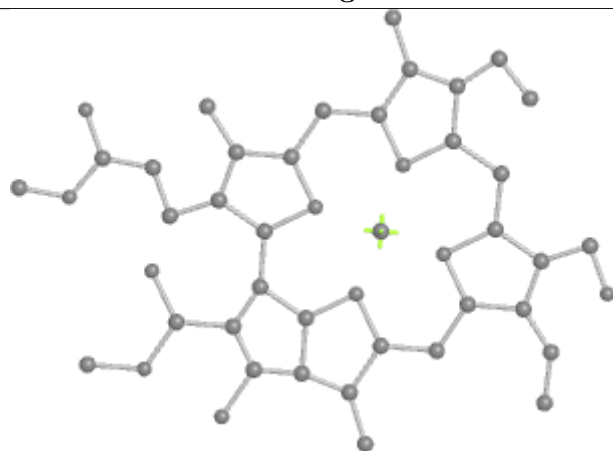
Bond lengths



Bond angles

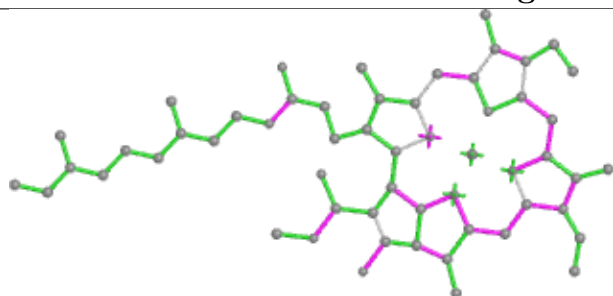


Torsions

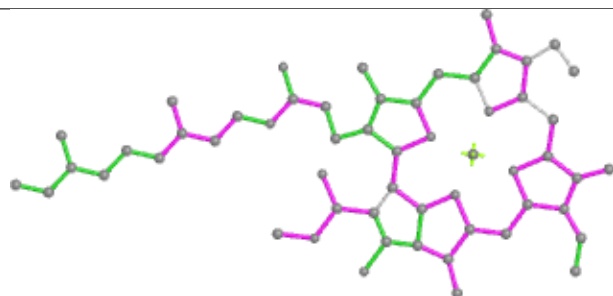


Rings

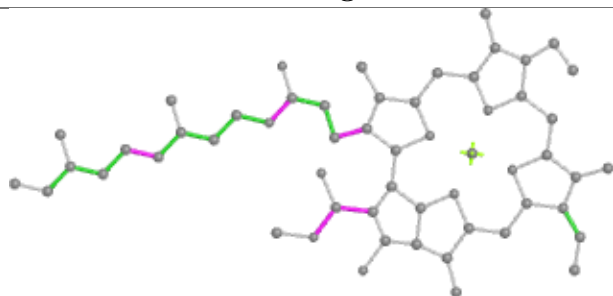
Ligand CHL 5 323



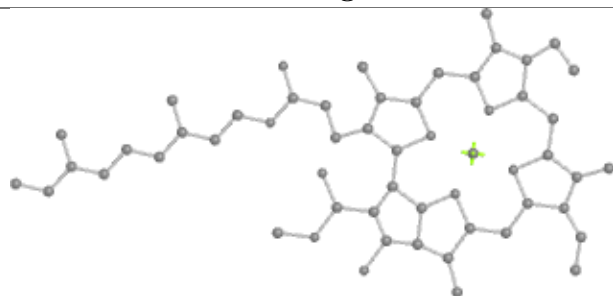
Bond lengths



Bond angles

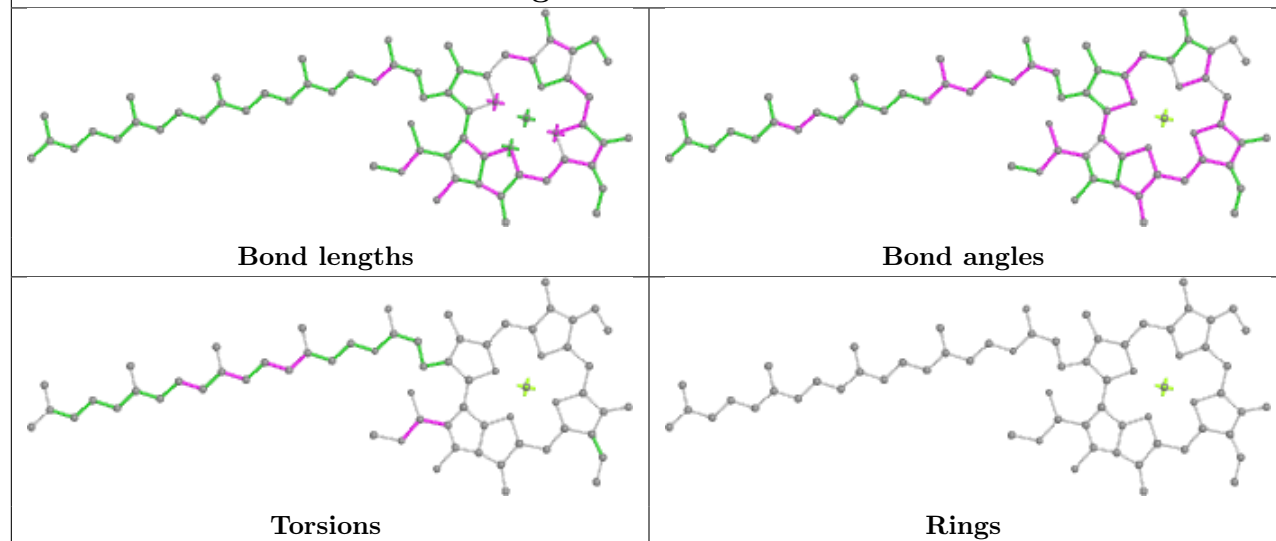


Torsions

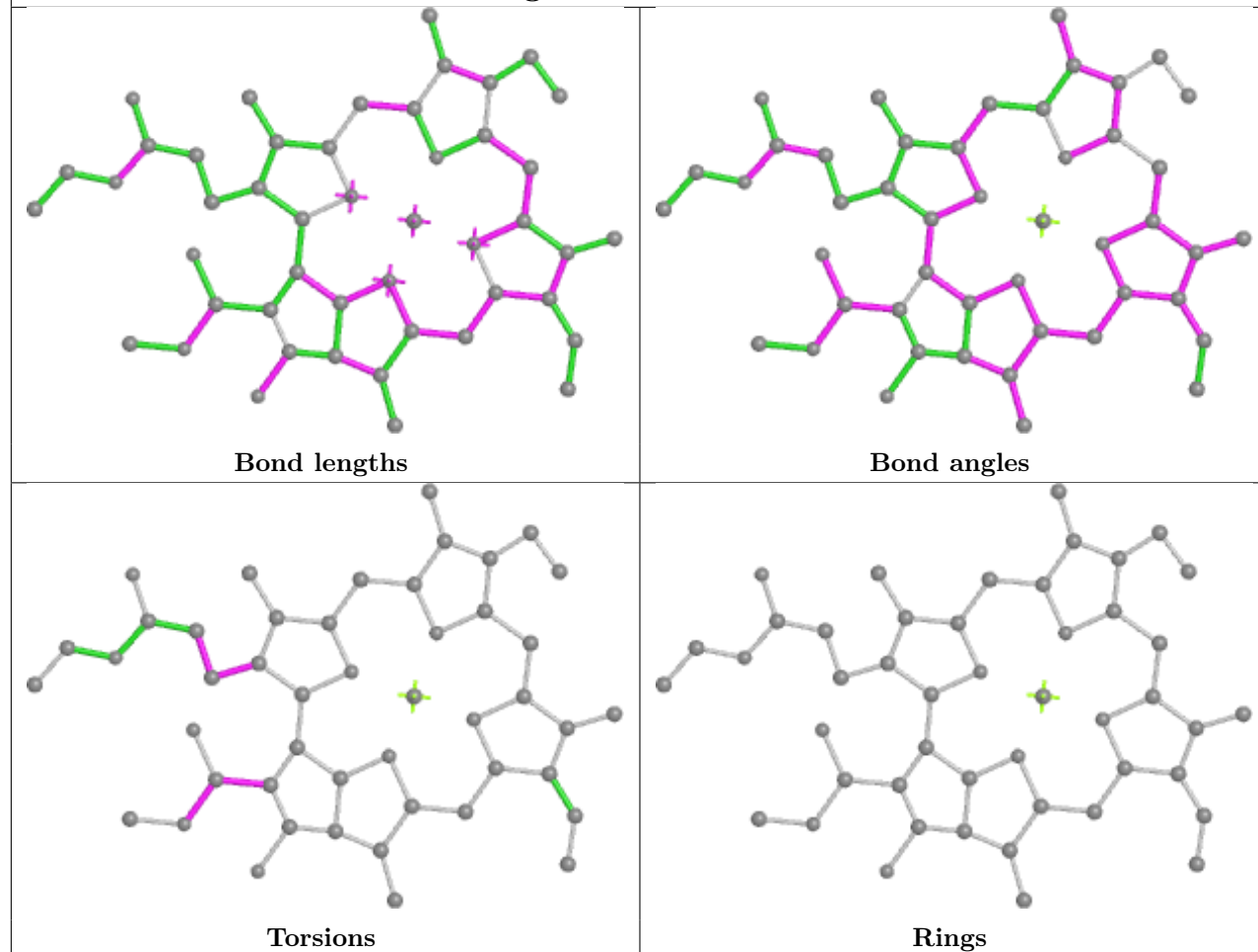


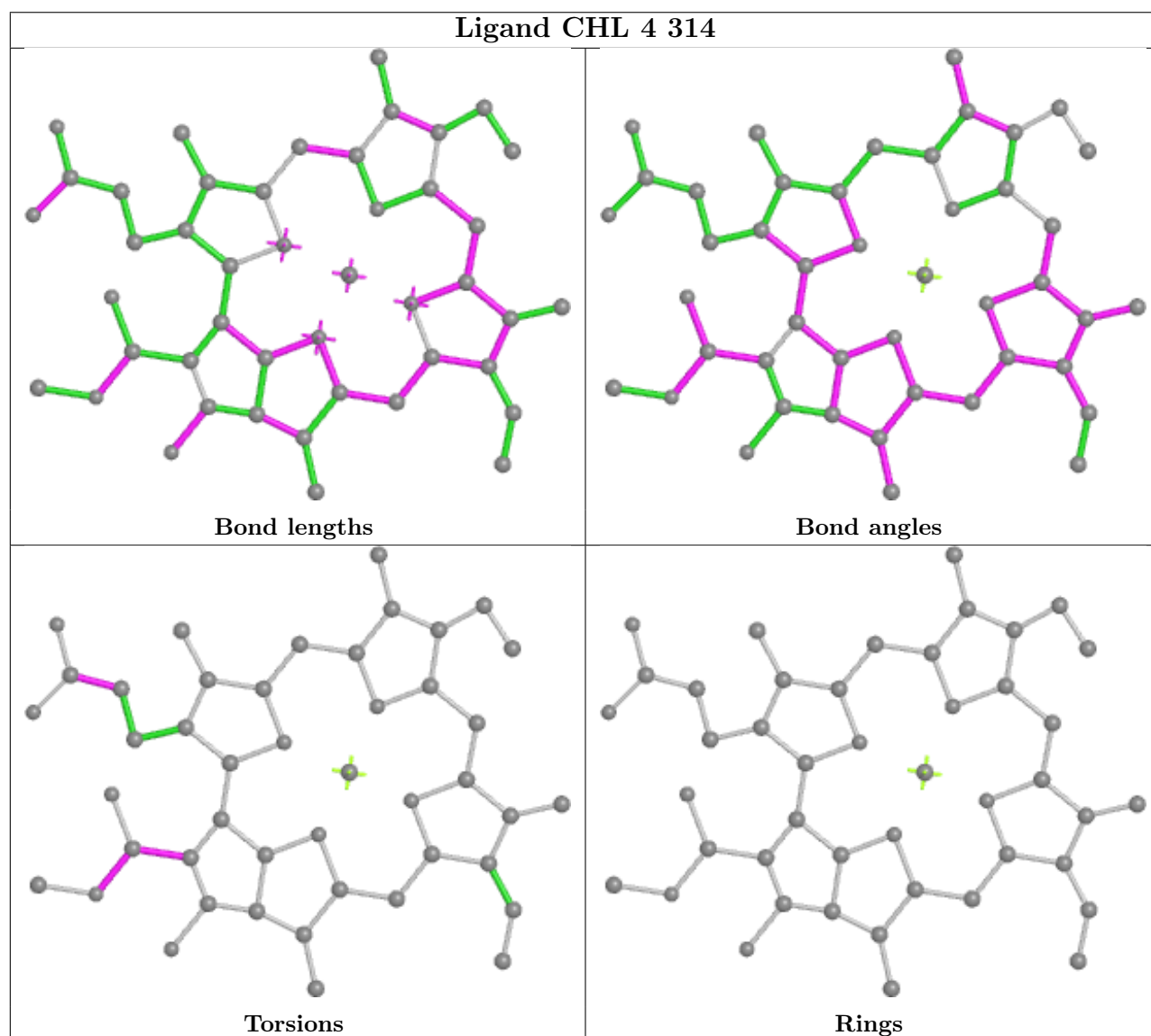
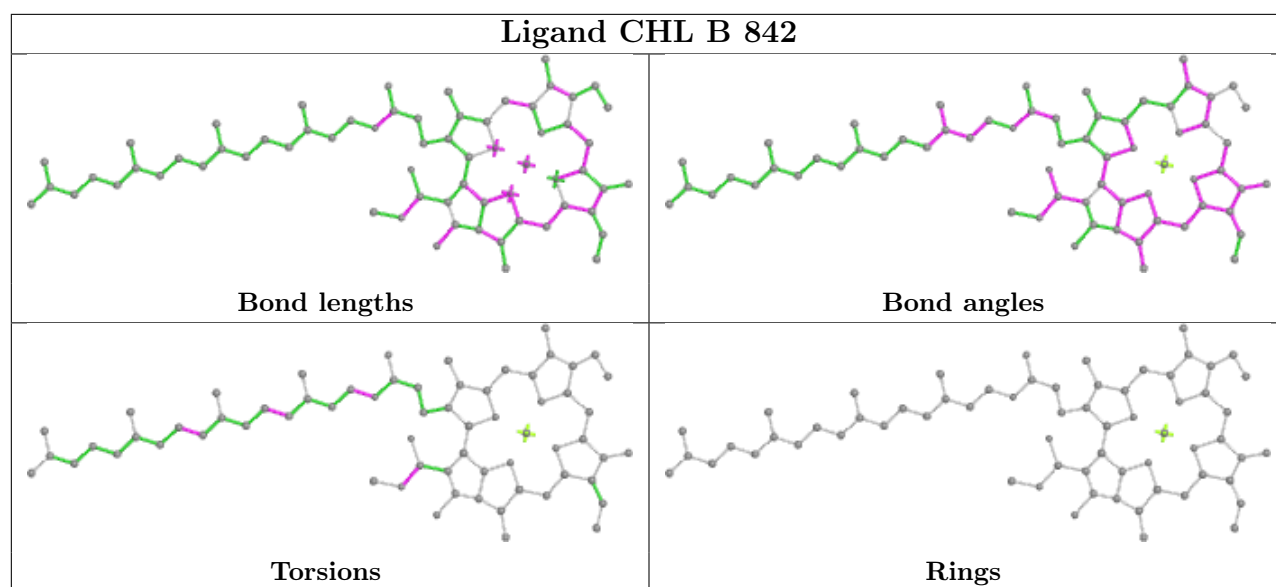
Rings

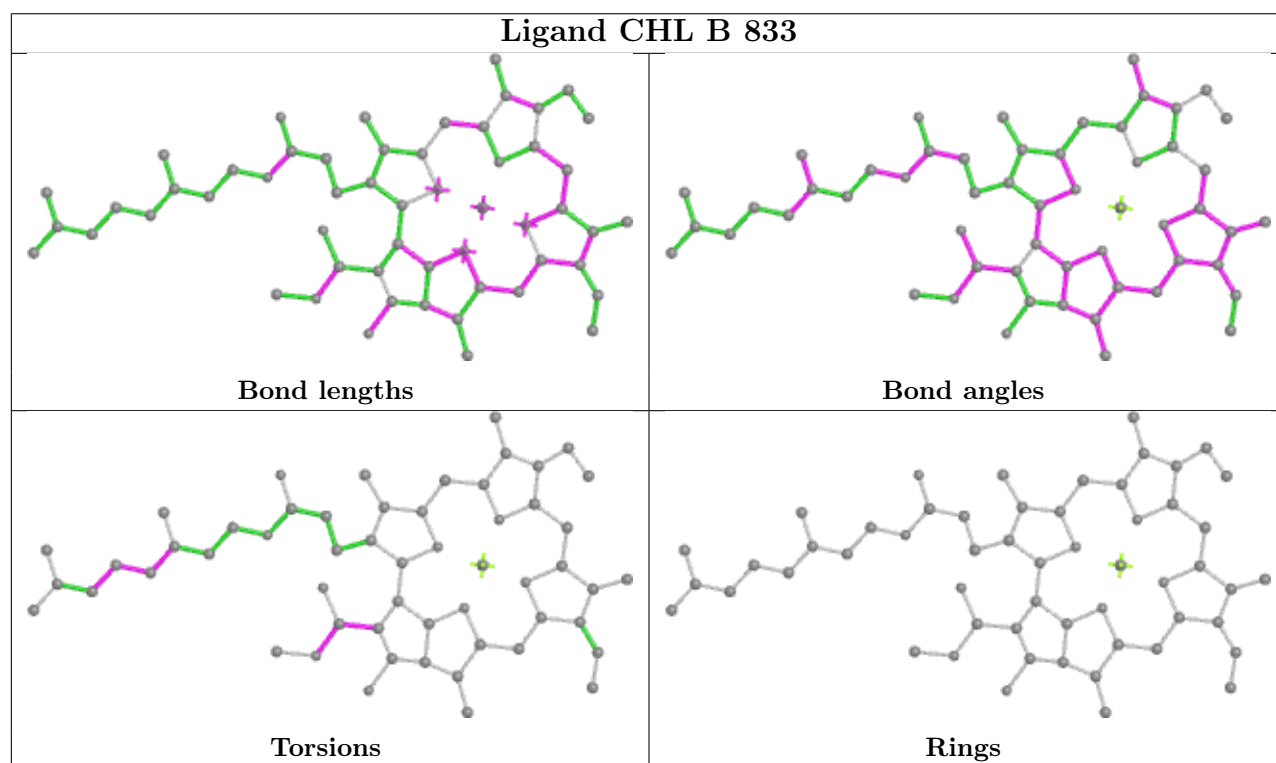
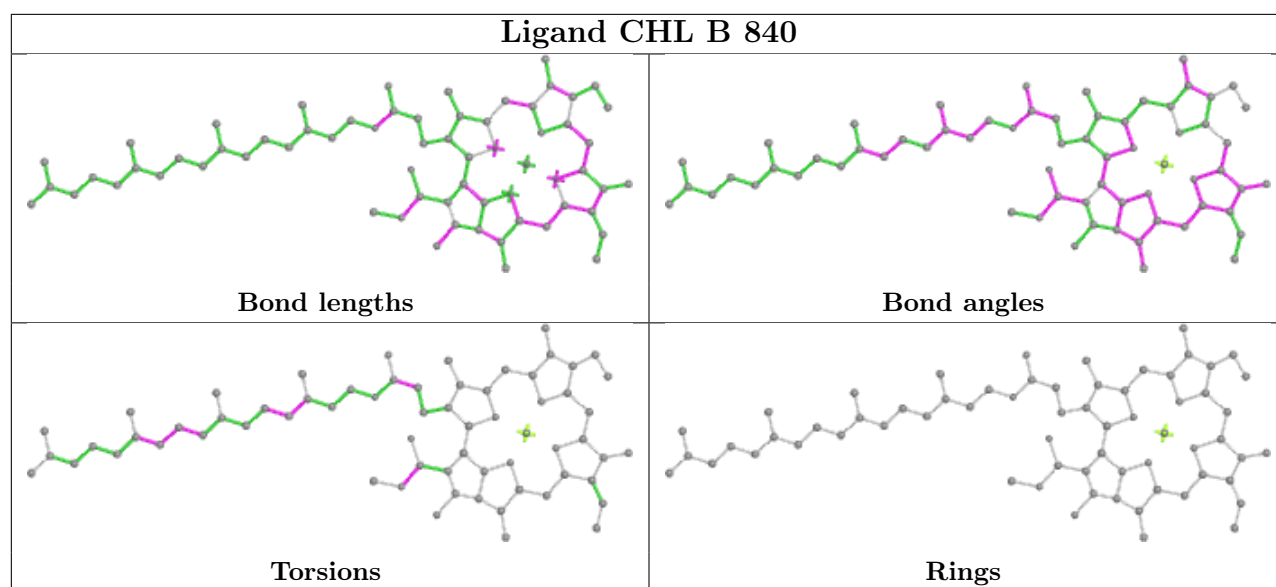
Ligand CHL B 817

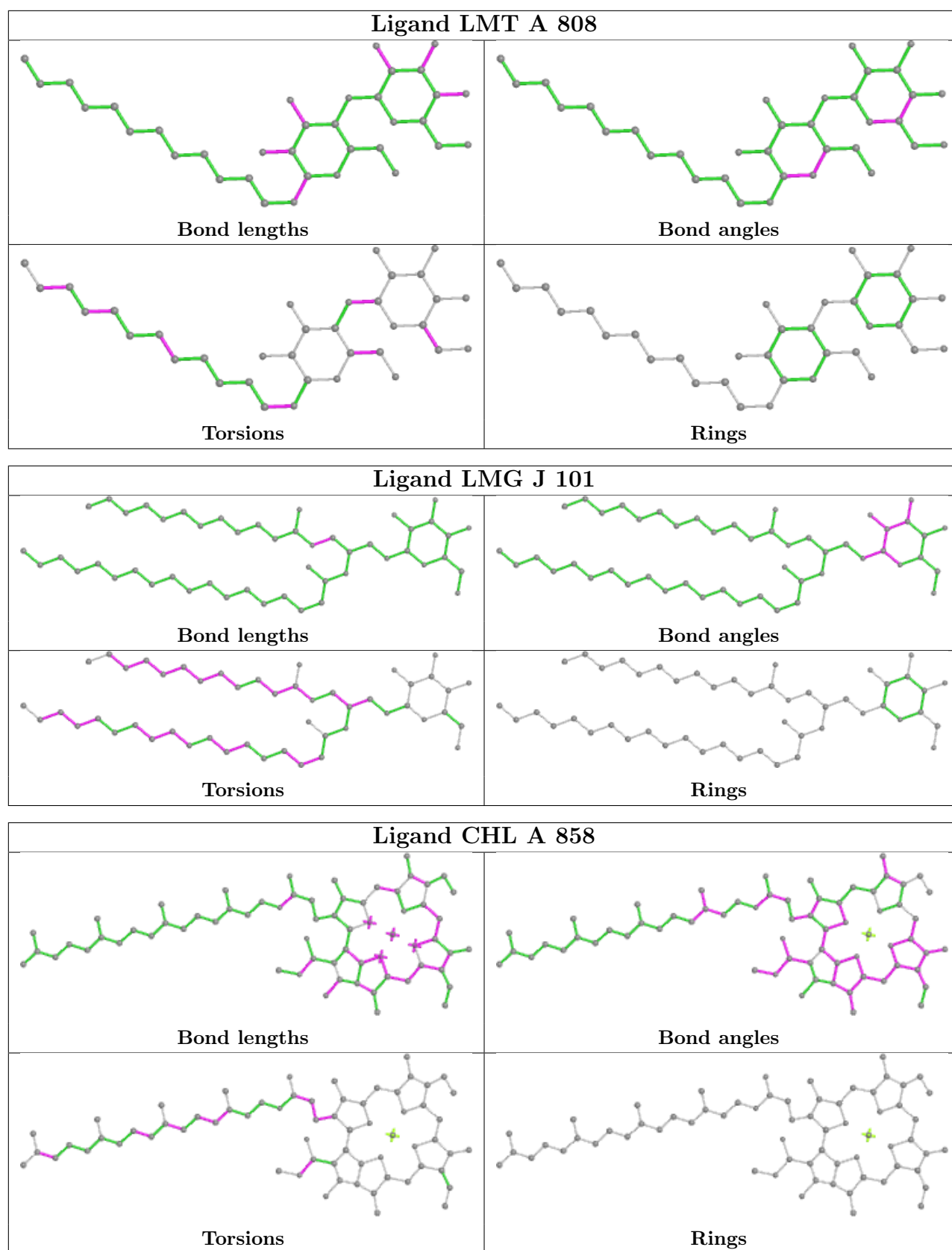


Ligand CHL A 835

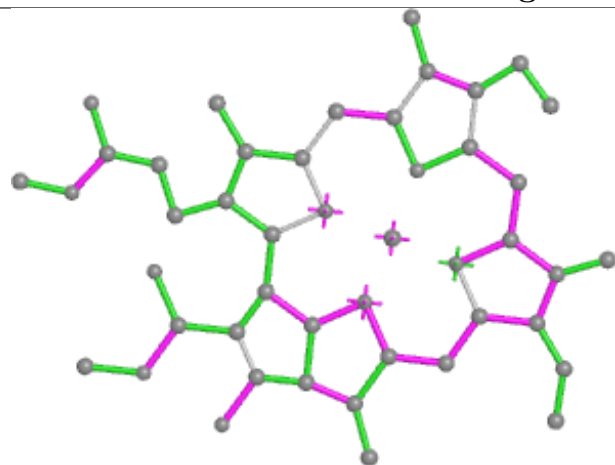




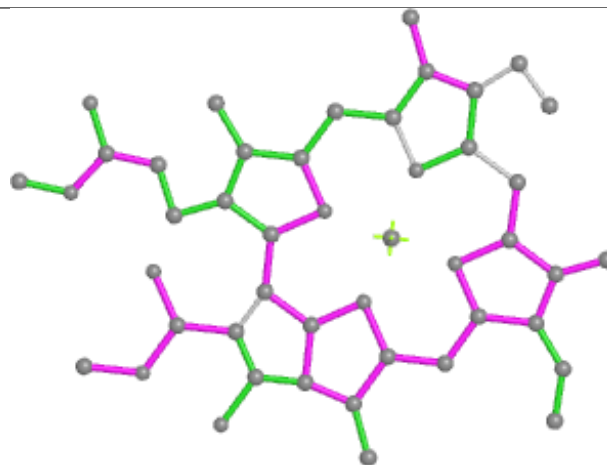




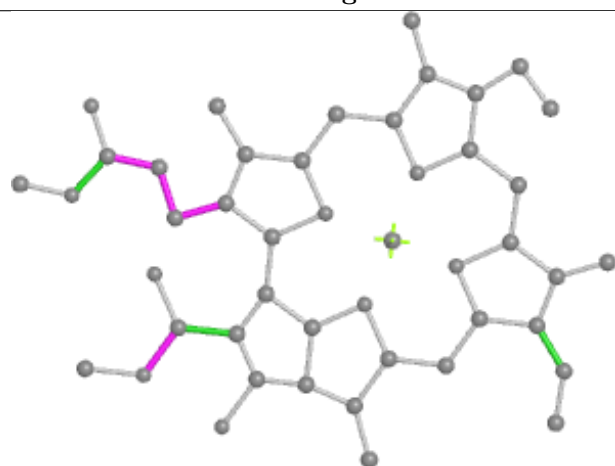
Ligand CHL b 313



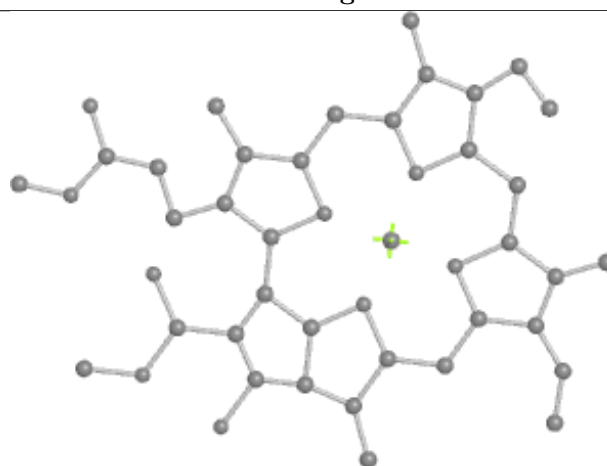
Bond lengths



Bond angles

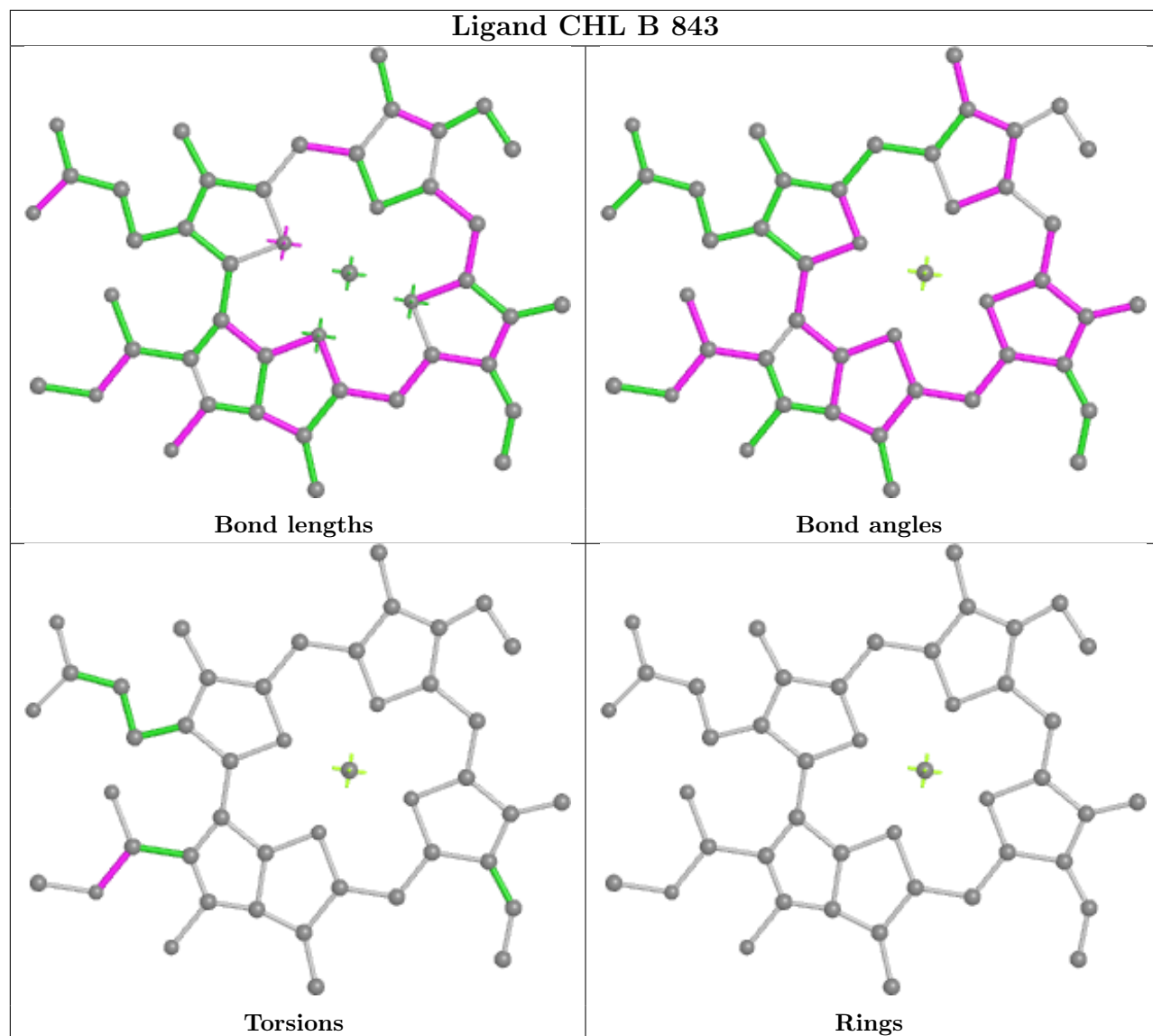


Torsions

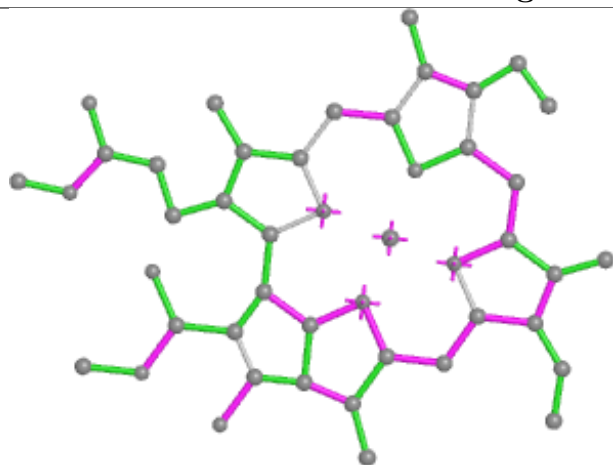


Rings

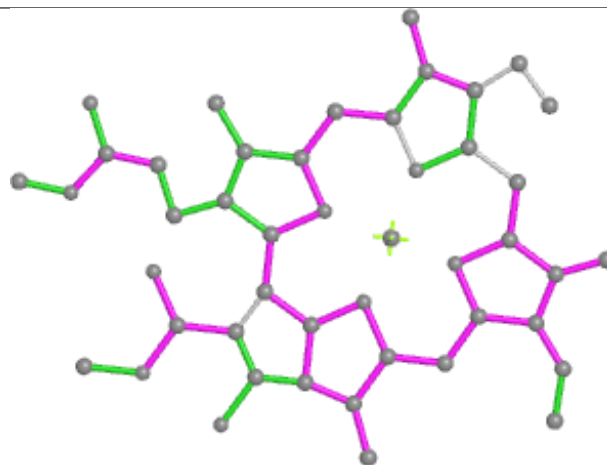
Ligand CHL B 843



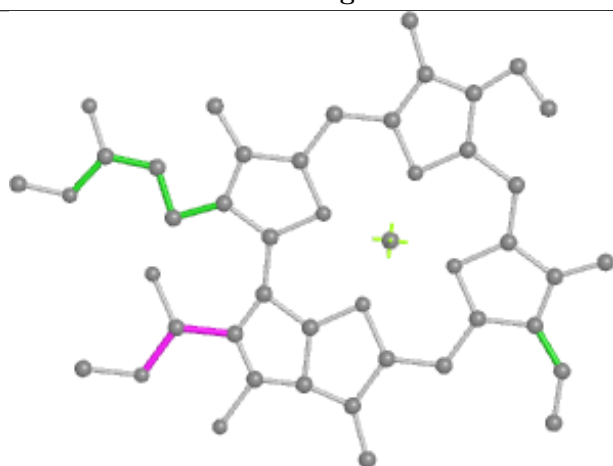
Ligand CHL b 314



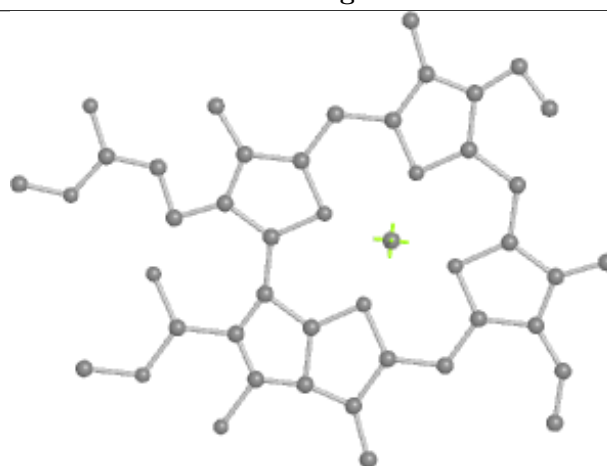
Bond lengths



Bond angles

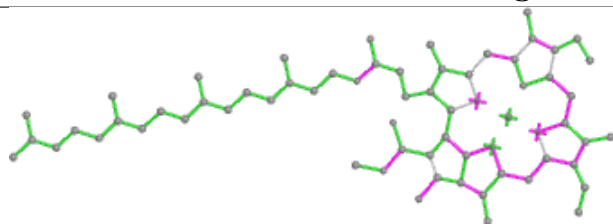


Torsions

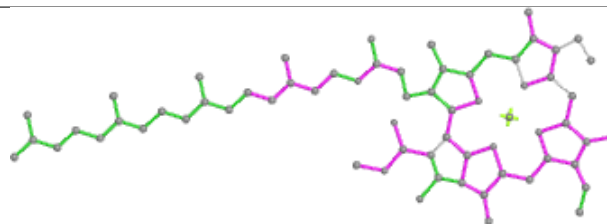


Rings

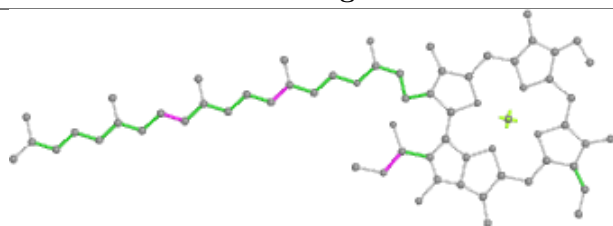
Ligand CHL A 856



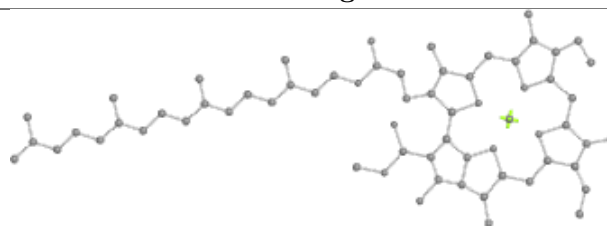
Bond lengths



Bond angles

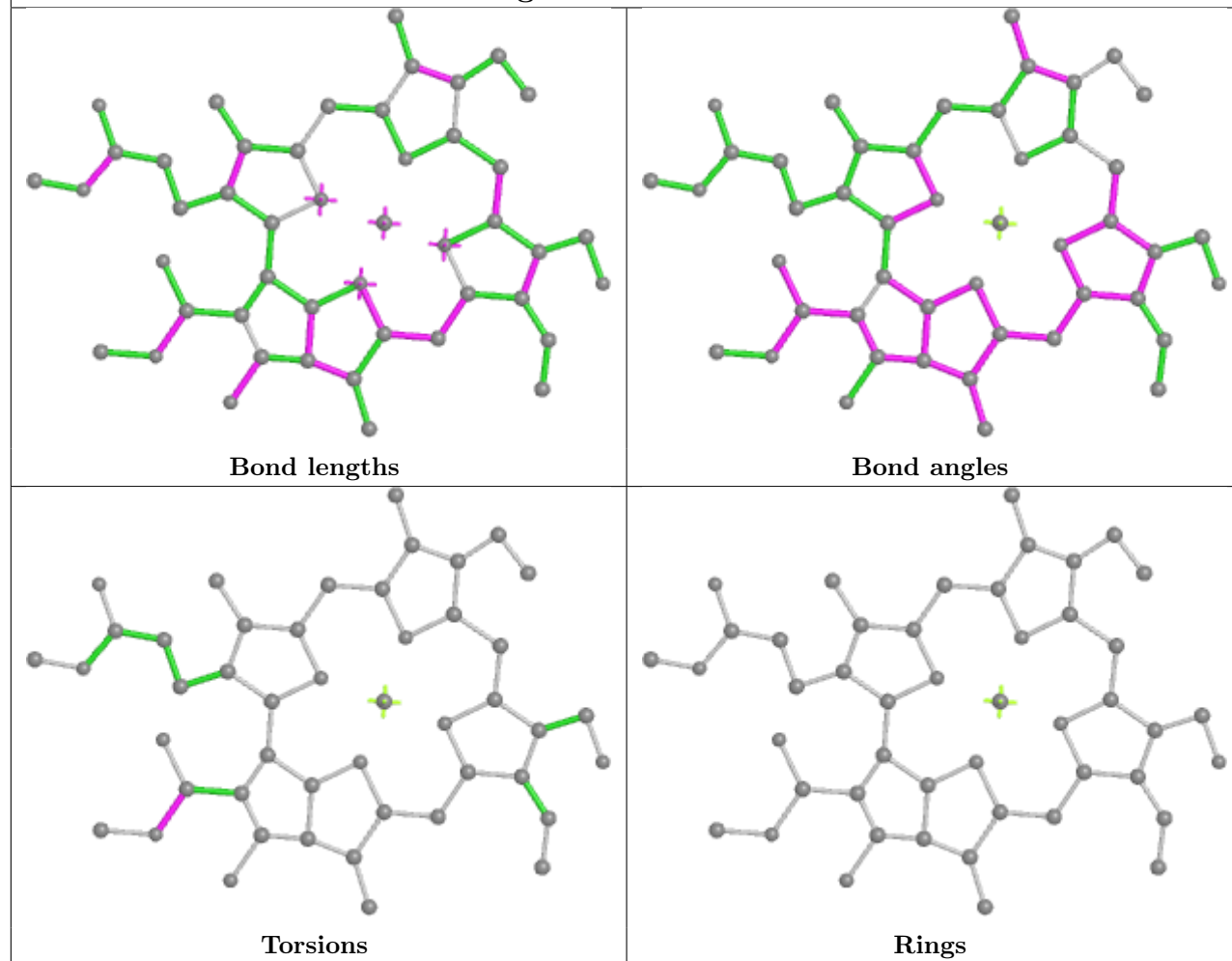


Torsions

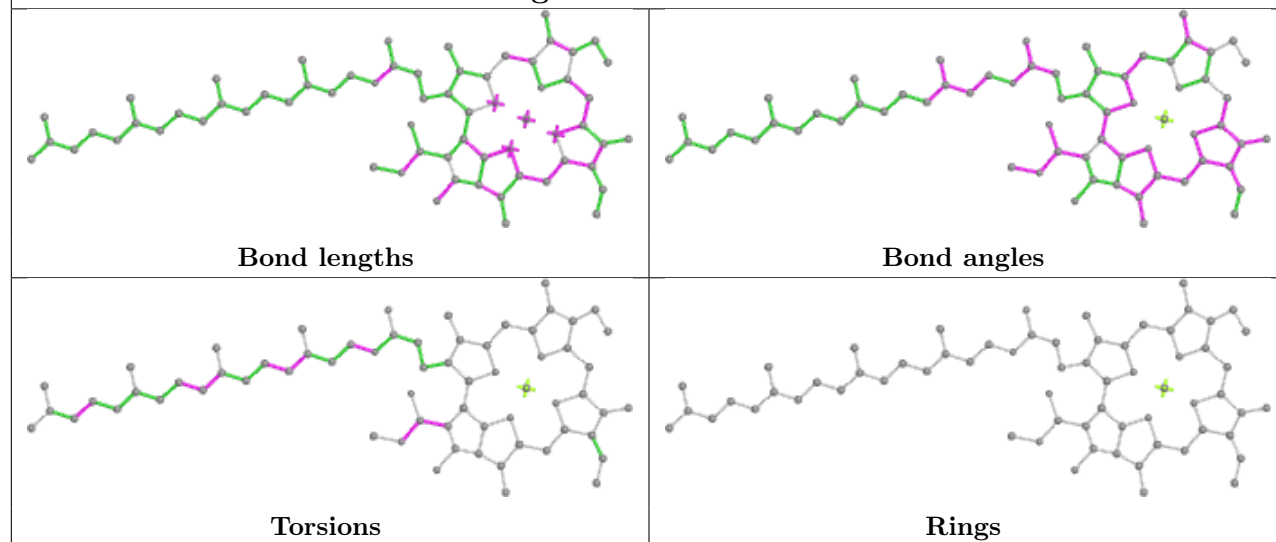


Rings

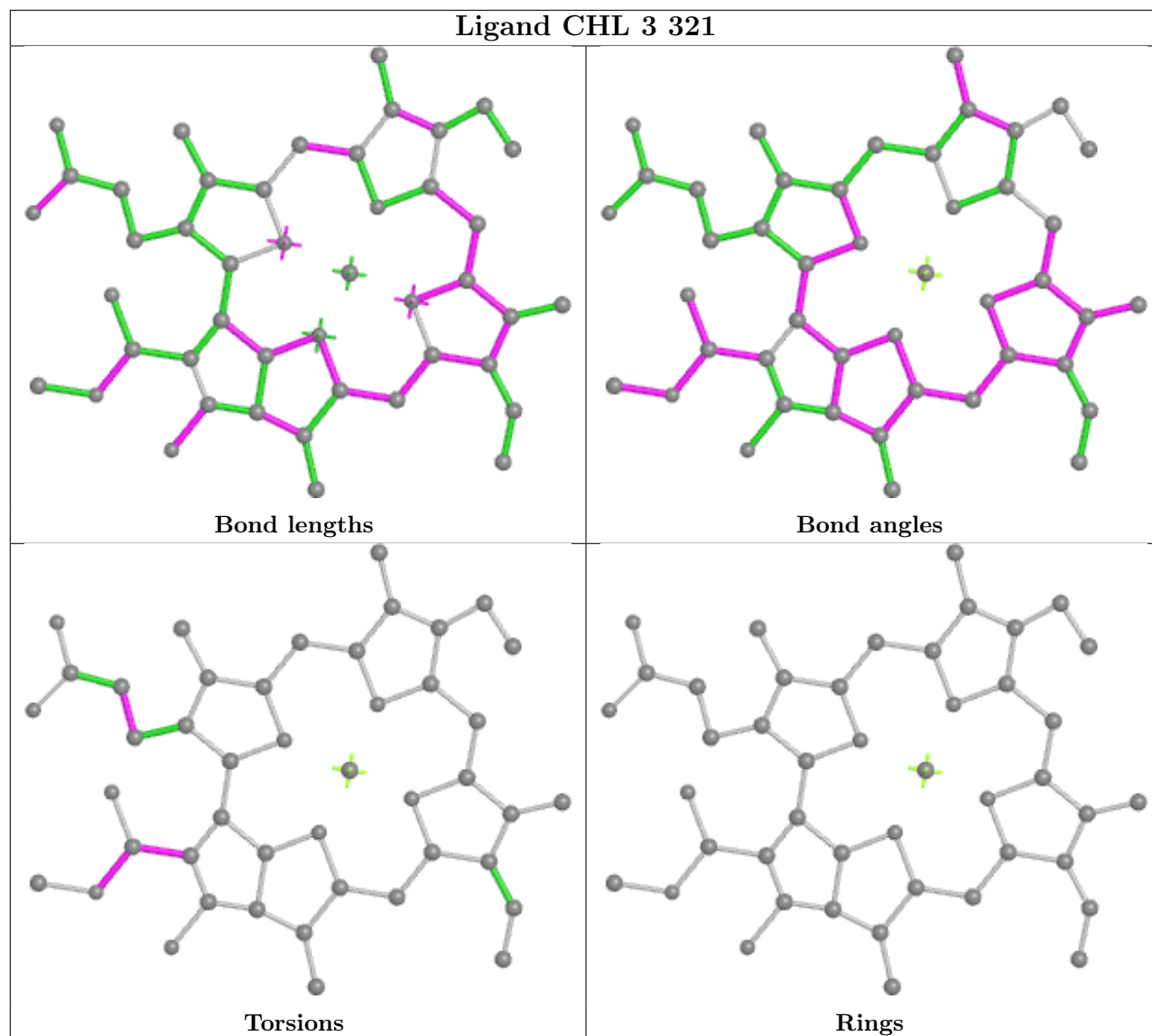
Ligand CHL 7 321



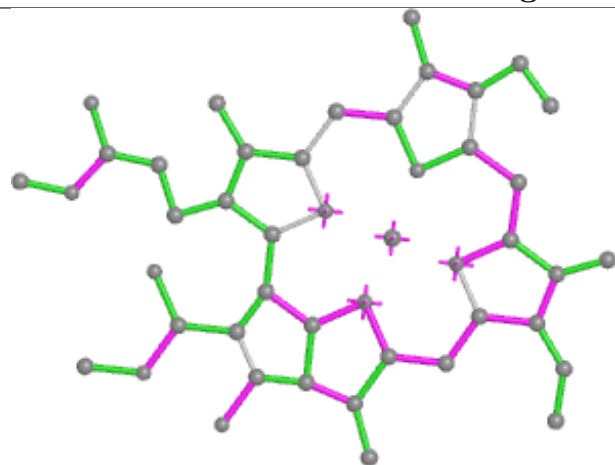
Ligand CHL A 855



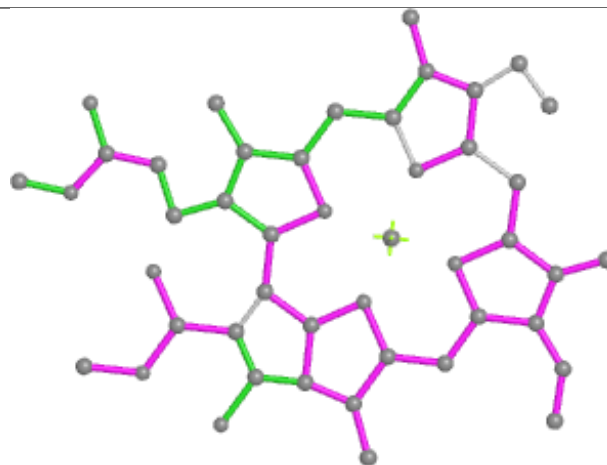
Ligand CHL 3 321



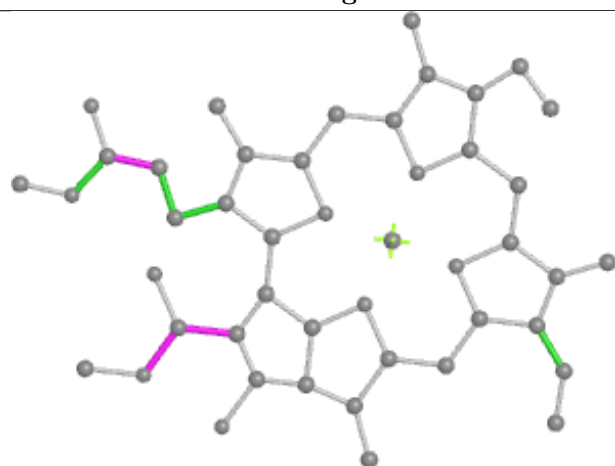
Ligand CHL 5 311



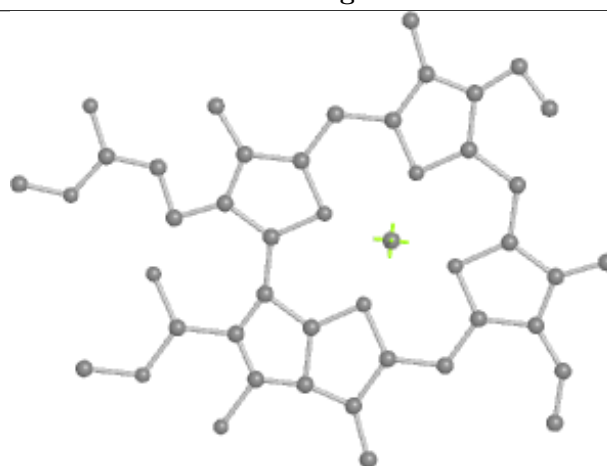
Bond lengths



Bond angles

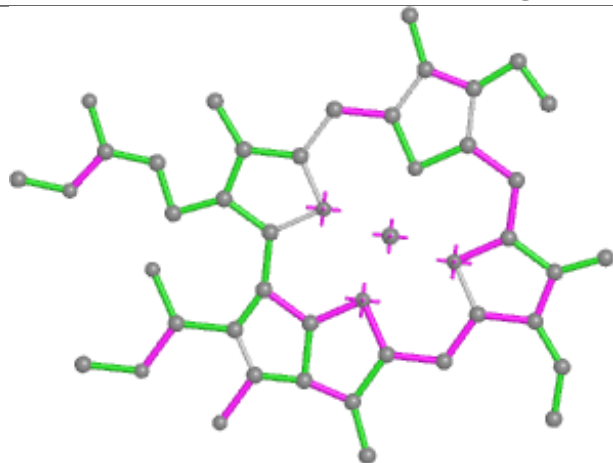


Torsions

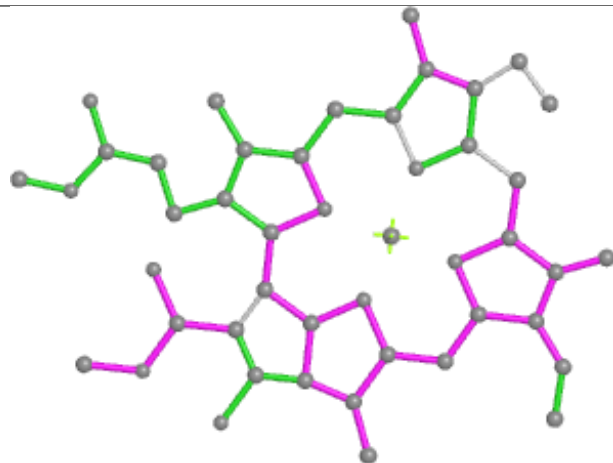


Rings

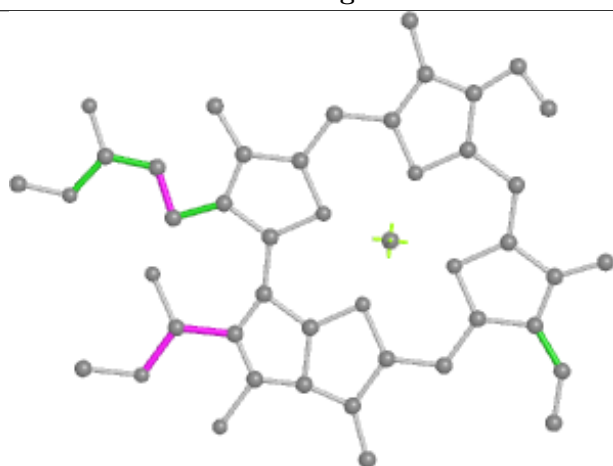
Ligand CHL b 305



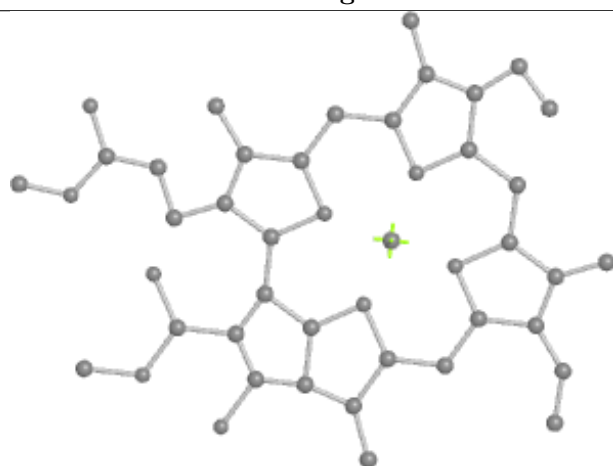
Bond lengths



Bond angles

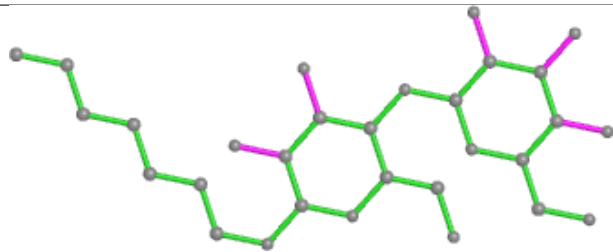


Torsions

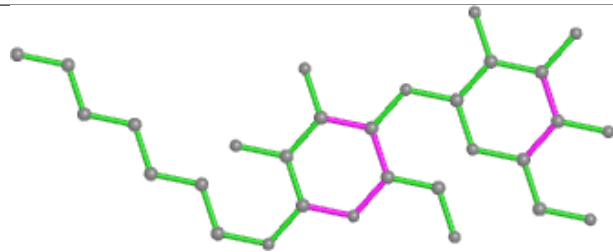


Rings

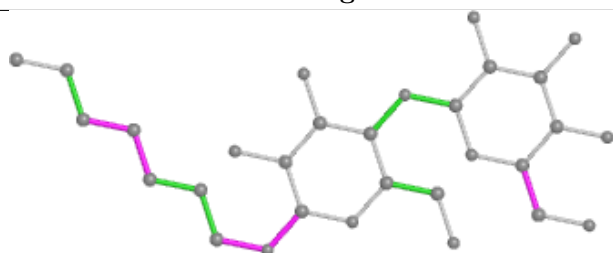
Ligand LMT 5 306



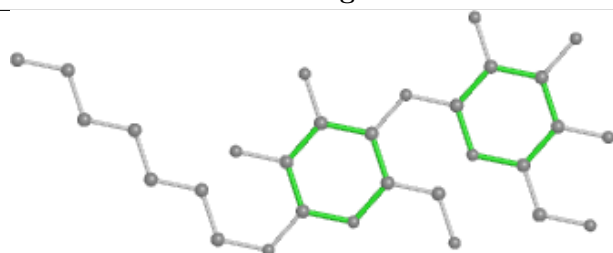
Bond lengths



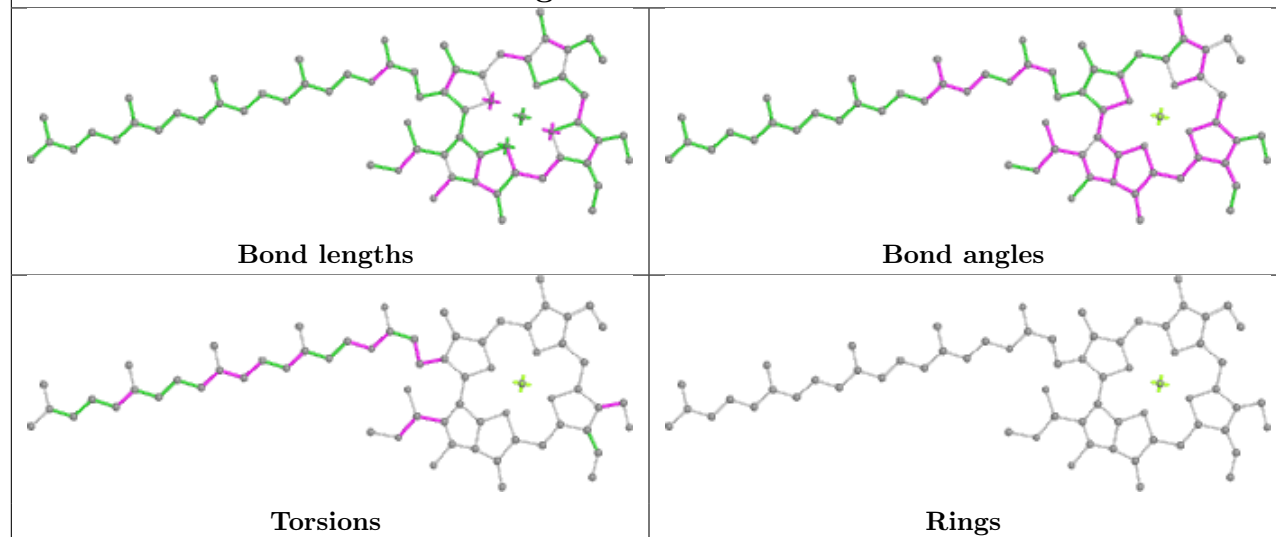
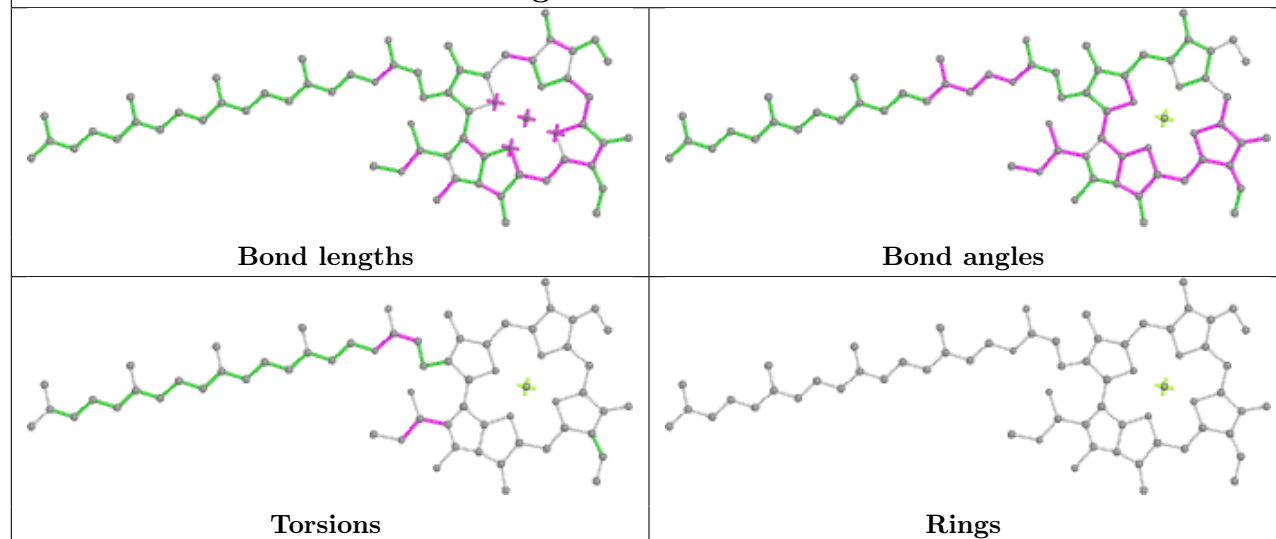
Bond angles



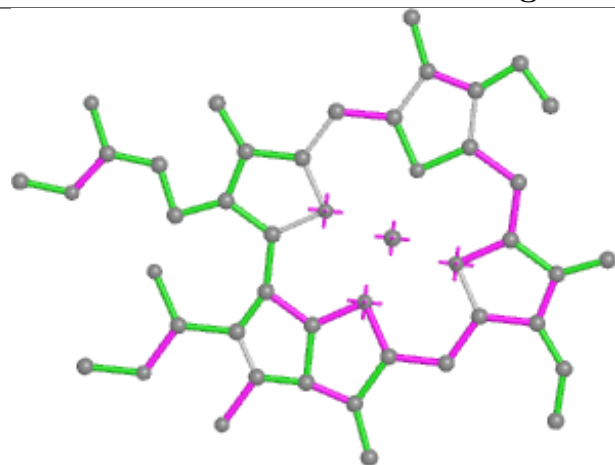
Torsions



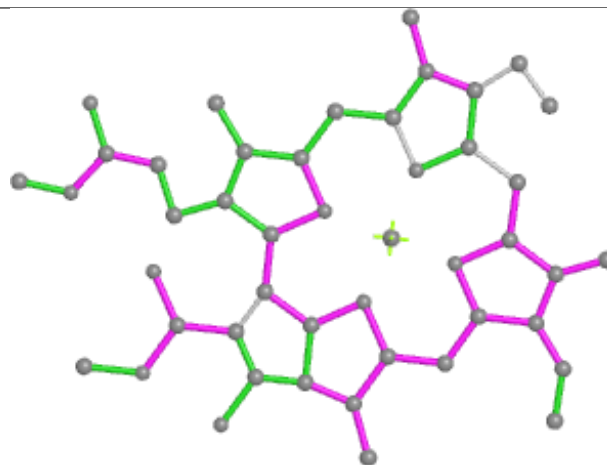
Rings

Ligand CHL 7 319**Ligand CHL B 811**

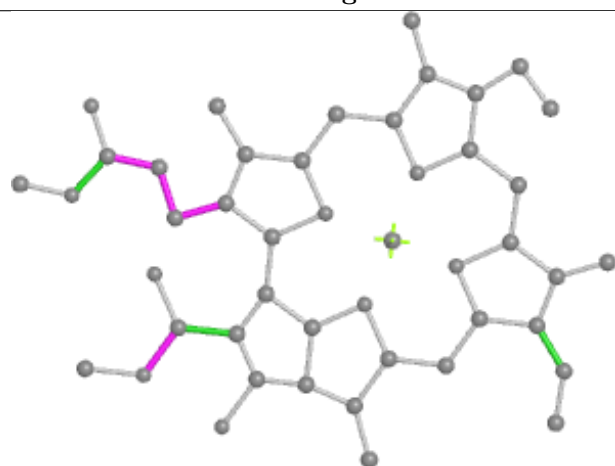
Ligand CHL 6 305



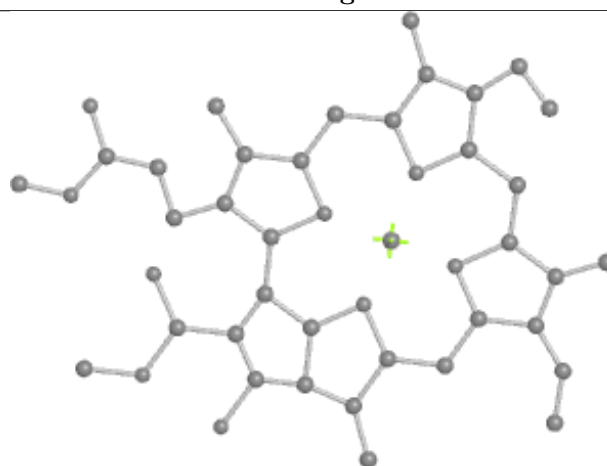
Bond lengths



Bond angles

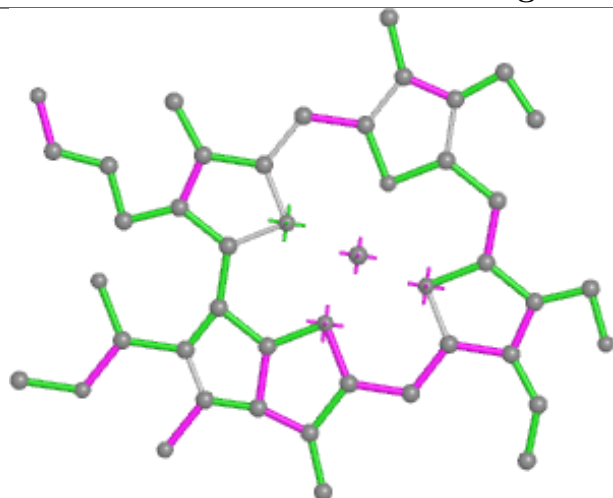


Torsions

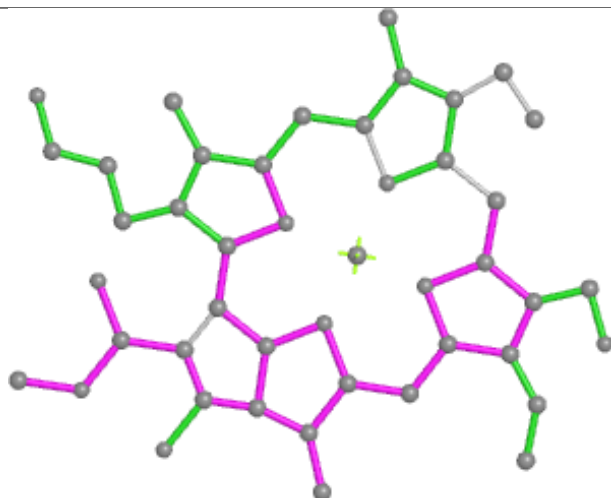


Rings

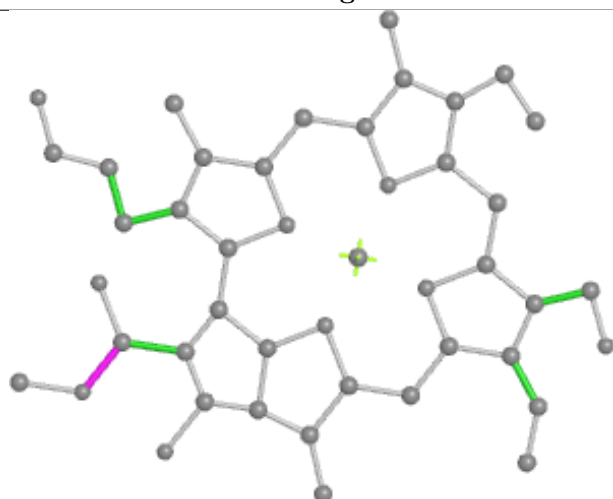
Ligand CHL 8 324



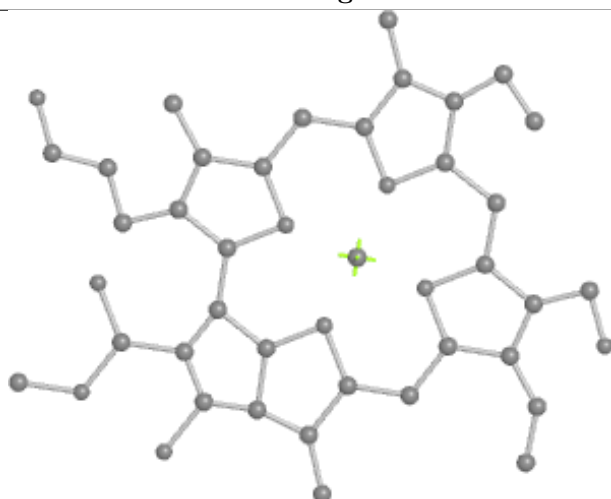
Bond lengths



Bond angles

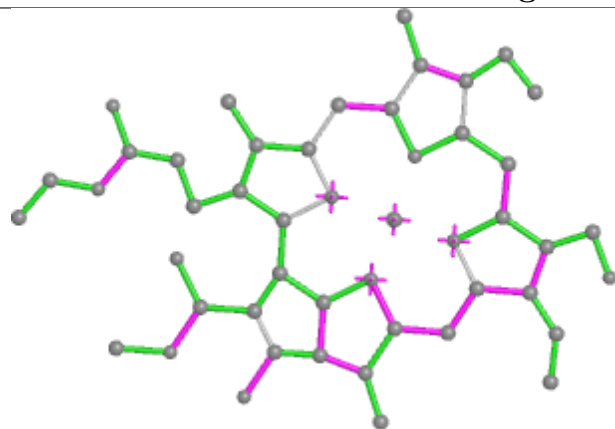


Torsions

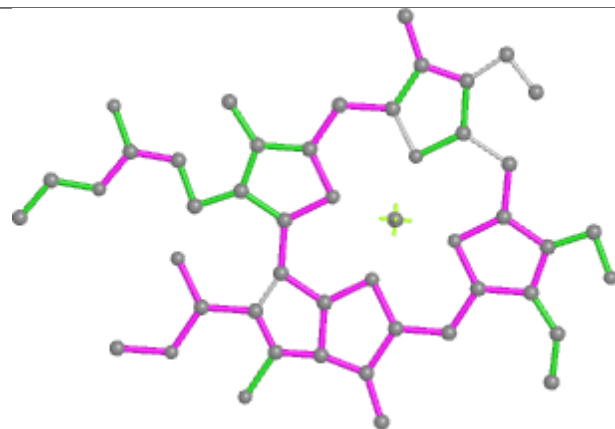


Rings

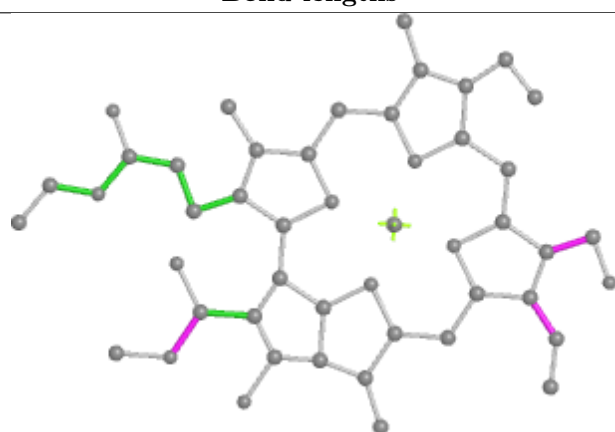
Ligand CHL b 316



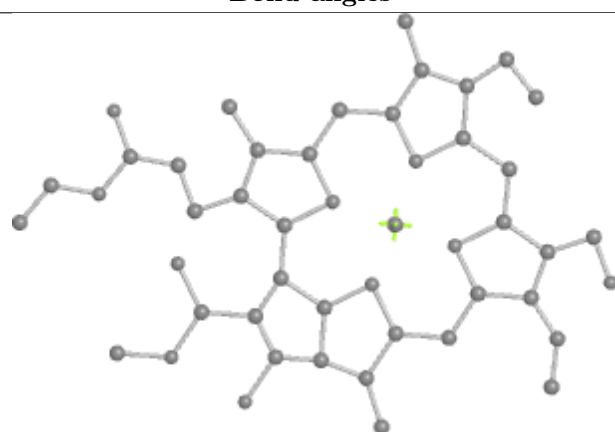
Bond lengths



Bond angles

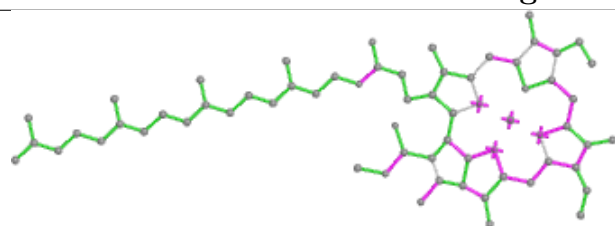


Torsions

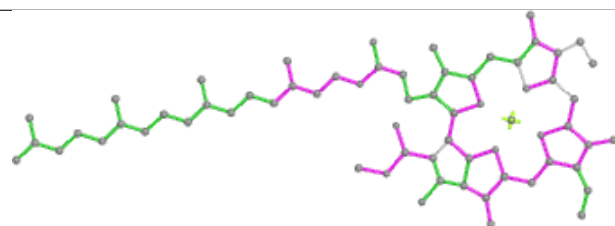


Rings

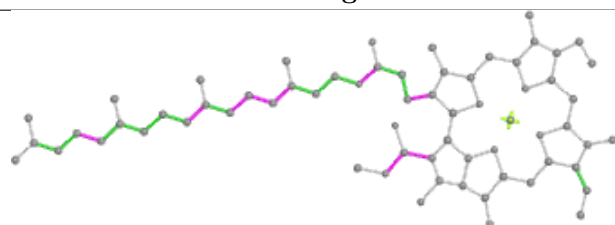
Ligand CHL 7 317



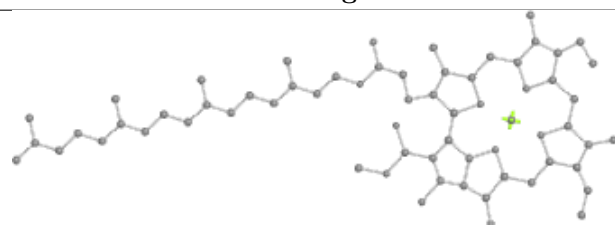
Bond lengths



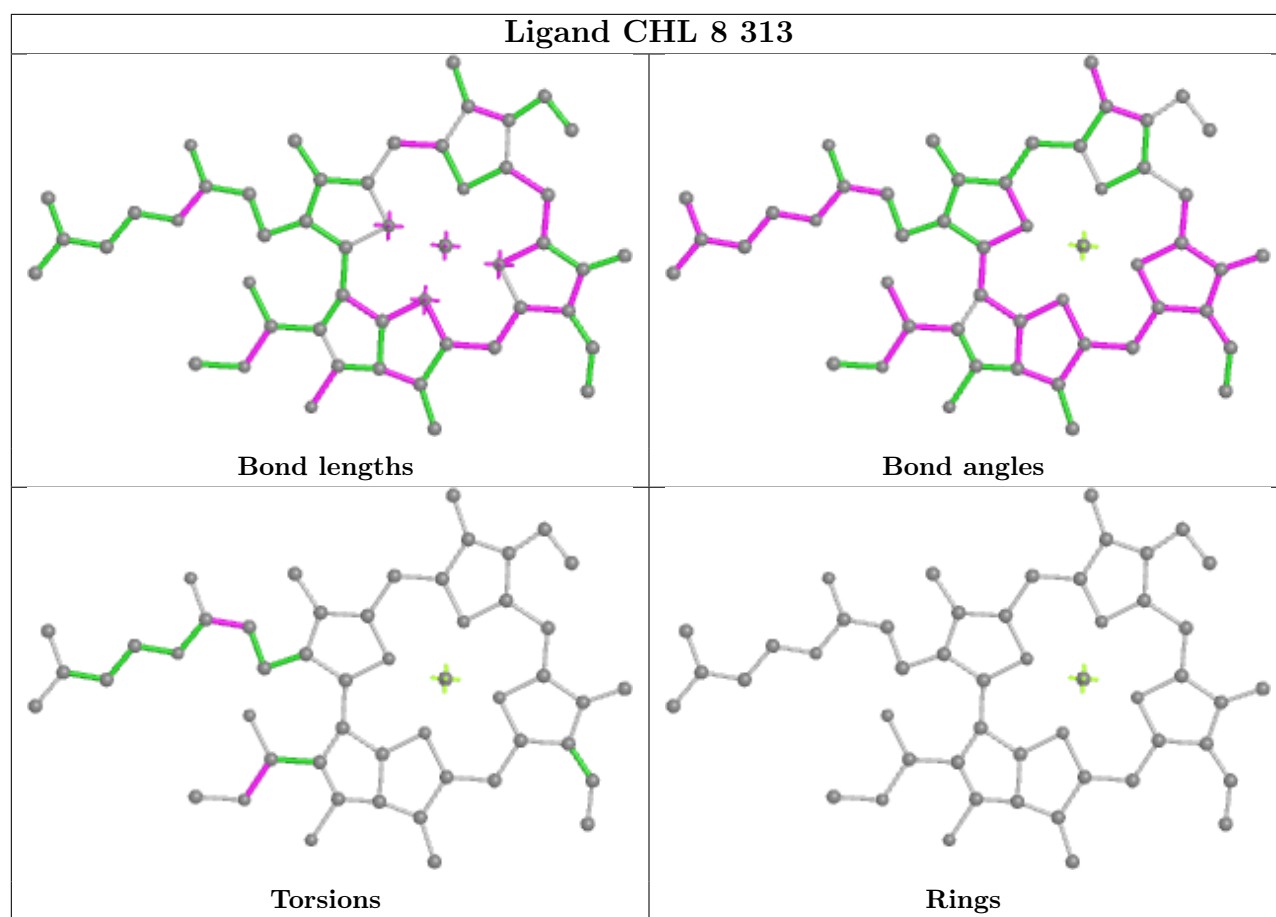
Bond angles



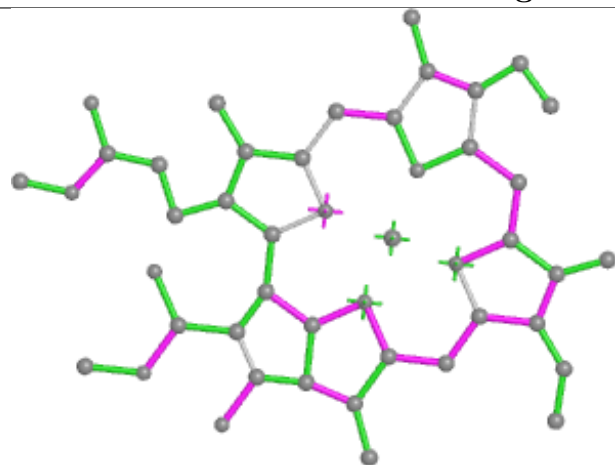
Torsions



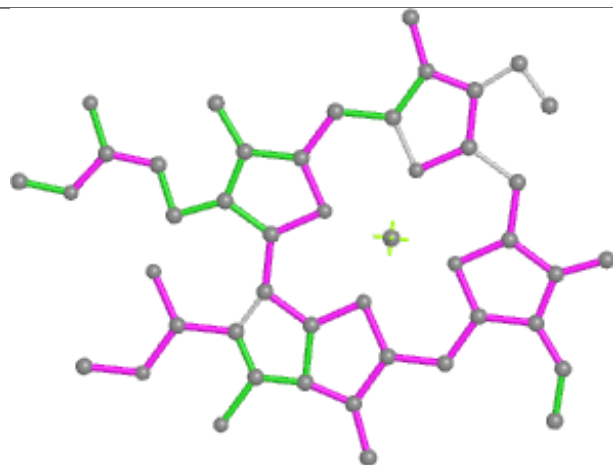
Rings



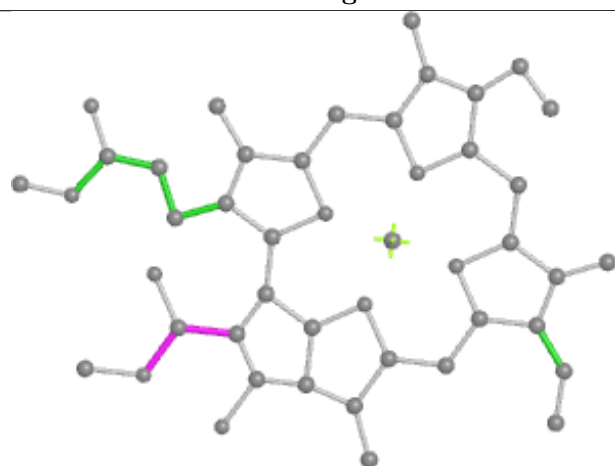
Ligand CHL A 857



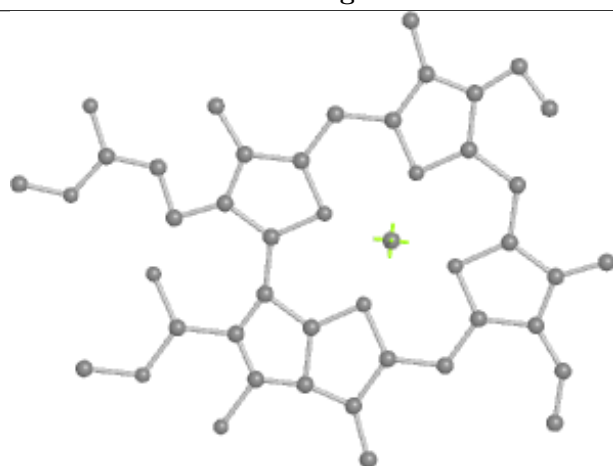
Bond lengths



Bond angles

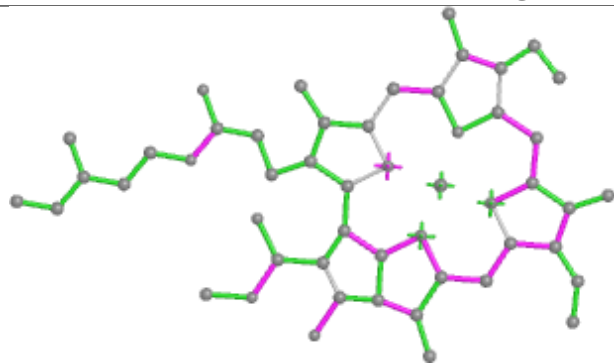


Torsions

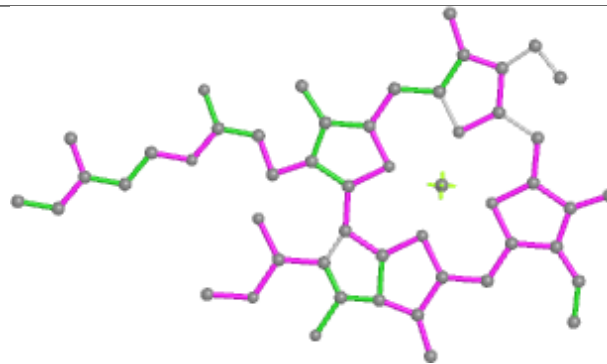


Rings

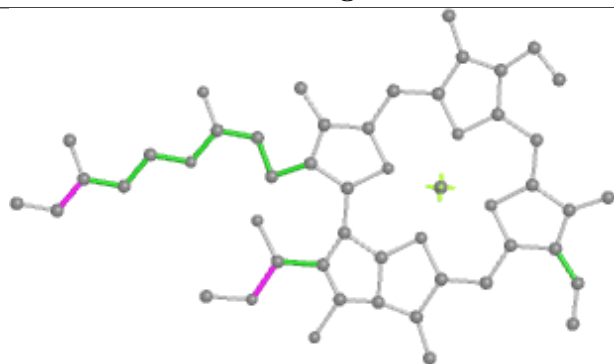
Ligand CHL A 852



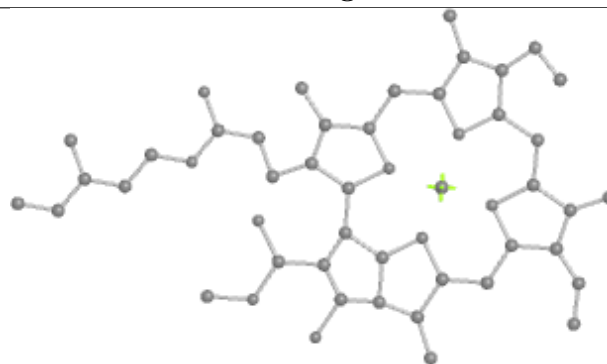
Bond lengths



Bond angles

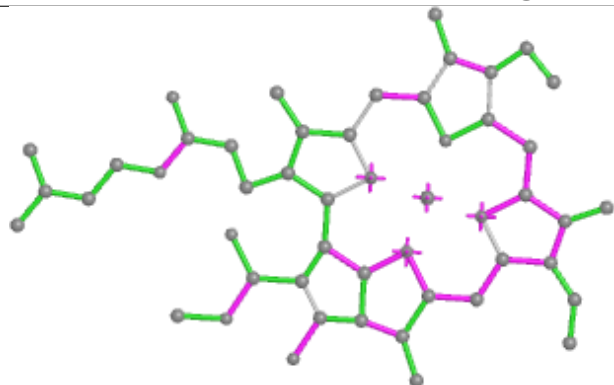


Torsions

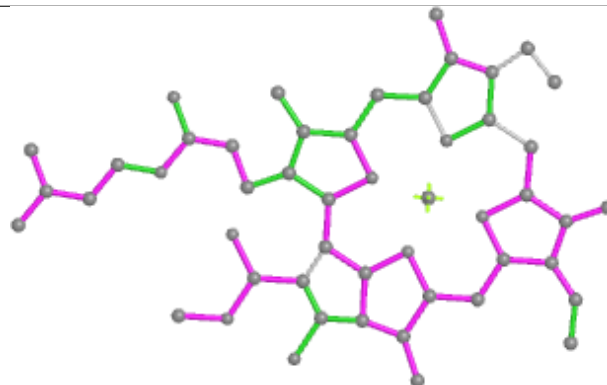


Rings

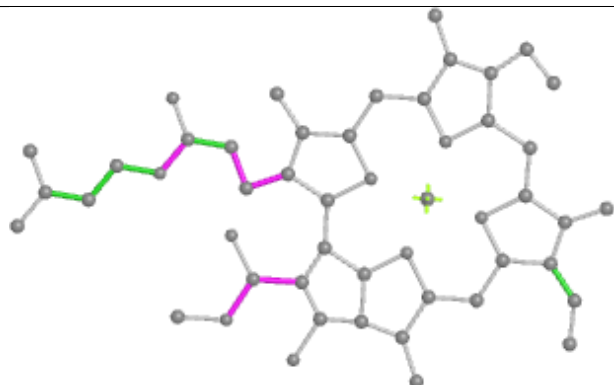
Ligand CHL 4 320



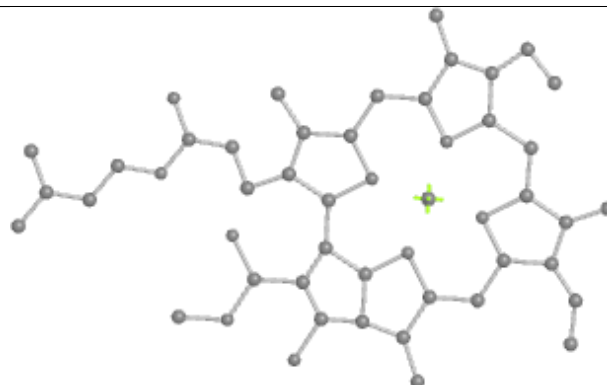
Bond lengths



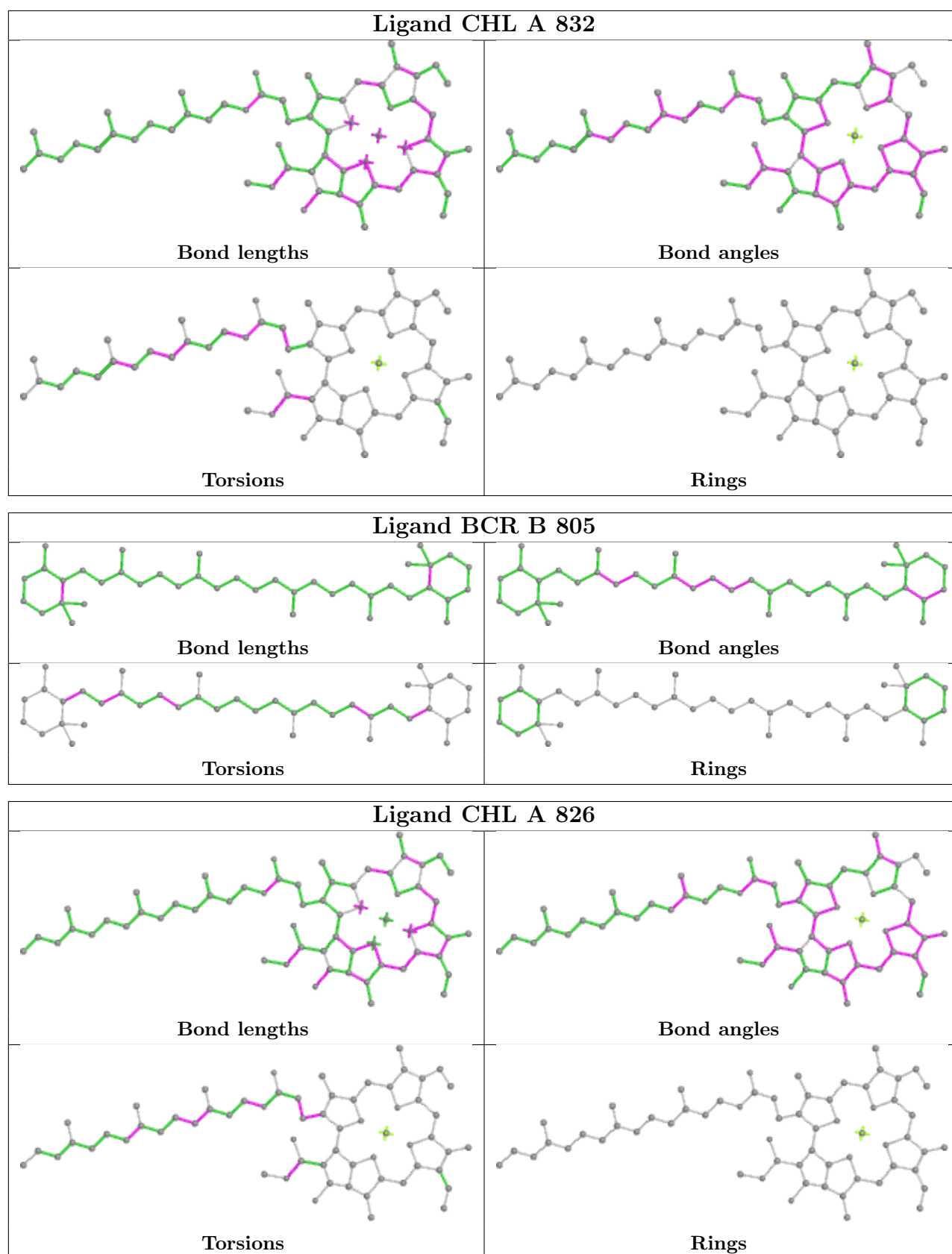
Bond angles

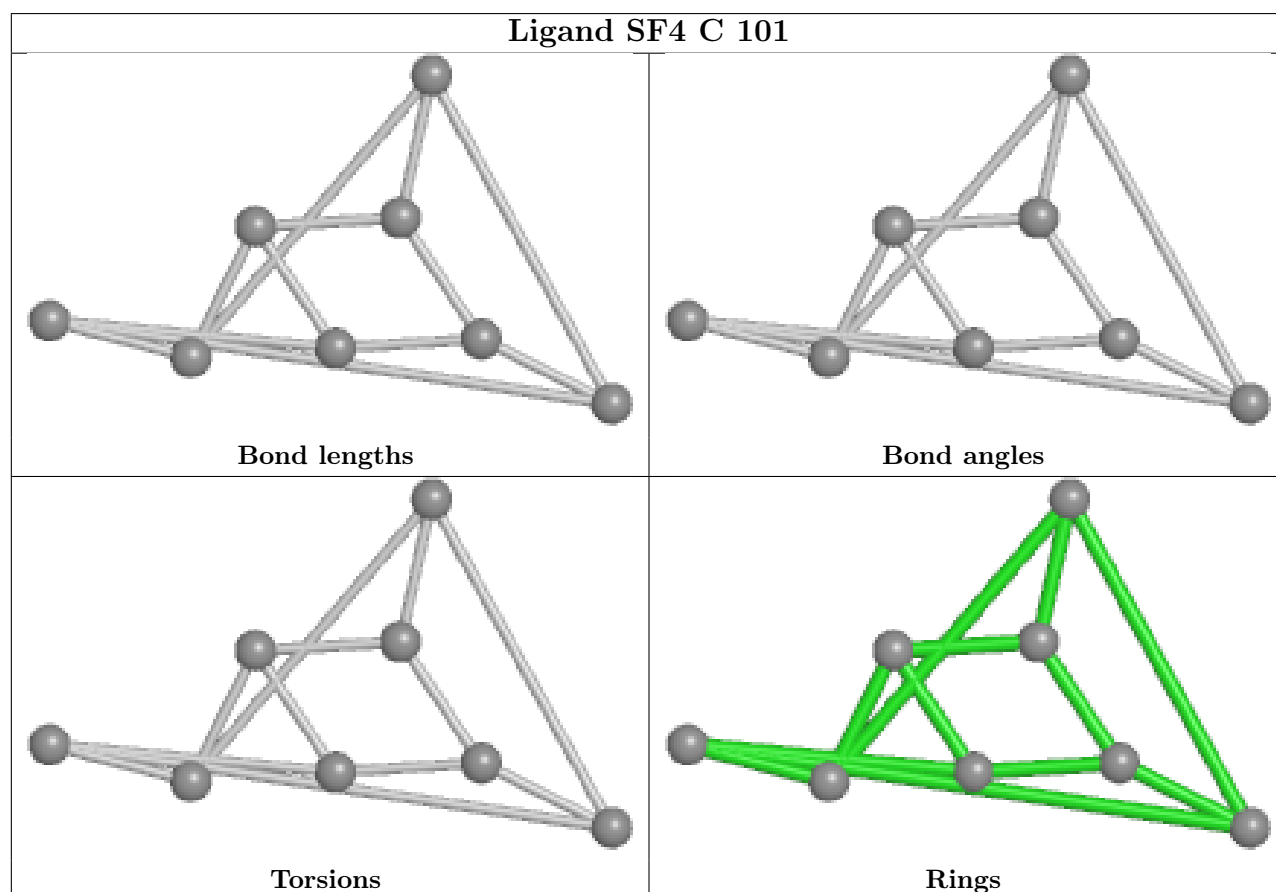
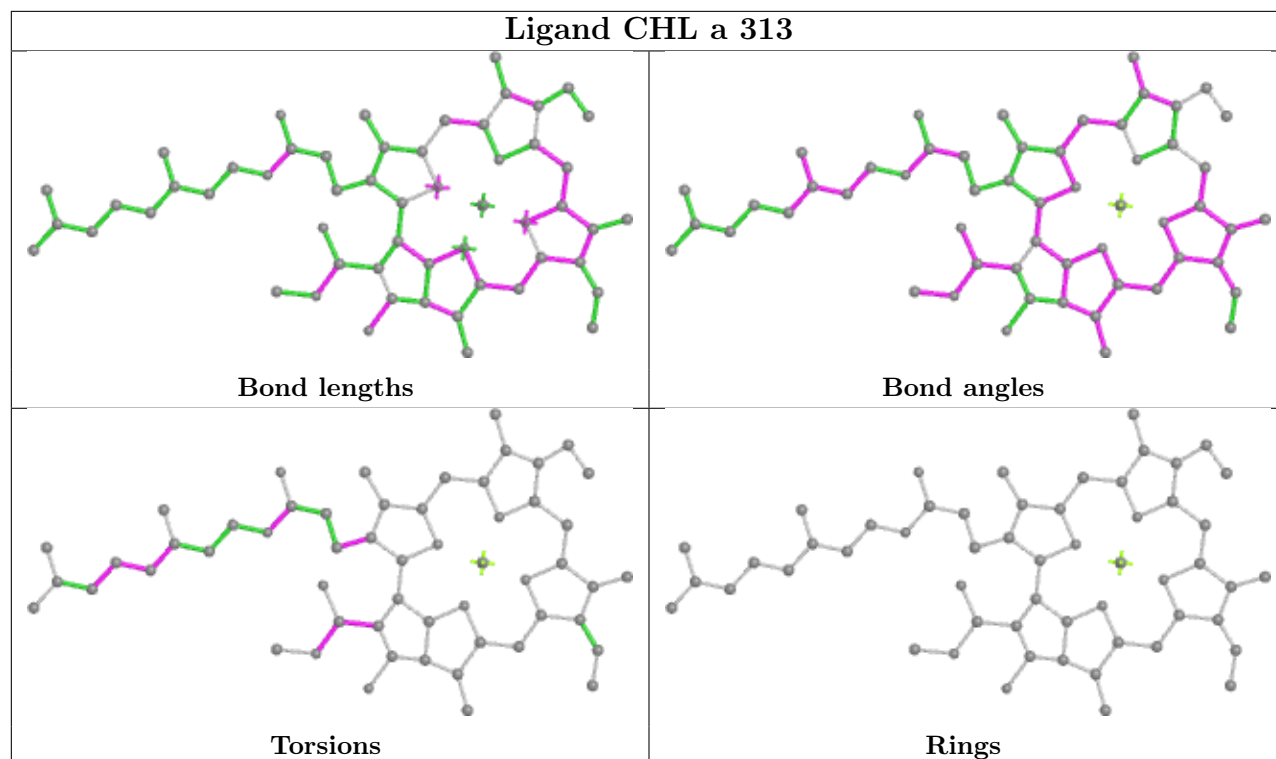


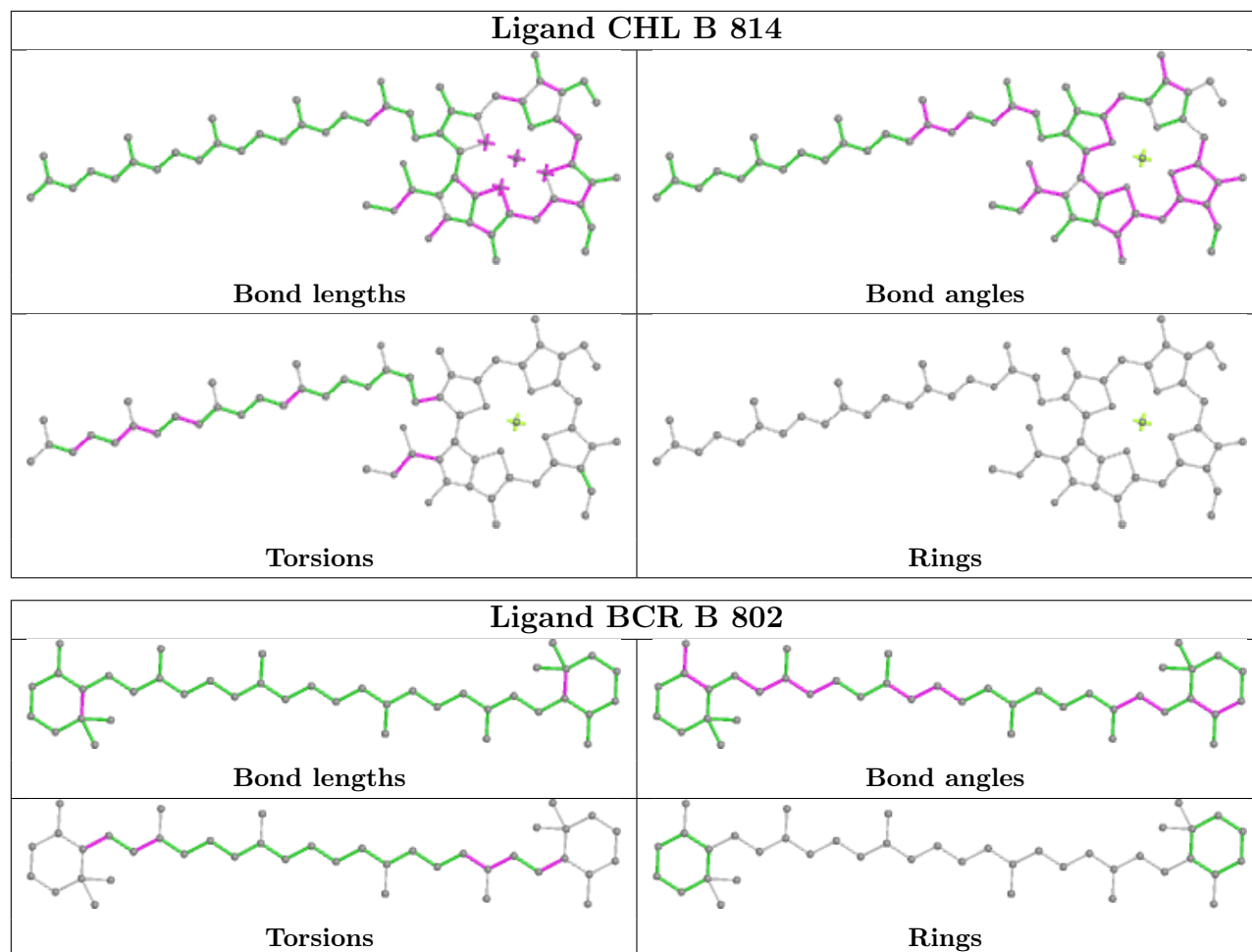
Torsions



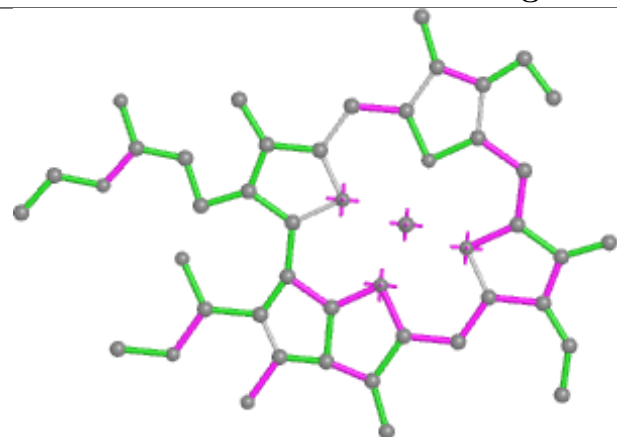
Rings



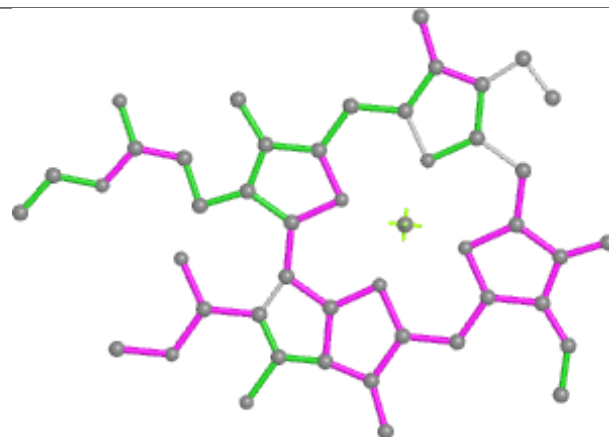




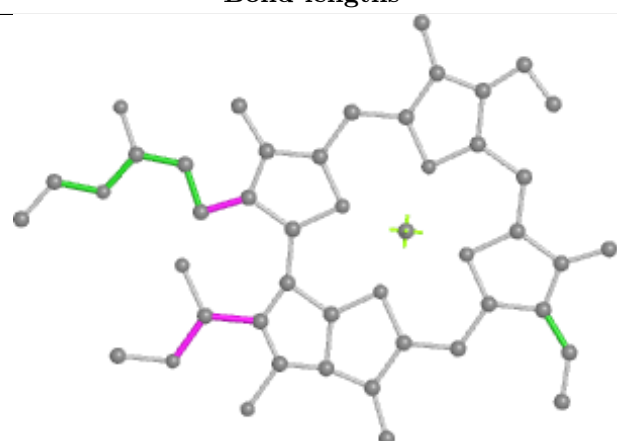
Ligand CHL 6 313



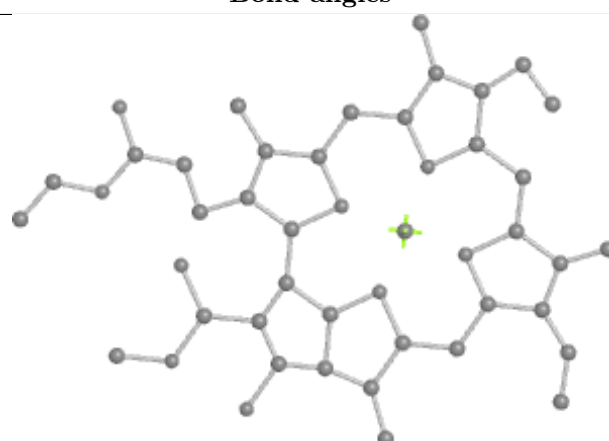
Bond lengths



Bond angles

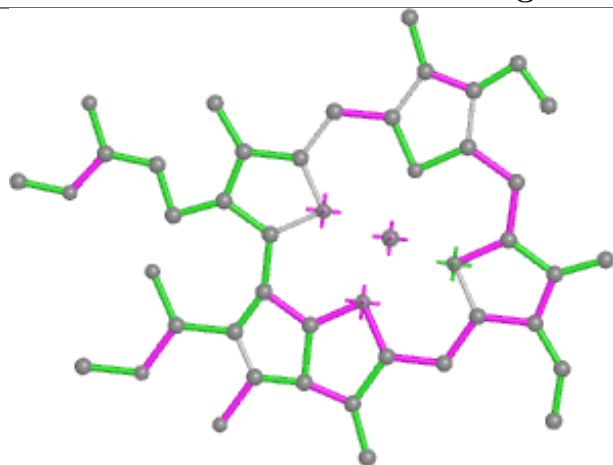


Torsions

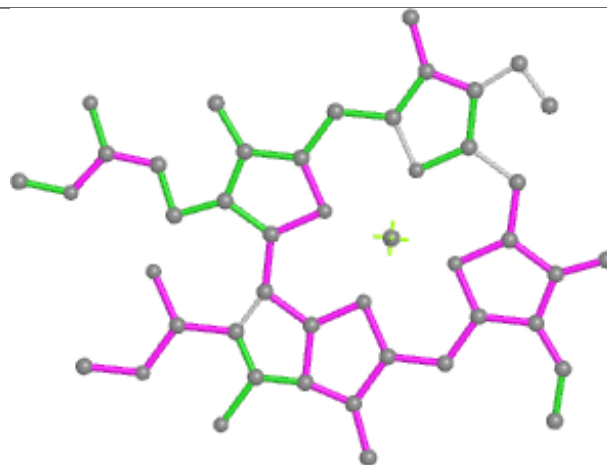


Rings

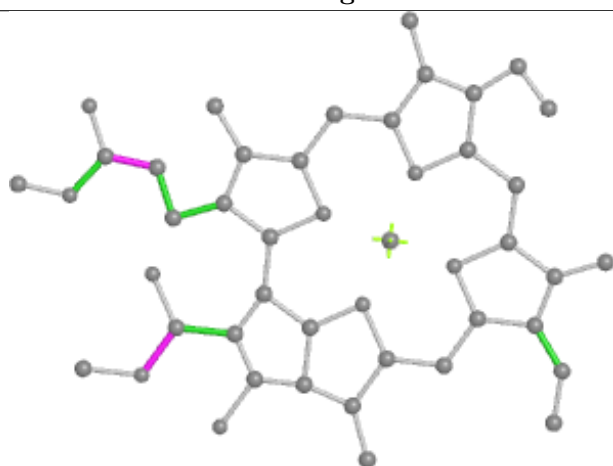
Ligand CHL b 312



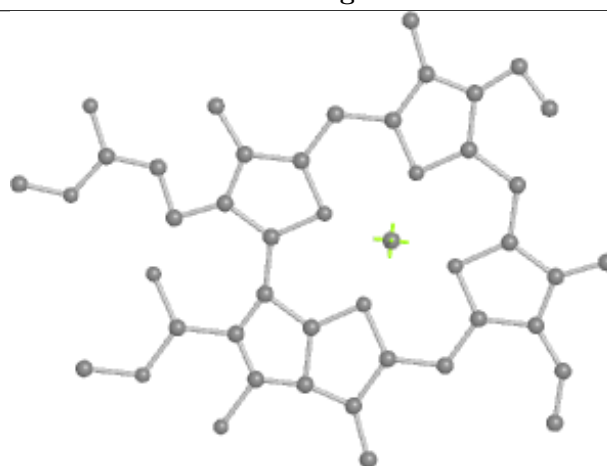
Bond lengths



Bond angles

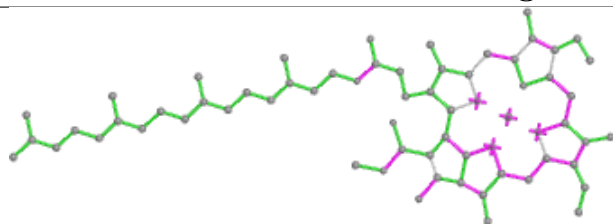


Torsions

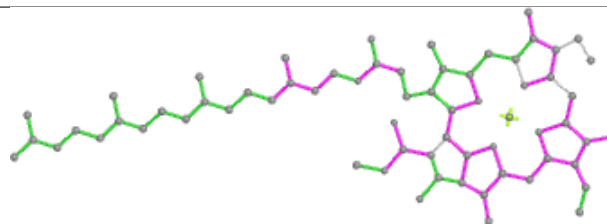


Rings

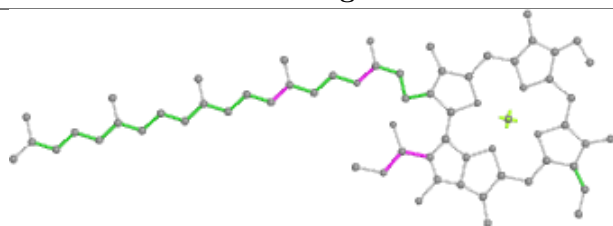
Ligand CHL 3 313



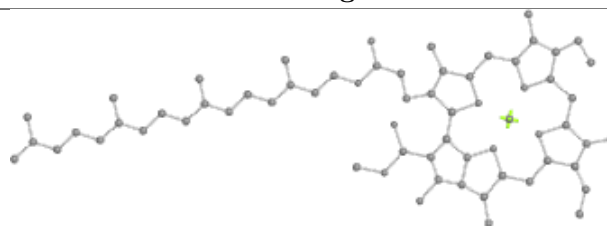
Bond lengths



Bond angles

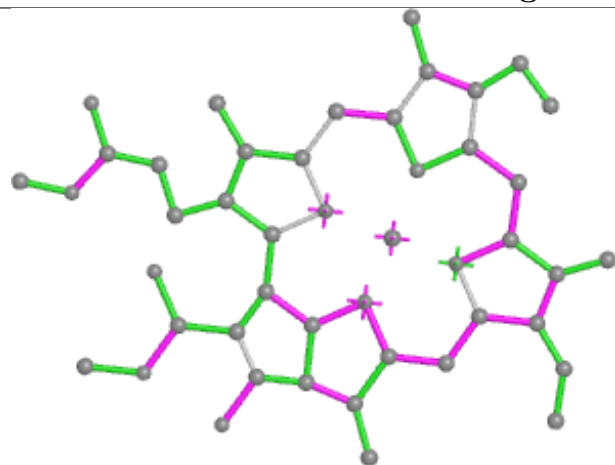


Torsions

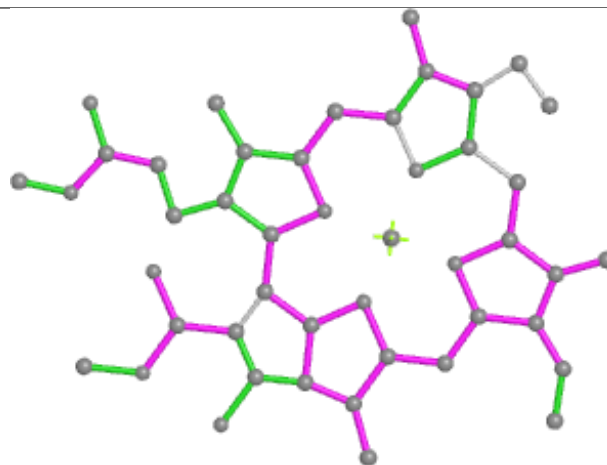


Rings

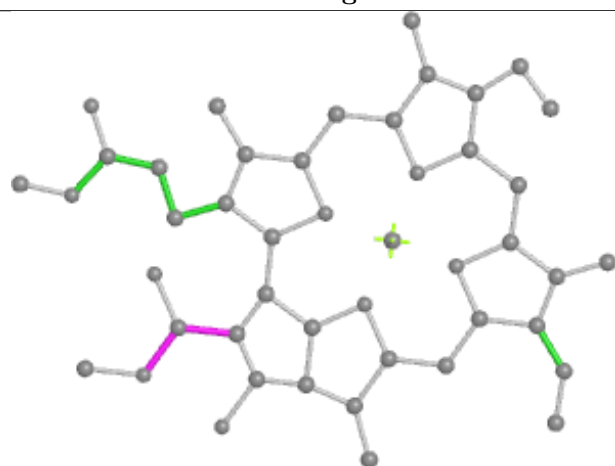
Ligand CHL 5 321



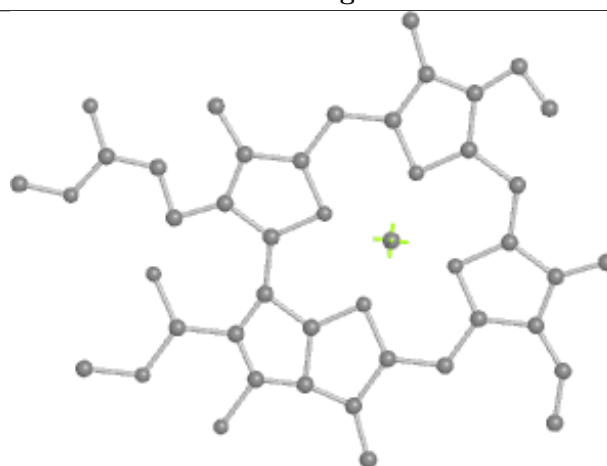
Bond lengths



Bond angles

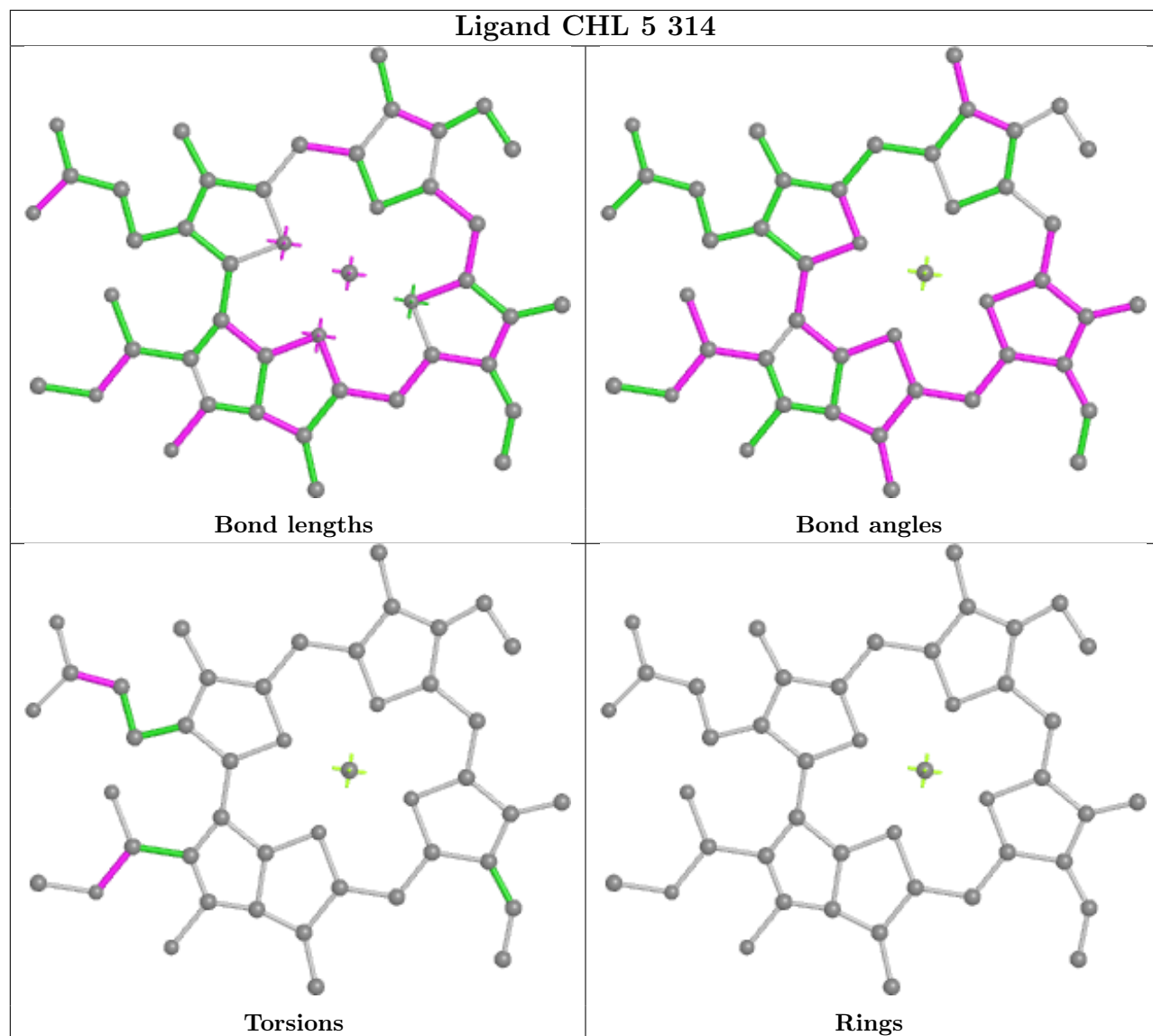


Torsions

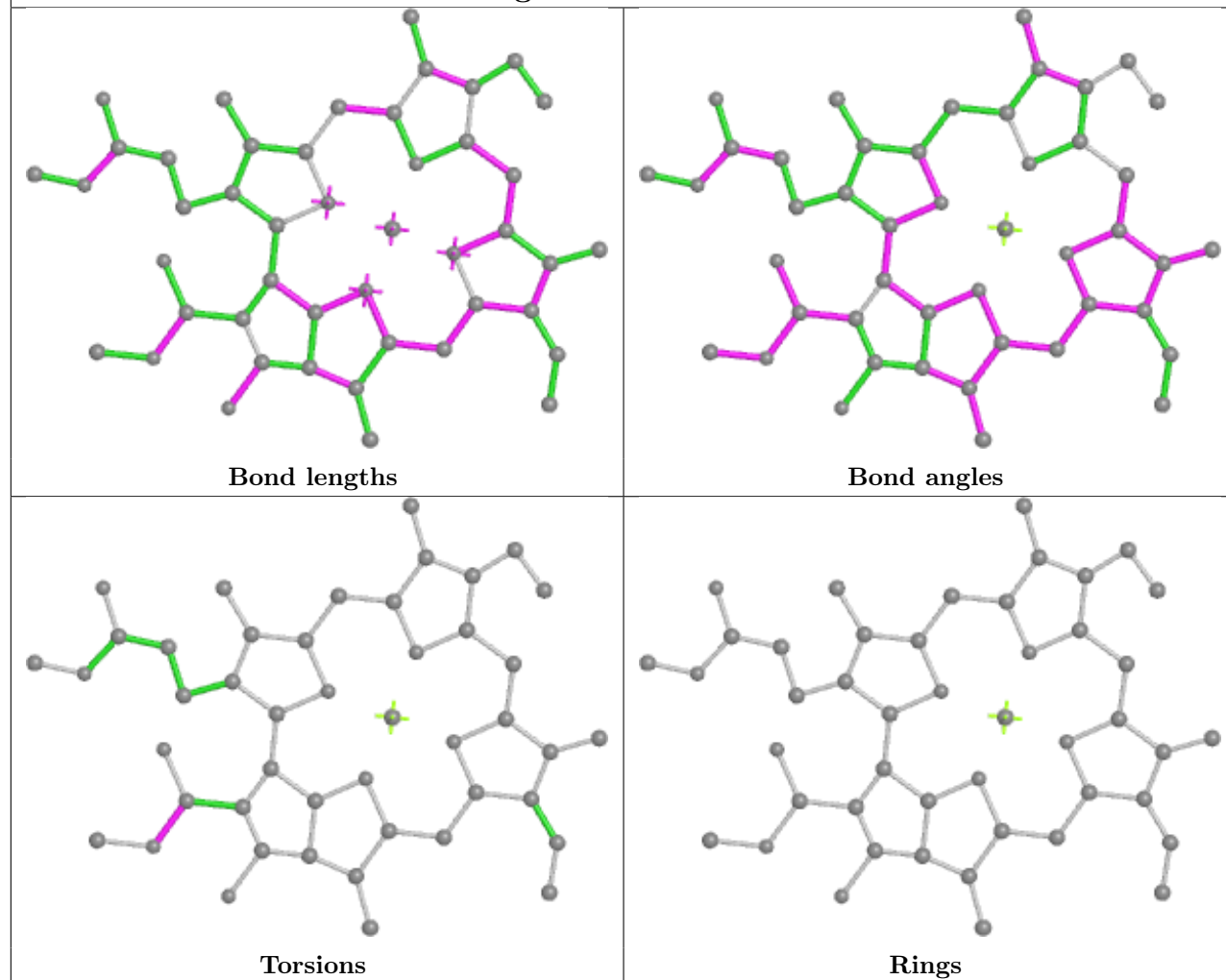


Rings

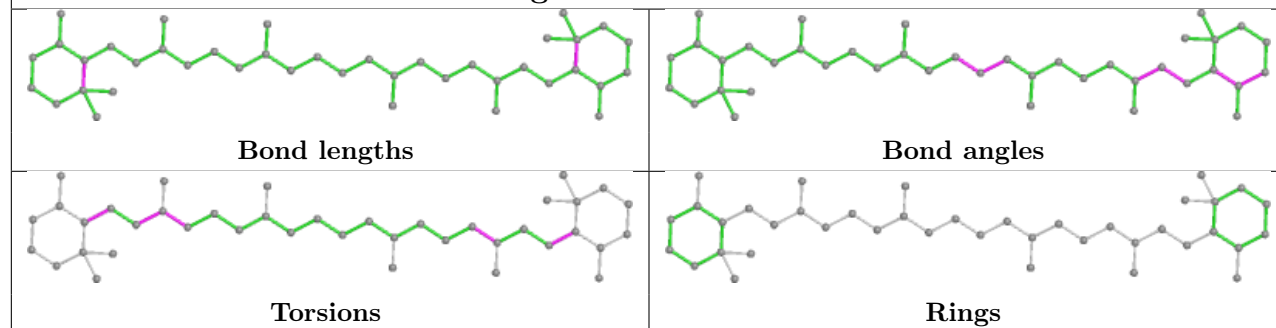
Ligand CHL 5 314

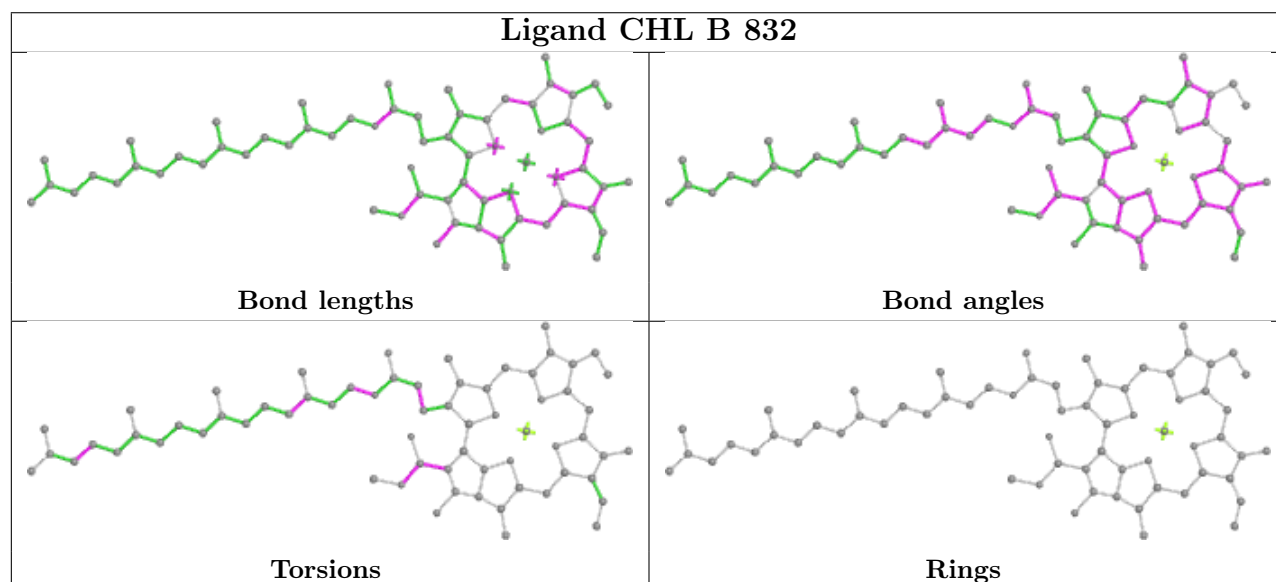
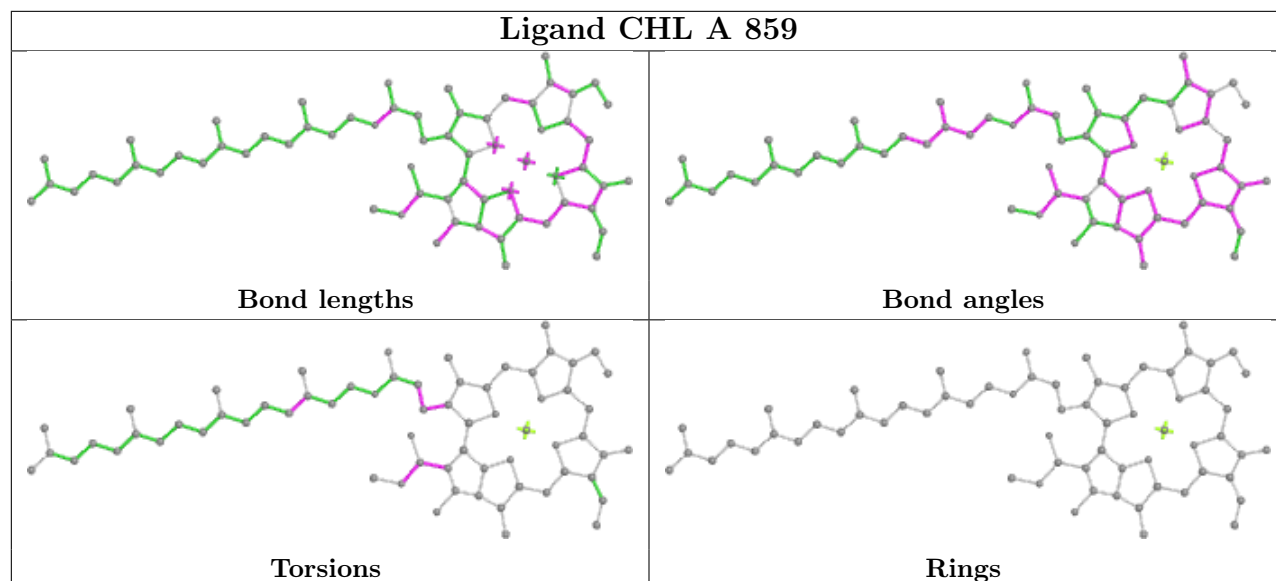
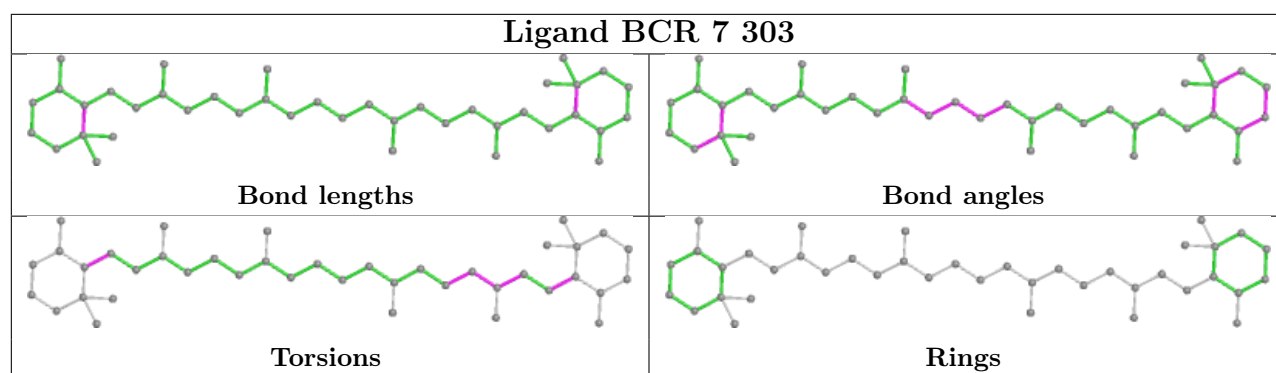


Ligand CHL 3 309

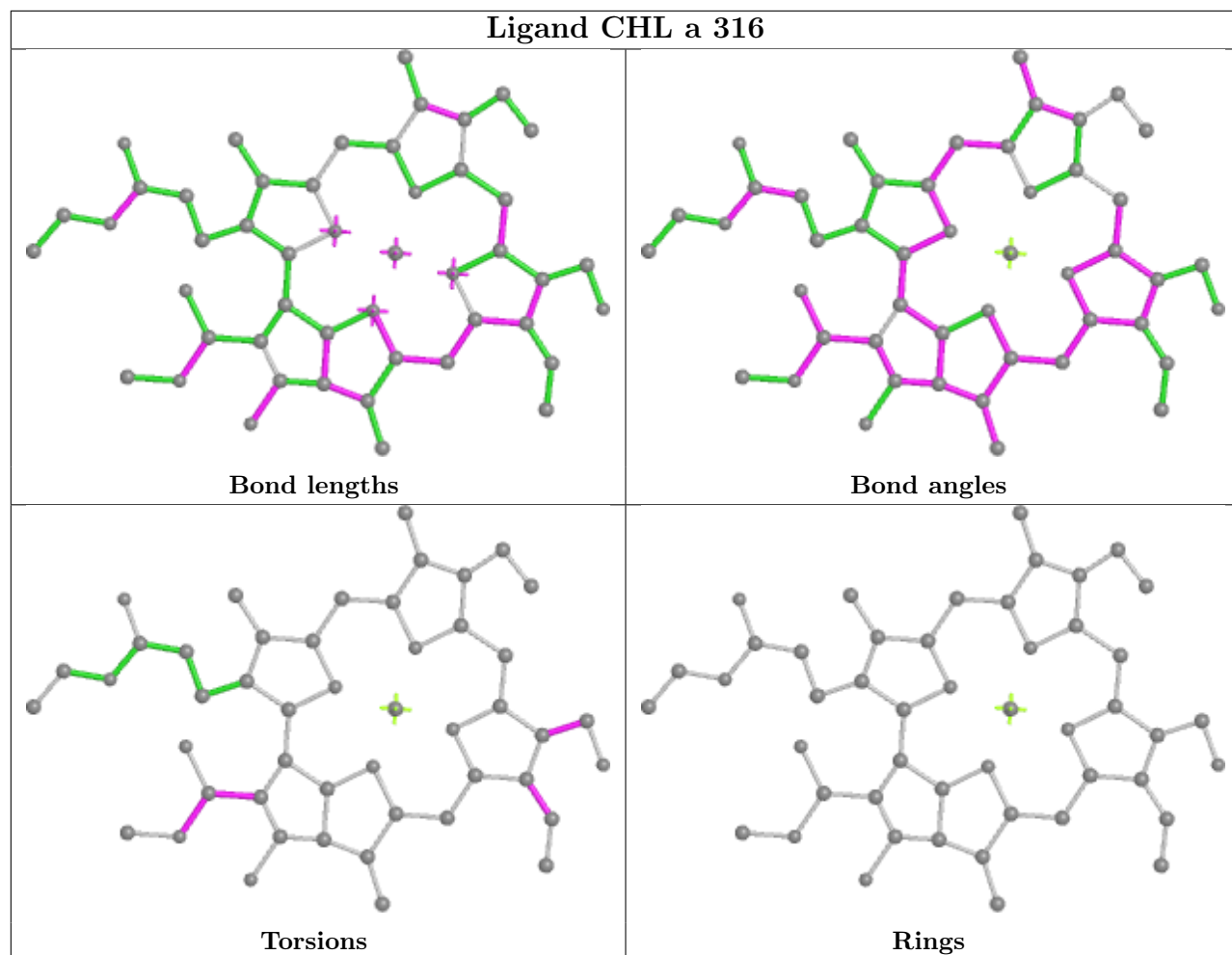


Ligand BCR B 804

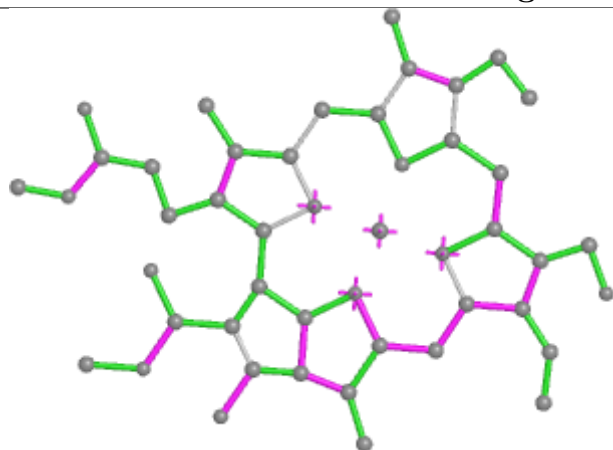




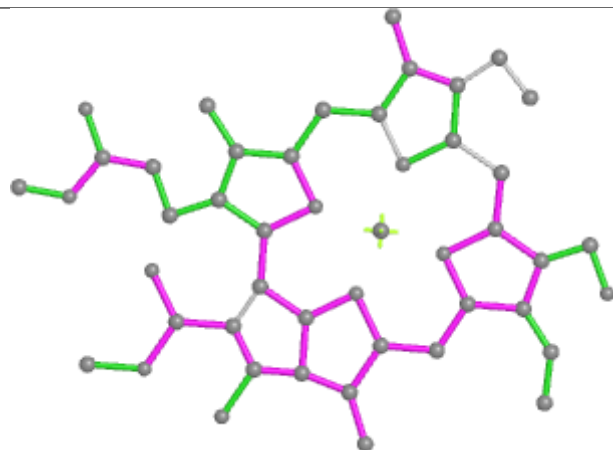
Ligand CHL a 316



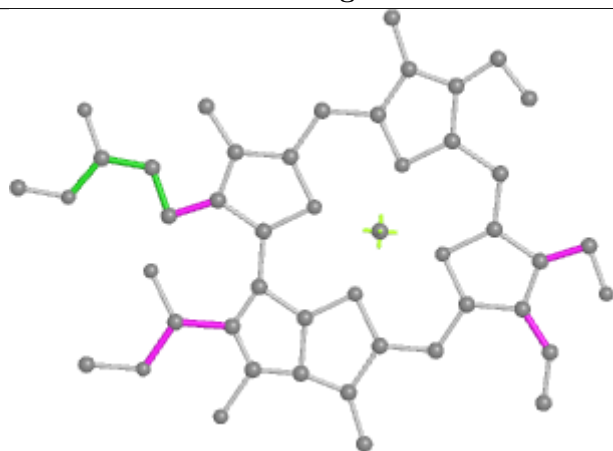
Ligand CHL 5 319



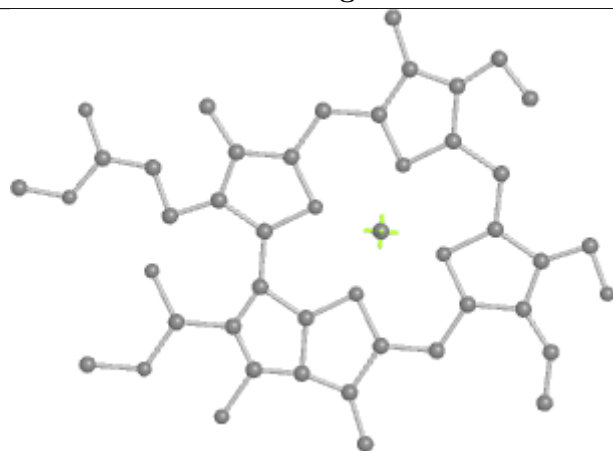
Bond lengths



Bond angles

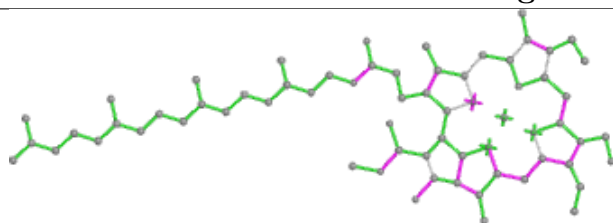


Torsions

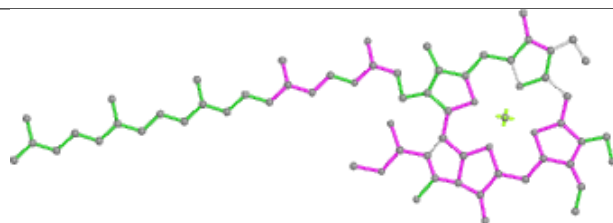


Rings

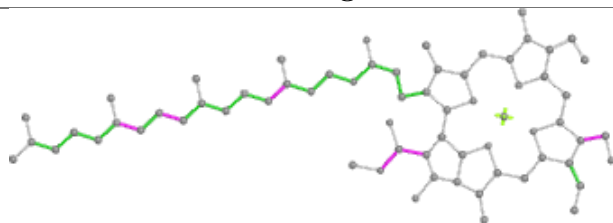
Ligand CHL 8 314



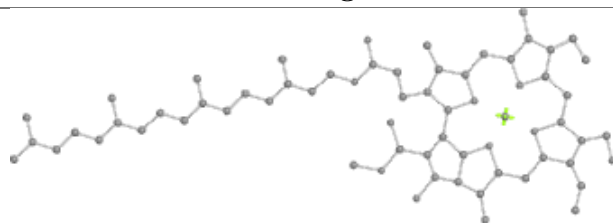
Bond lengths



Bond angles

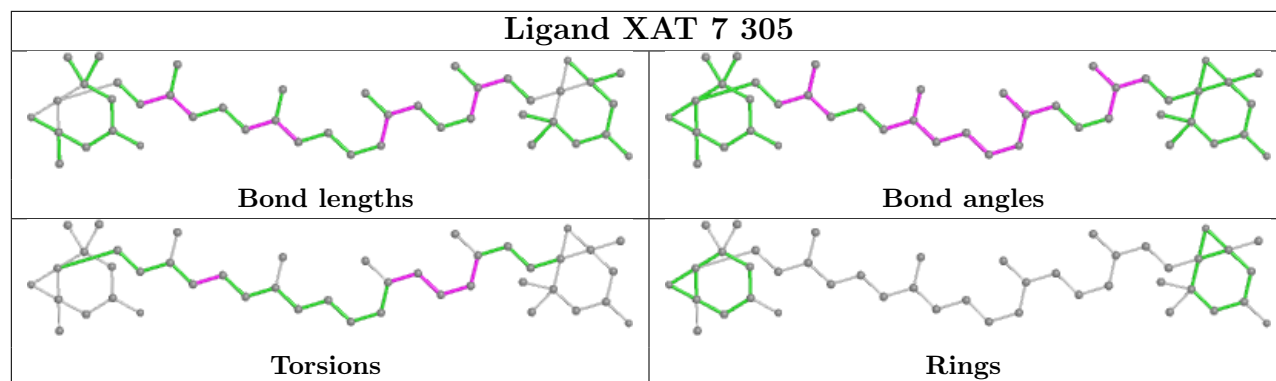


Torsions

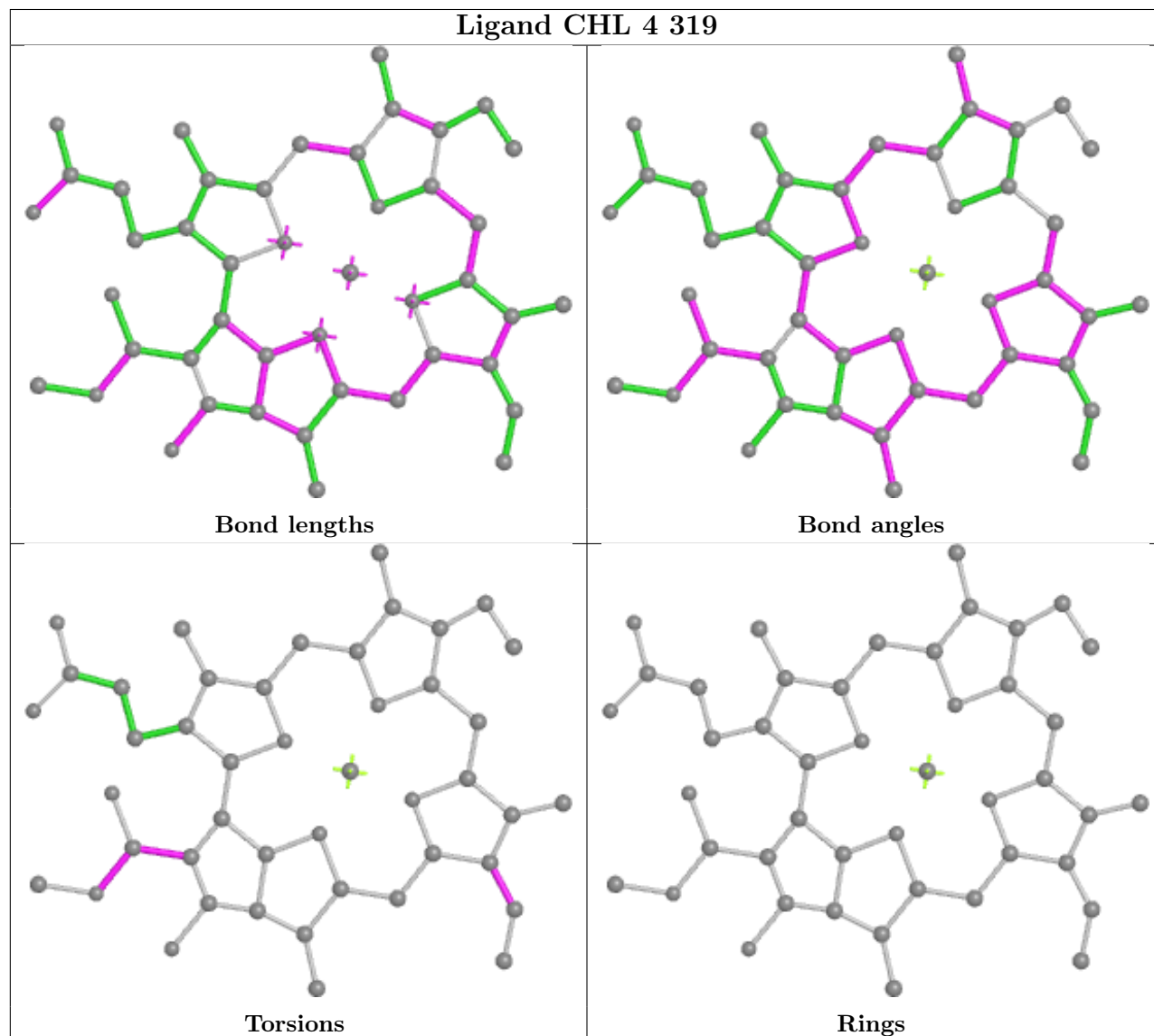


Rings

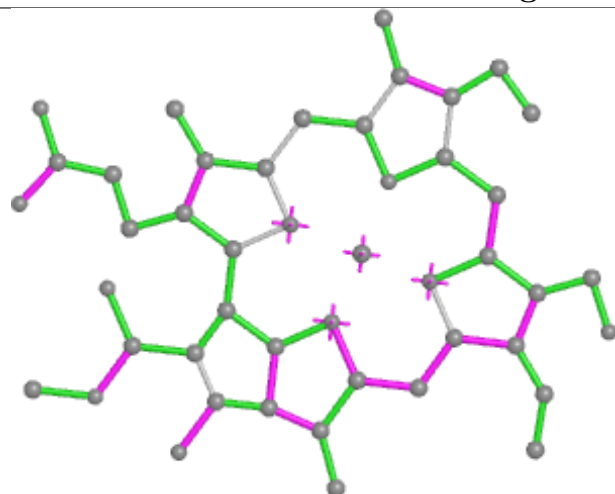
Ligand XAT 7 305



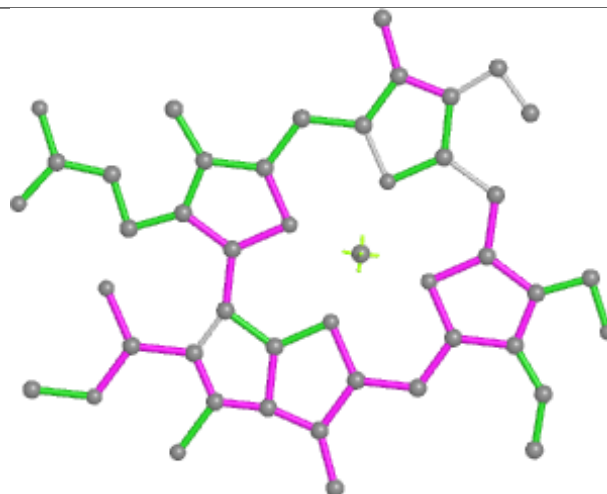
Ligand CHL 4 319



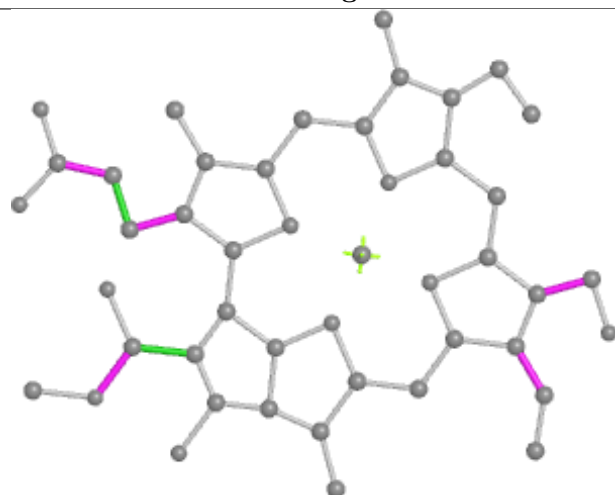
Ligand CHL 6 316



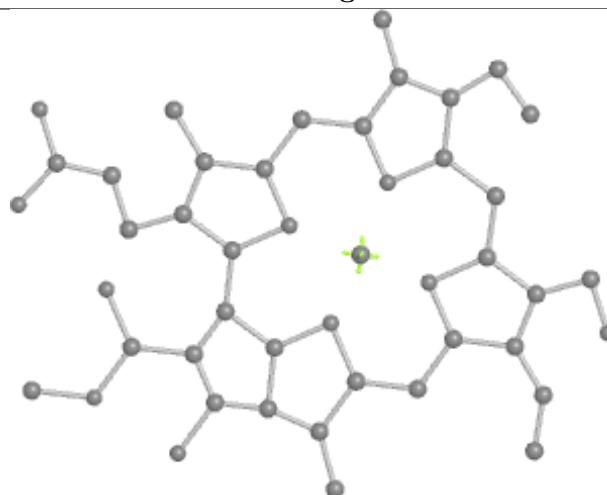
Bond lengths



Bond angles

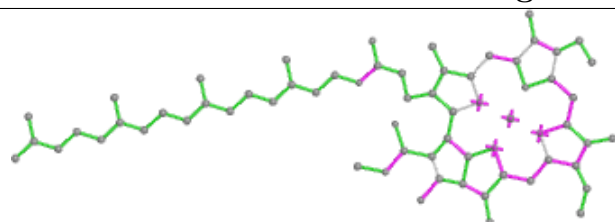


Torsions

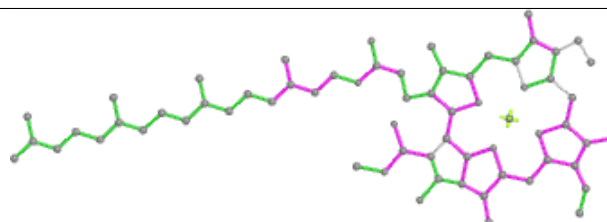


Rings

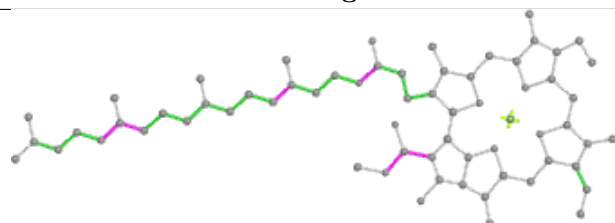
Ligand CHL B 844



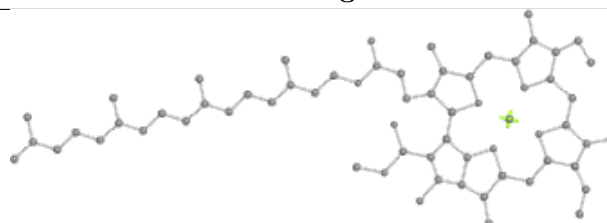
Bond lengths



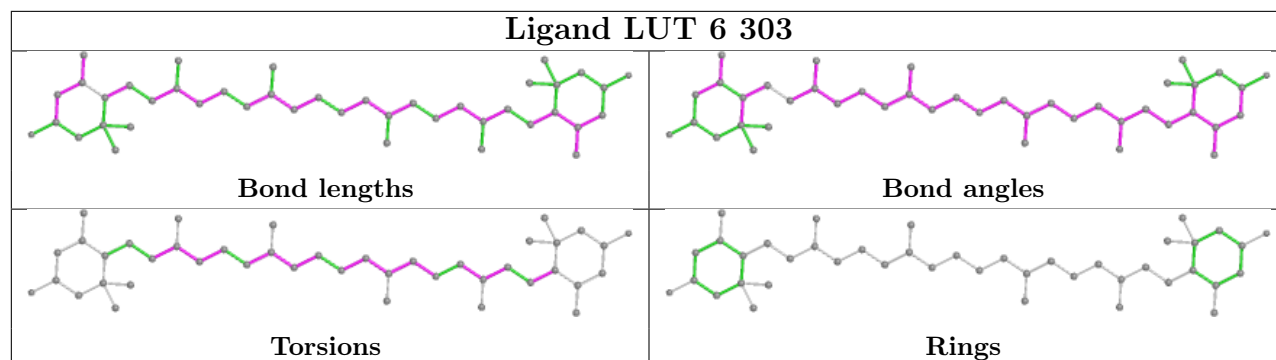
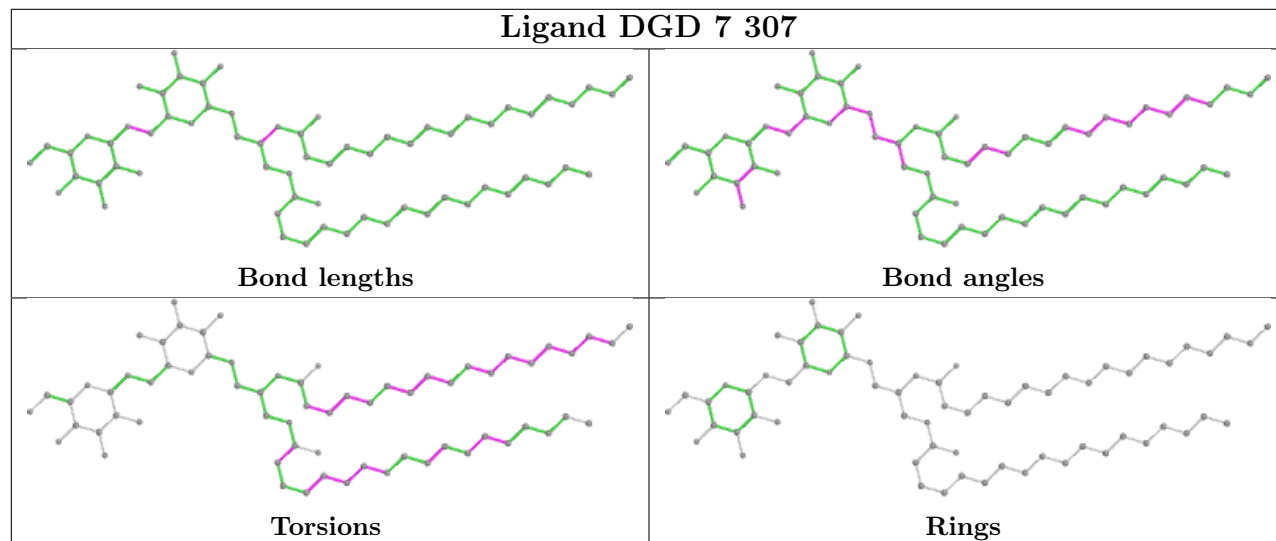
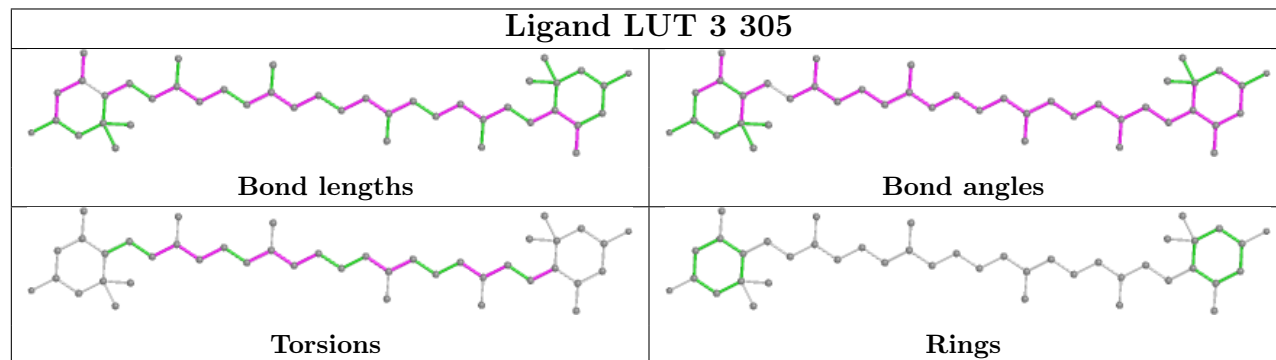
Bond angles

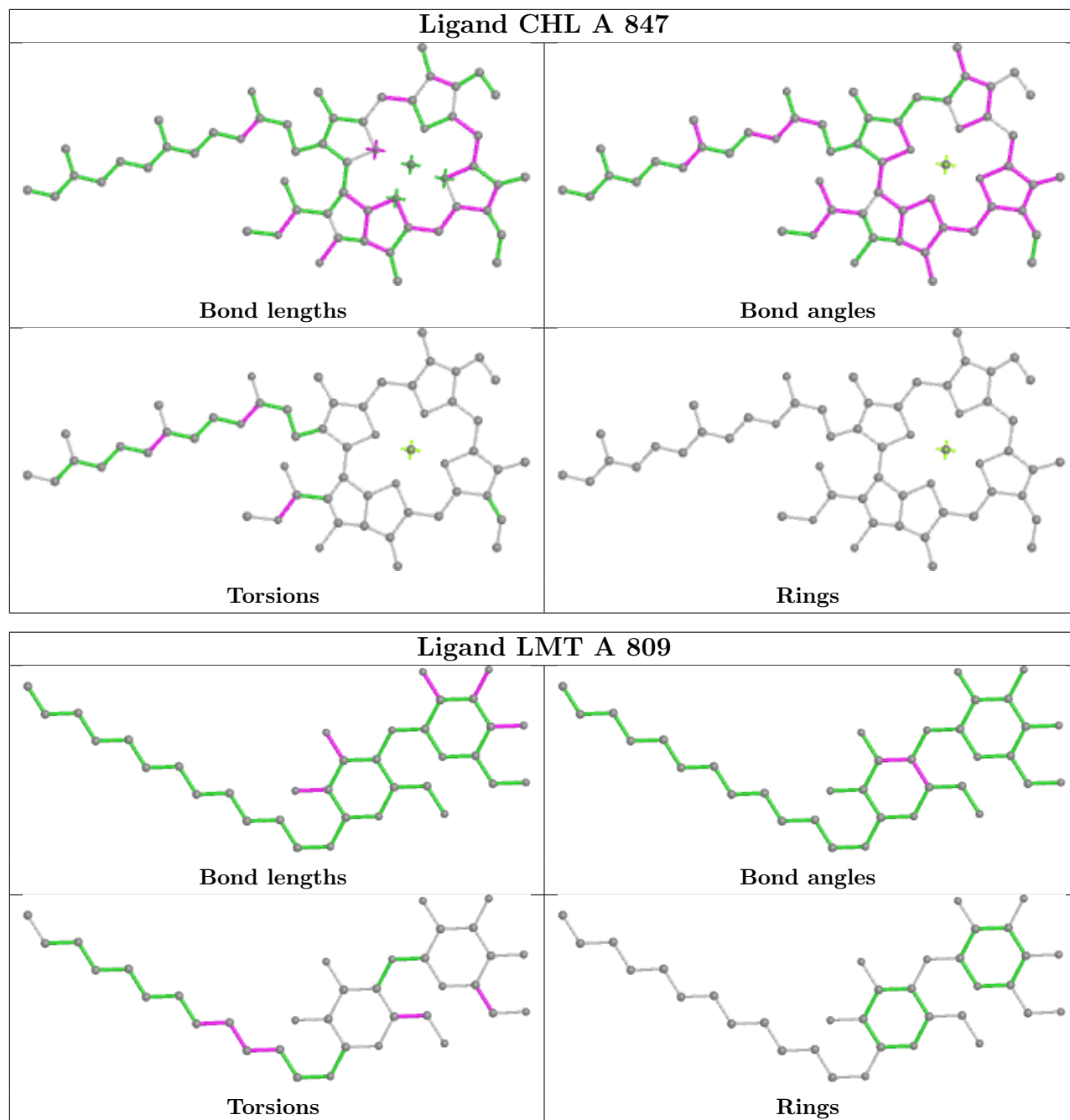


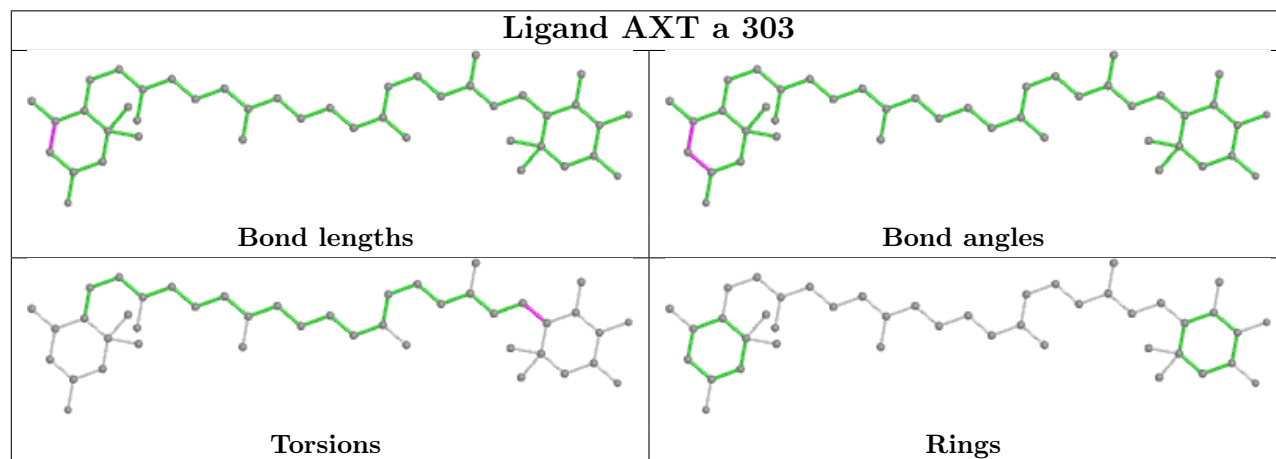
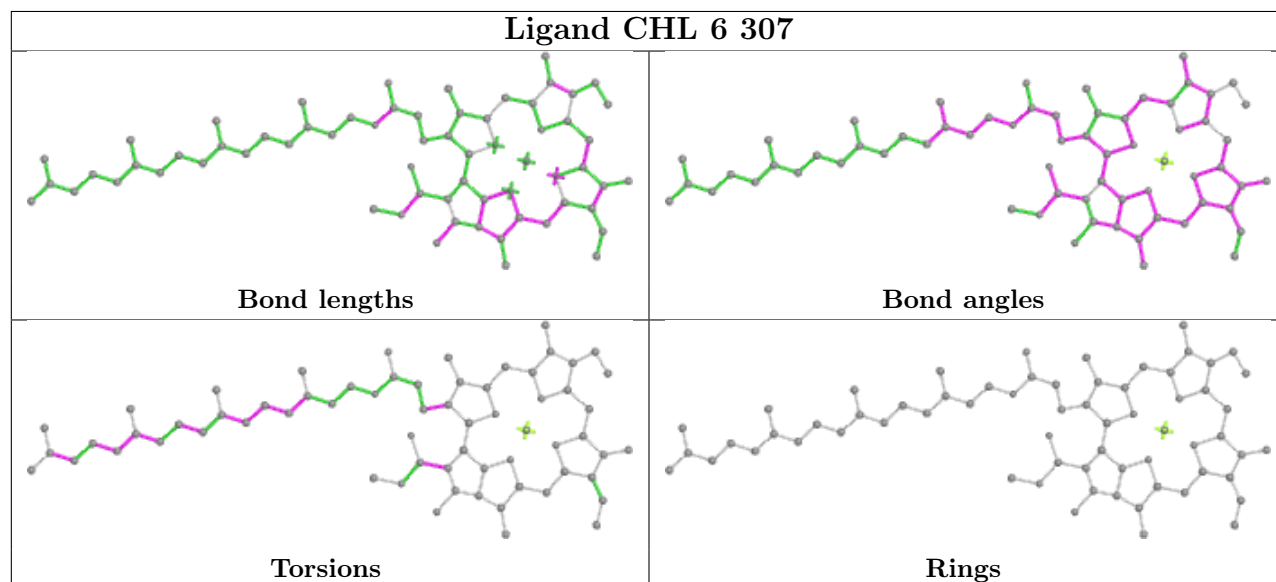
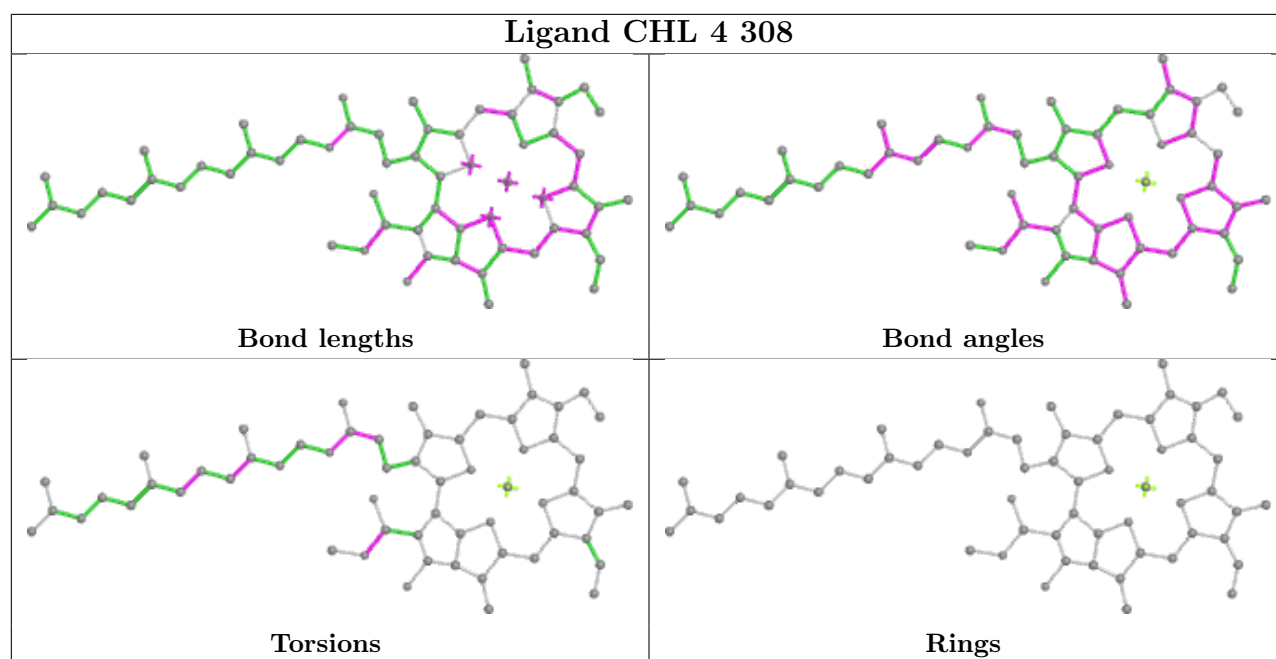
Torsions

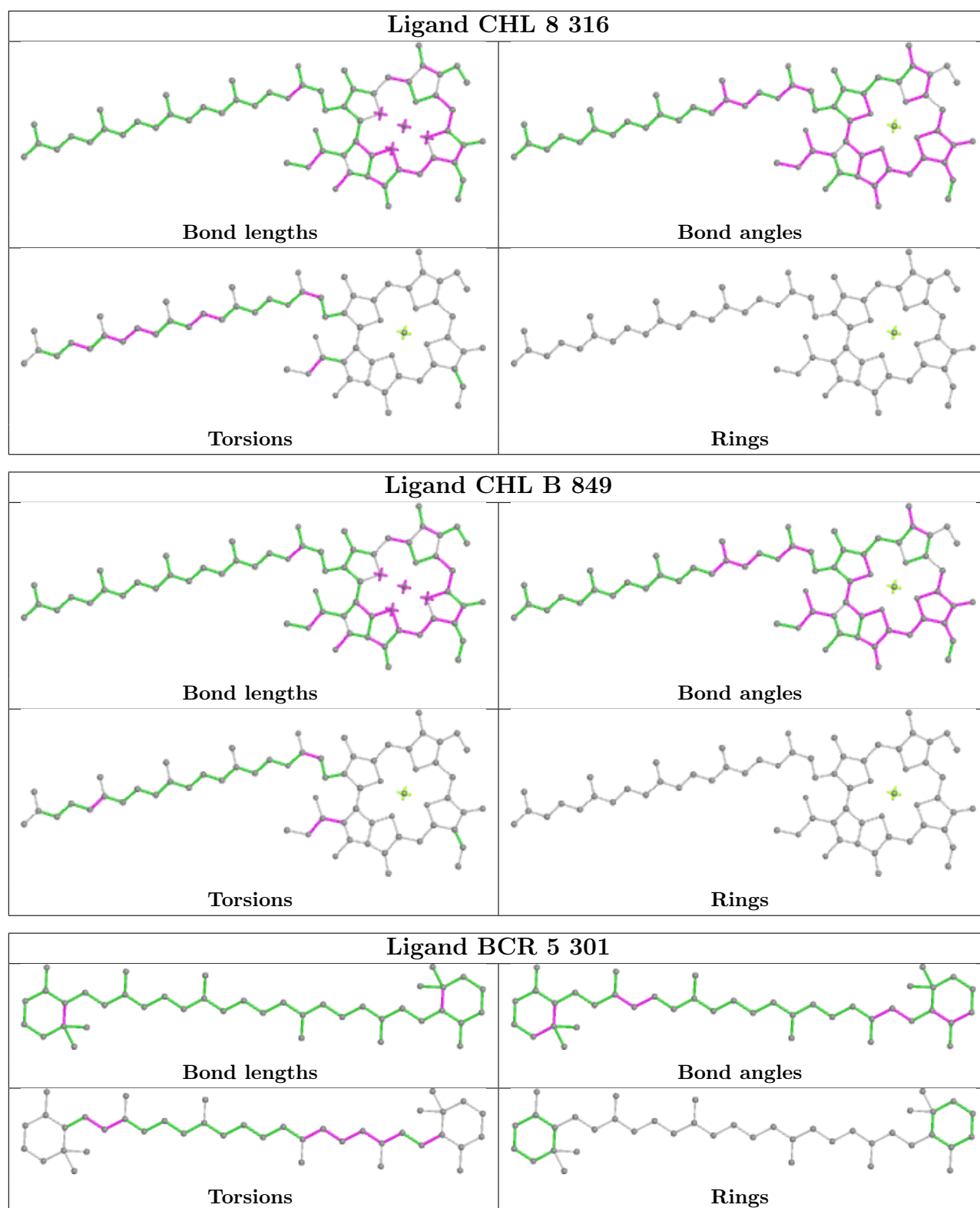


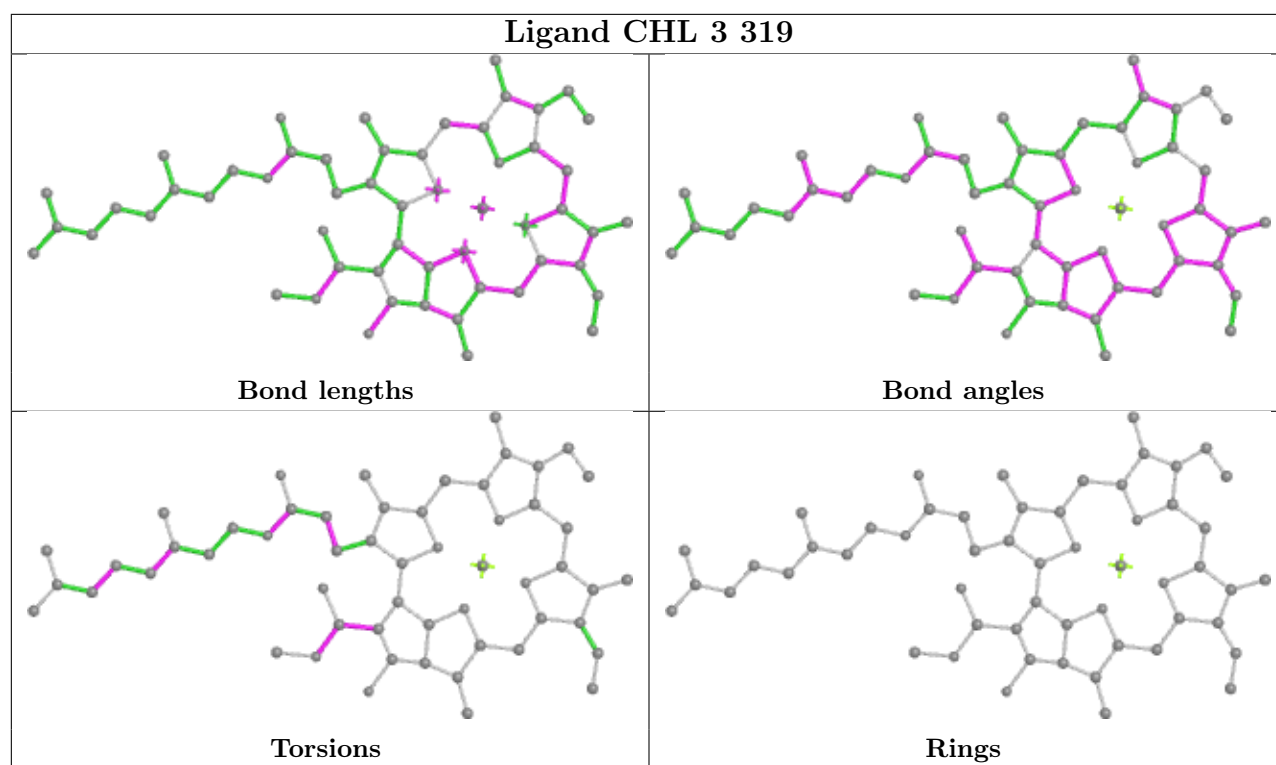
Rings

Ligand LUT 6 303**Ligand DGD 7 307****Ligand LUT 3 305**

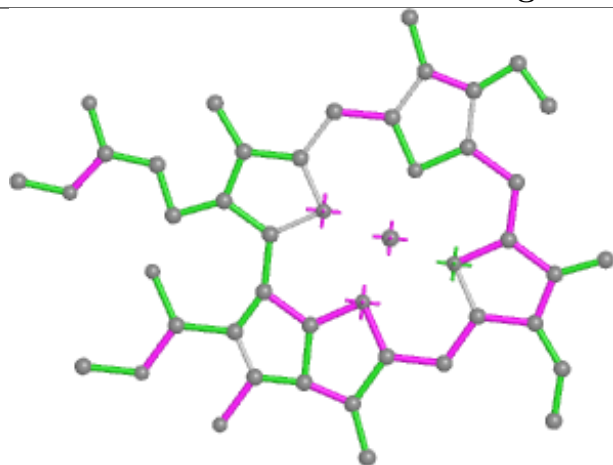




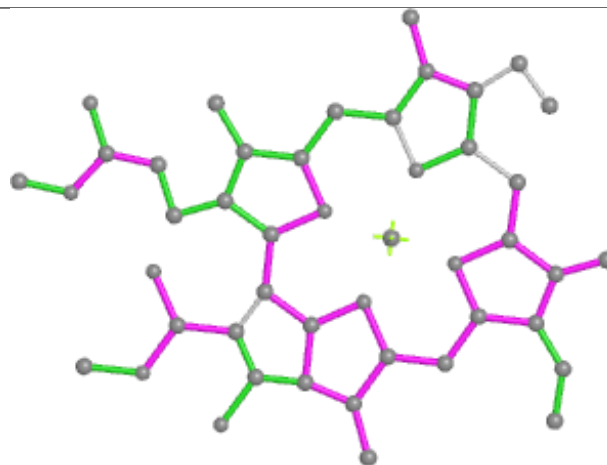




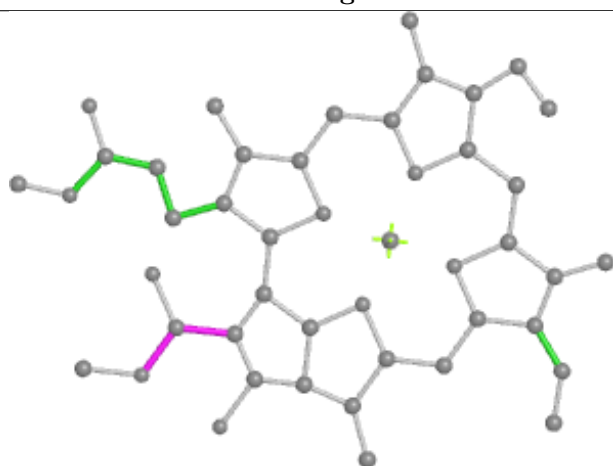
Ligand CHL 6 314



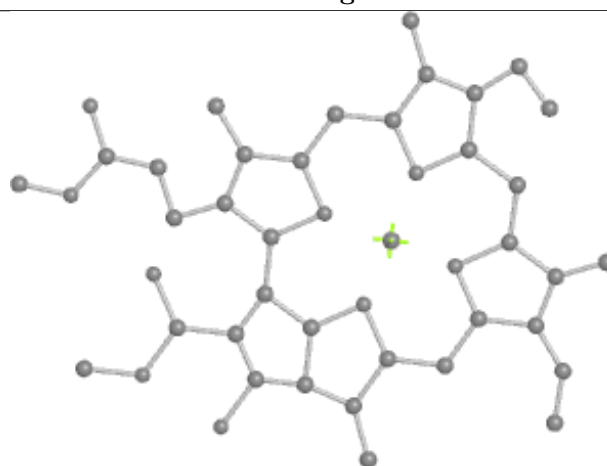
Bond lengths



Bond angles

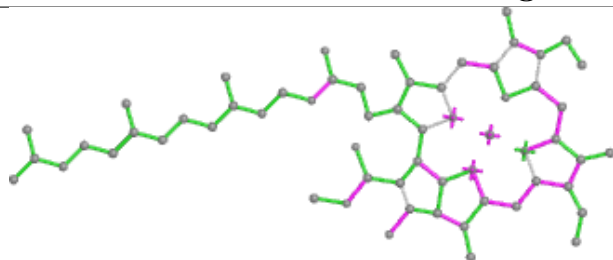


Torsions

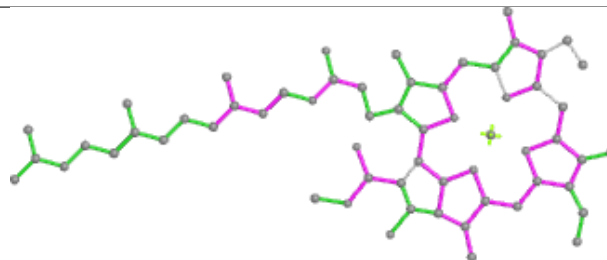


Rings

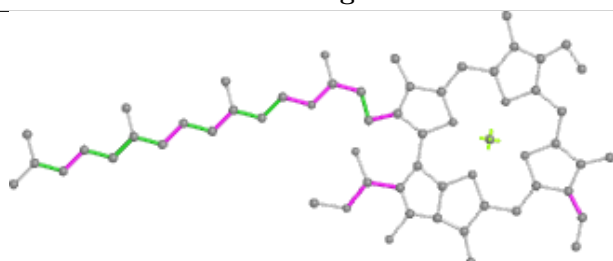
Ligand CHL 3 311



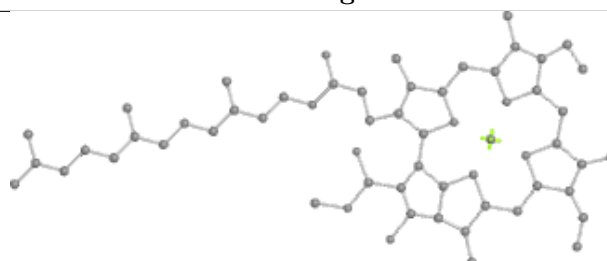
Bond lengths



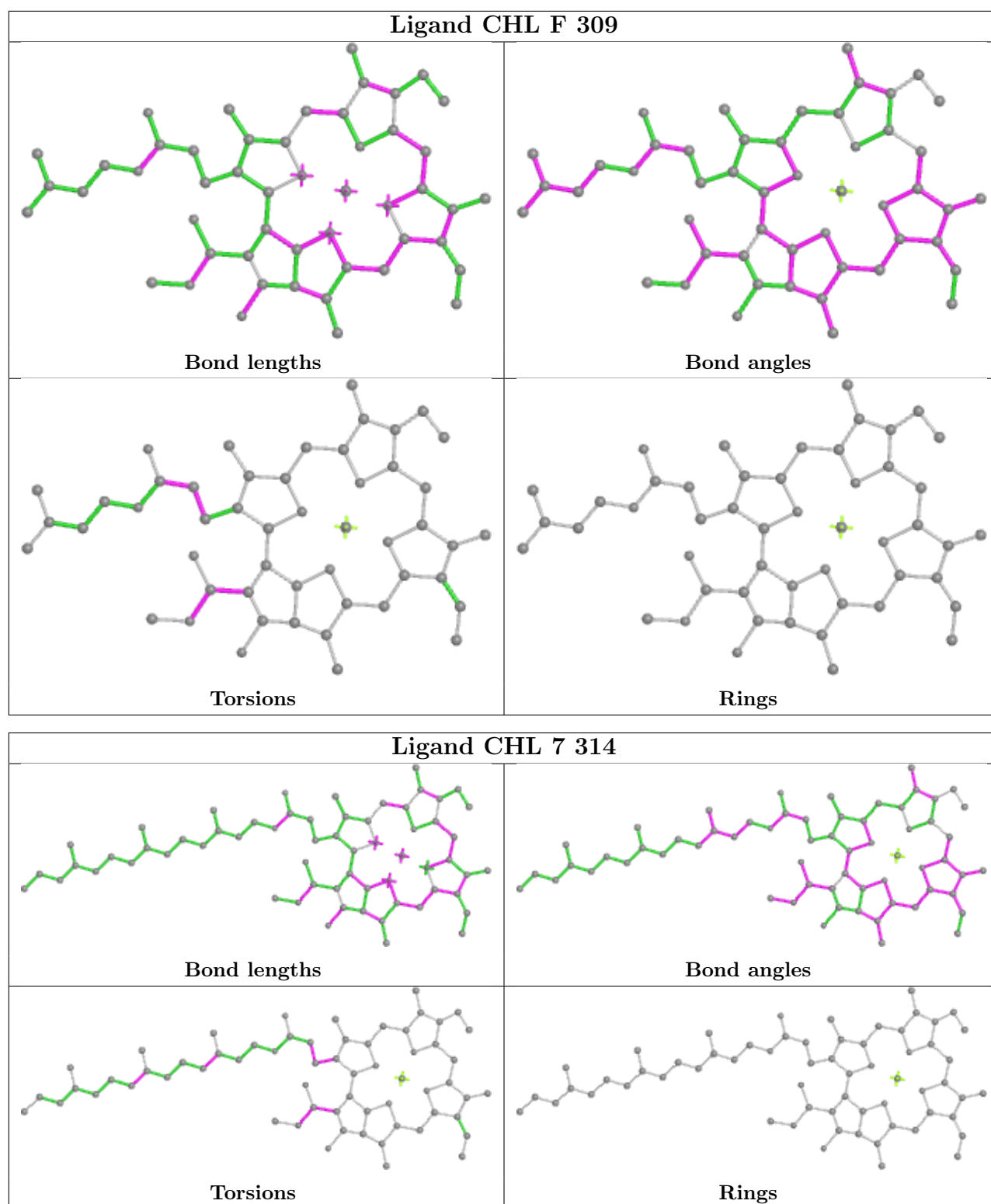
Bond angles



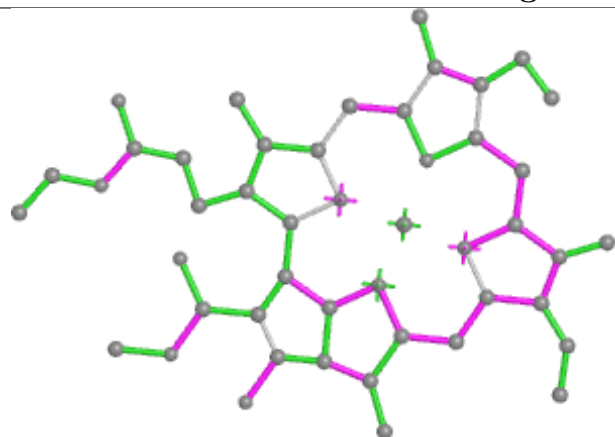
Torsions



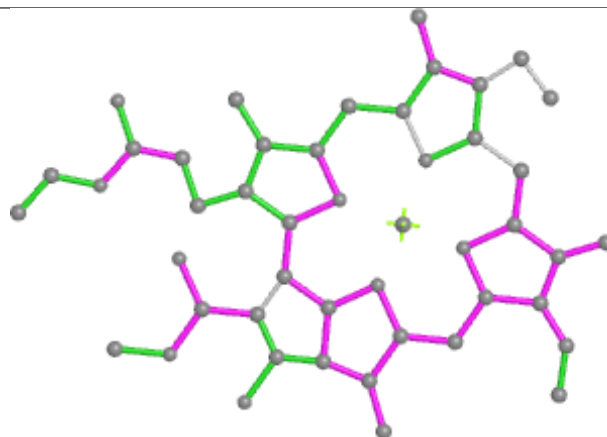
Rings



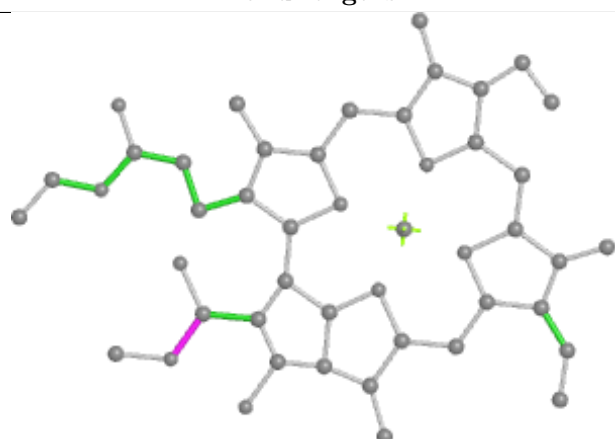
Ligand CHL 4 315



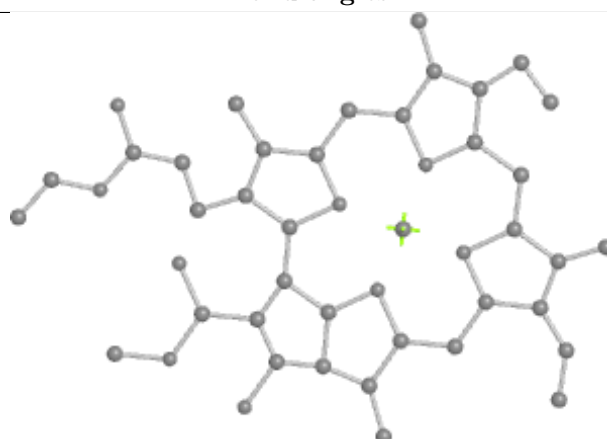
Bond lengths



Bond angles

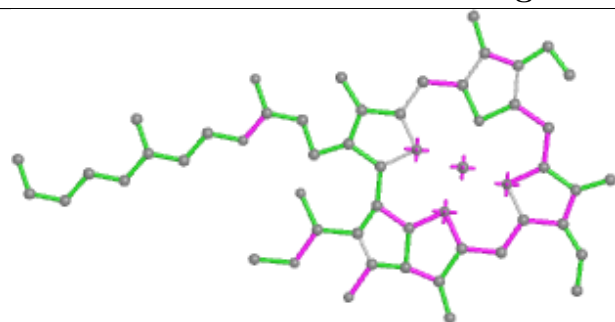


Torsions

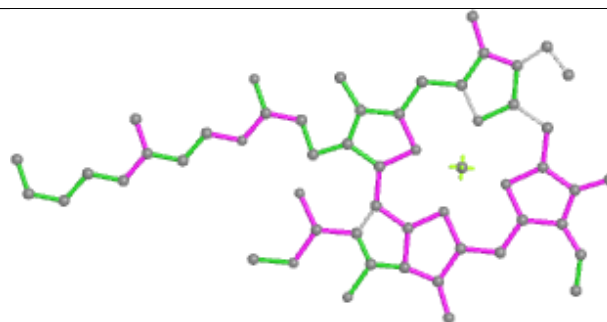


Rings

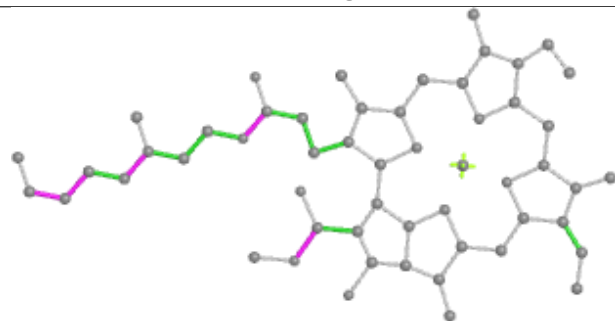
Ligand CHL A 827



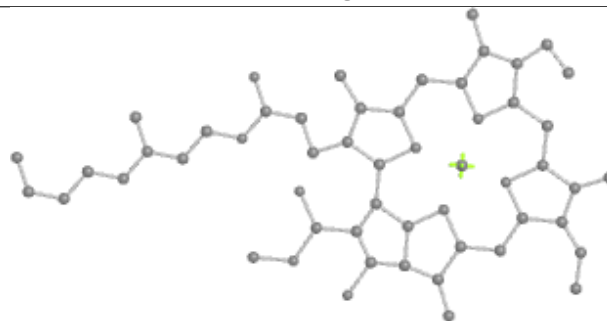
Bond lengths



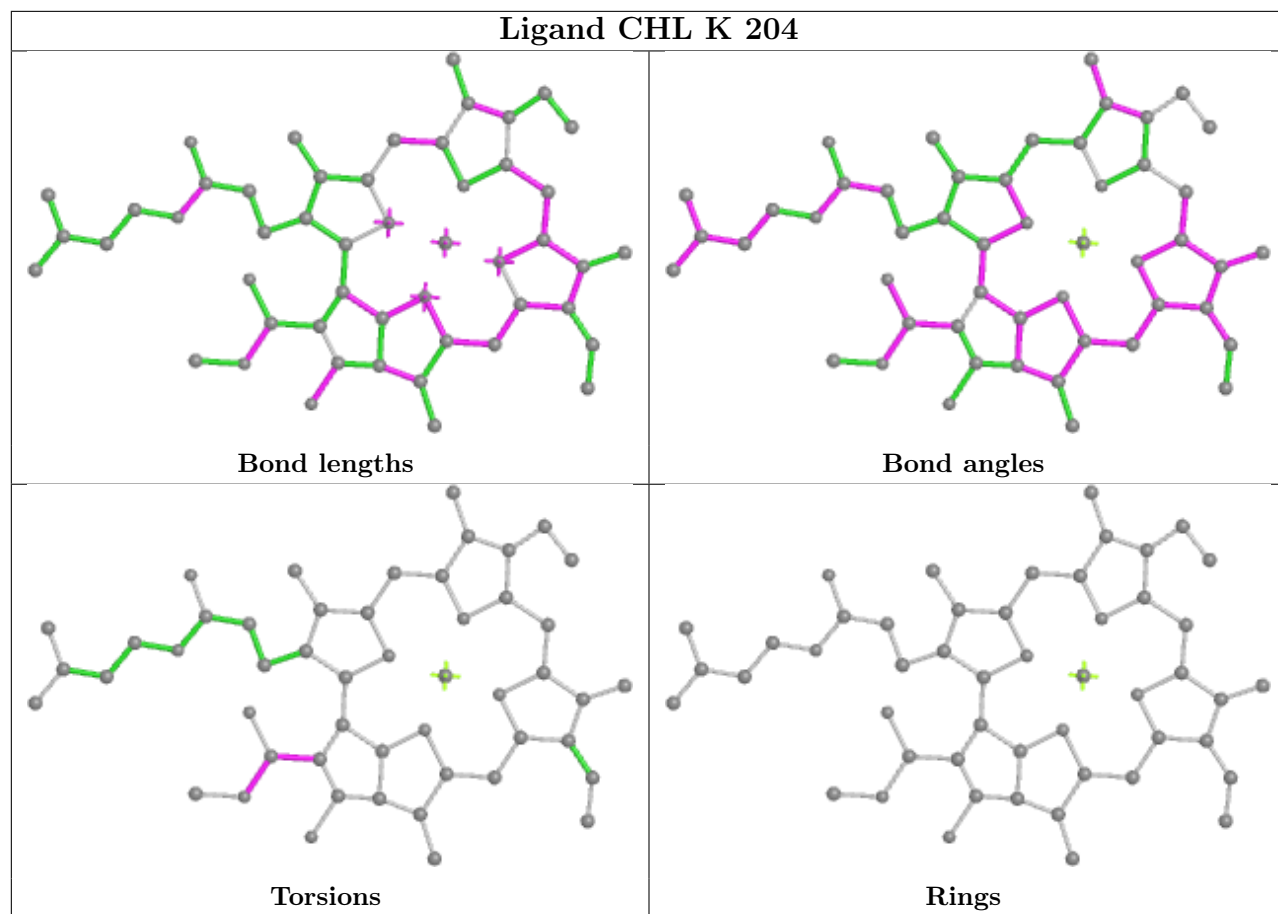
Bond angles



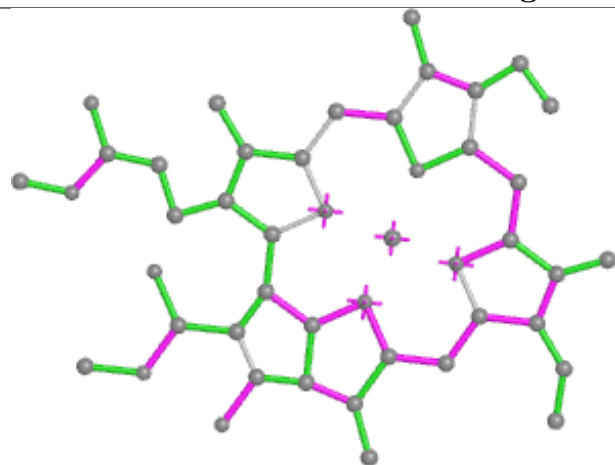
Torsions



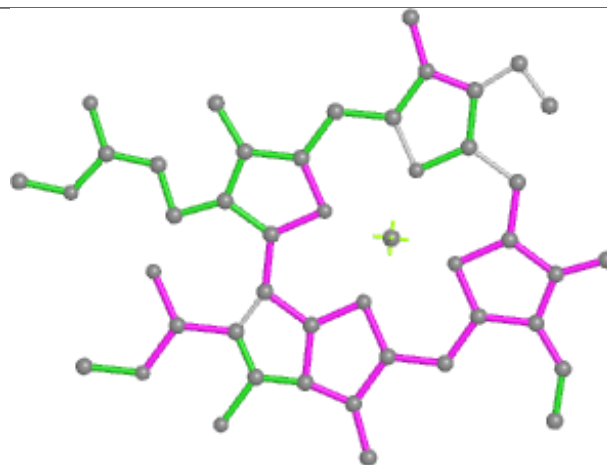
Rings



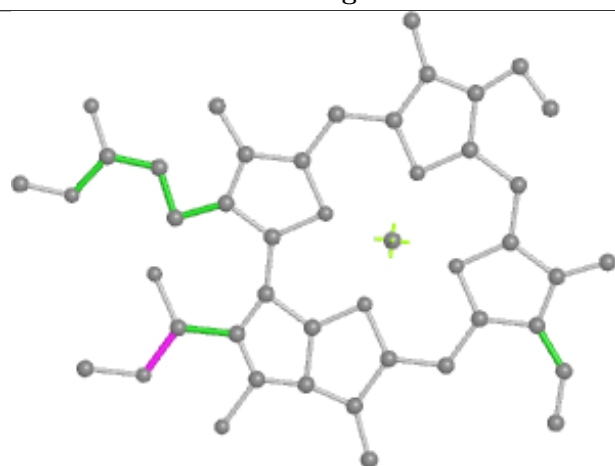
Ligand CHL 8 311



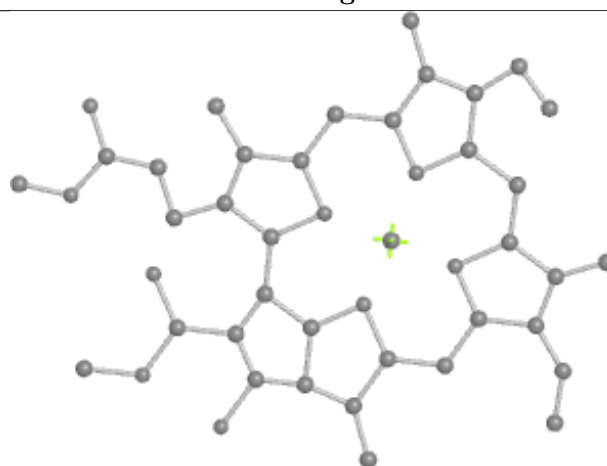
Bond lengths



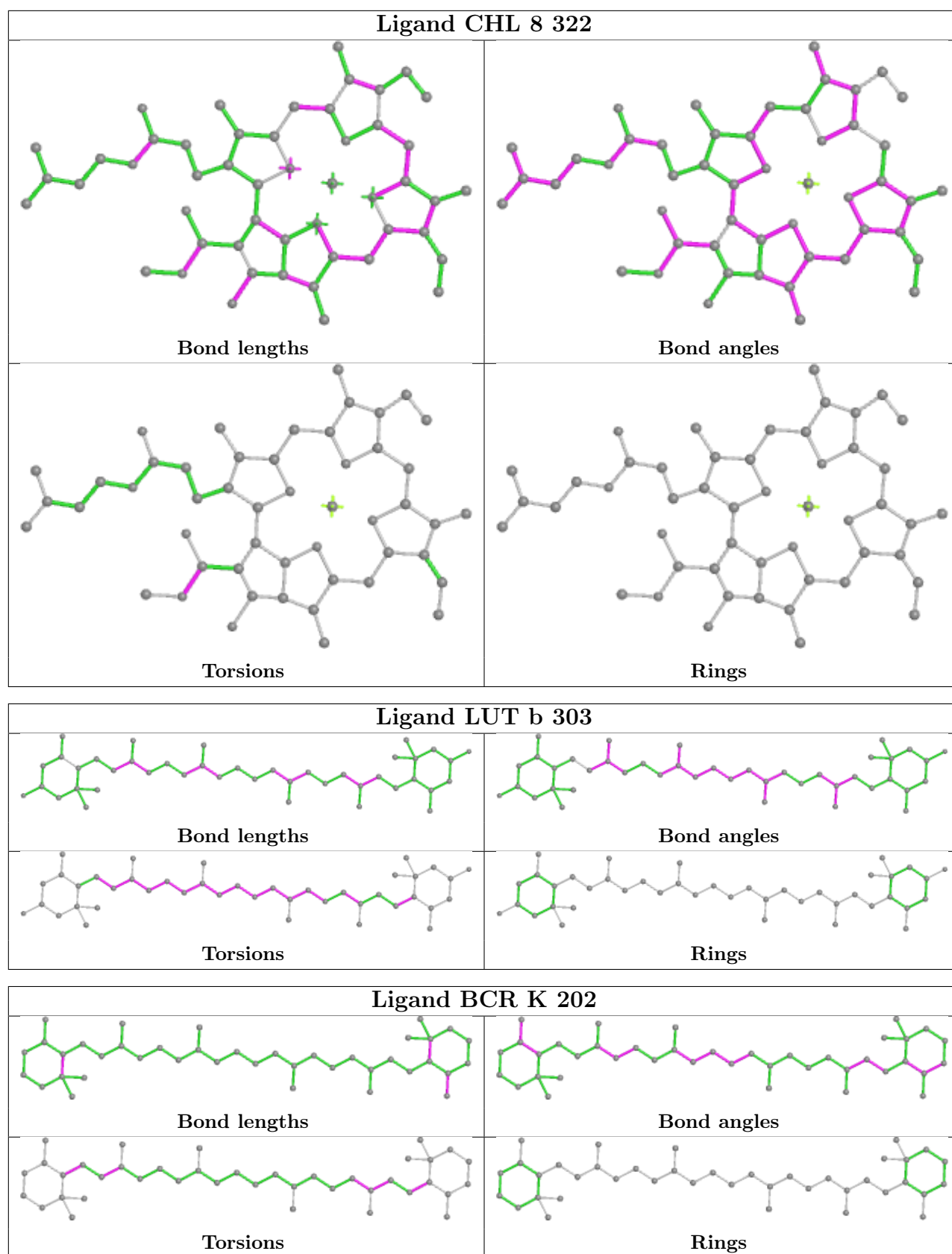
Bond angles

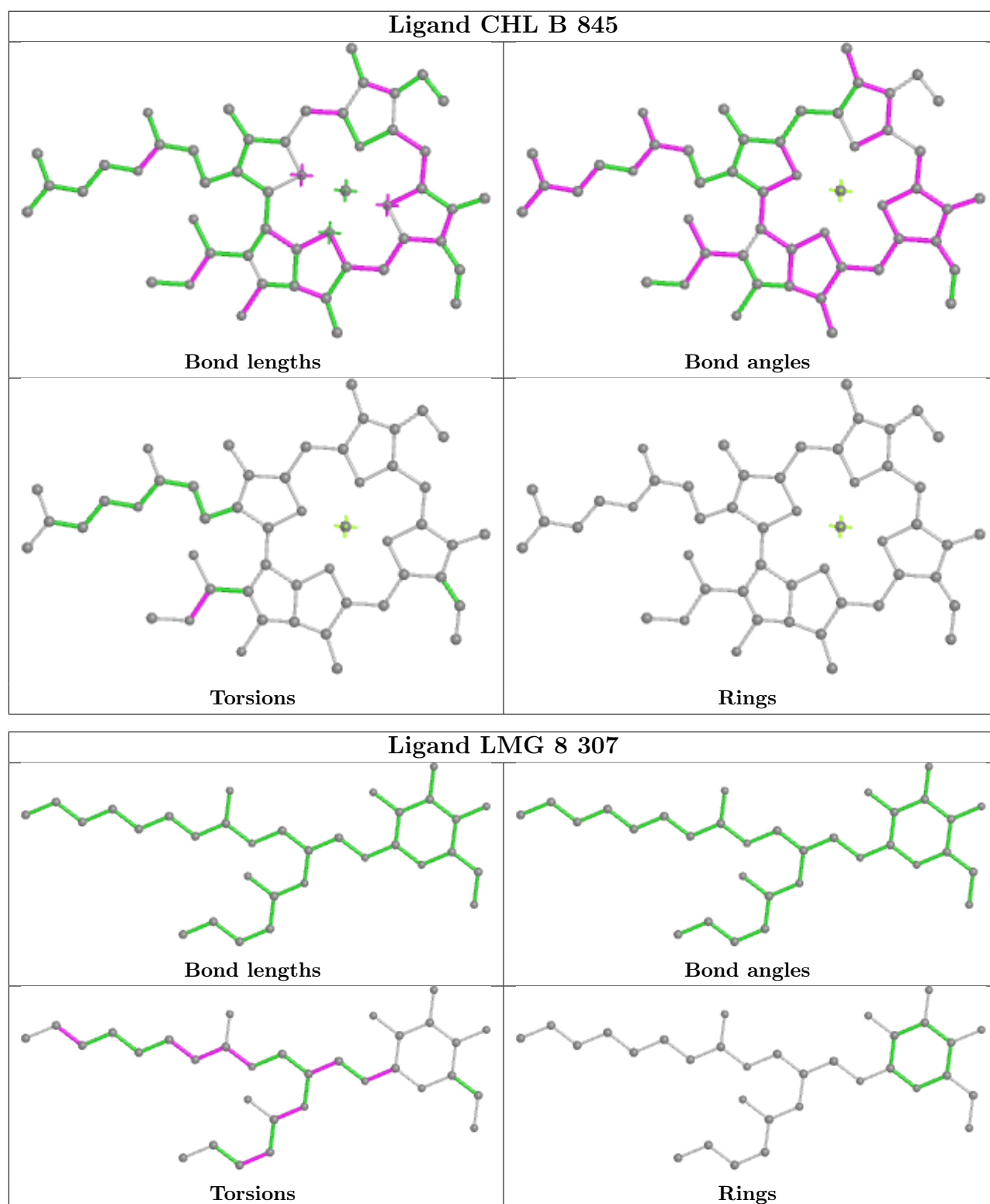


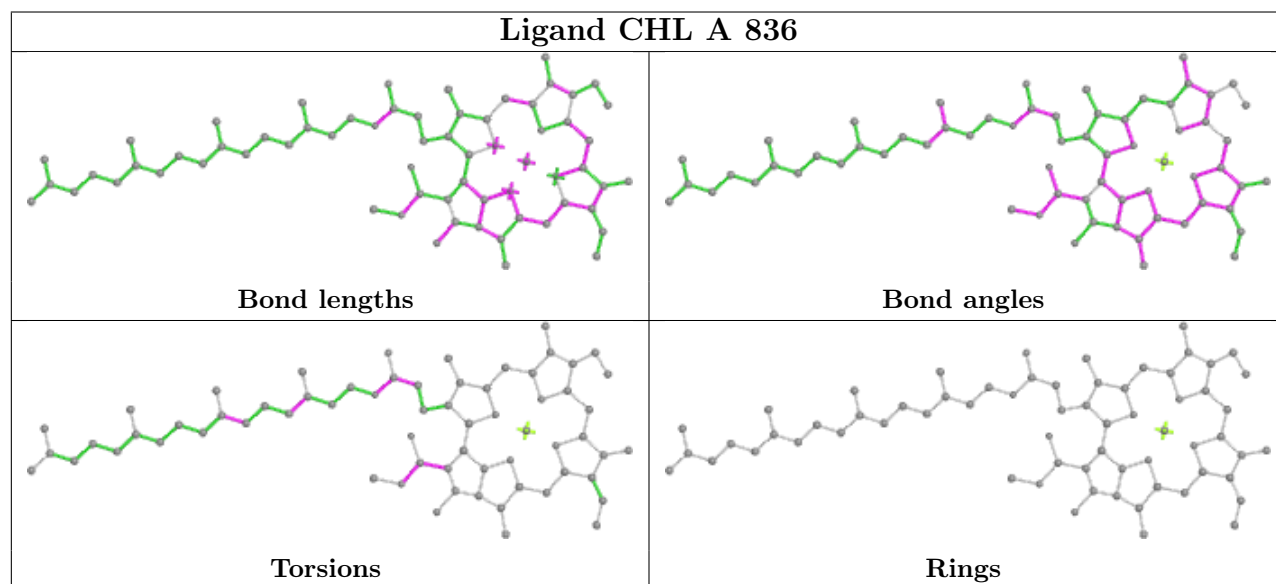
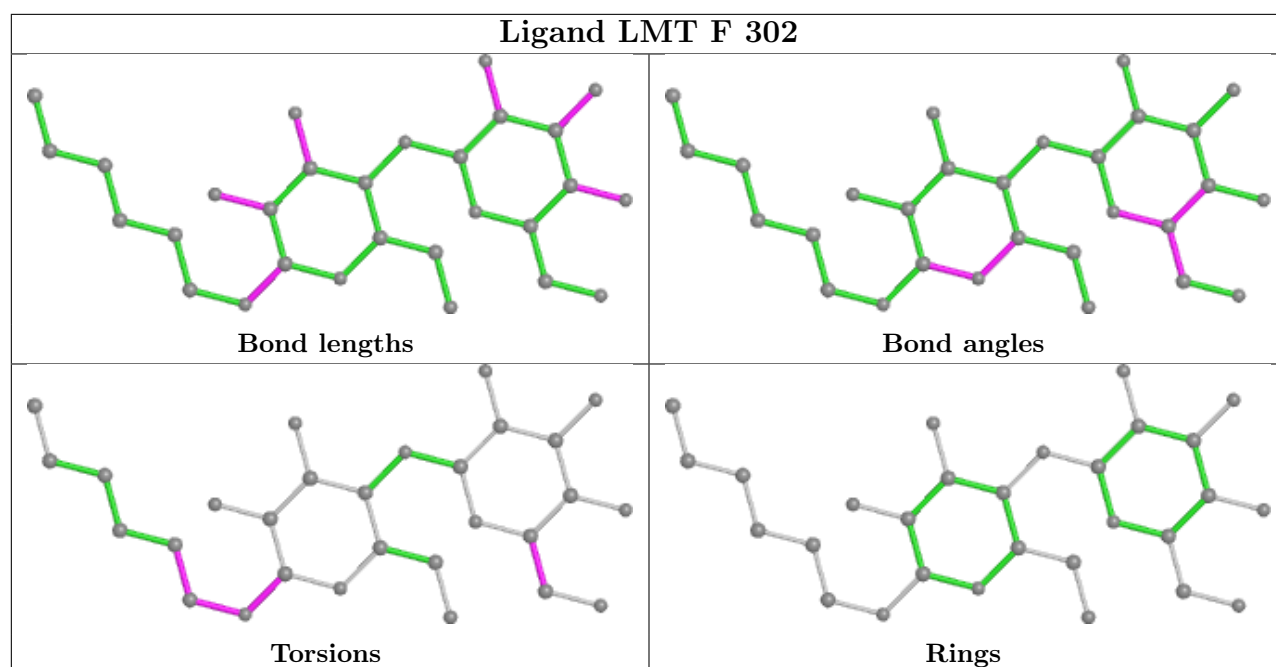
Torsions

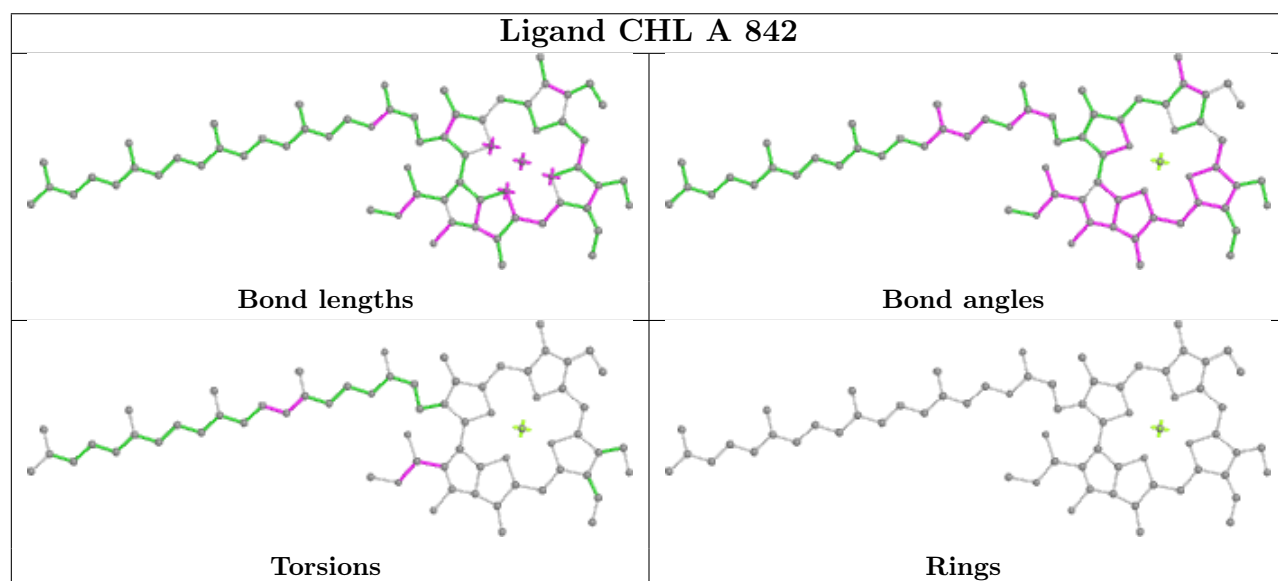
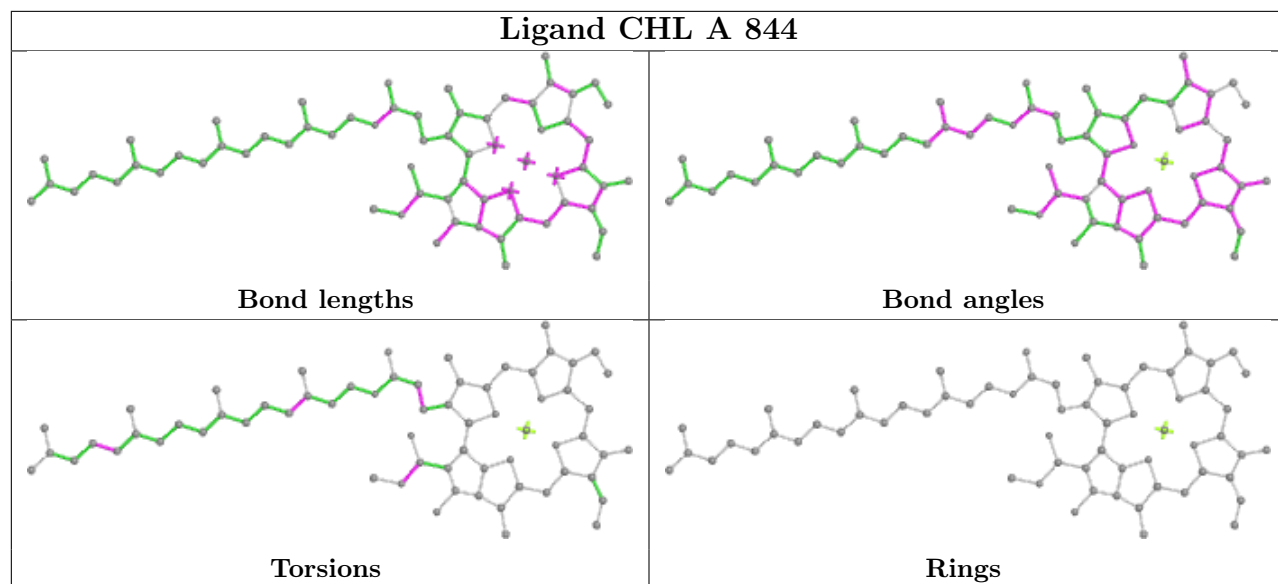


Rings

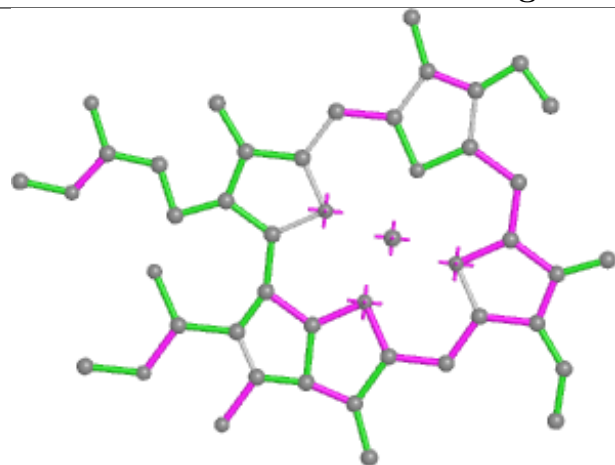




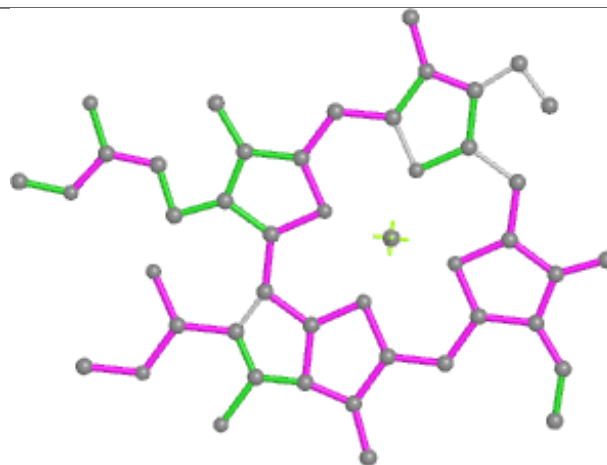




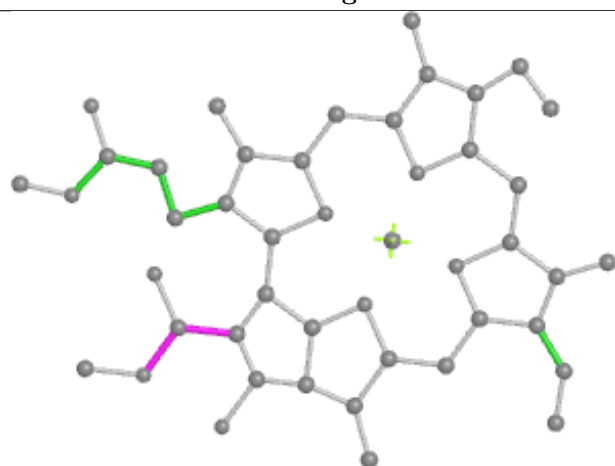
Ligand CHL b 310



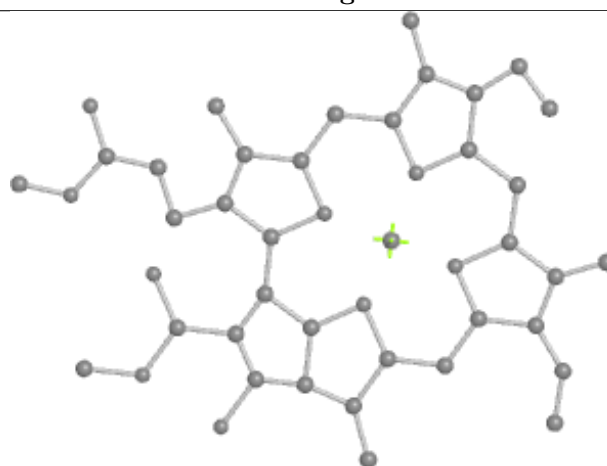
Bond lengths



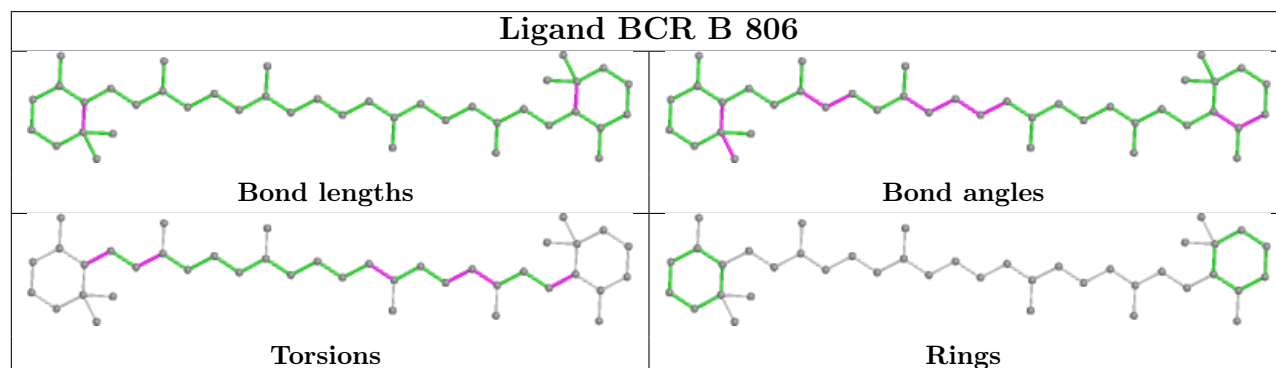
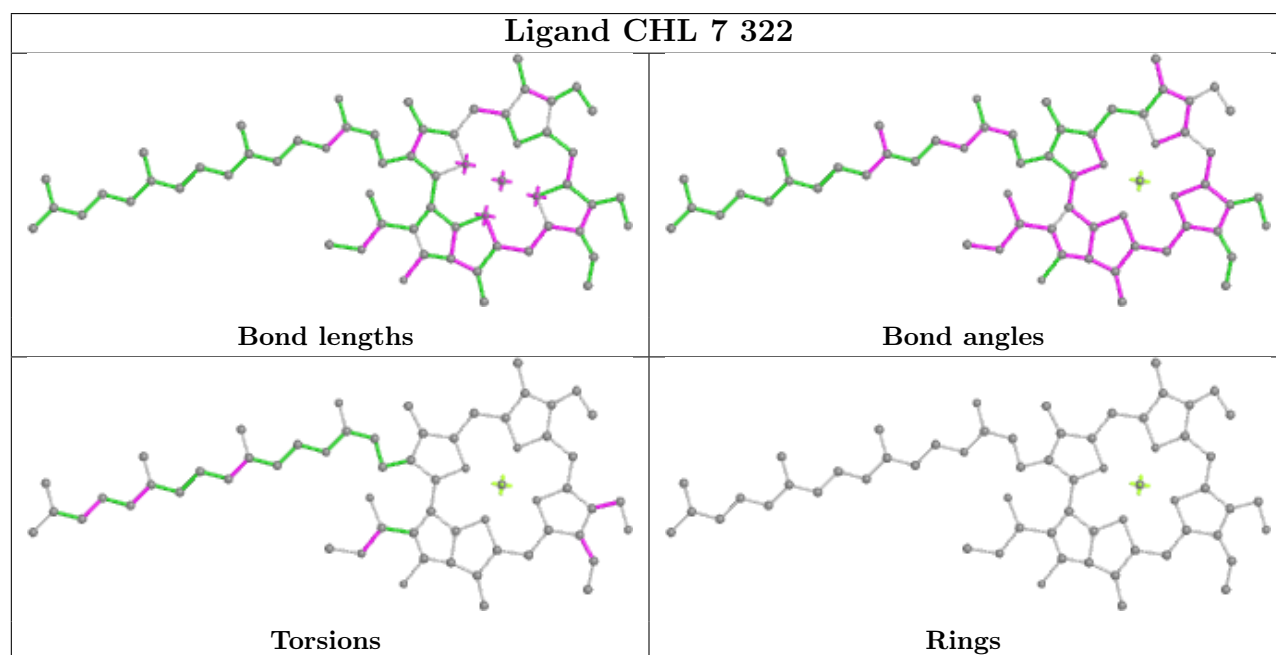
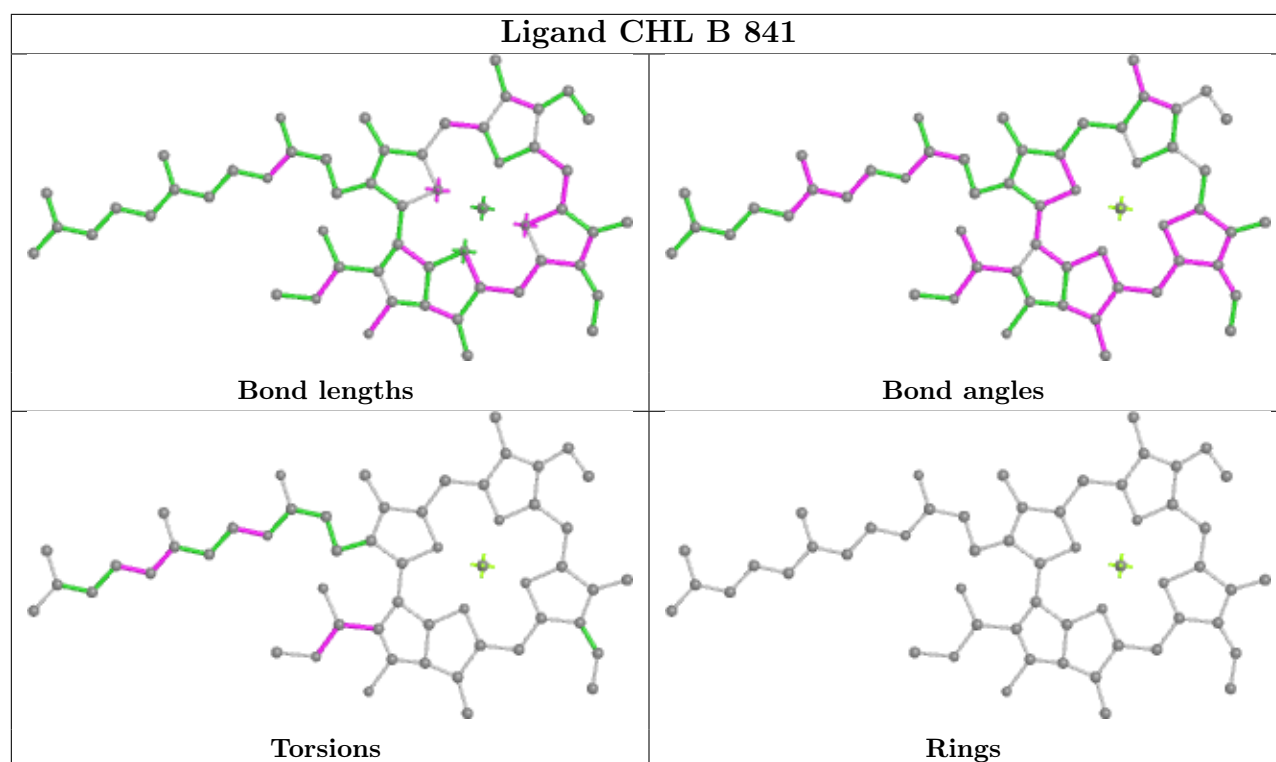
Bond angles

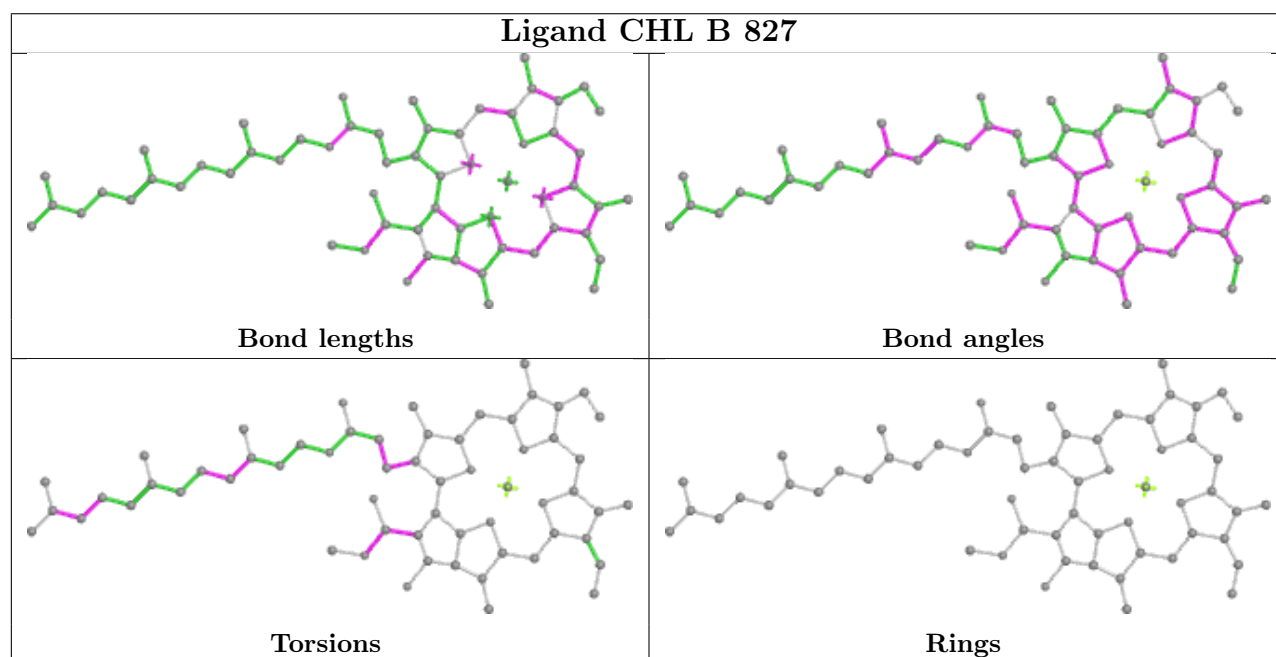
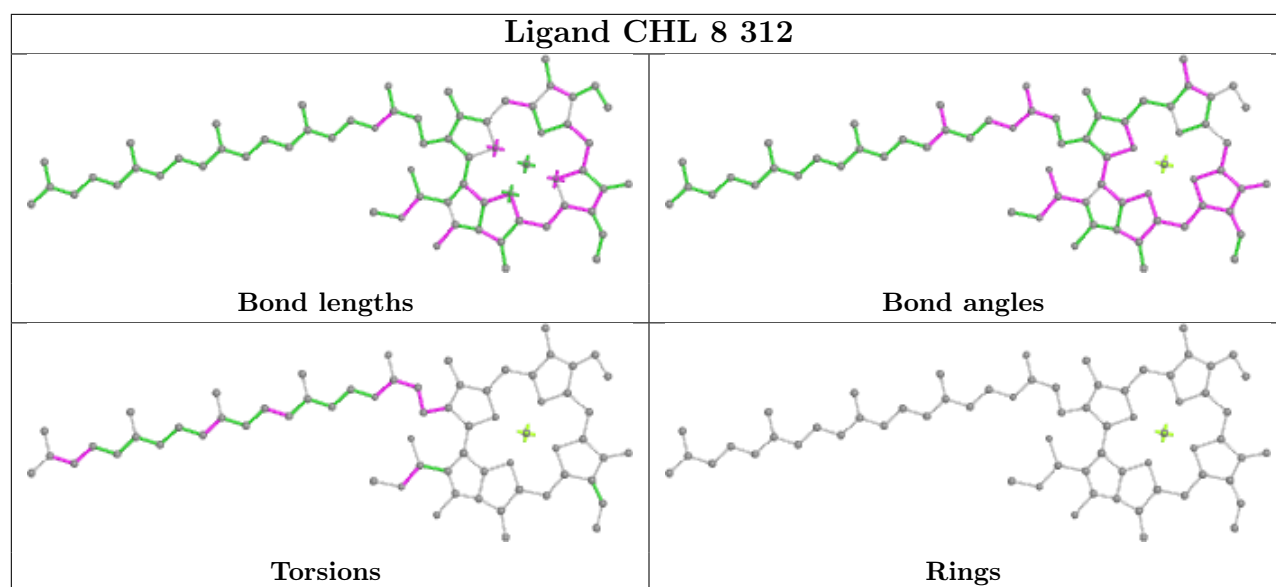


Torsions

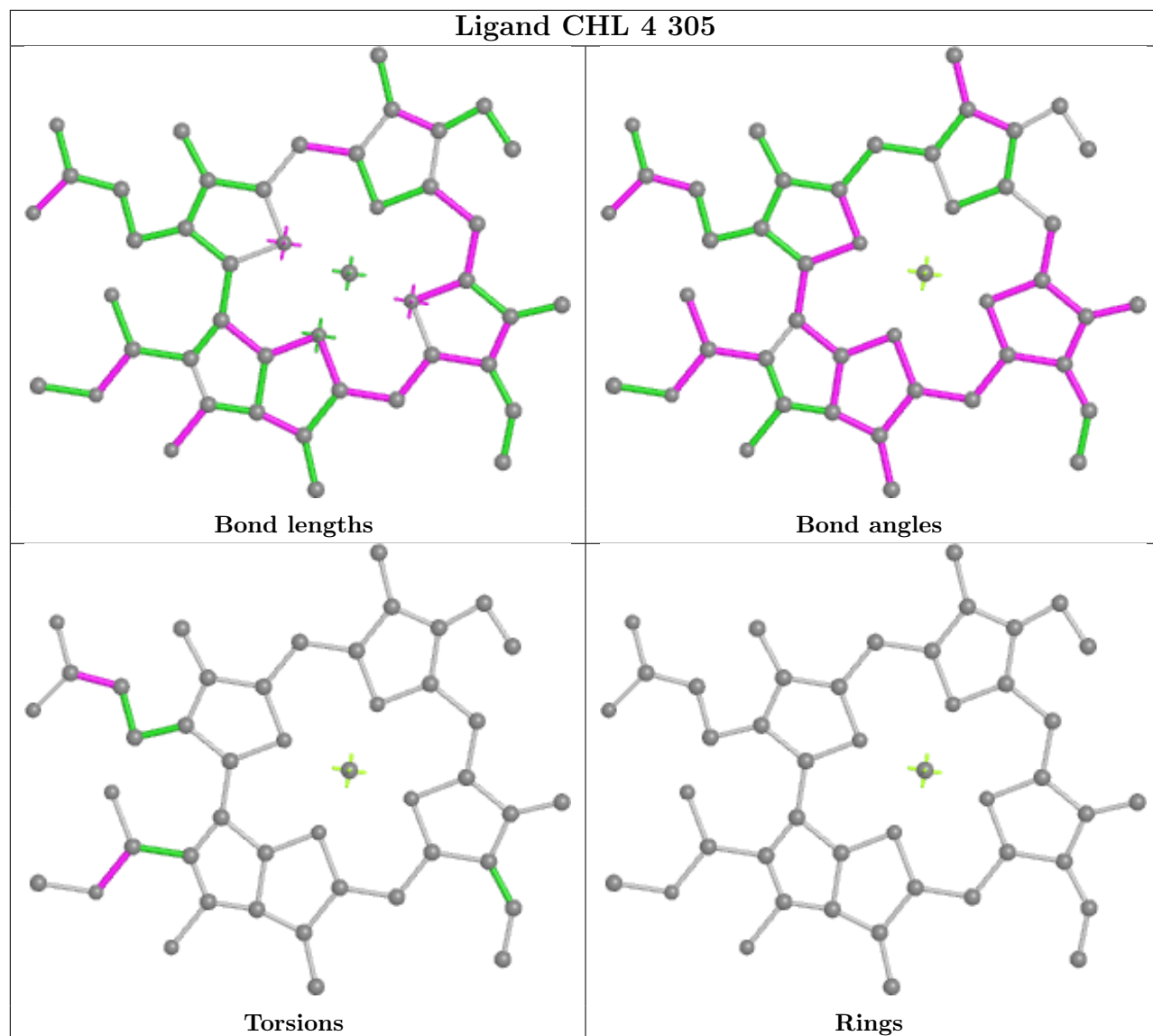


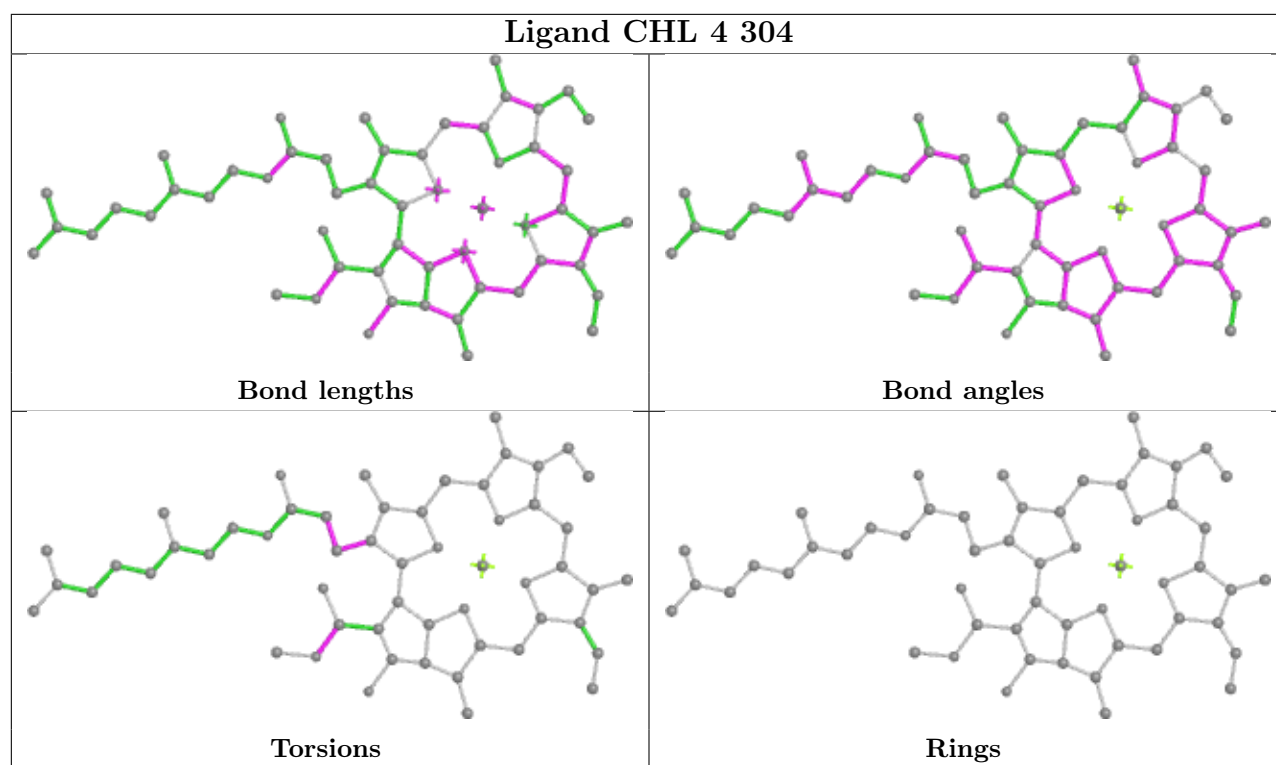
Rings



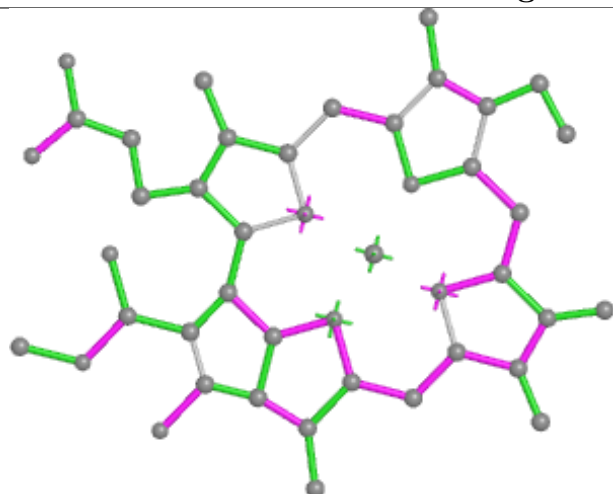


Ligand CHL 4 305

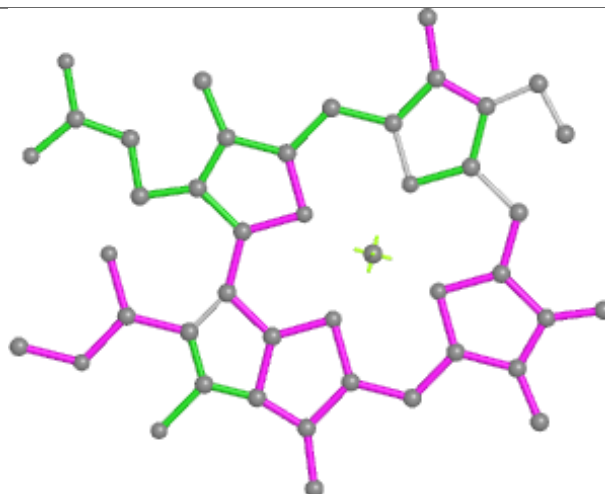




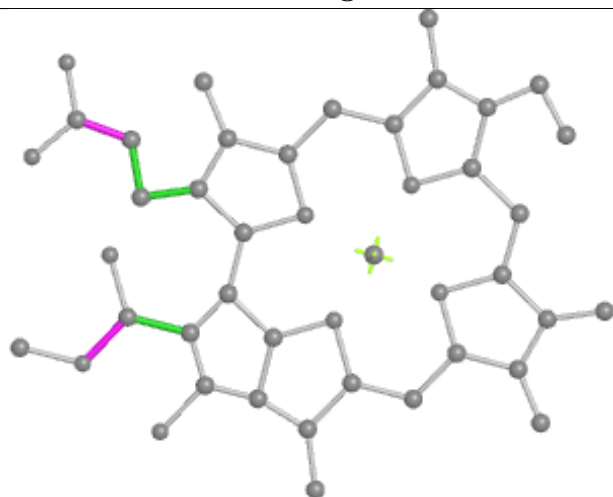
Ligand CHL 7 312



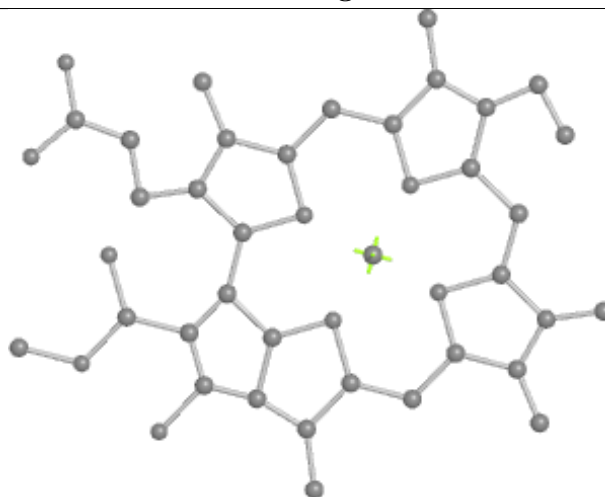
Bond lengths



Bond angles

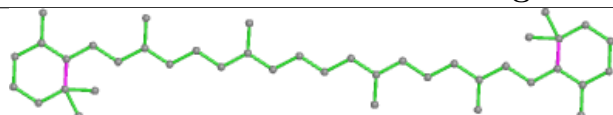


Torsions

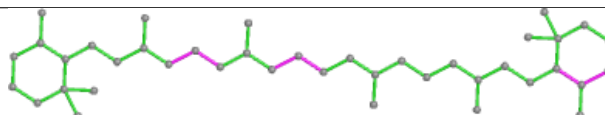


Rings

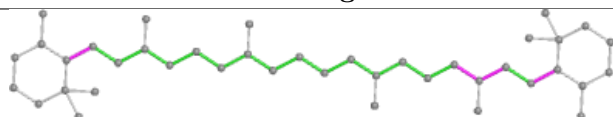
Ligand BCR B 807



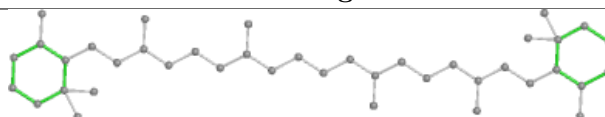
Bond lengths



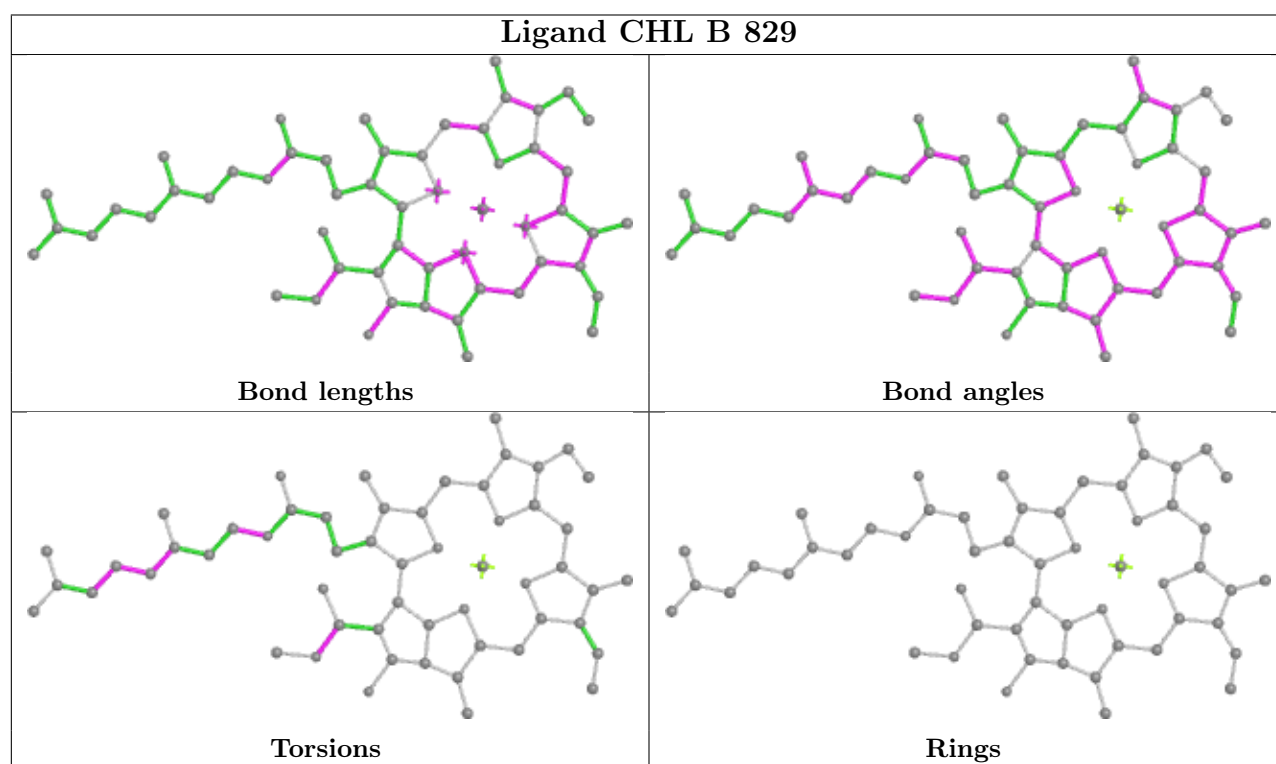
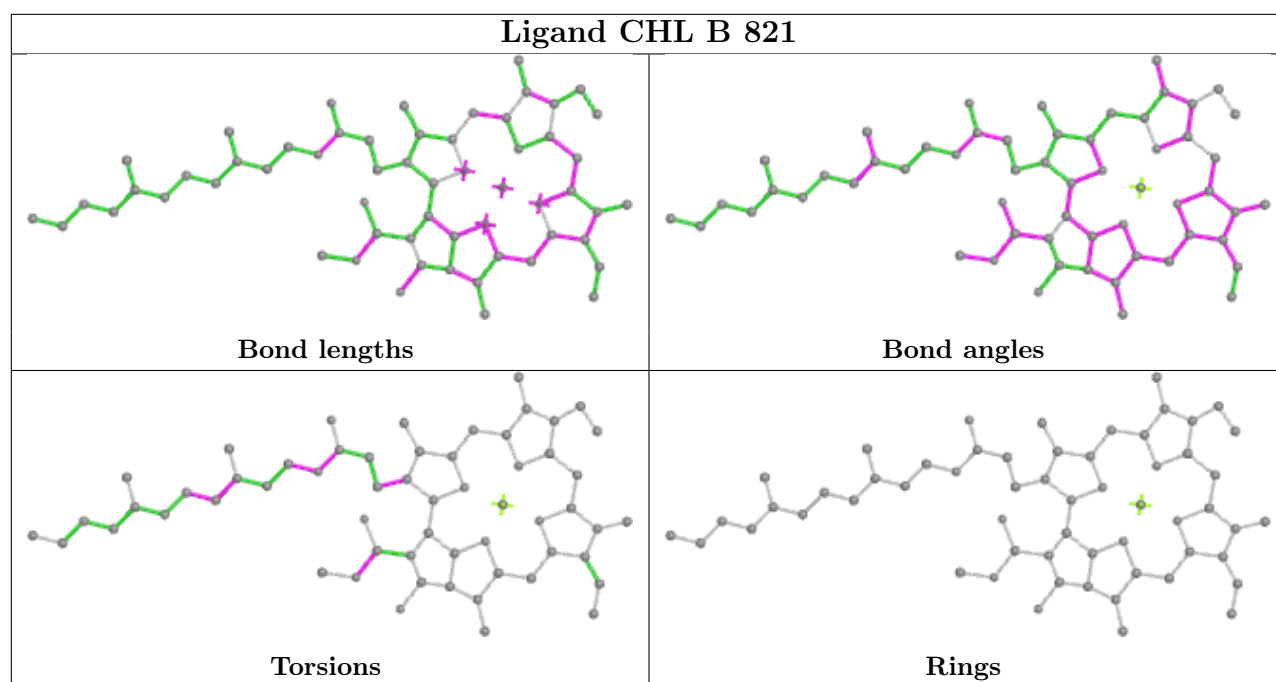
Bond angles

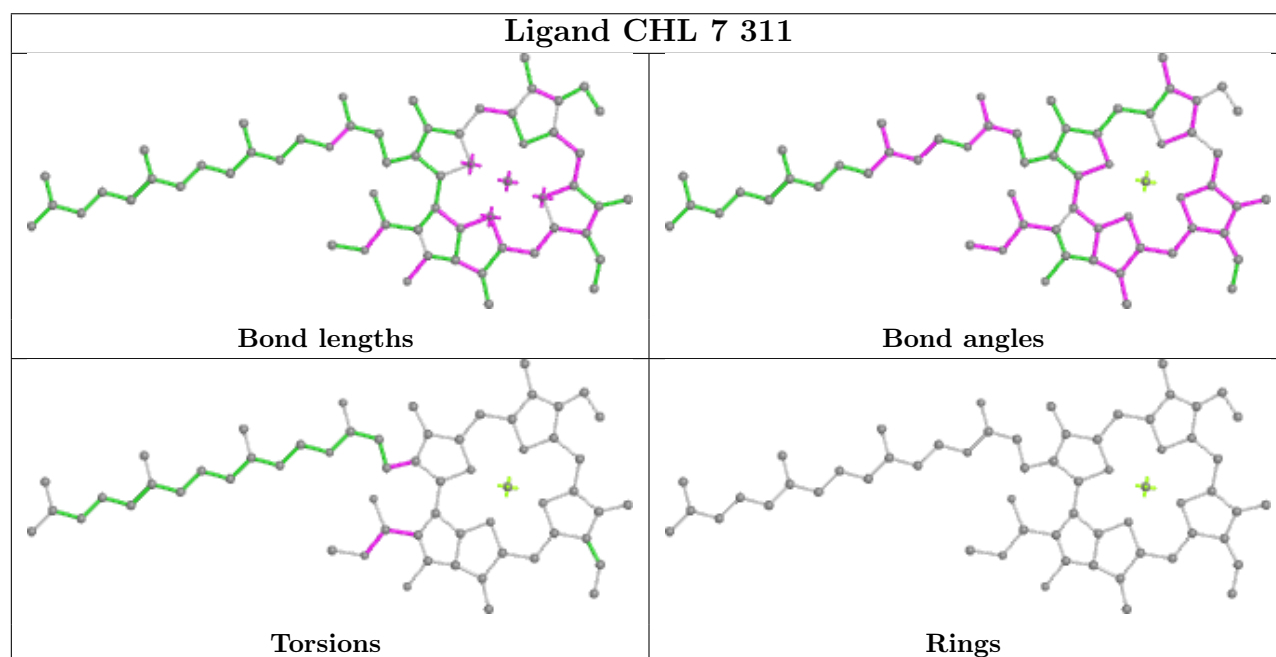
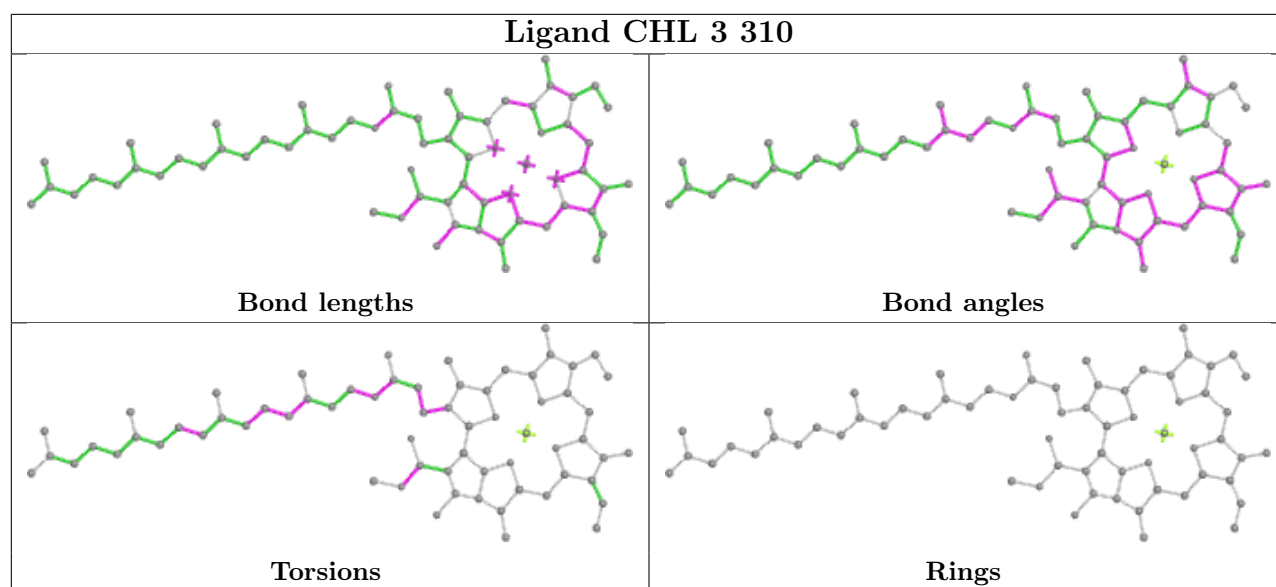


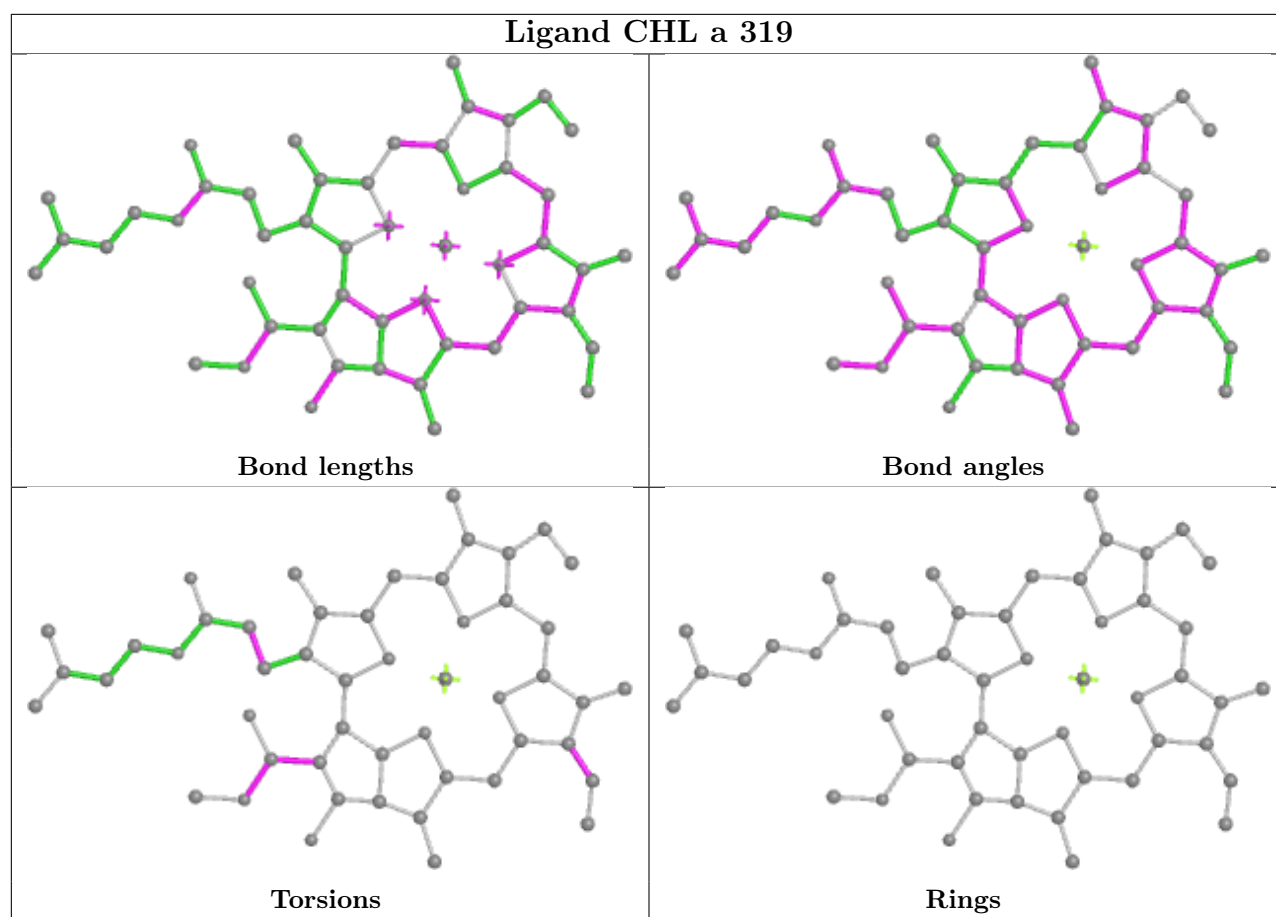
Torsions



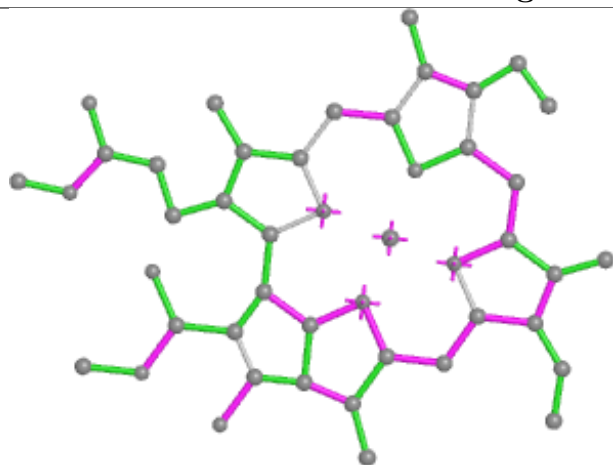
Rings



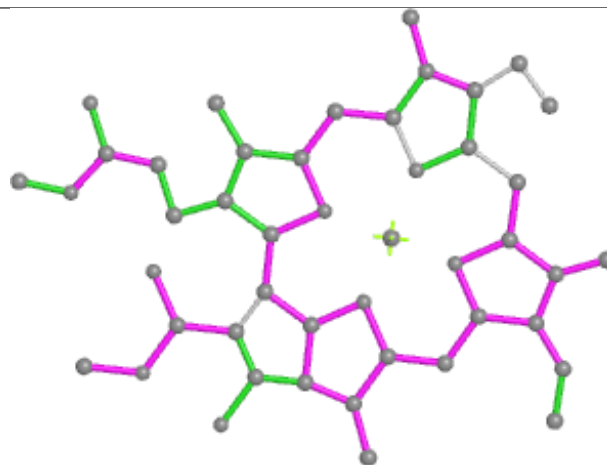




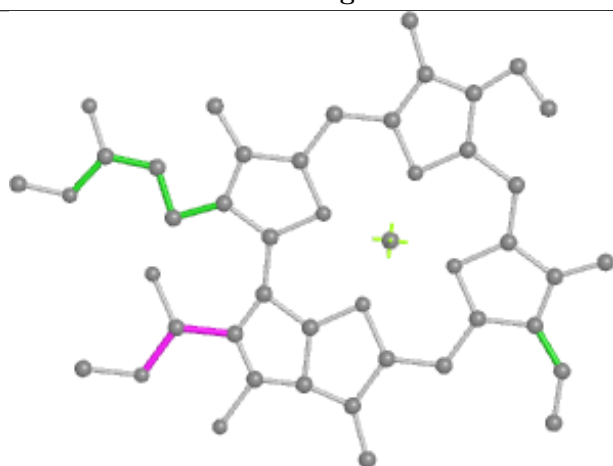
Ligand CHL b 309



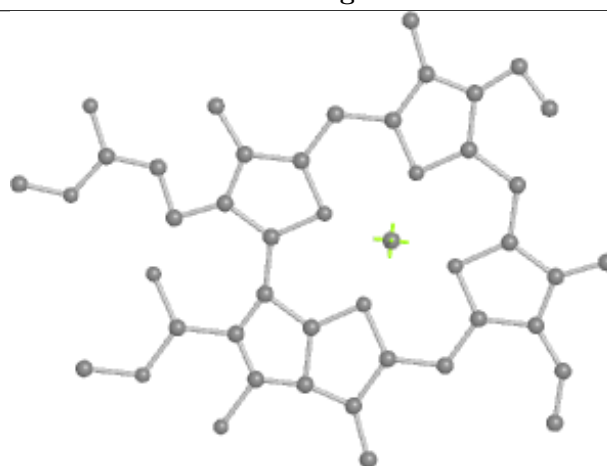
Bond lengths



Bond angles

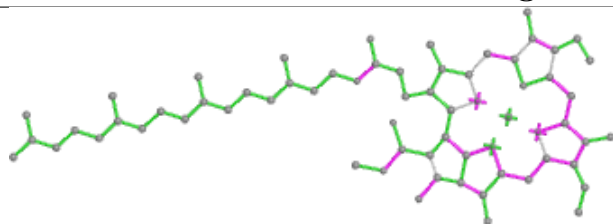


Torsions

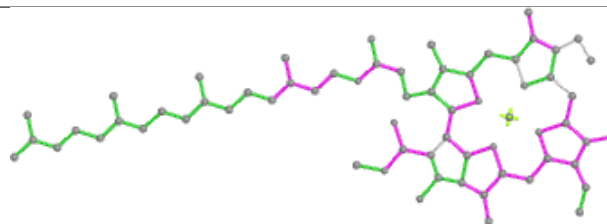


Rings

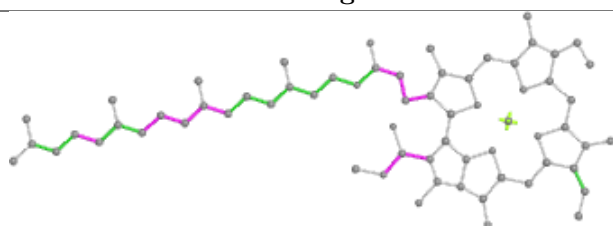
Ligand CHL 8 315



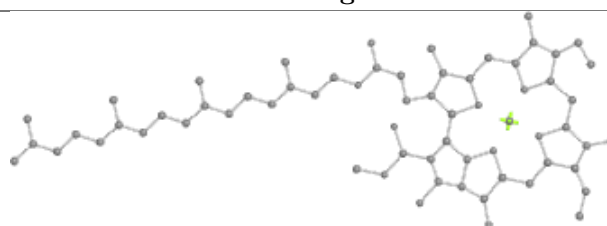
Bond lengths



Bond angles

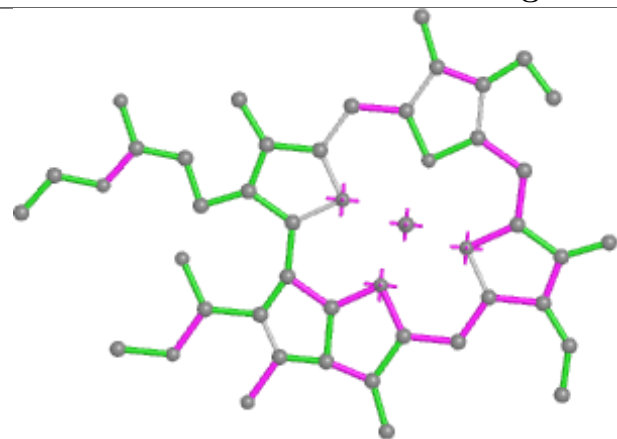


Torsions

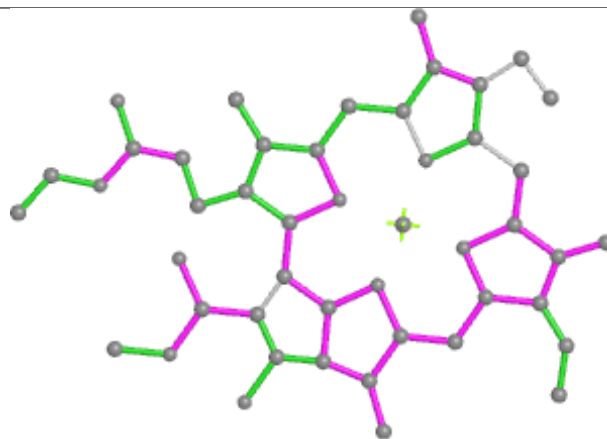


Rings

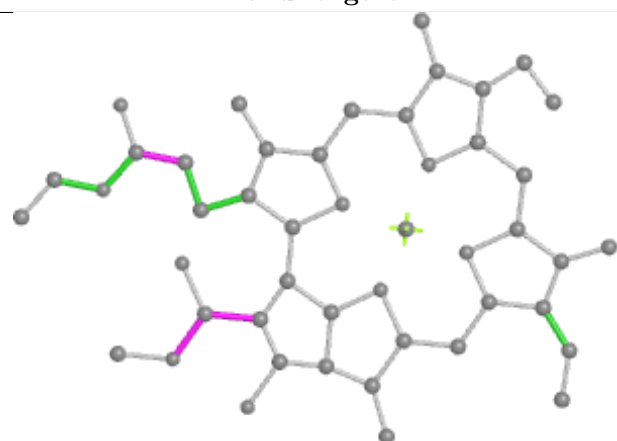
Ligand CHL 6 309



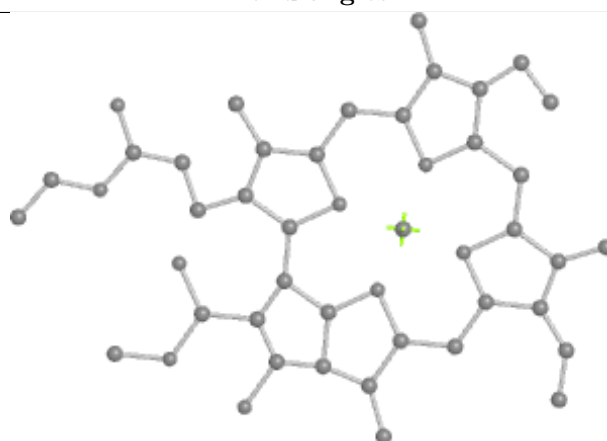
Bond lengths



Bond angles

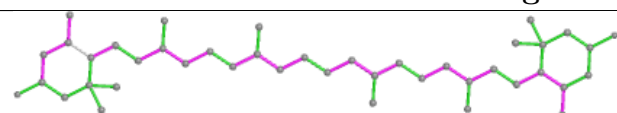


Torsions

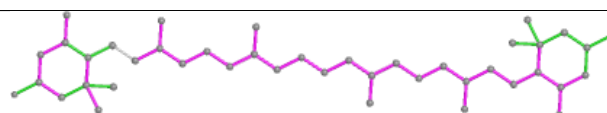


Rings

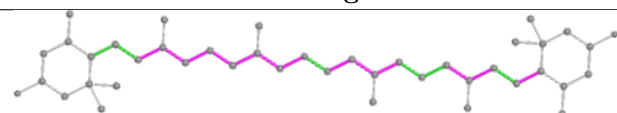
Ligand LUT 6 302



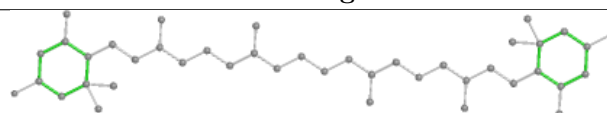
Bond lengths



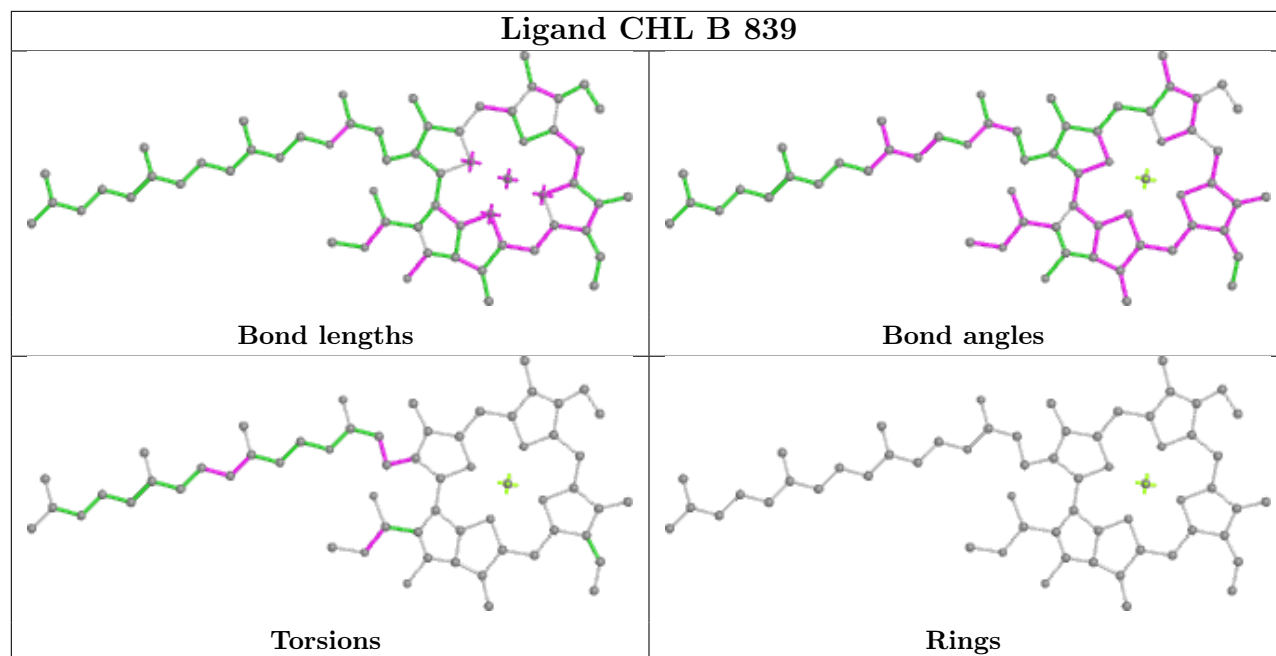
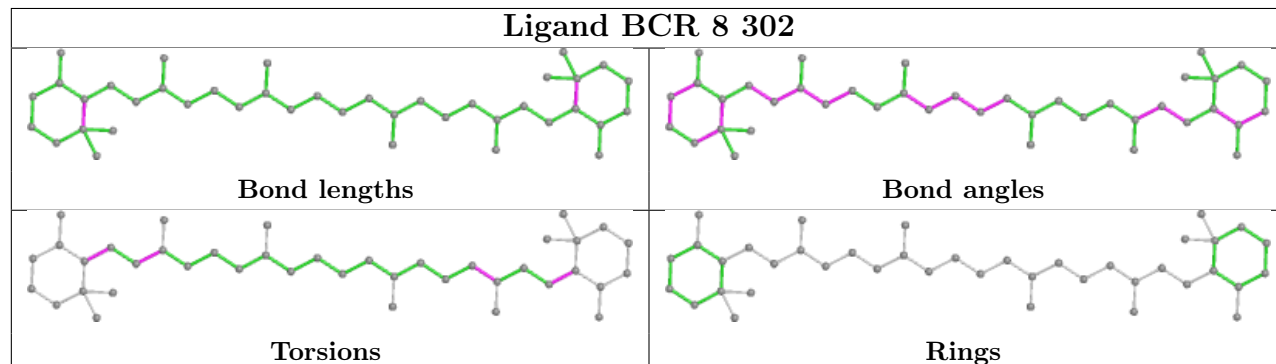
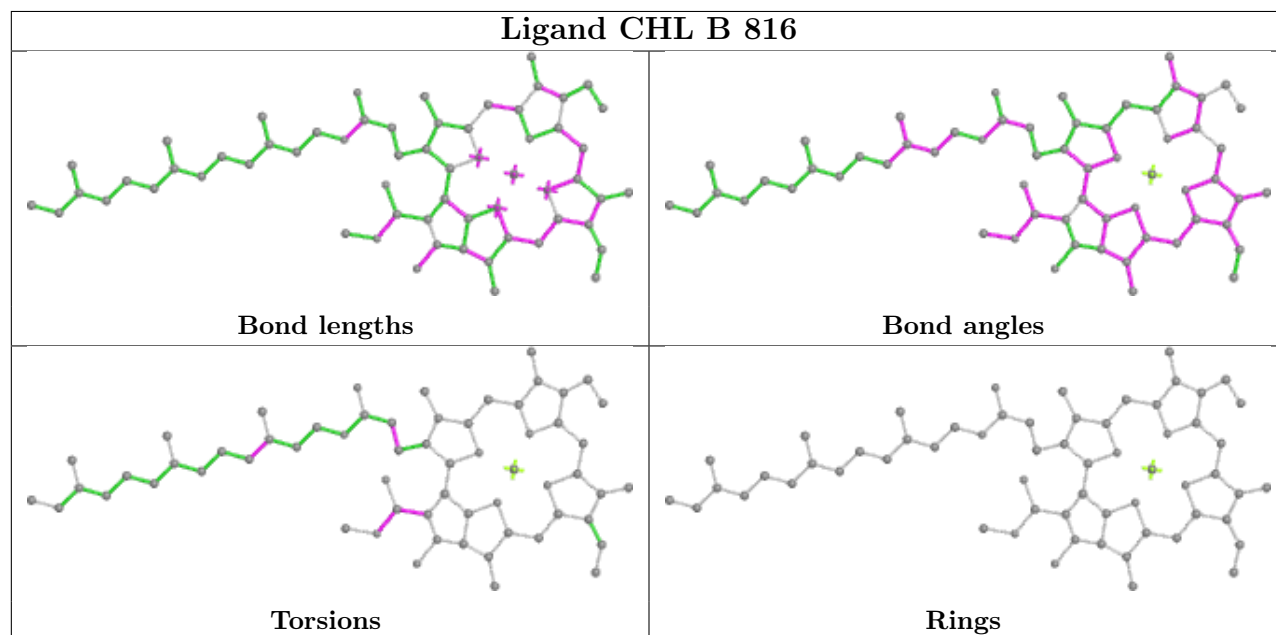
Bond angles

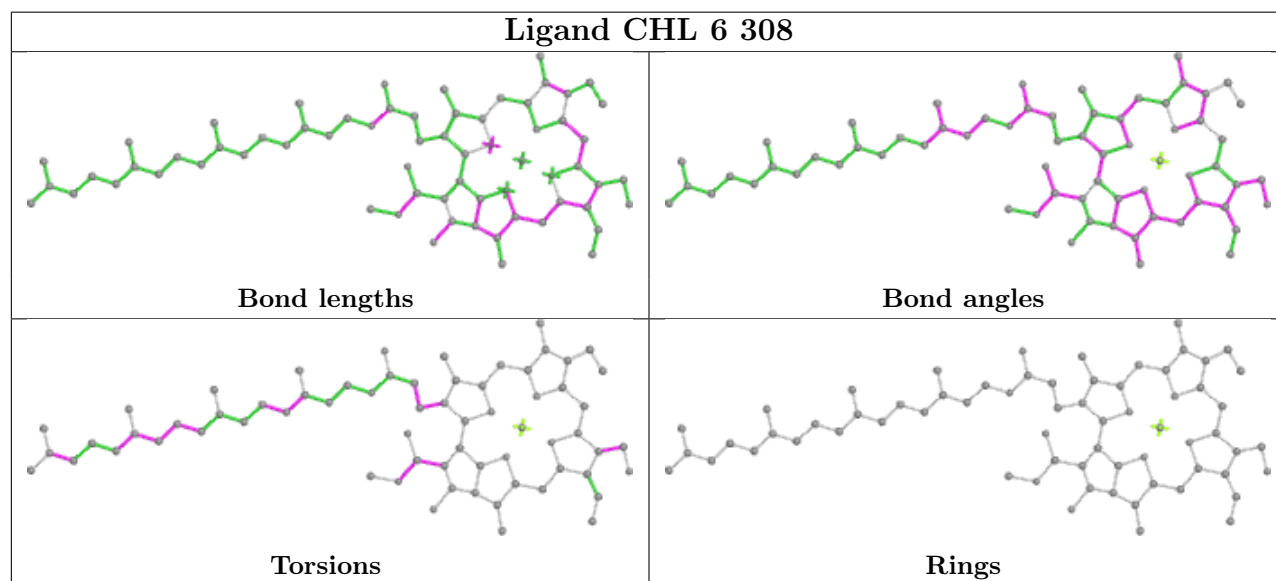
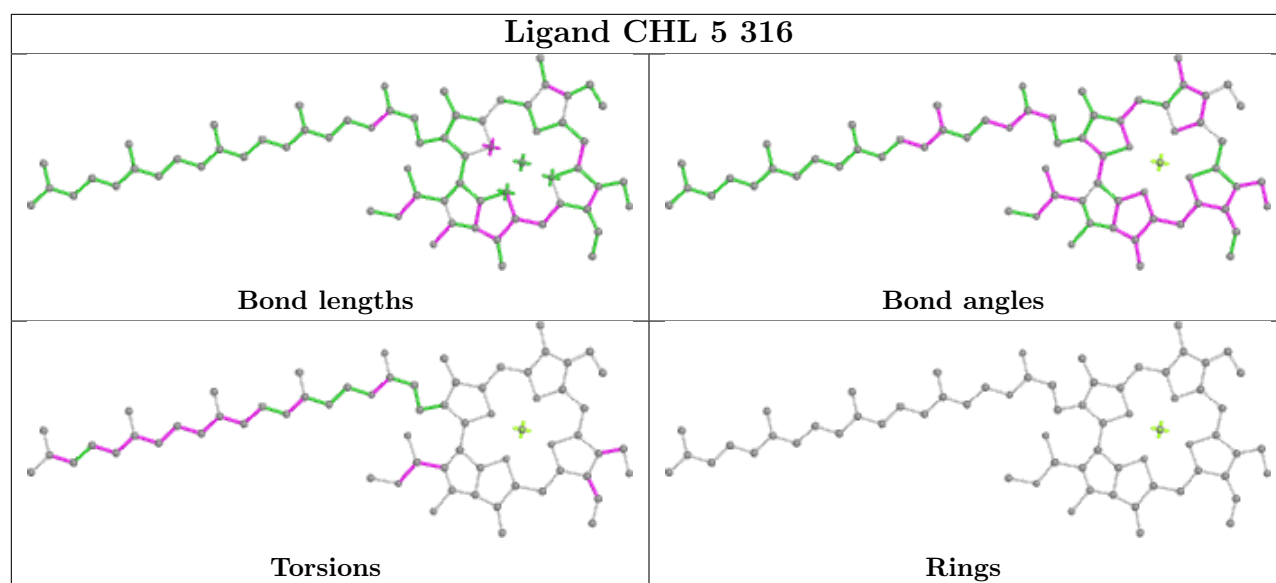


Torsions

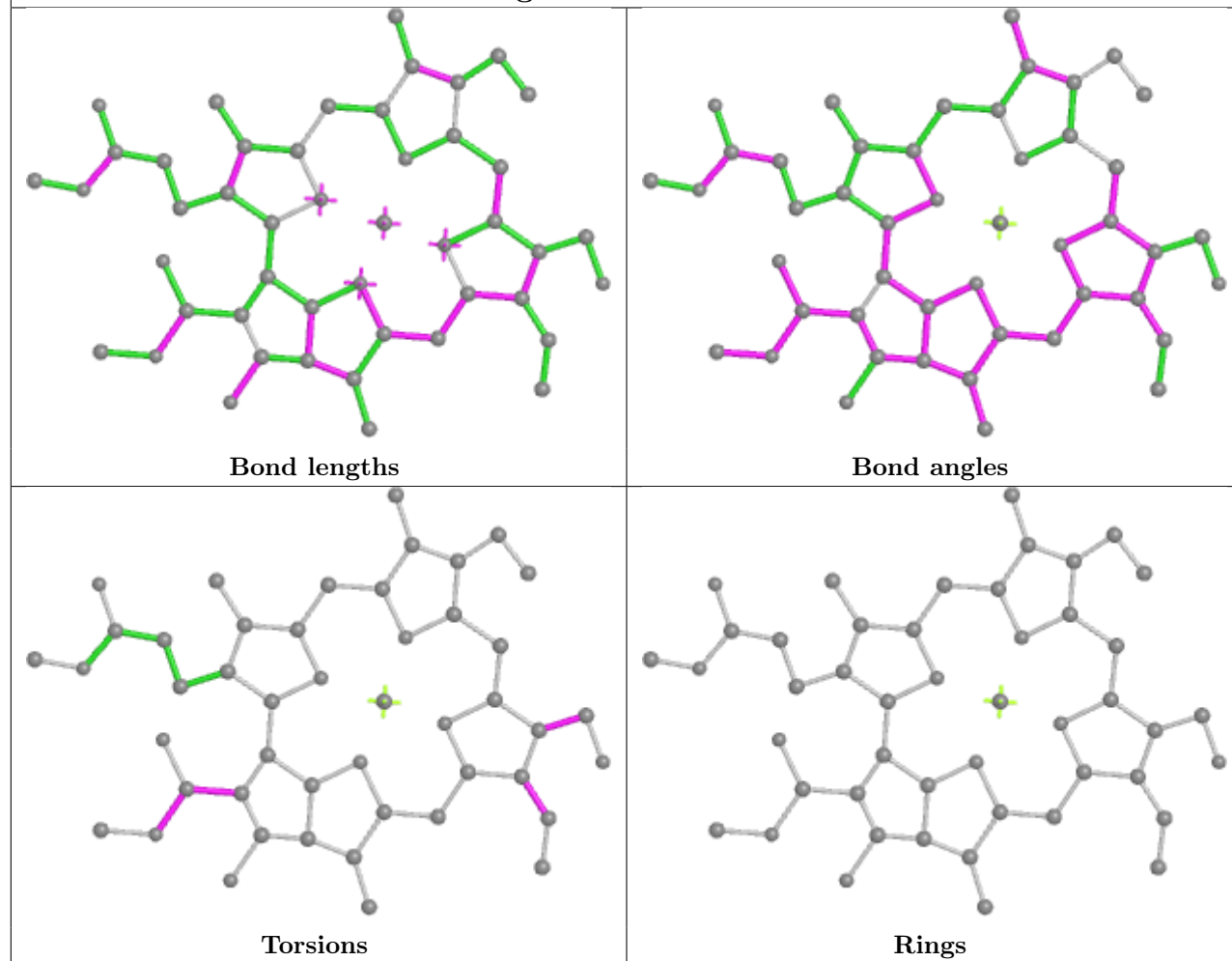


Rings

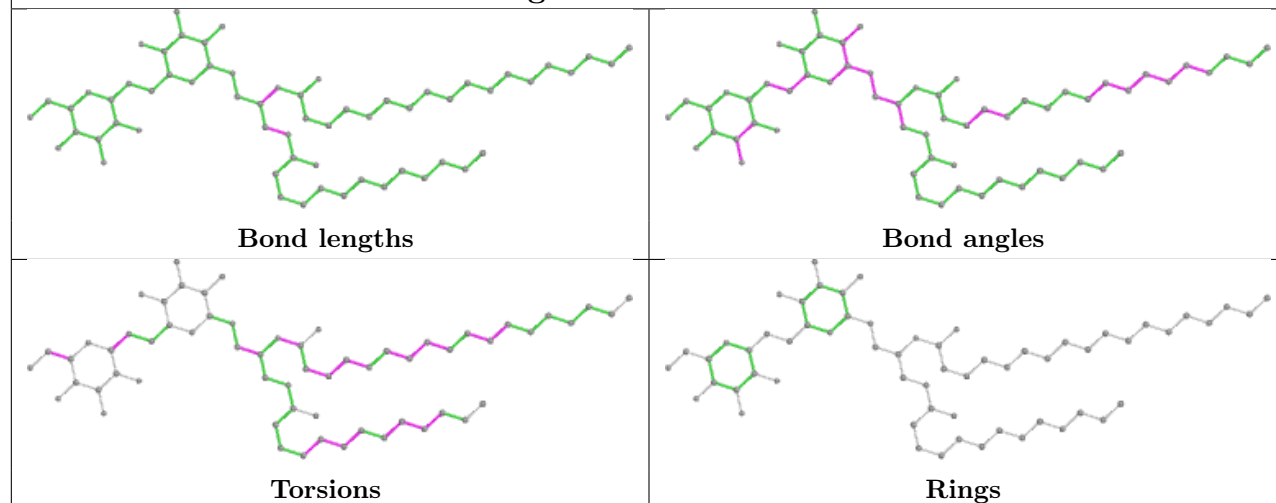
Ligand CHL B 839**Ligand BCR 8 302****Ligand CHL B 816**

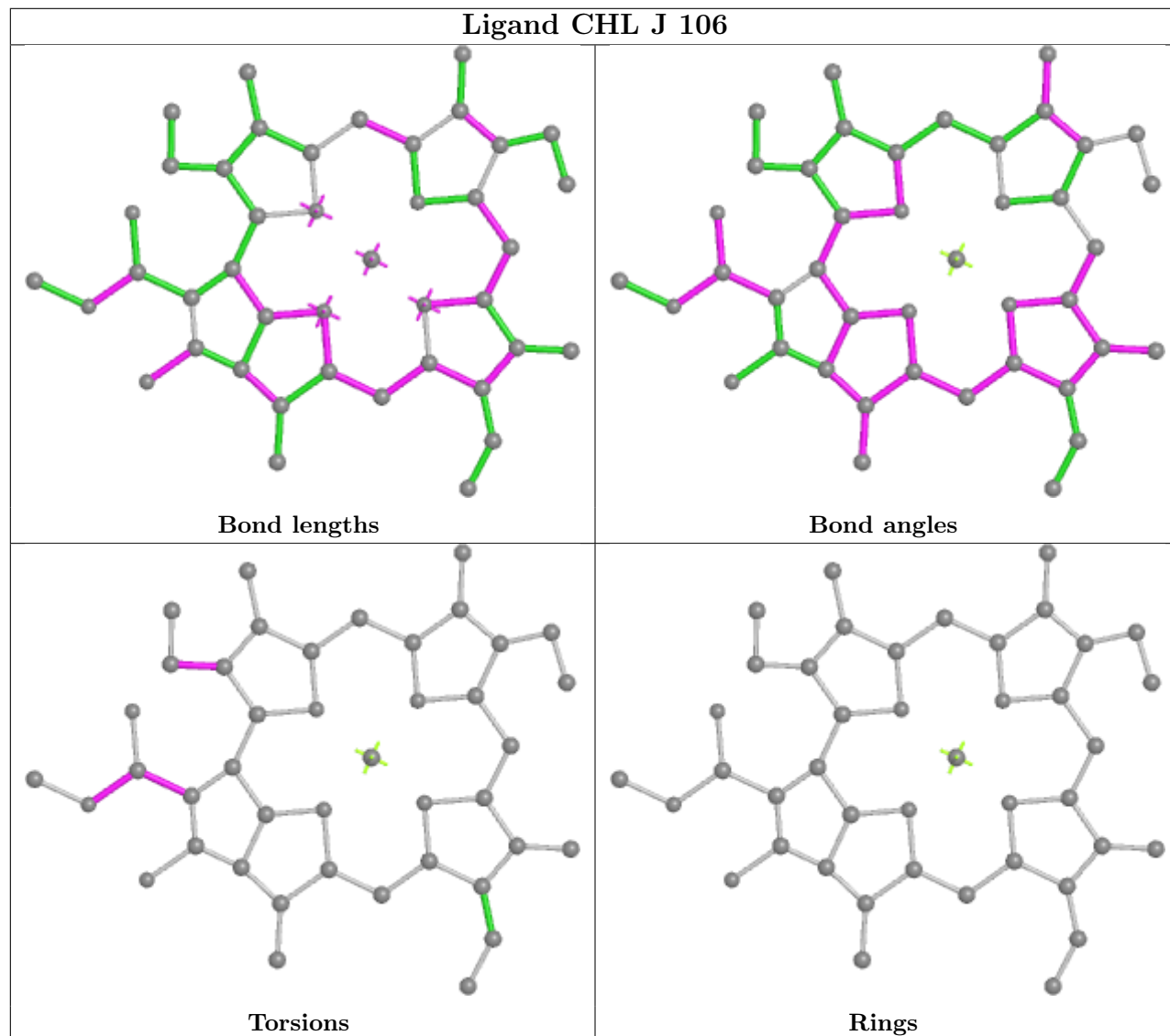
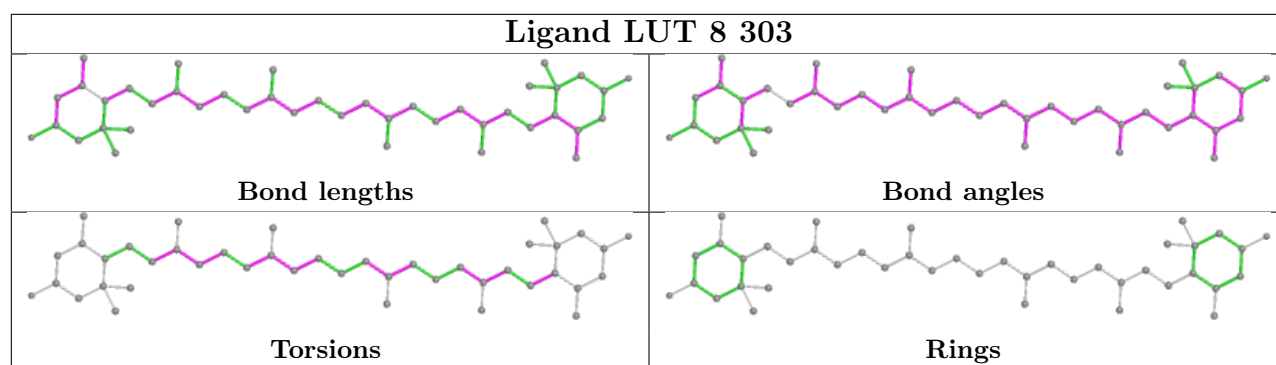


Ligand CHL b 311

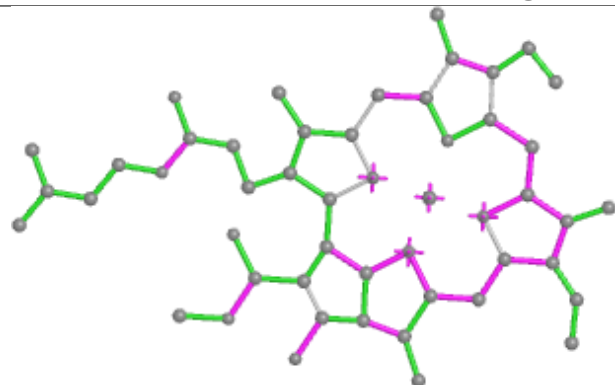


Ligand DGD B 809

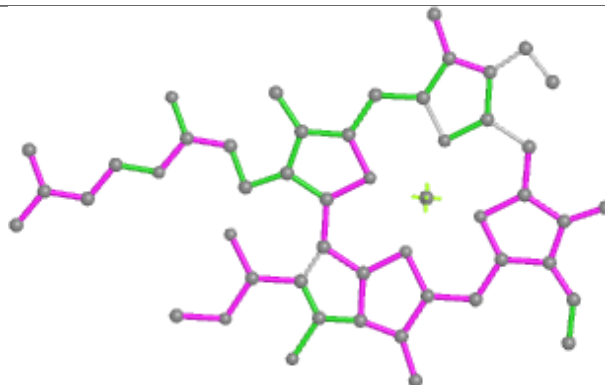




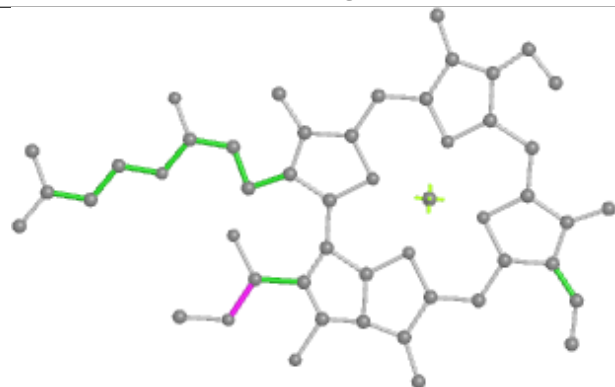
Ligand CHL 6 315



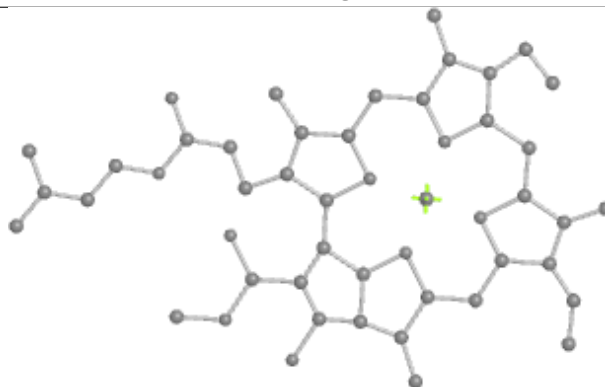
Bond lengths



Bond angles

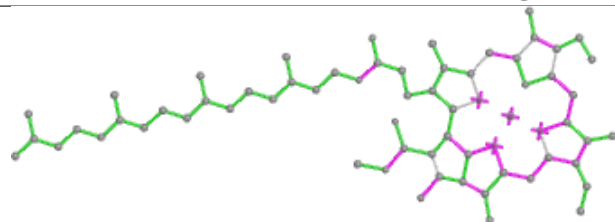


Torsions

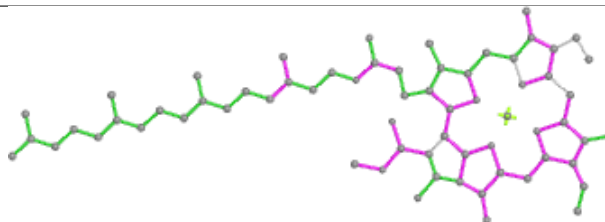


Rings

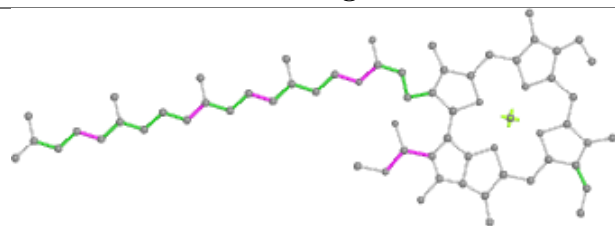
Ligand CHL A 853



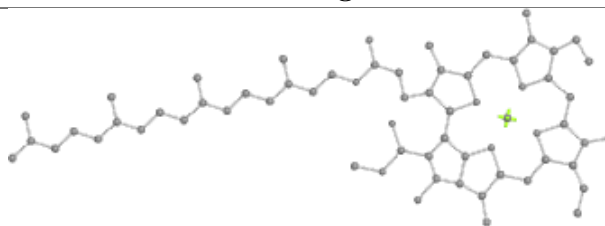
Bond lengths



Bond angles

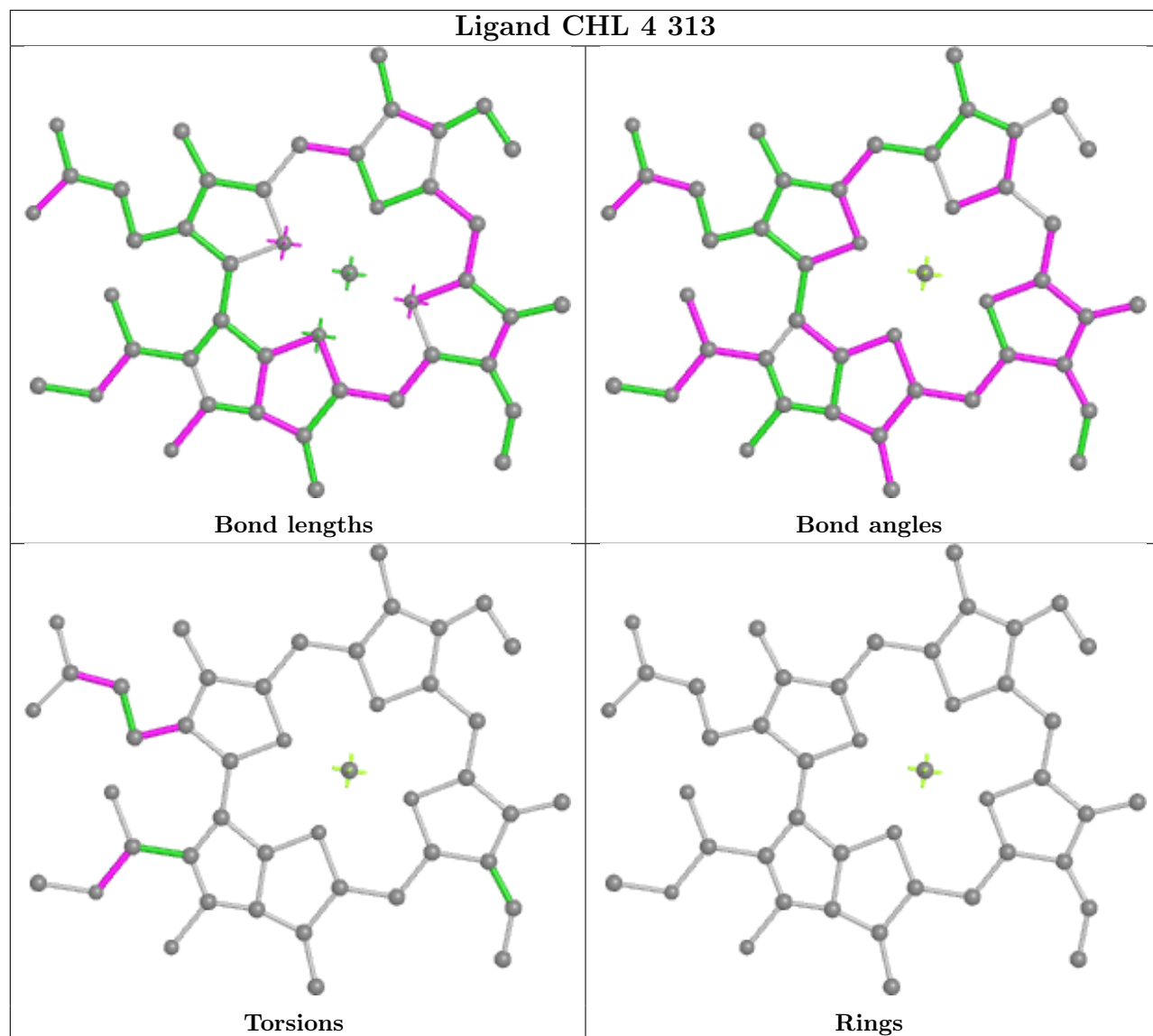


Torsions

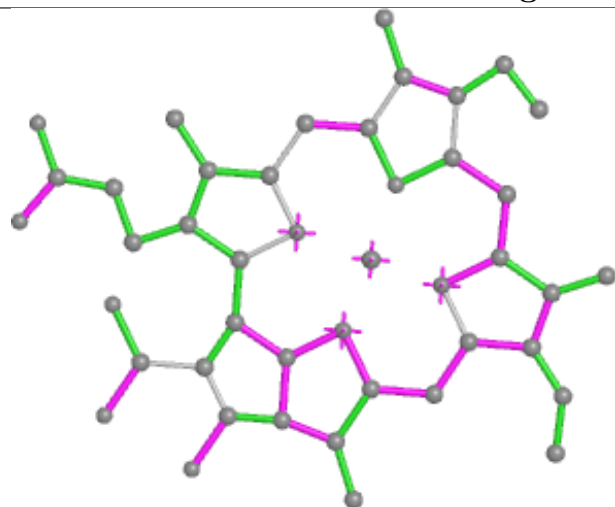


Rings

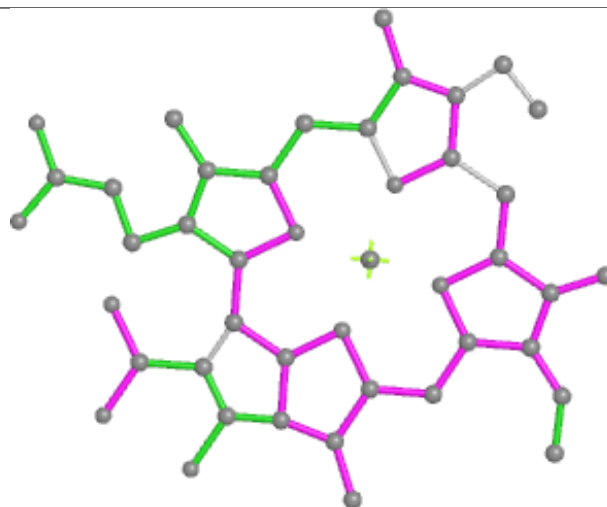
Ligand CHL 4 313



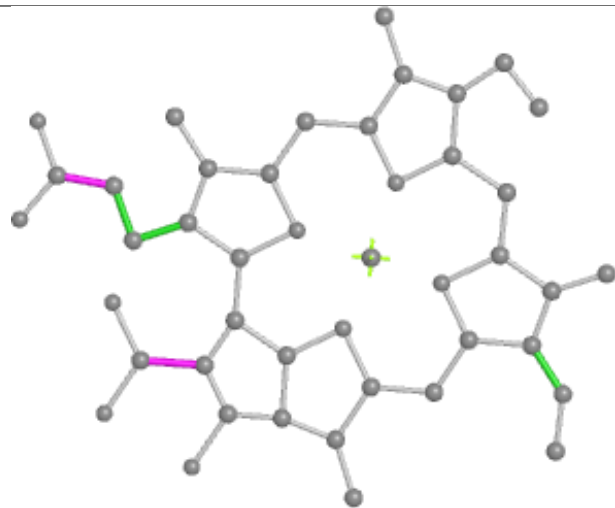
Ligand CHL 7 315



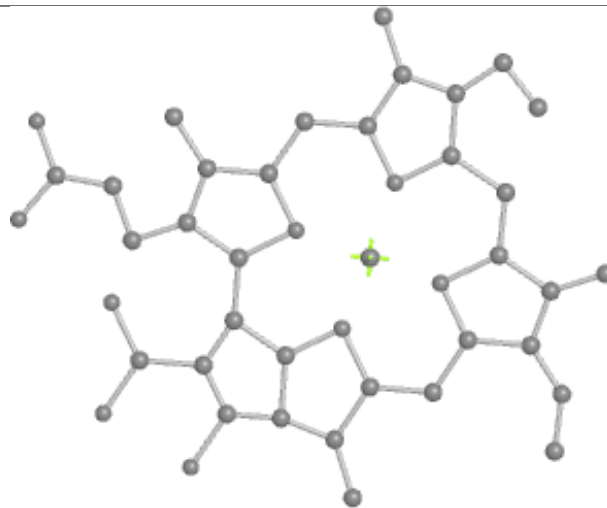
Bond lengths



Bond angles

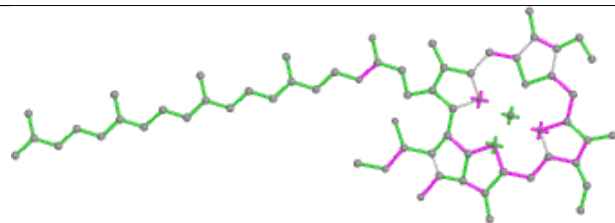


Torsions

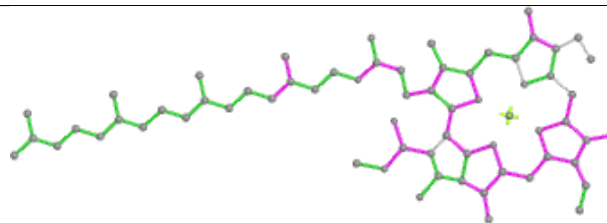


Rings

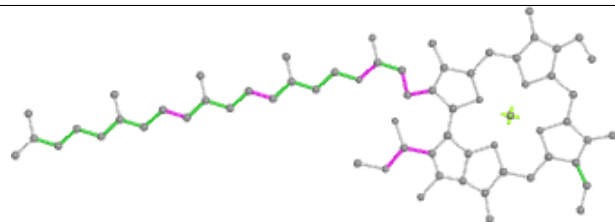
Ligand CHL 8 325



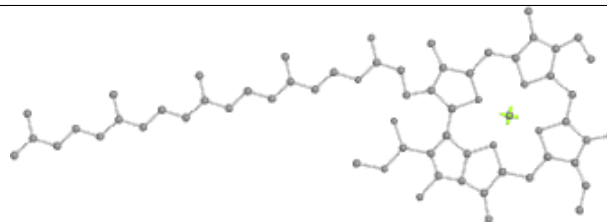
Bond lengths



Bond angles

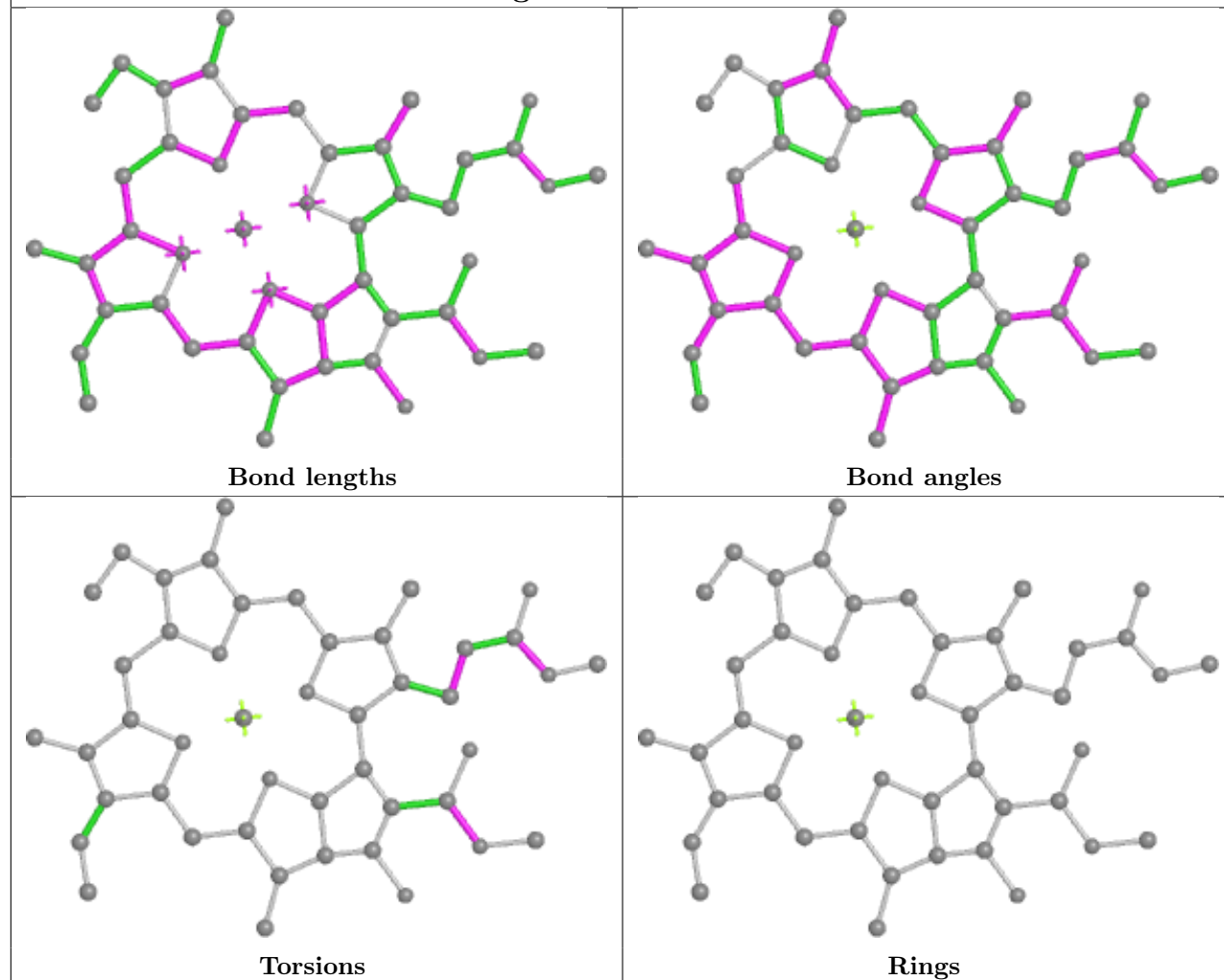


Torsions

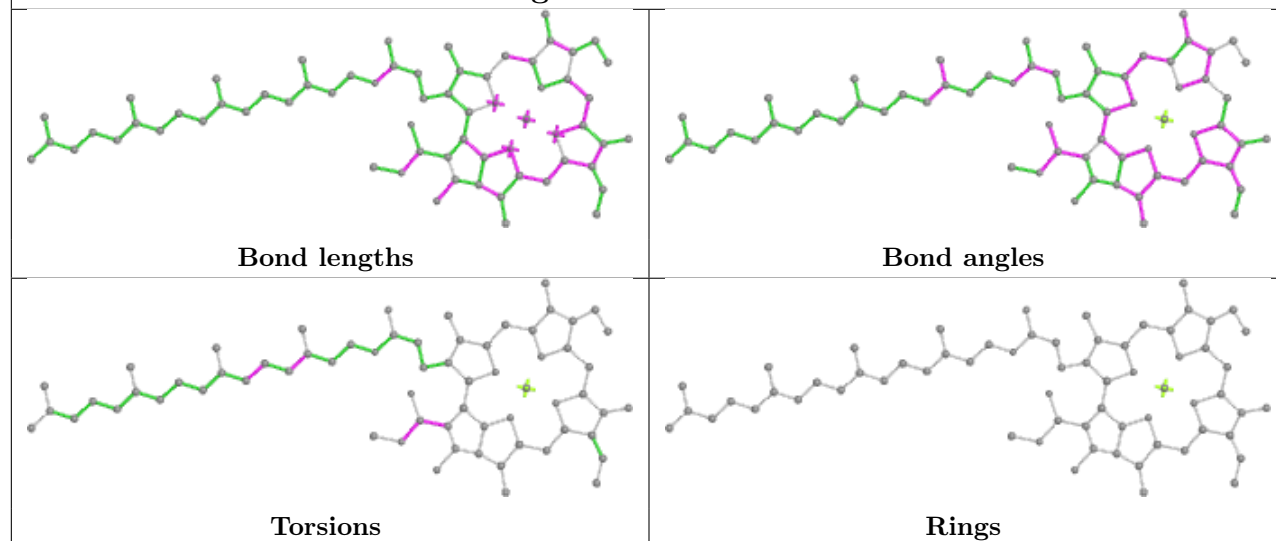


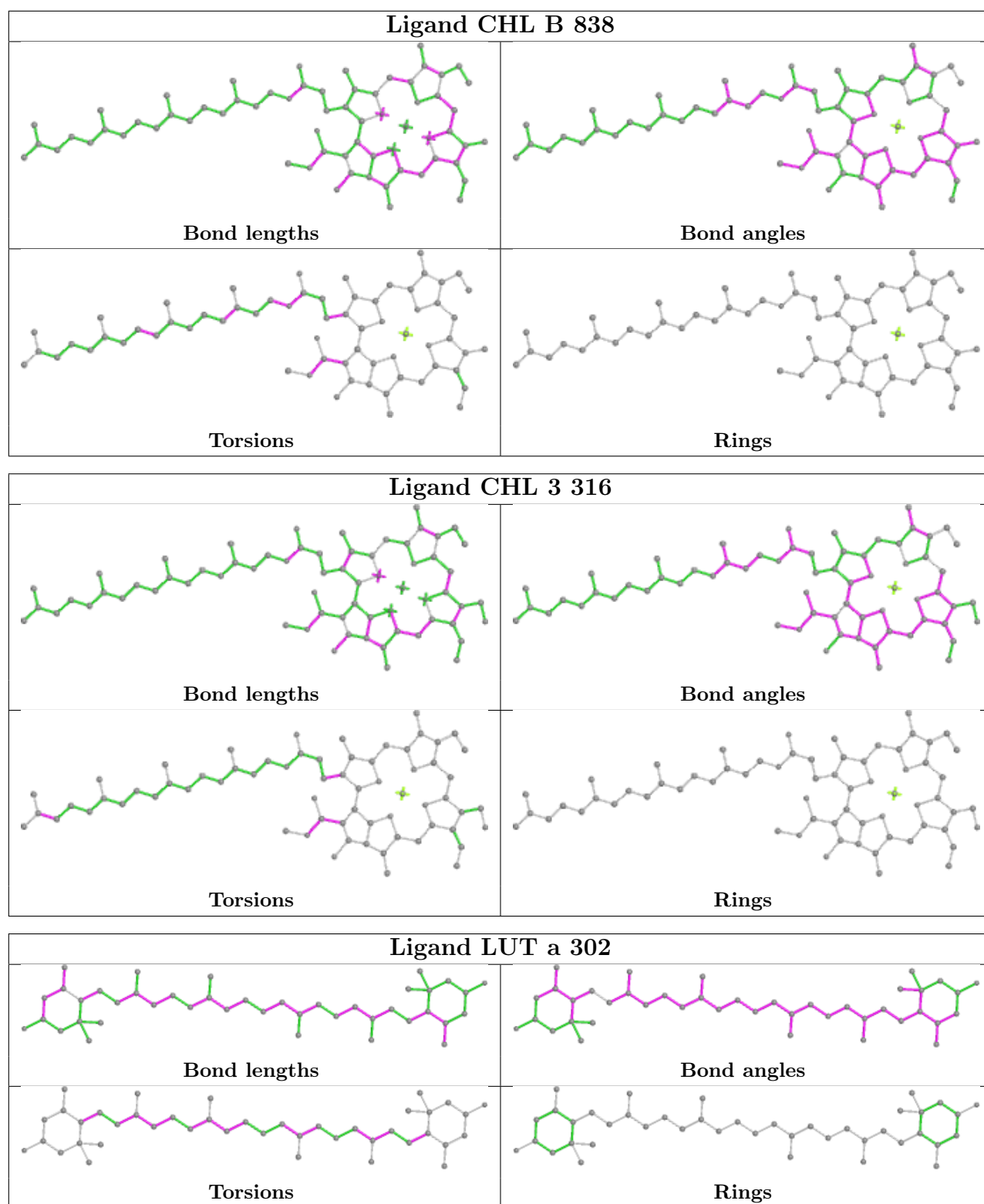
Rings

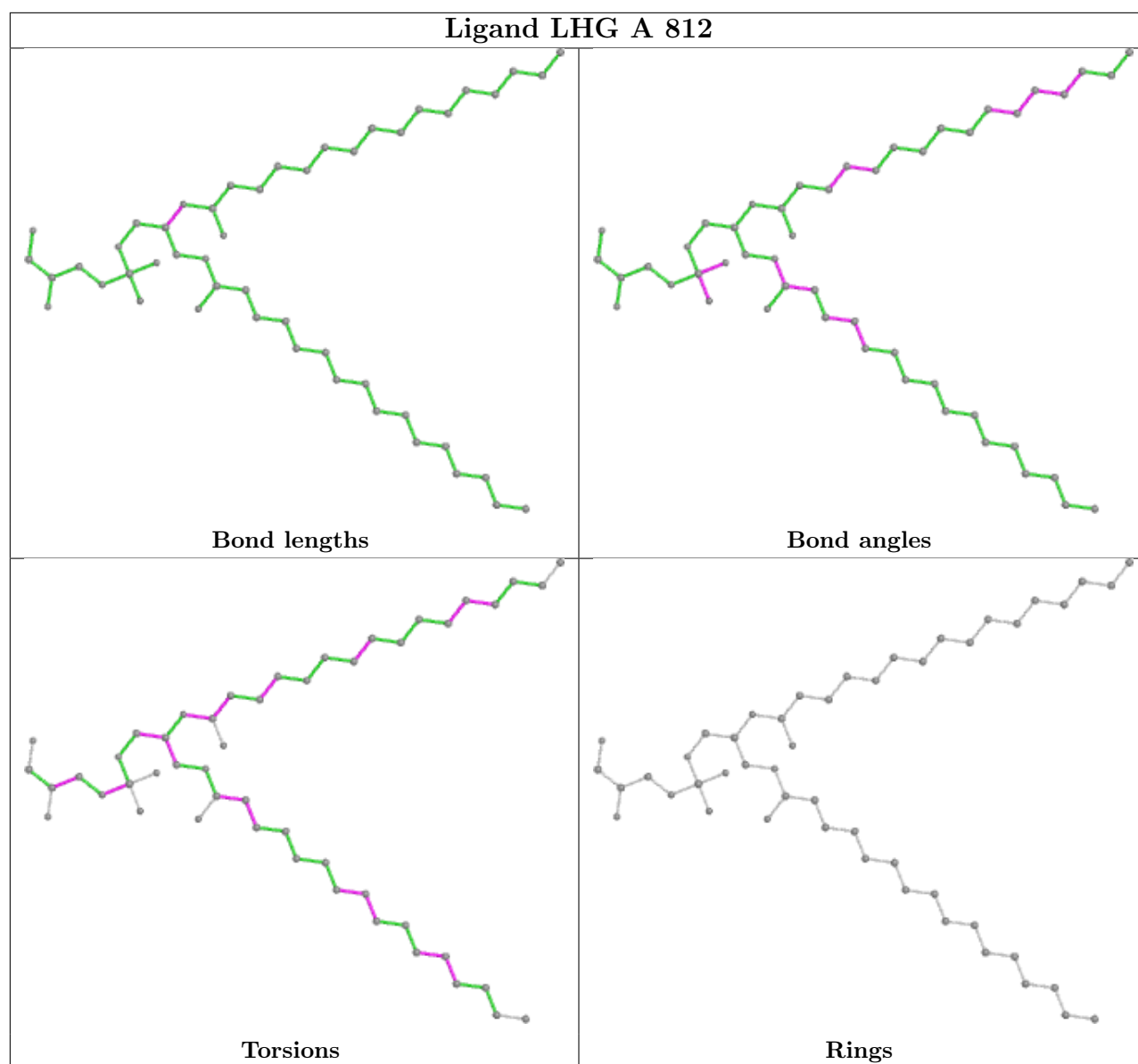
Ligand CHL b 308



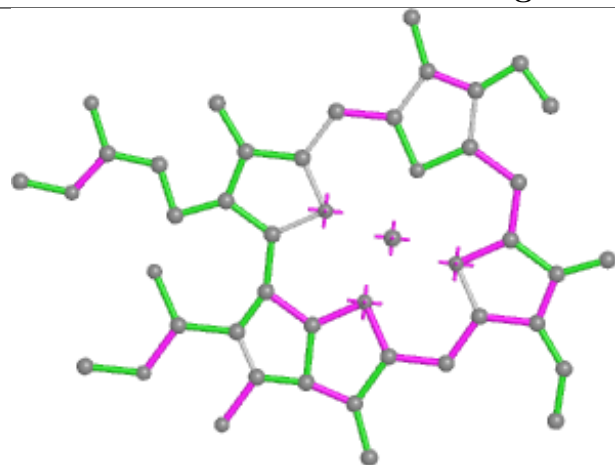
Ligand CHL A 849



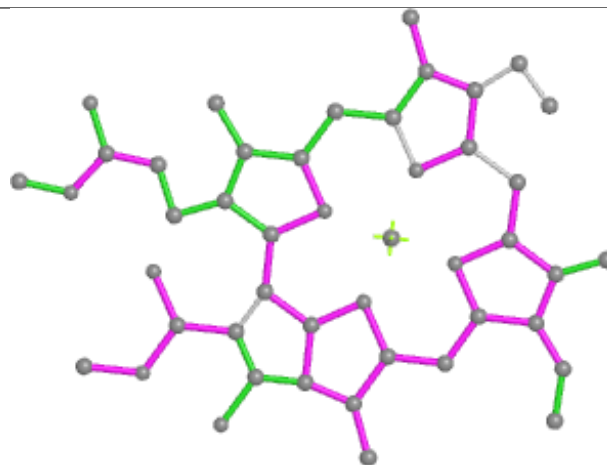




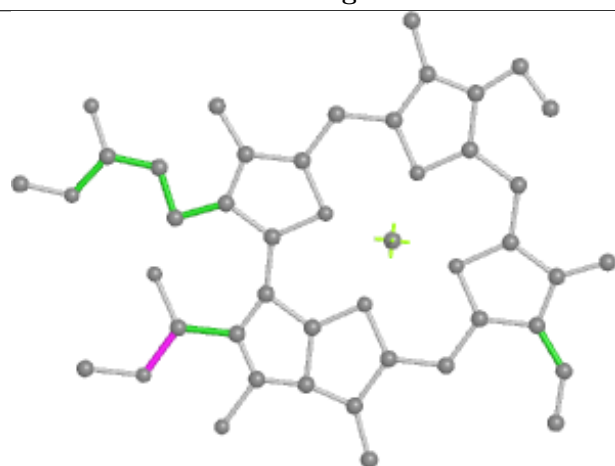
Ligand CHL K 206



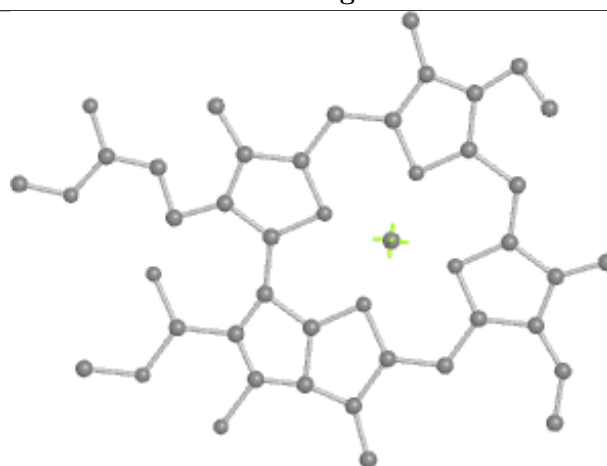
Bond lengths



Bond angles

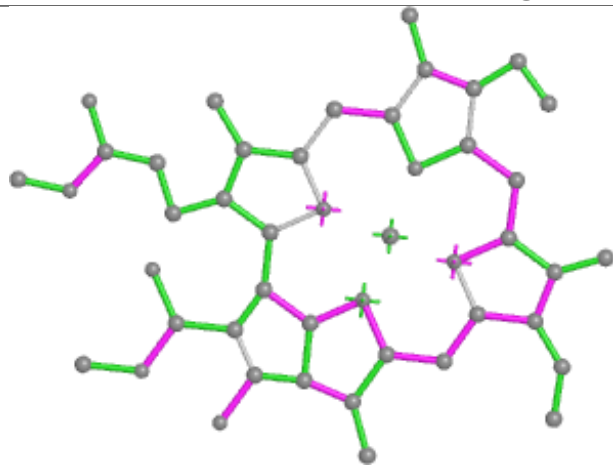


Torsions

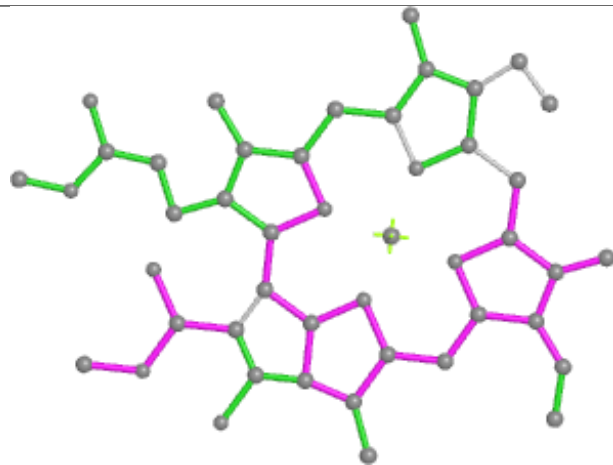


Rings

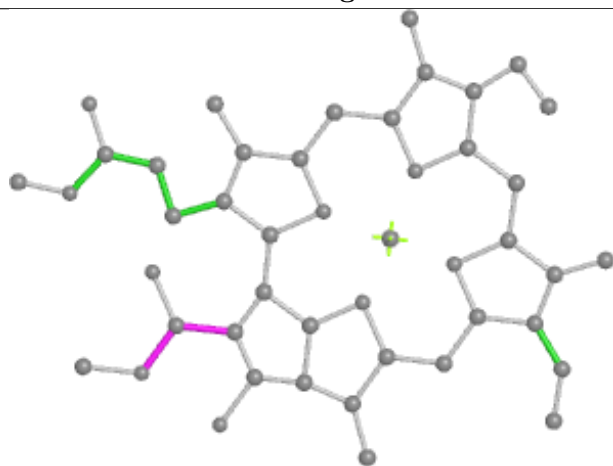
Ligand CHL 5 308



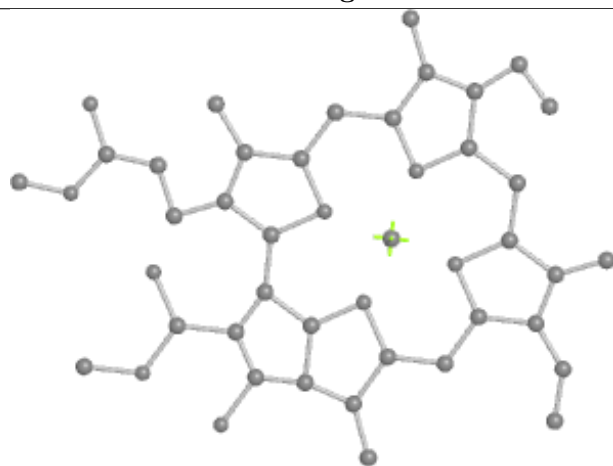
Bond lengths



Bond angles

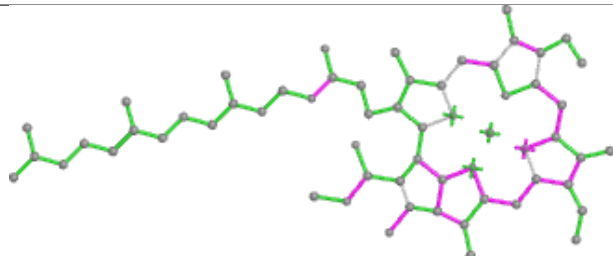


Torsions

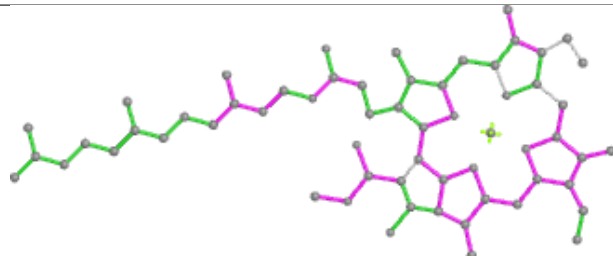


Rings

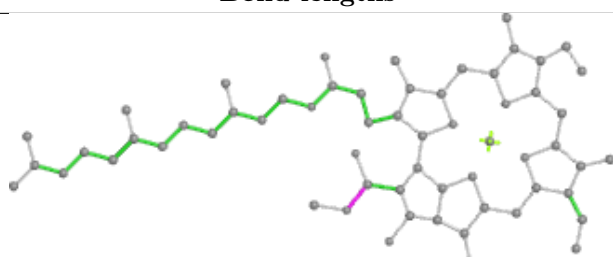
Ligand CHL B 828



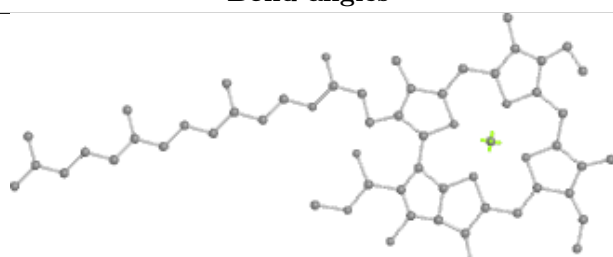
Bond lengths



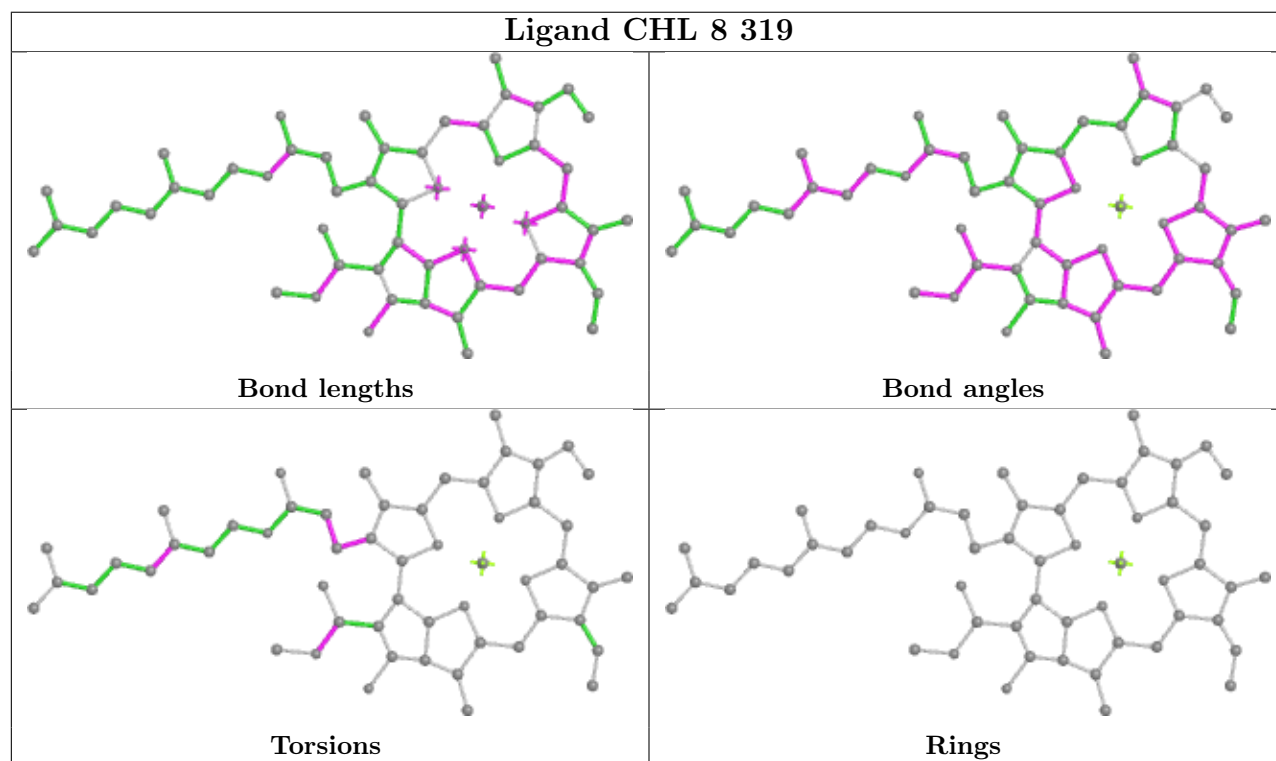
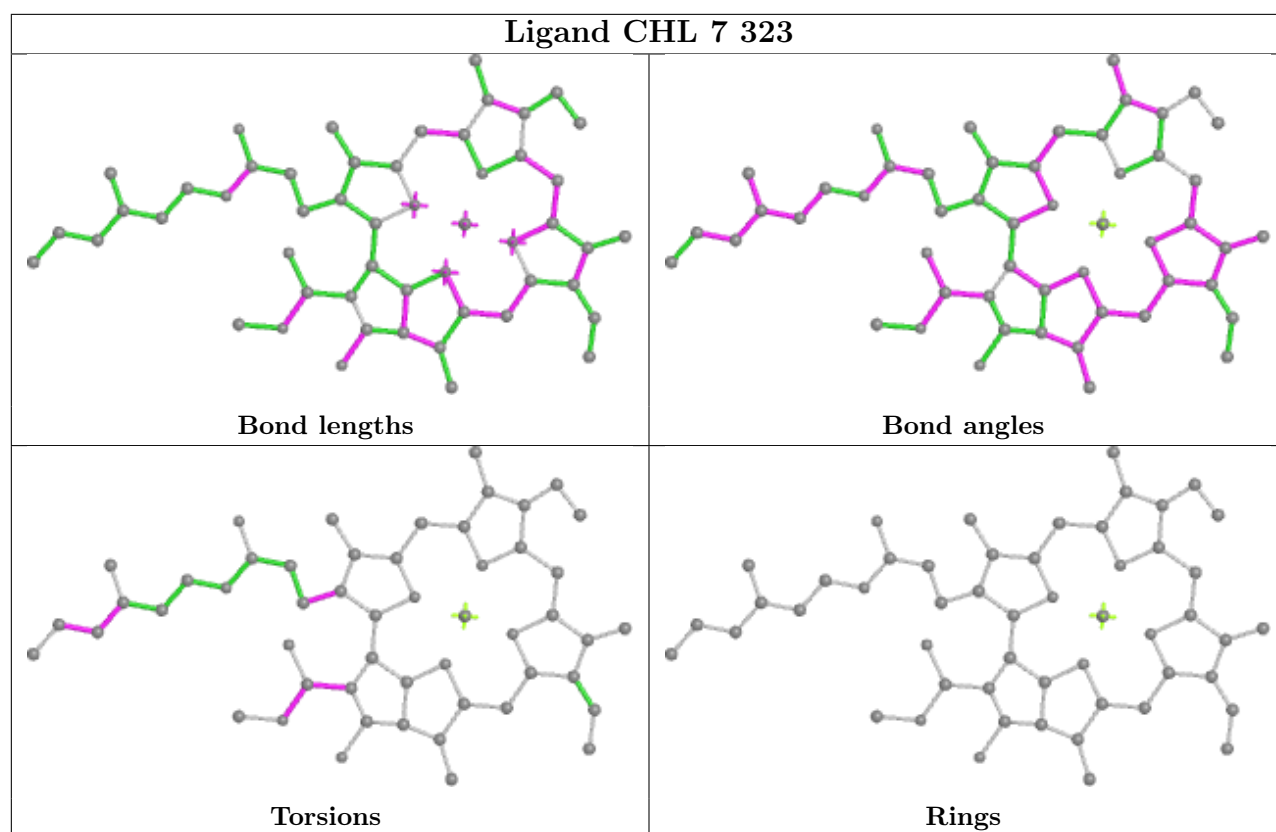
Bond angles

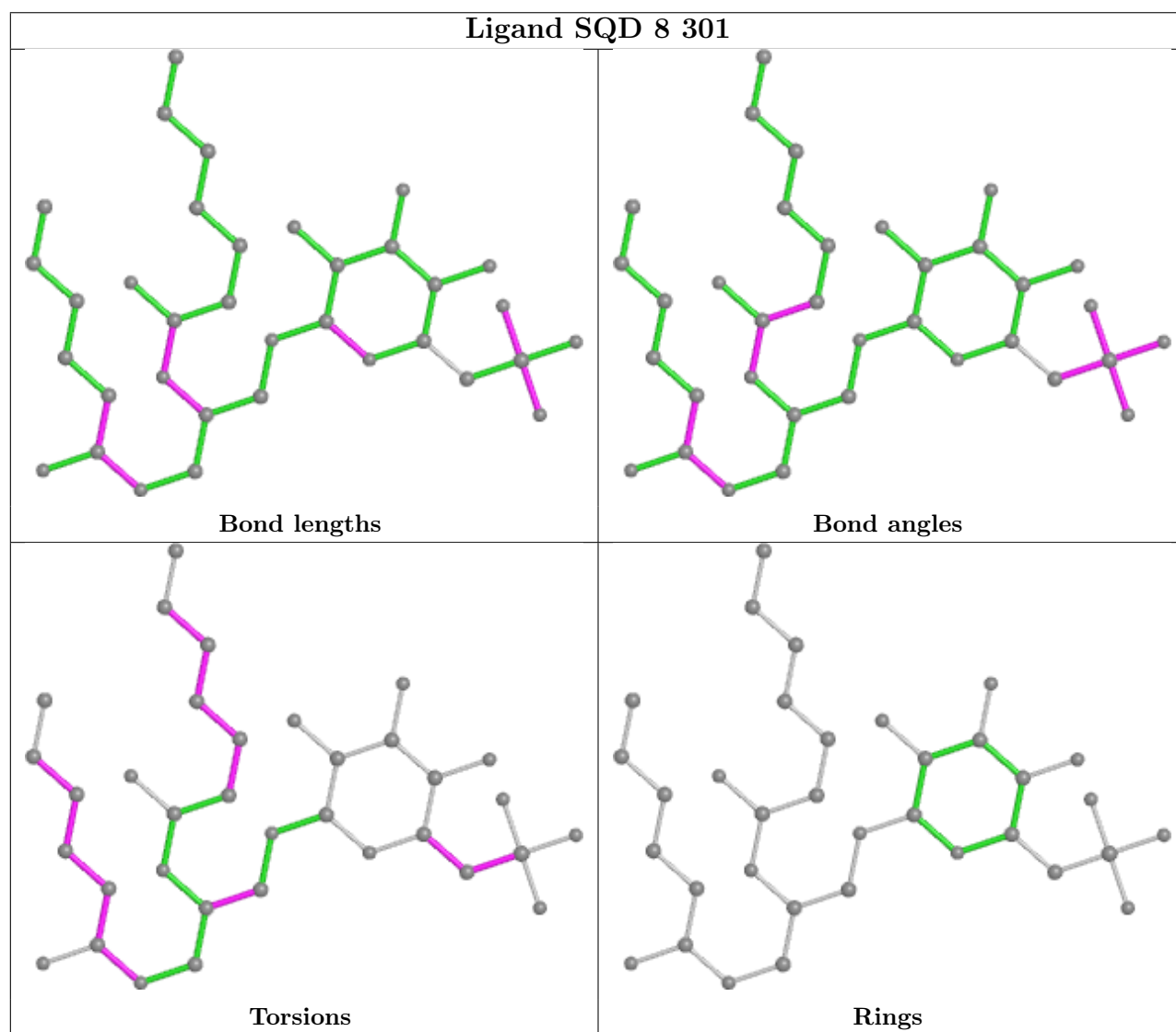
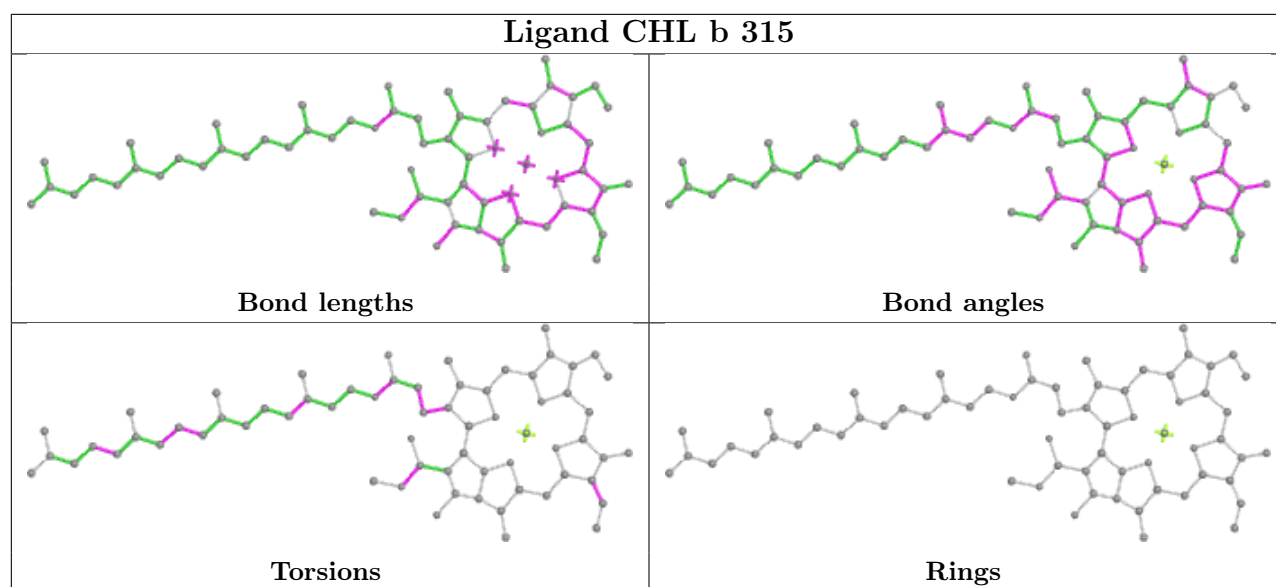


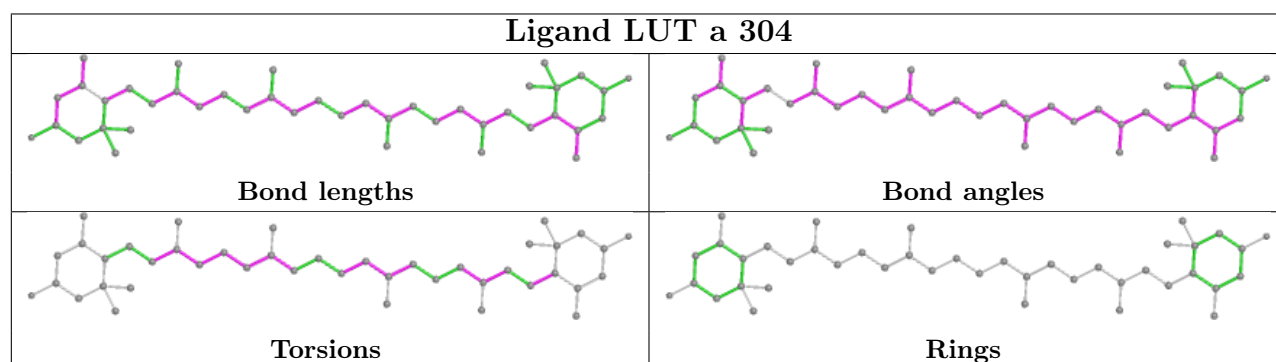
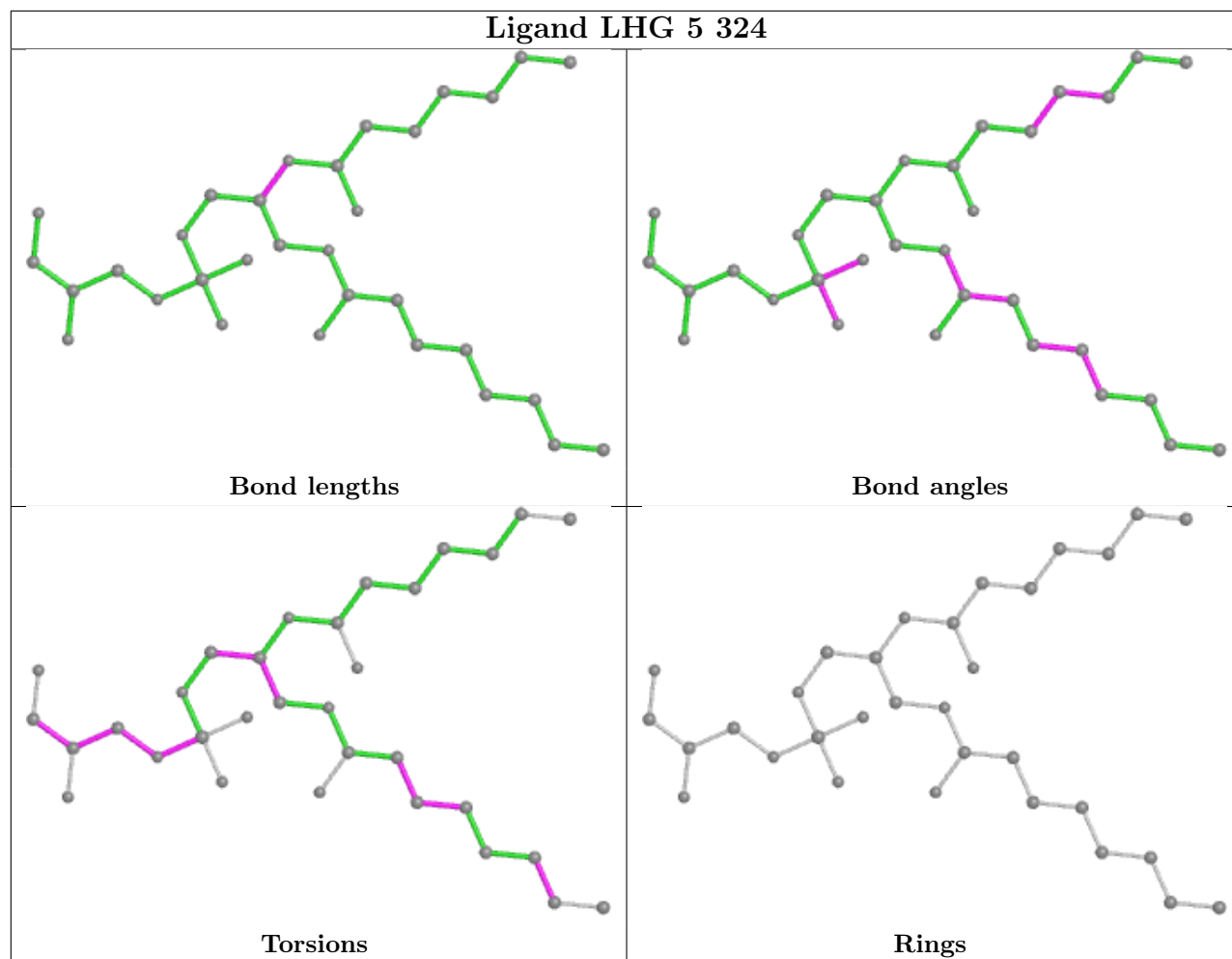
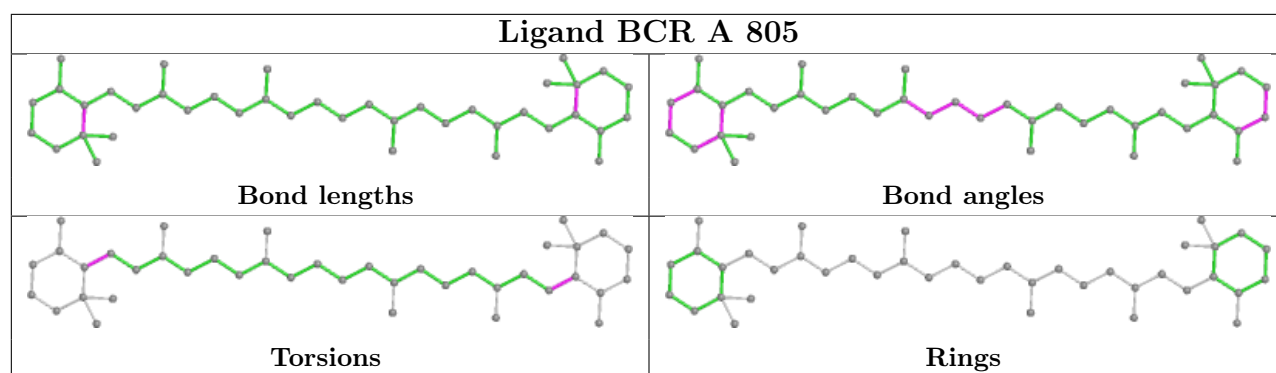
Torsions

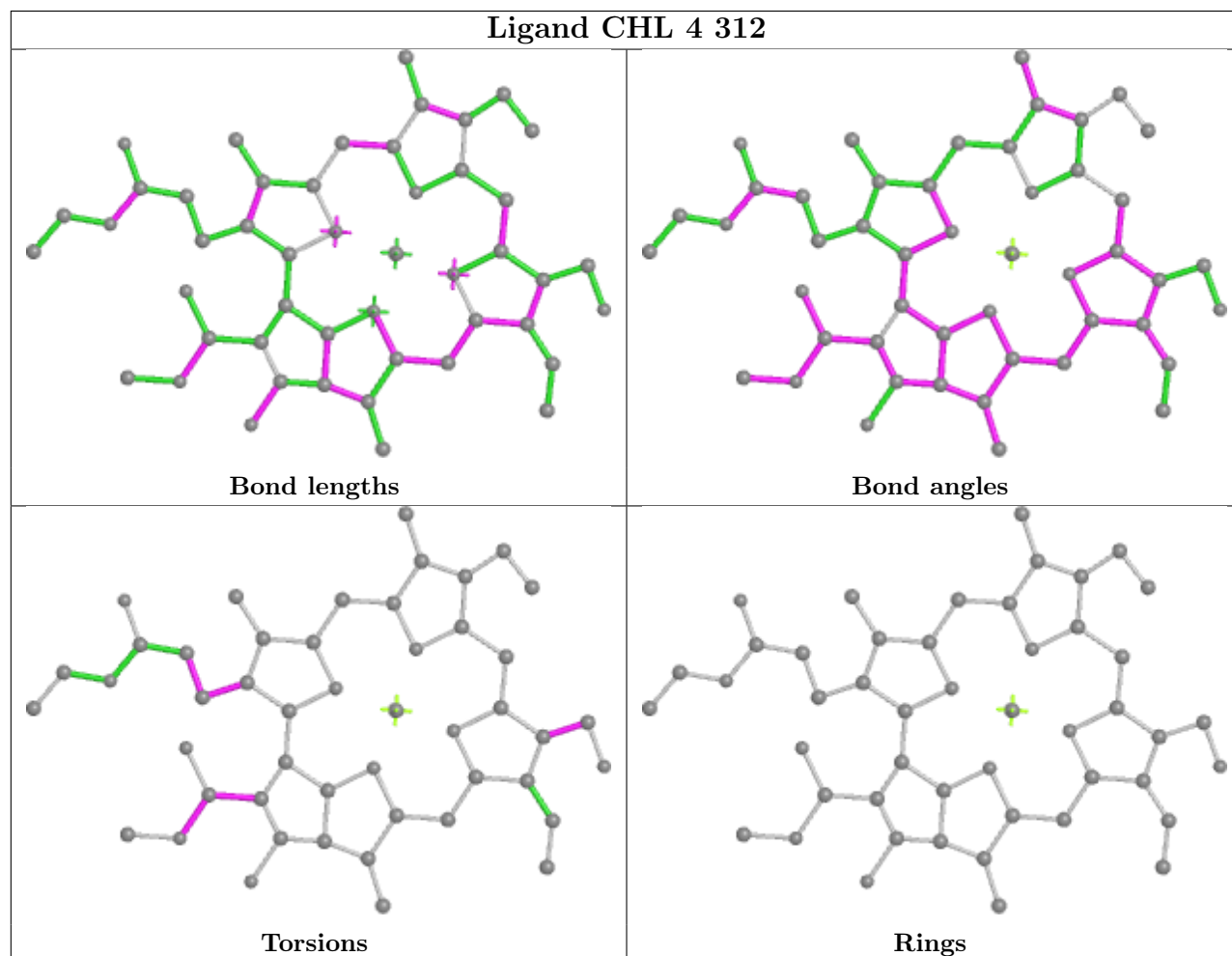
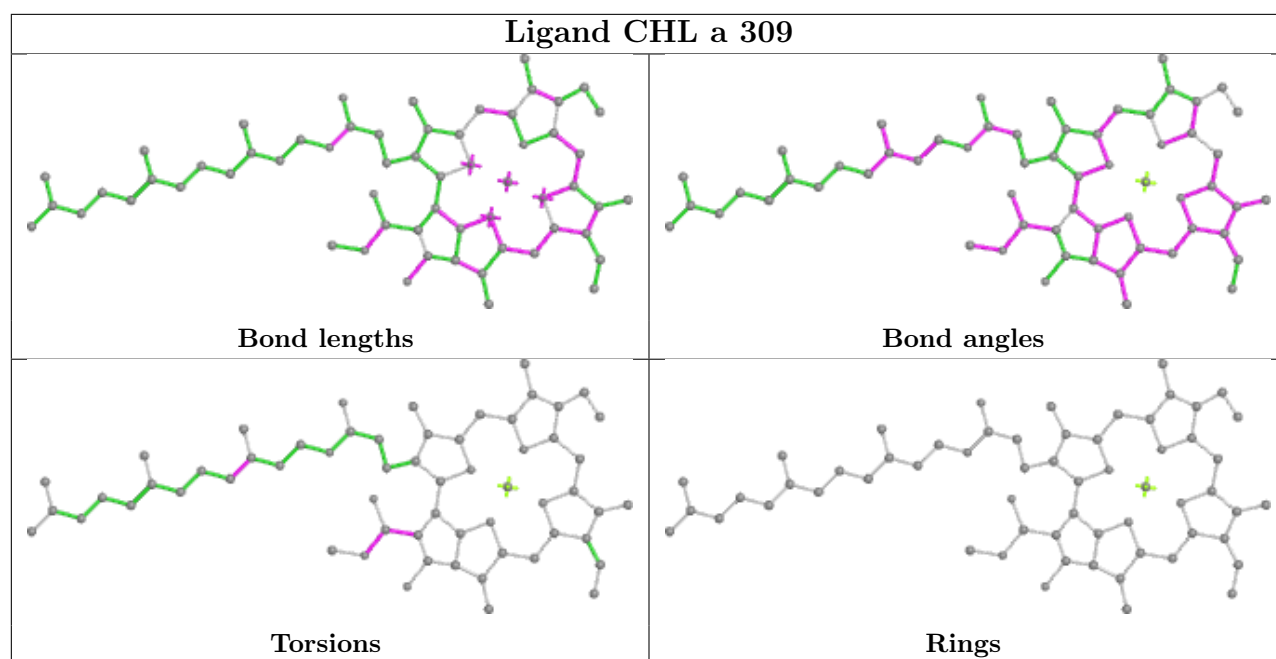


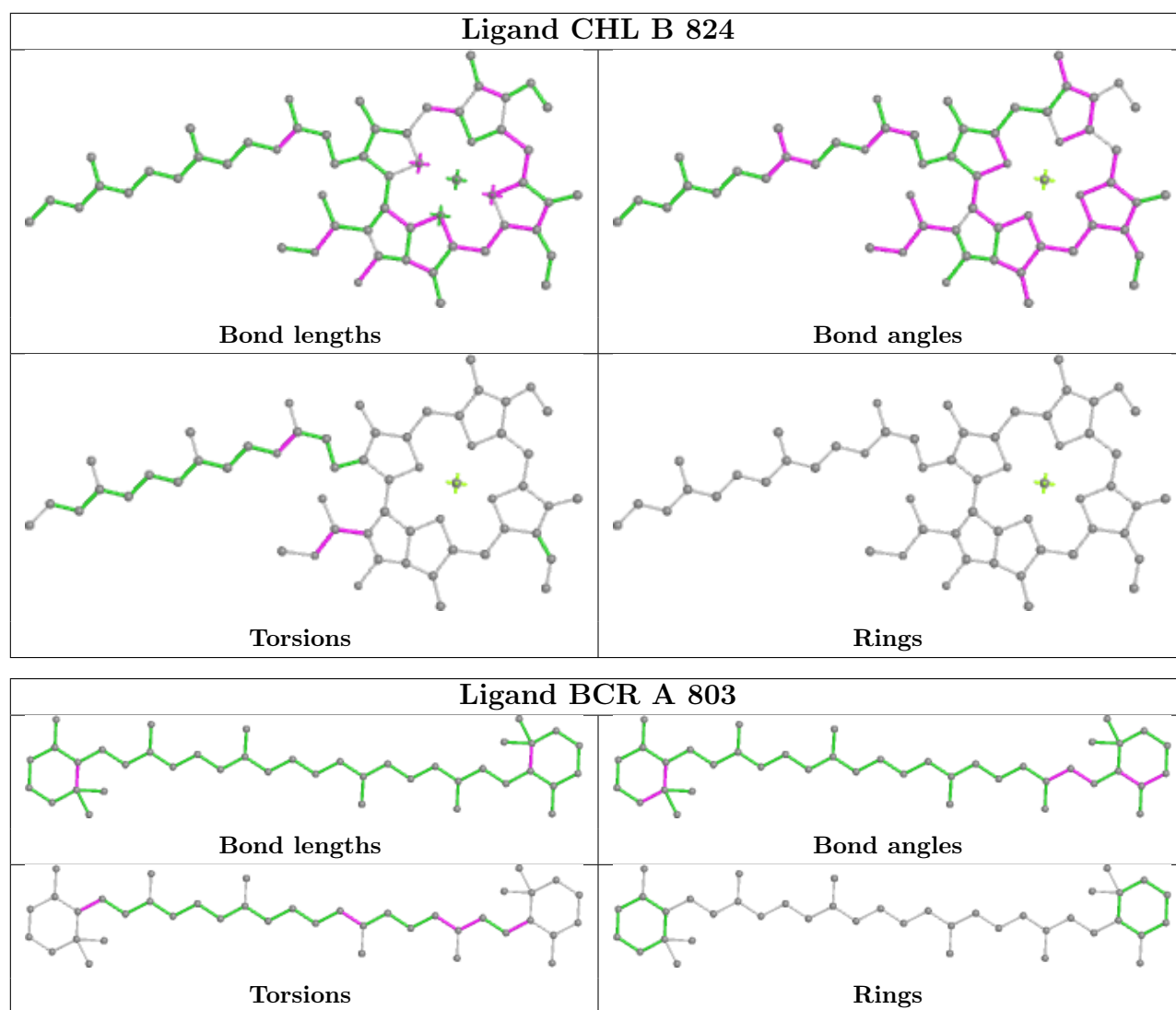
Rings



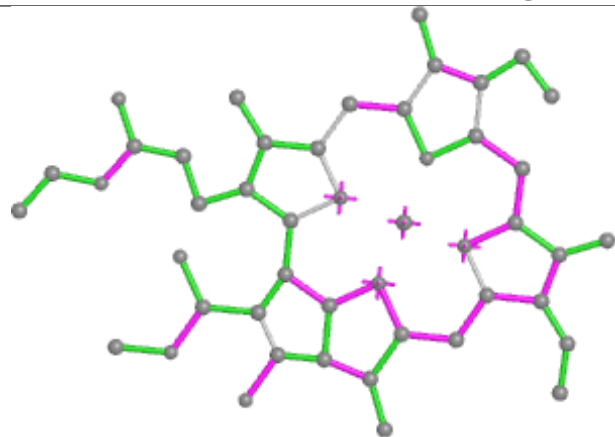




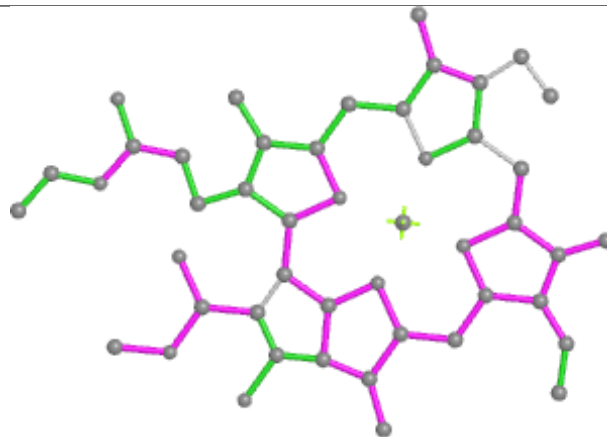




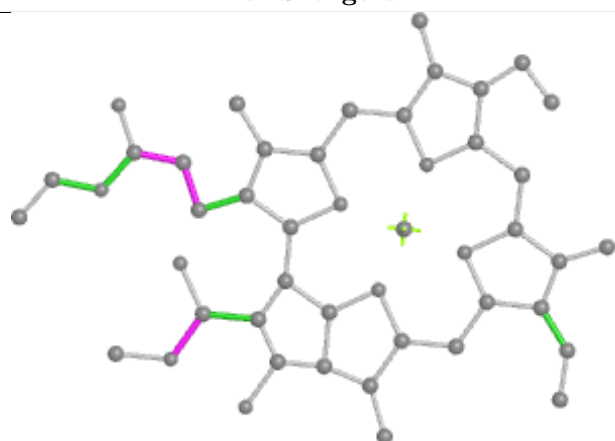
Ligand CHL 4 311



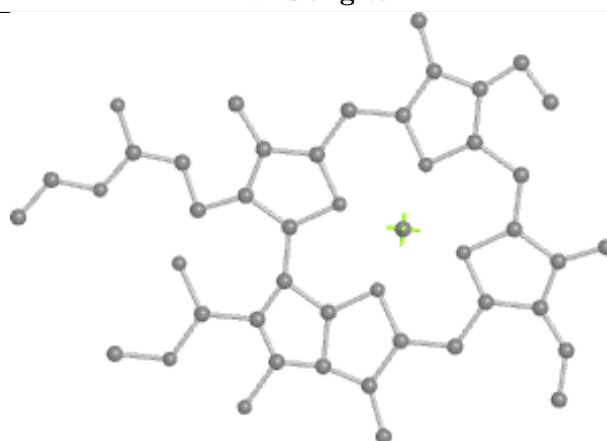
Bond lengths



Bond angles

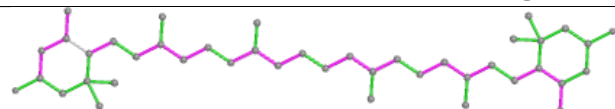


Torsions

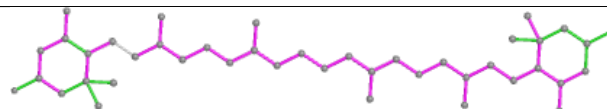


Rings

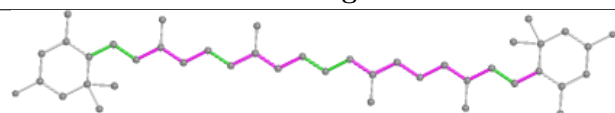
Ligand LUT F 303



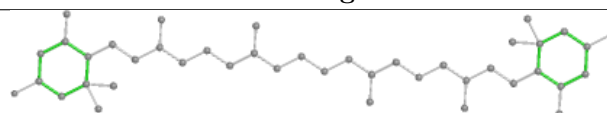
Bond lengths



Bond angles

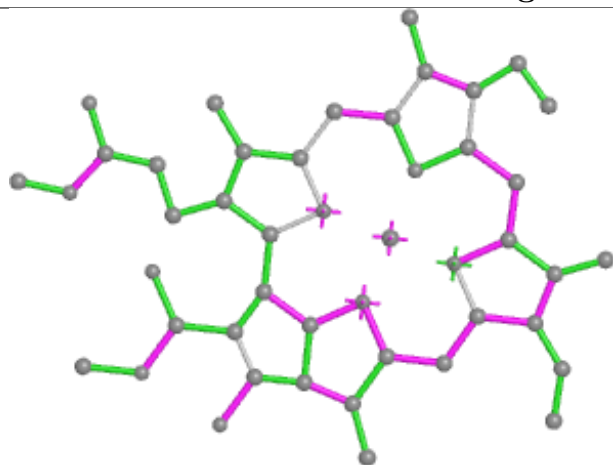


Torsions

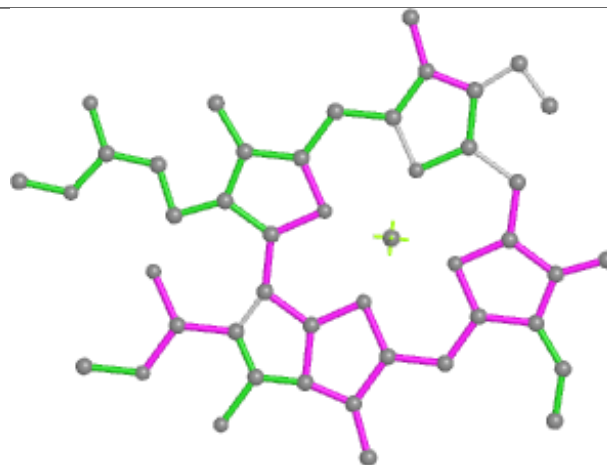


Rings

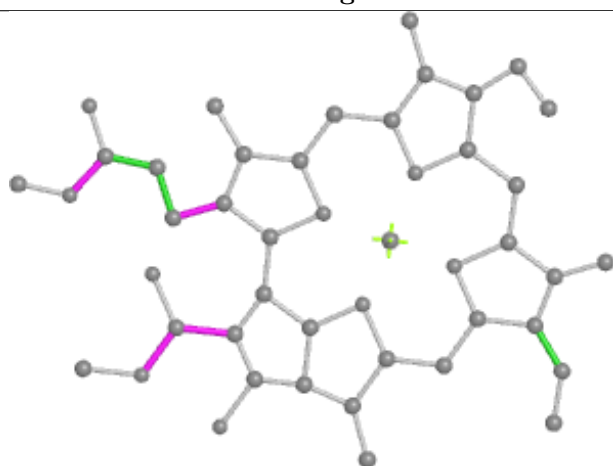
Ligand CHL 8 318



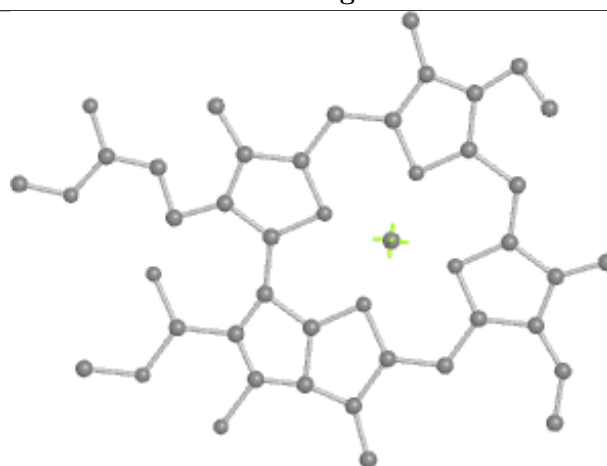
Bond lengths



Bond angles

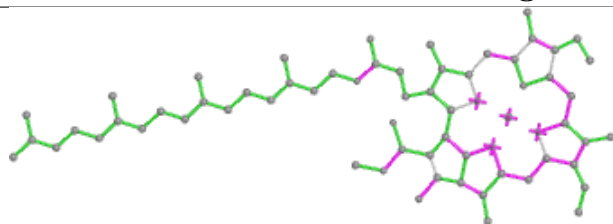


Torsions

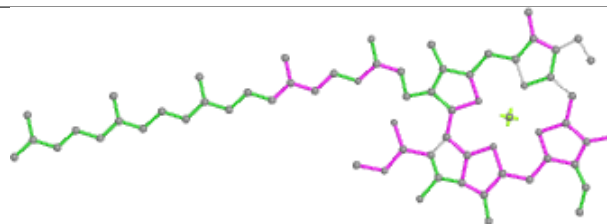


Rings

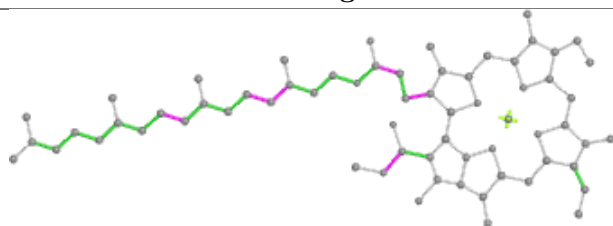
Ligand CHL a 317



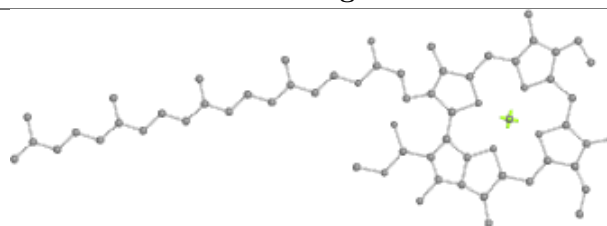
Bond lengths



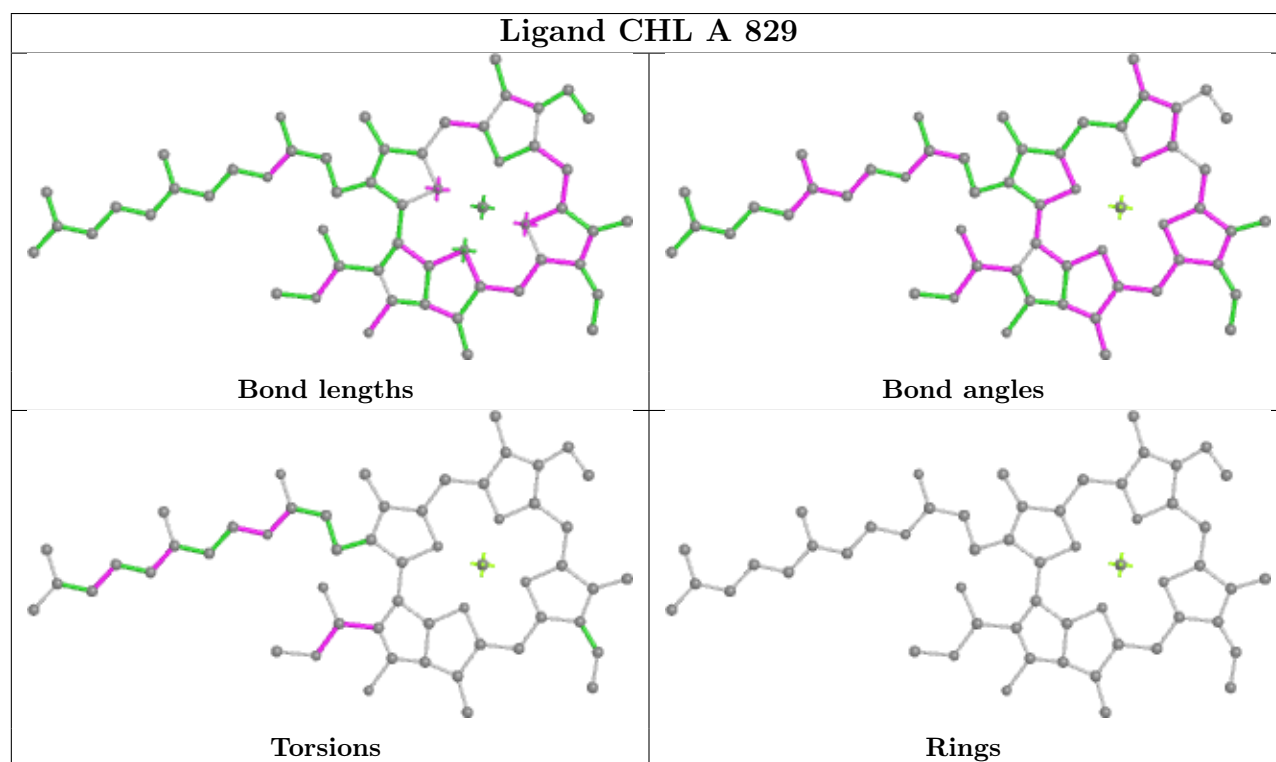
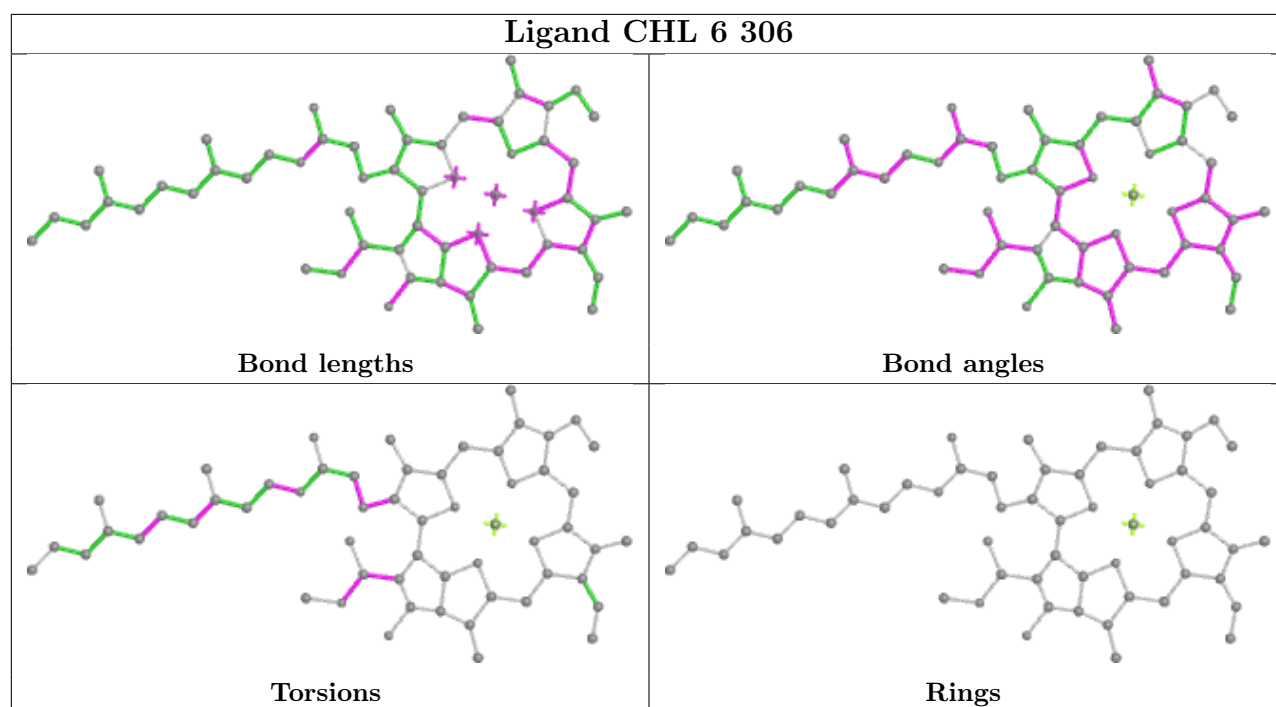
Bond angles

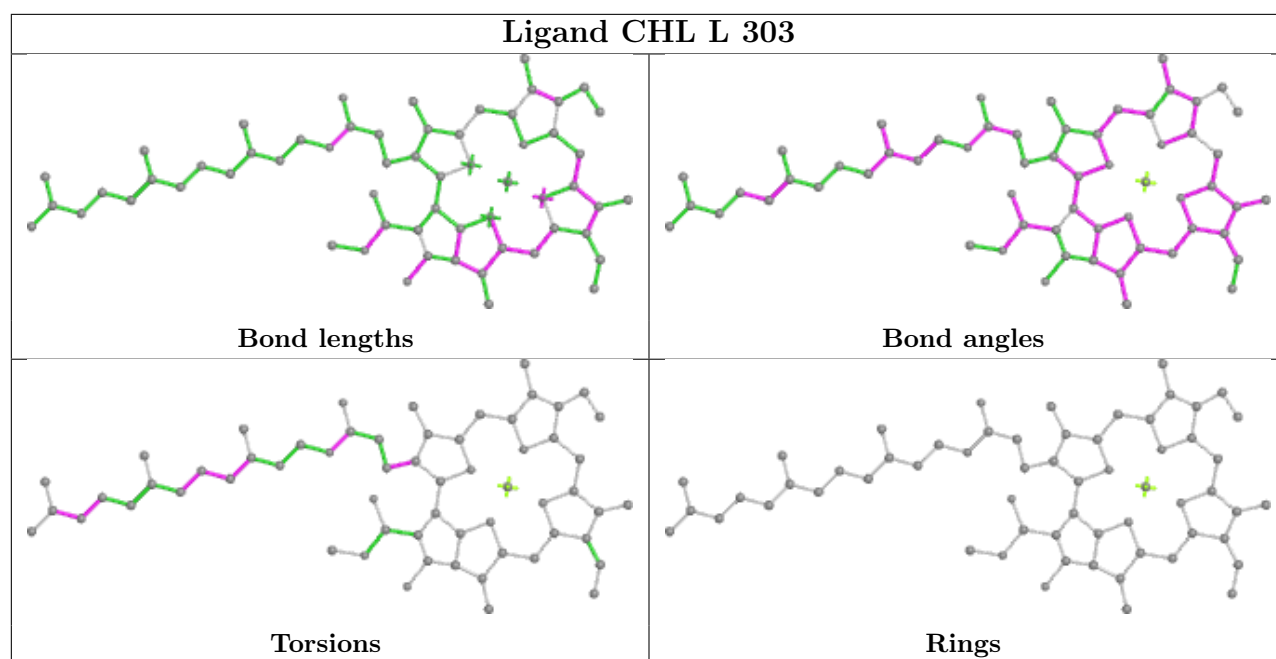


Torsions

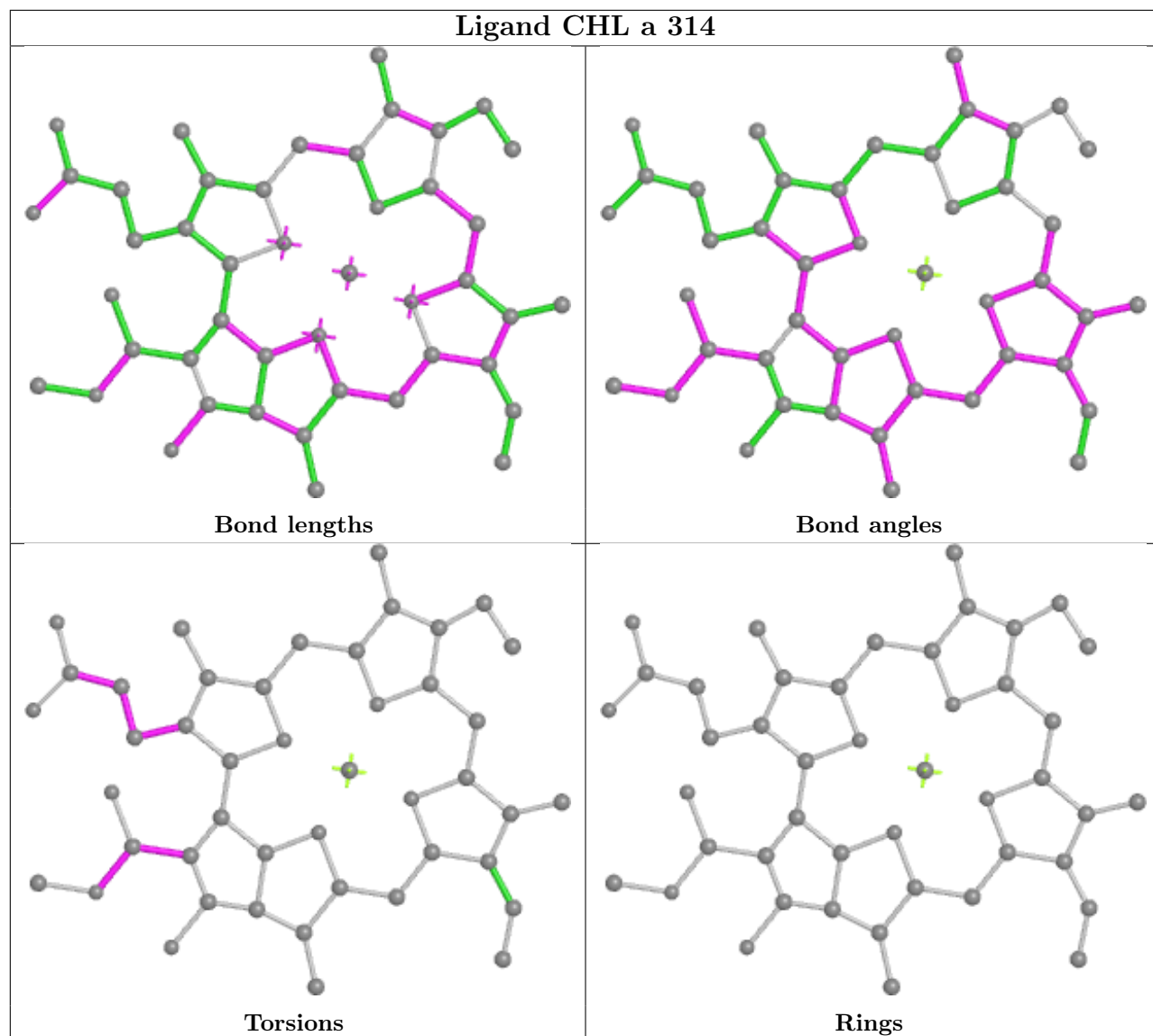


Rings

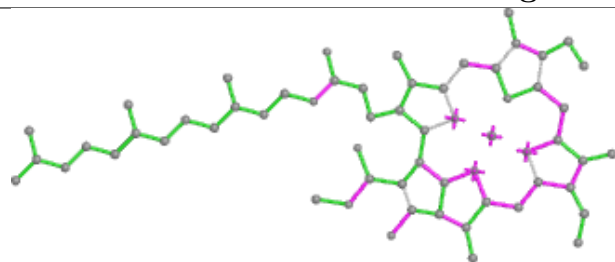




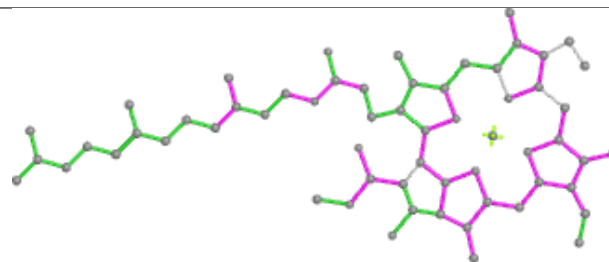
Ligand CHL a 314



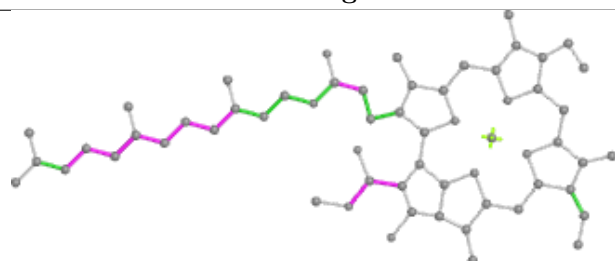
Ligand CHL 5 309



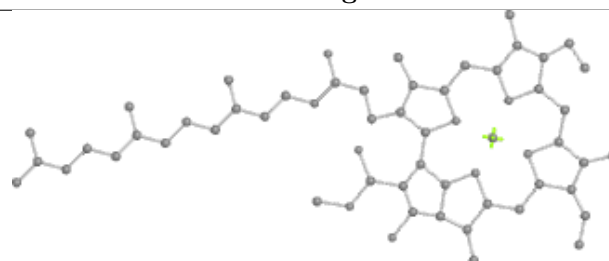
Bond lengths



Bond angles

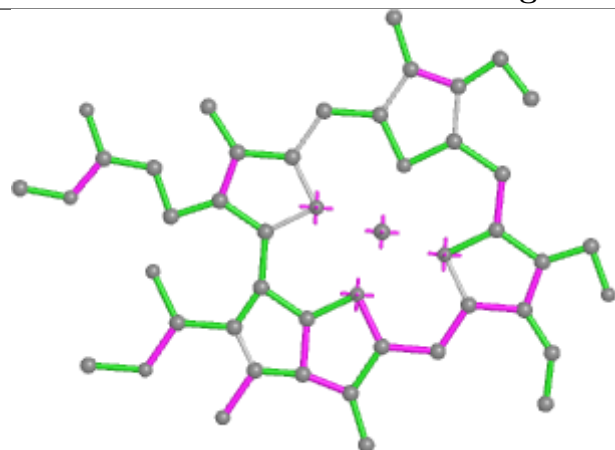


Torsions

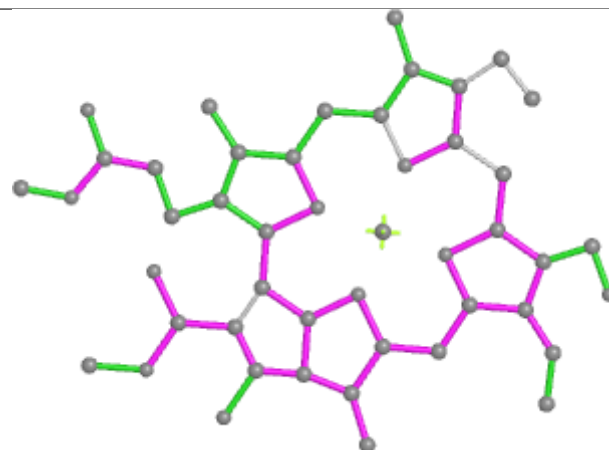


Rings

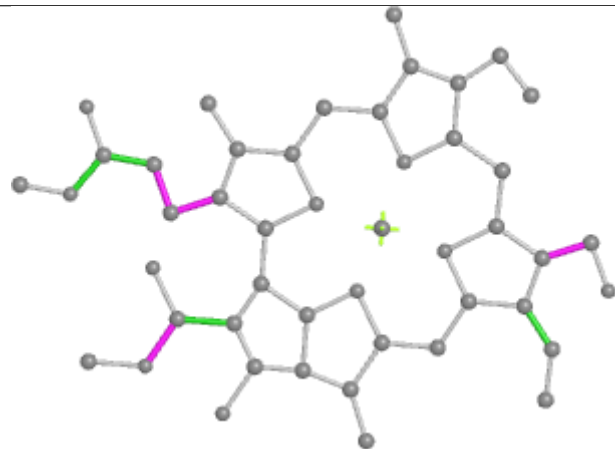
Ligand CHL 6 317



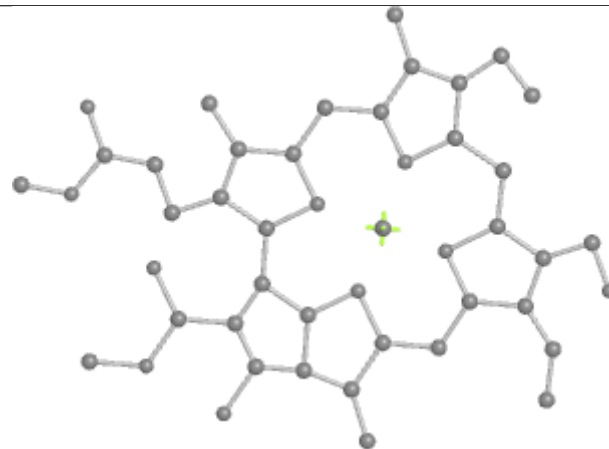
Bond lengths



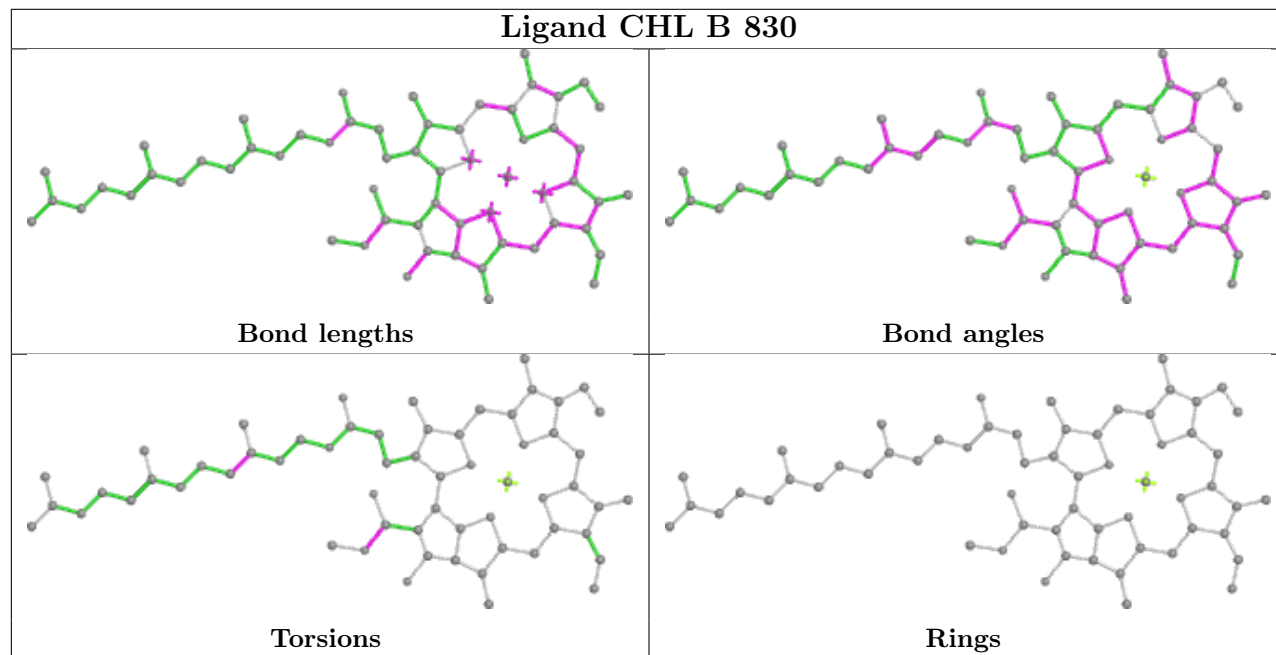
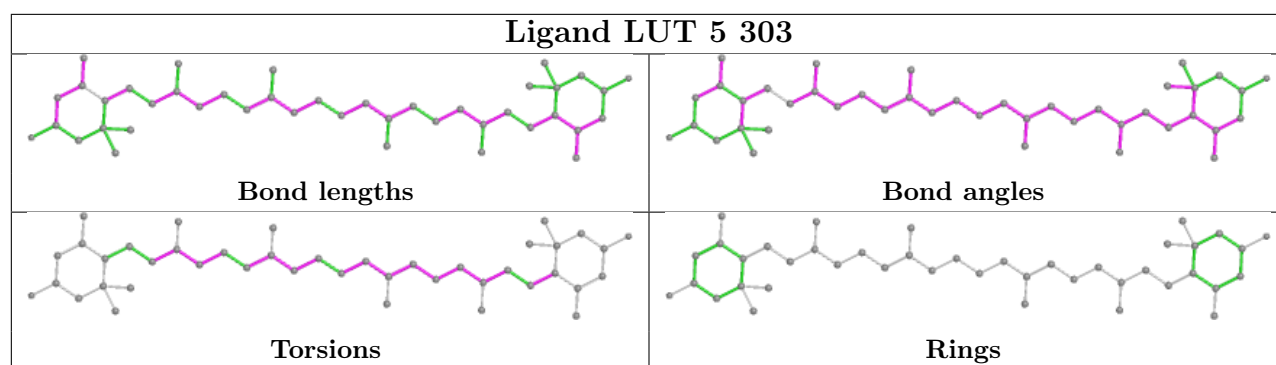
Bond angles

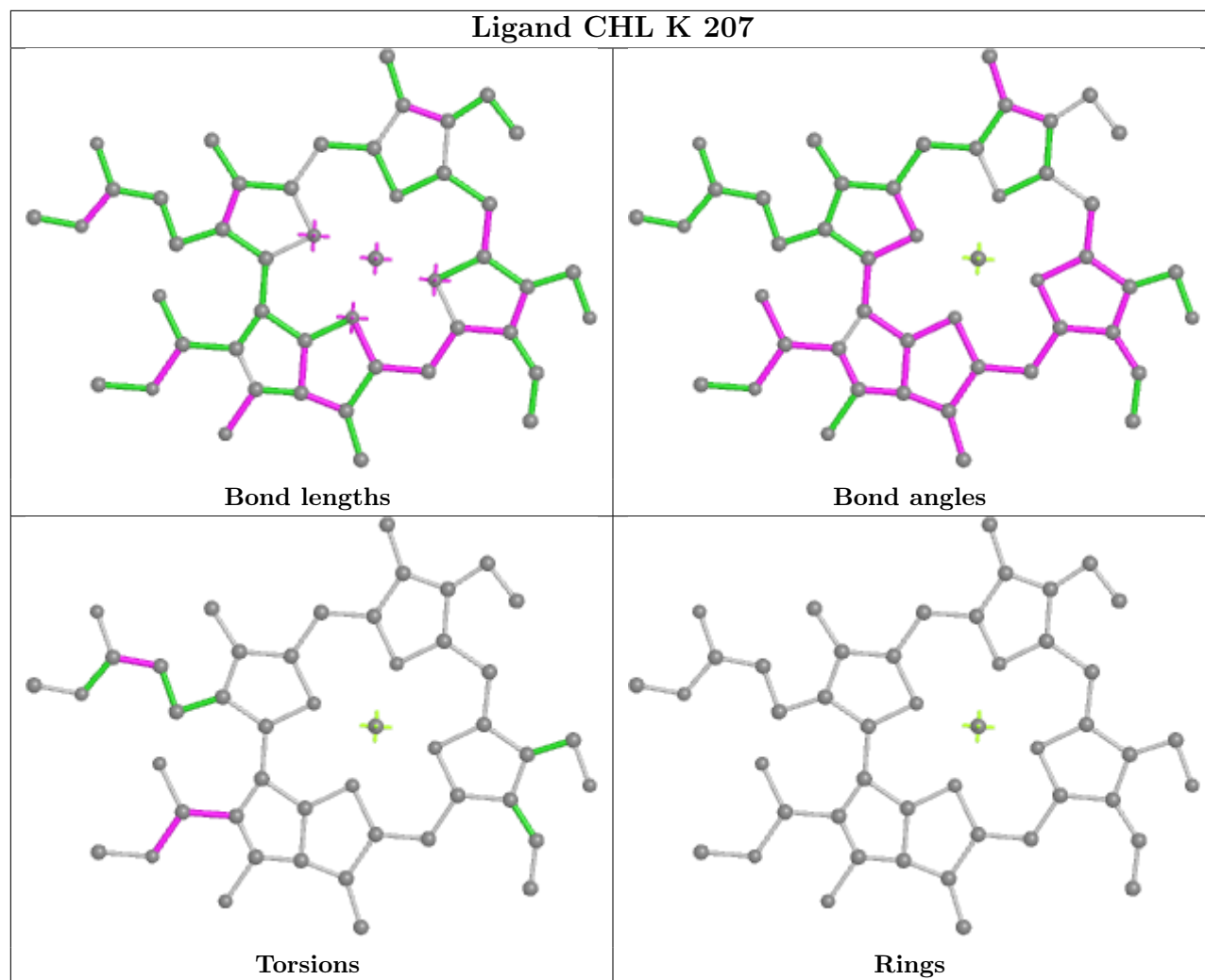


Torsions

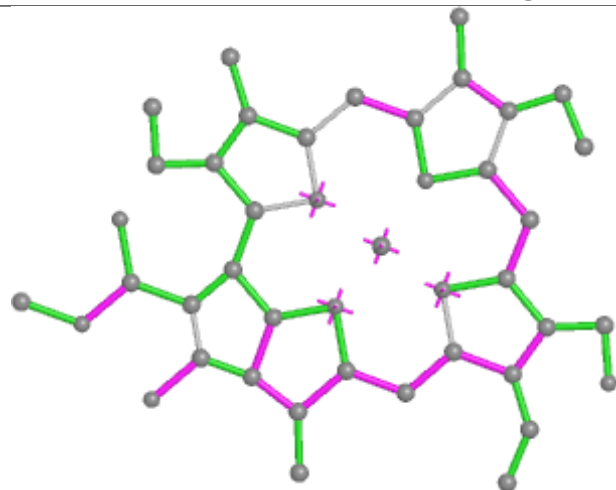


Rings

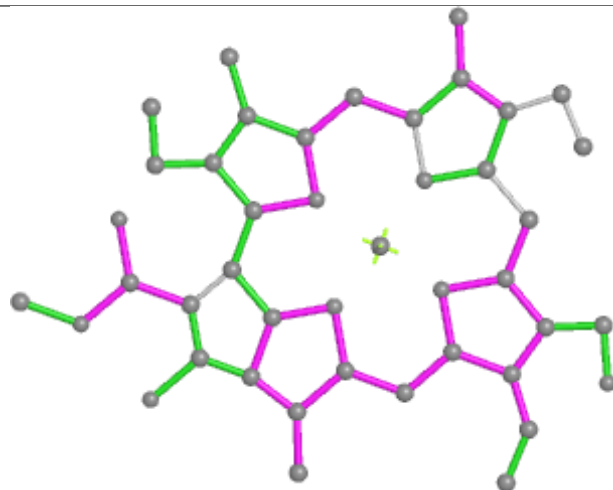




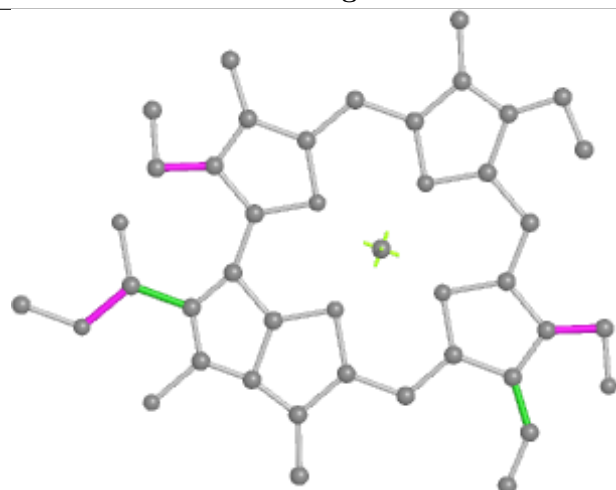
Ligand CHL 6 319



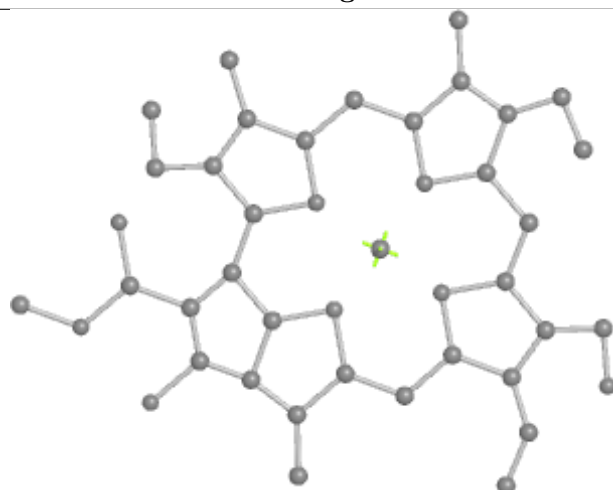
Bond lengths



Bond angles

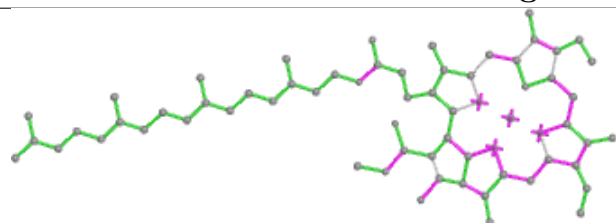


Torsions

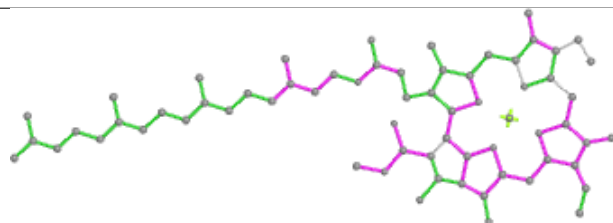


Rings

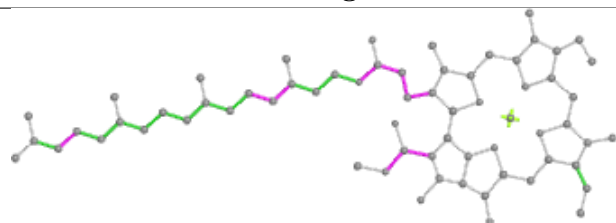
Ligand CHL 8 317



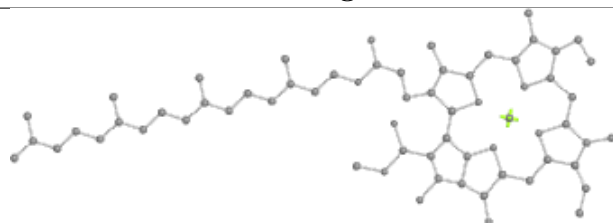
Bond lengths



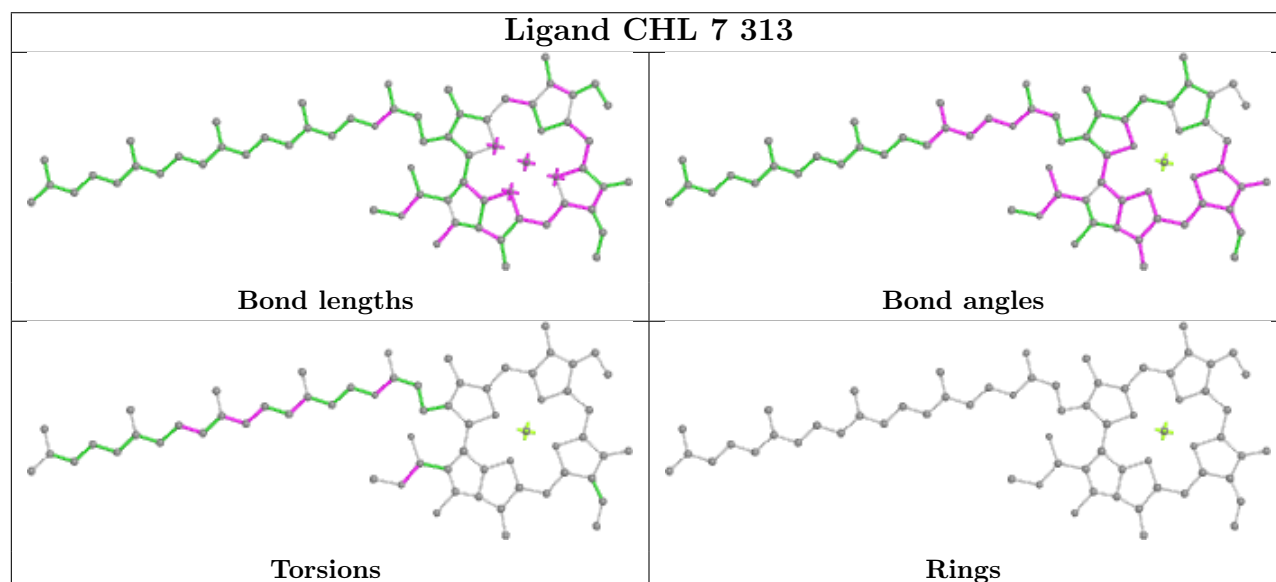
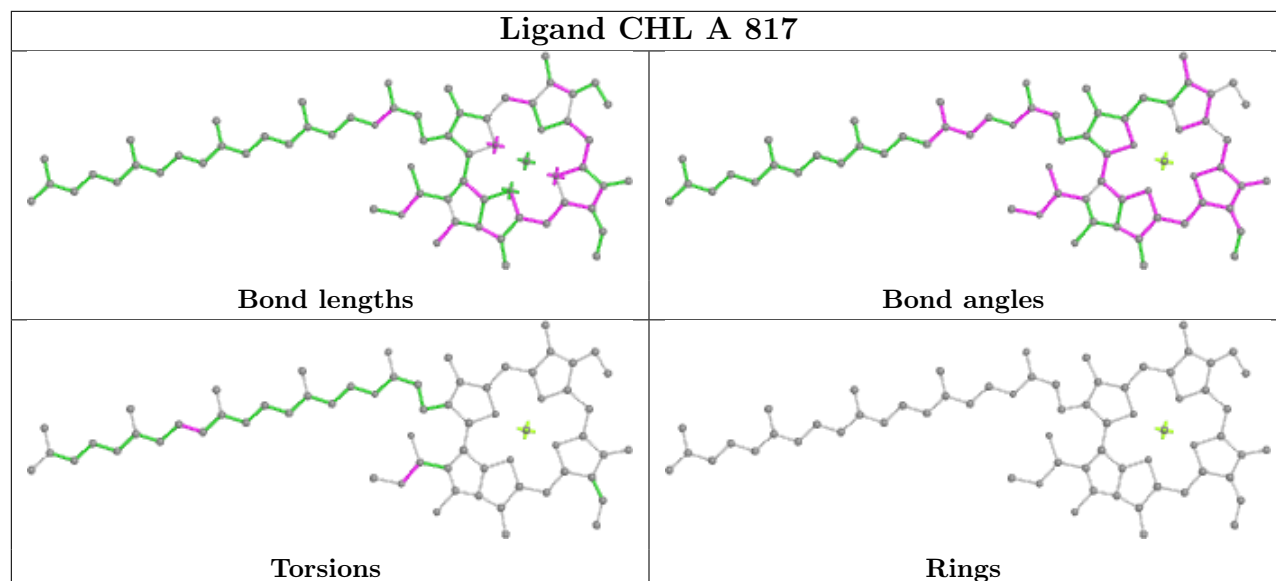
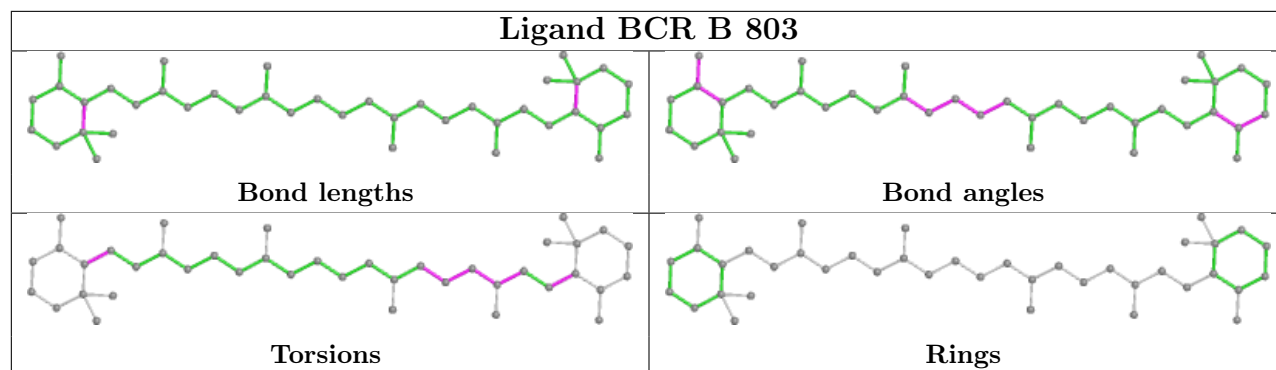
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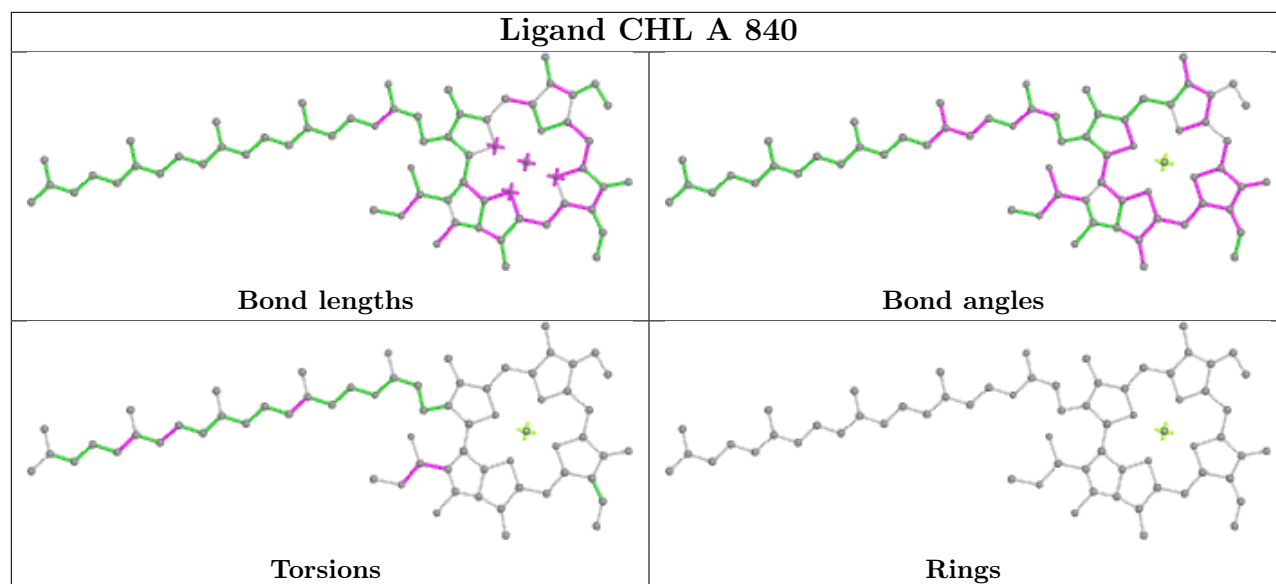
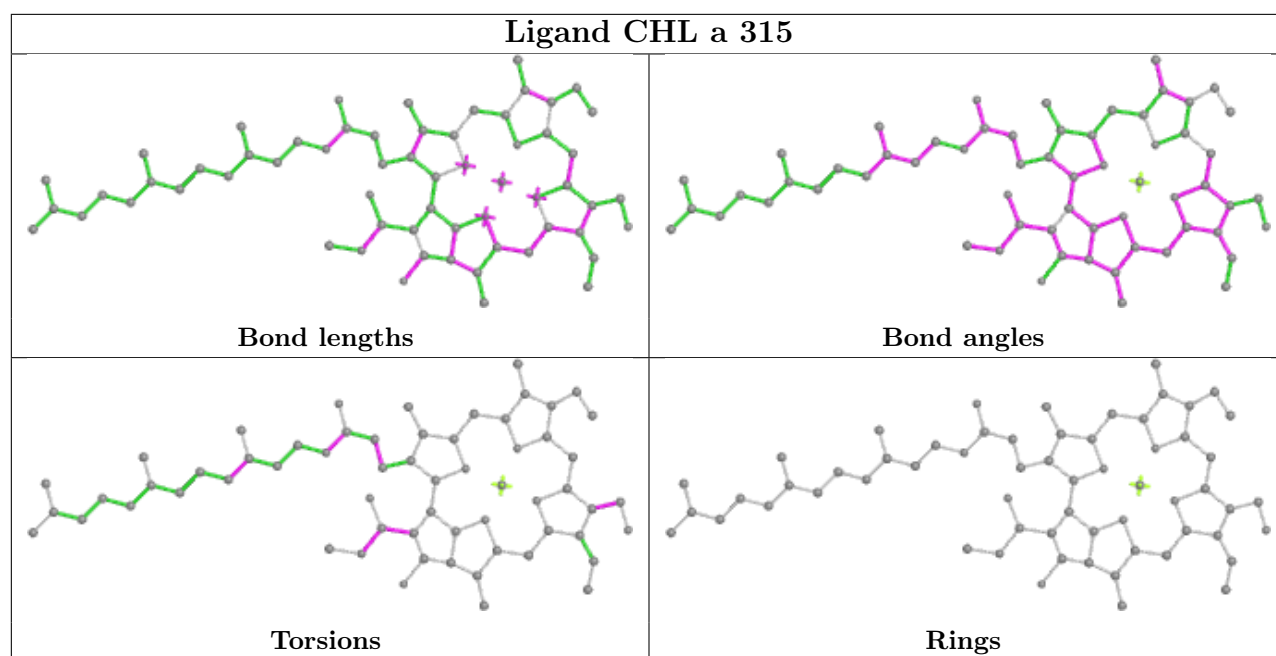


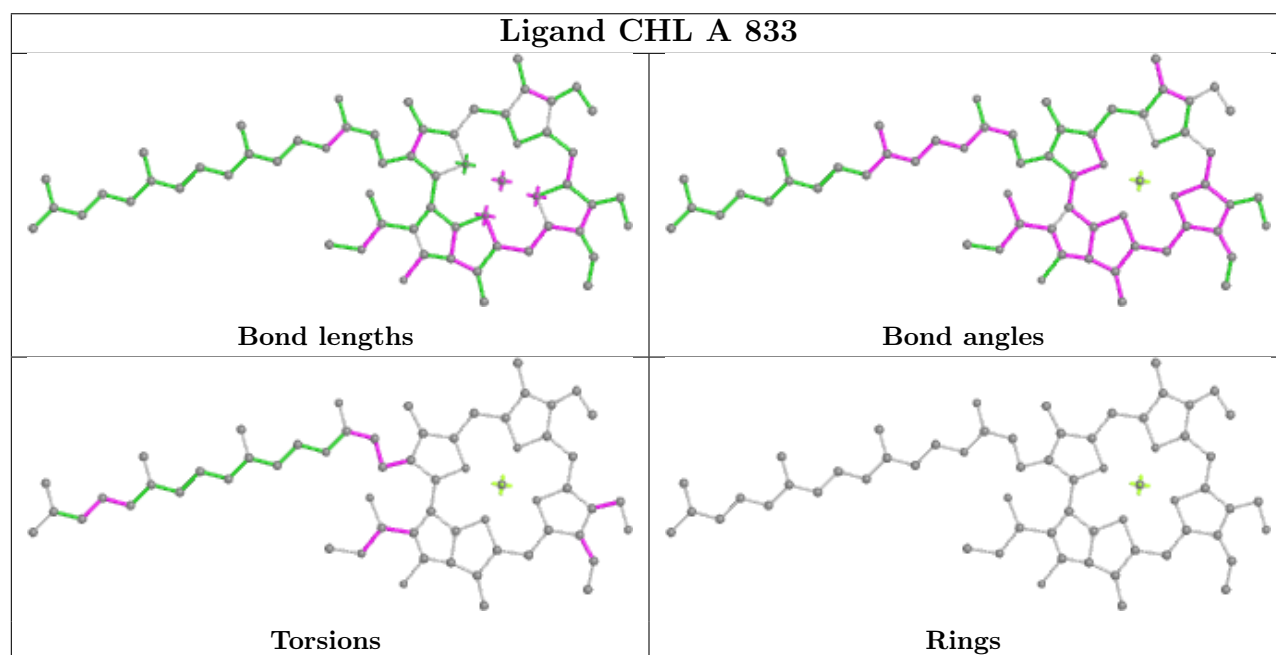
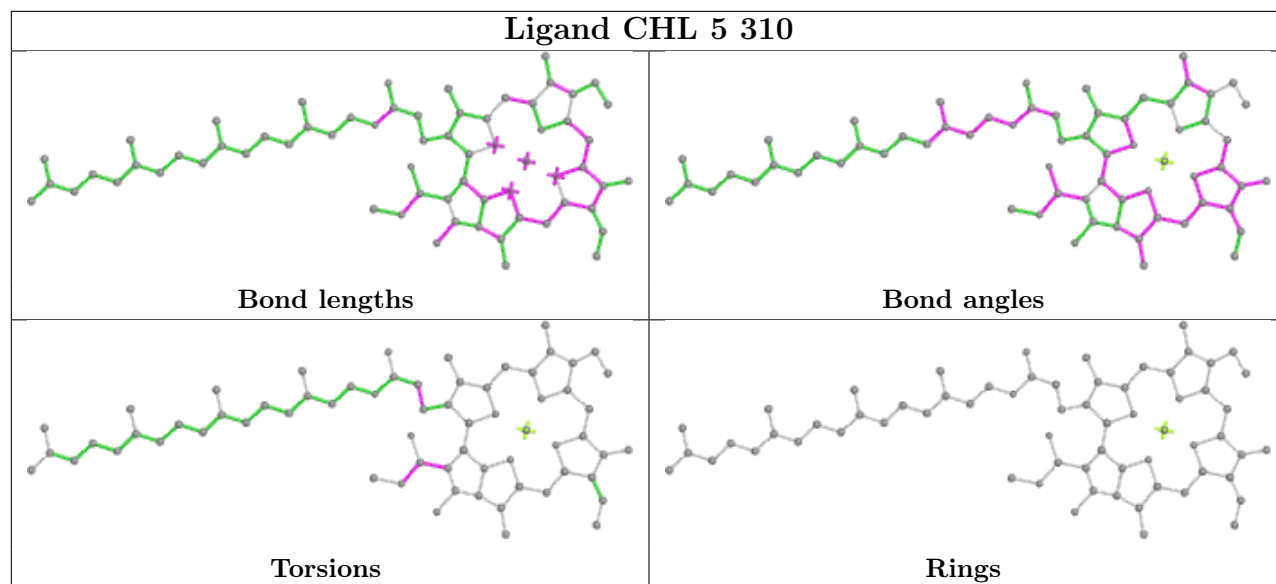
Torsions

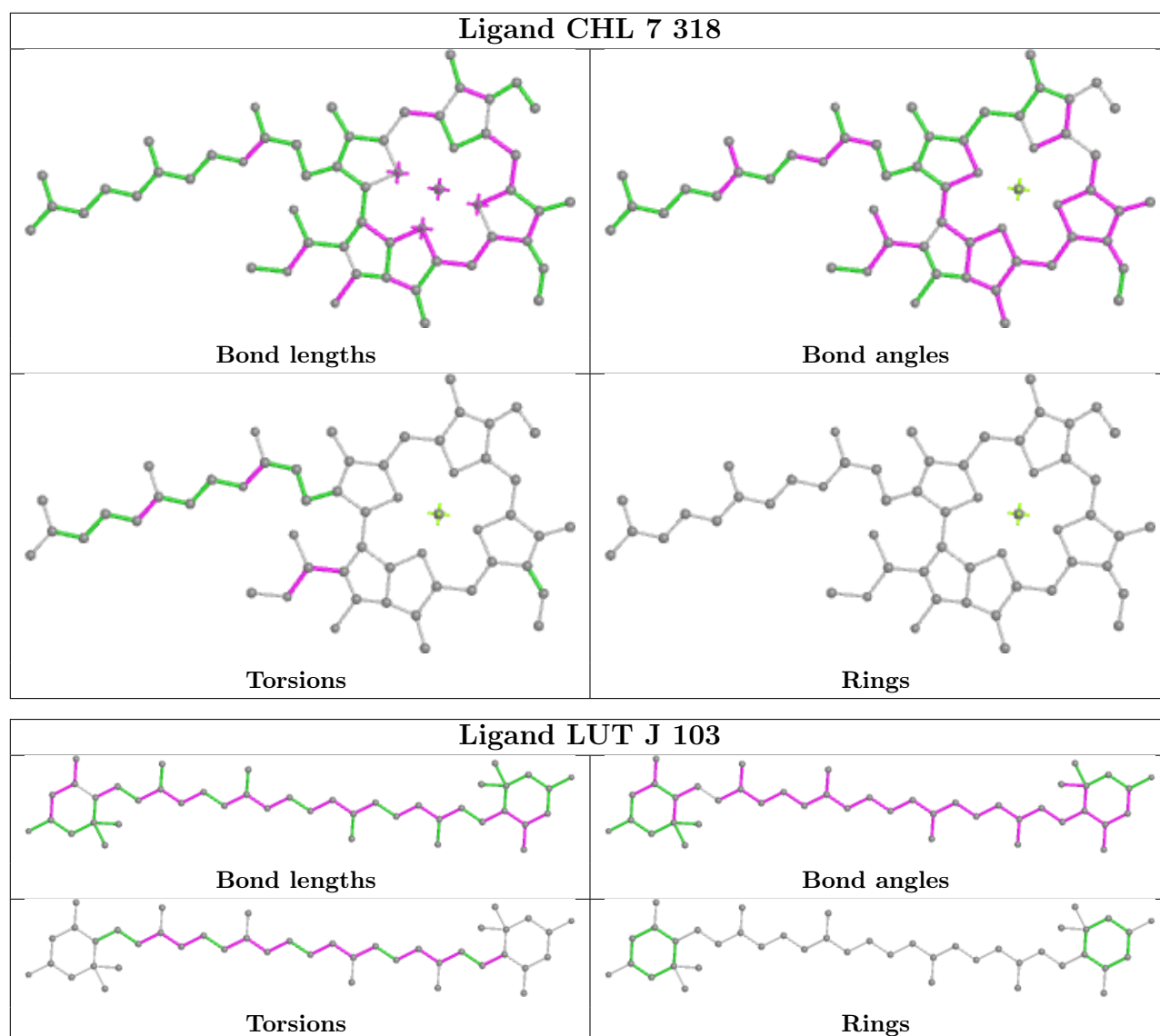


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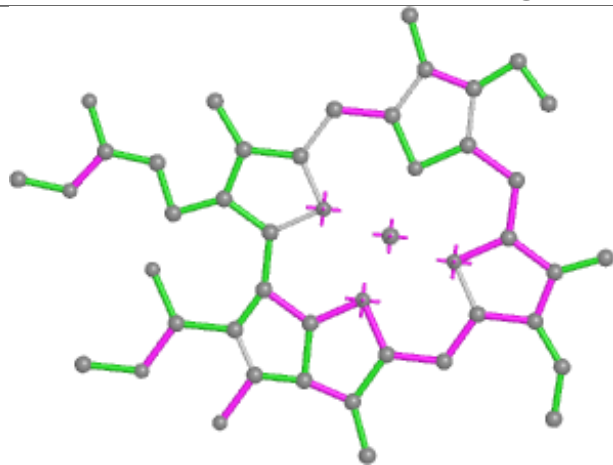




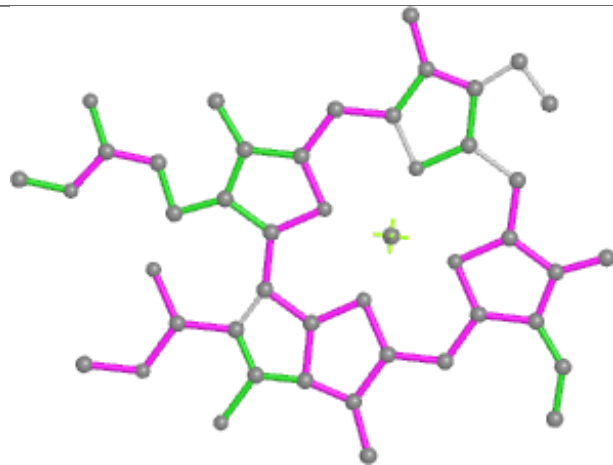




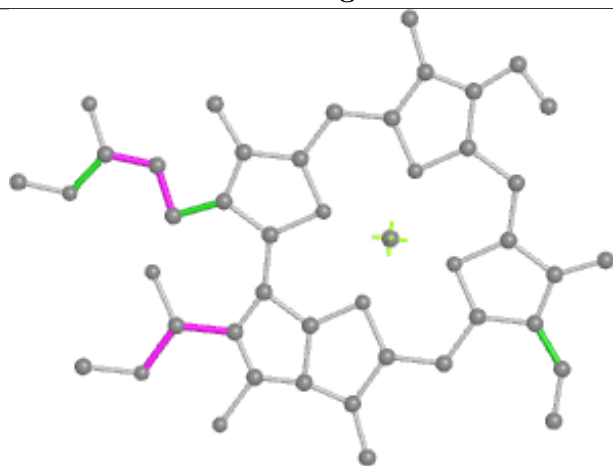
Ligand CHL 4 310



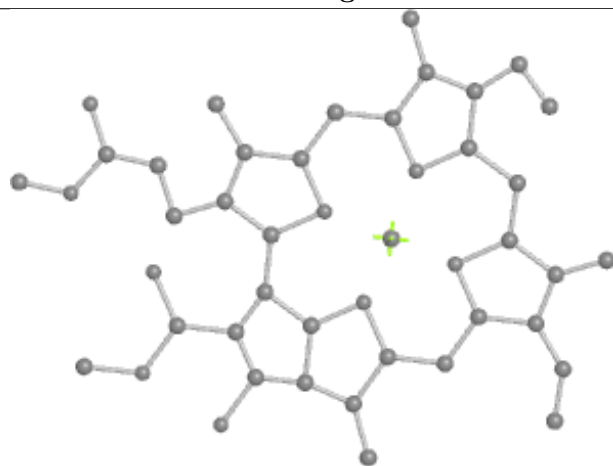
Bond lengths



Bond angles

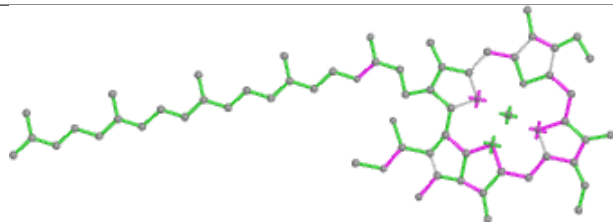


Torsions

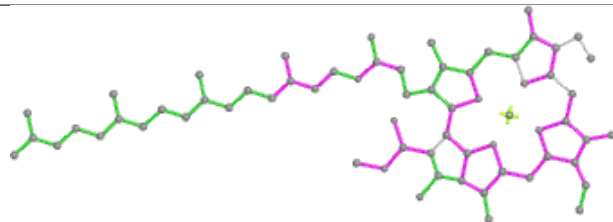


Rings

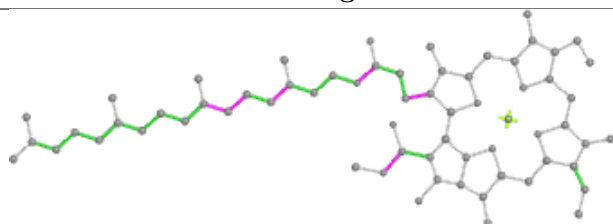
Ligand CHL A 850



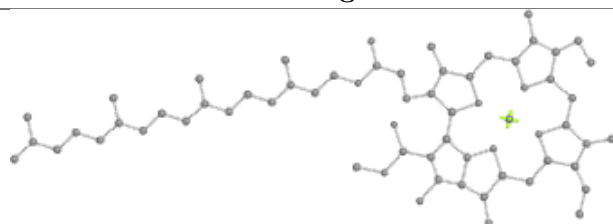
Bond lengths



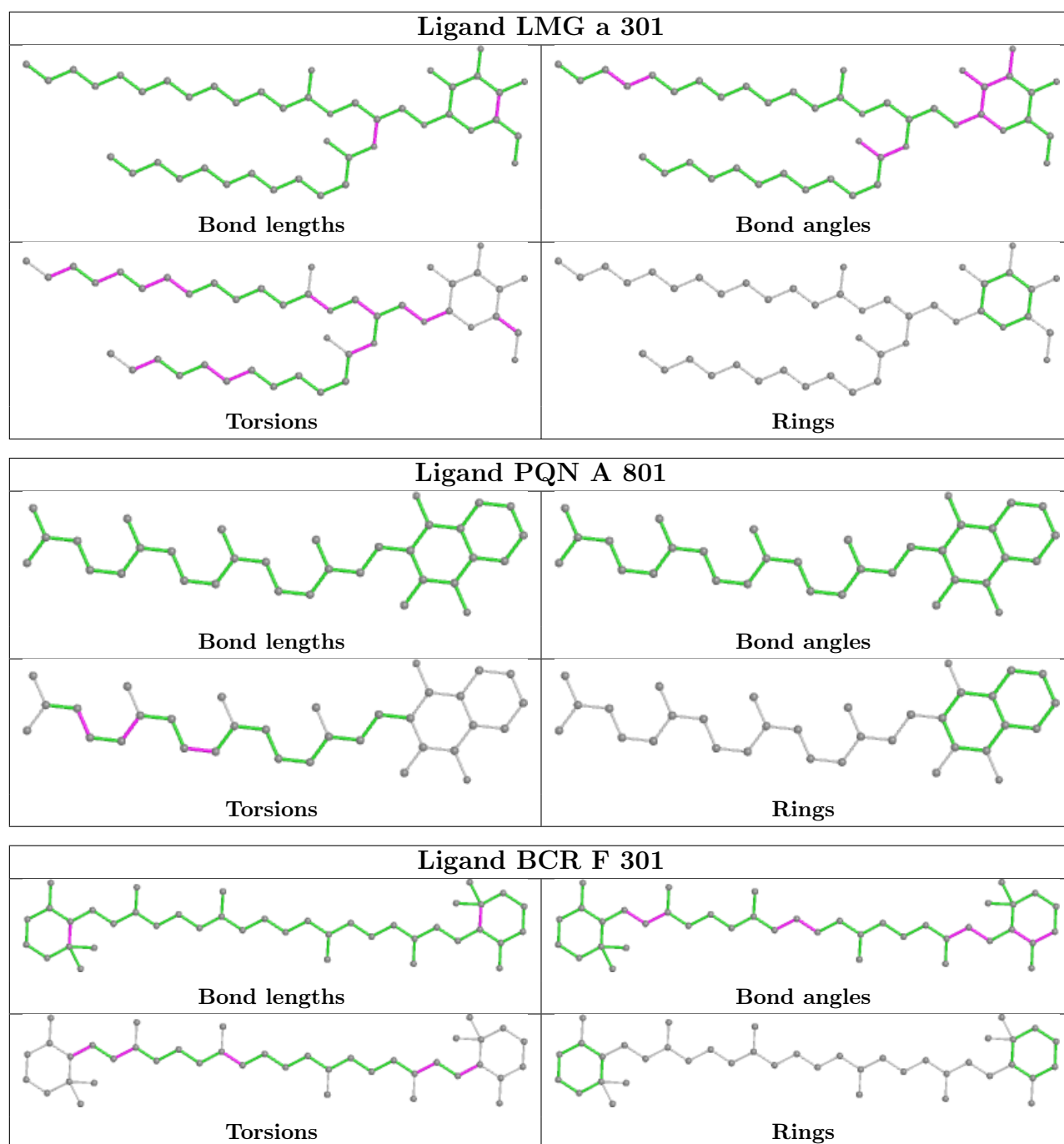
Bond angles



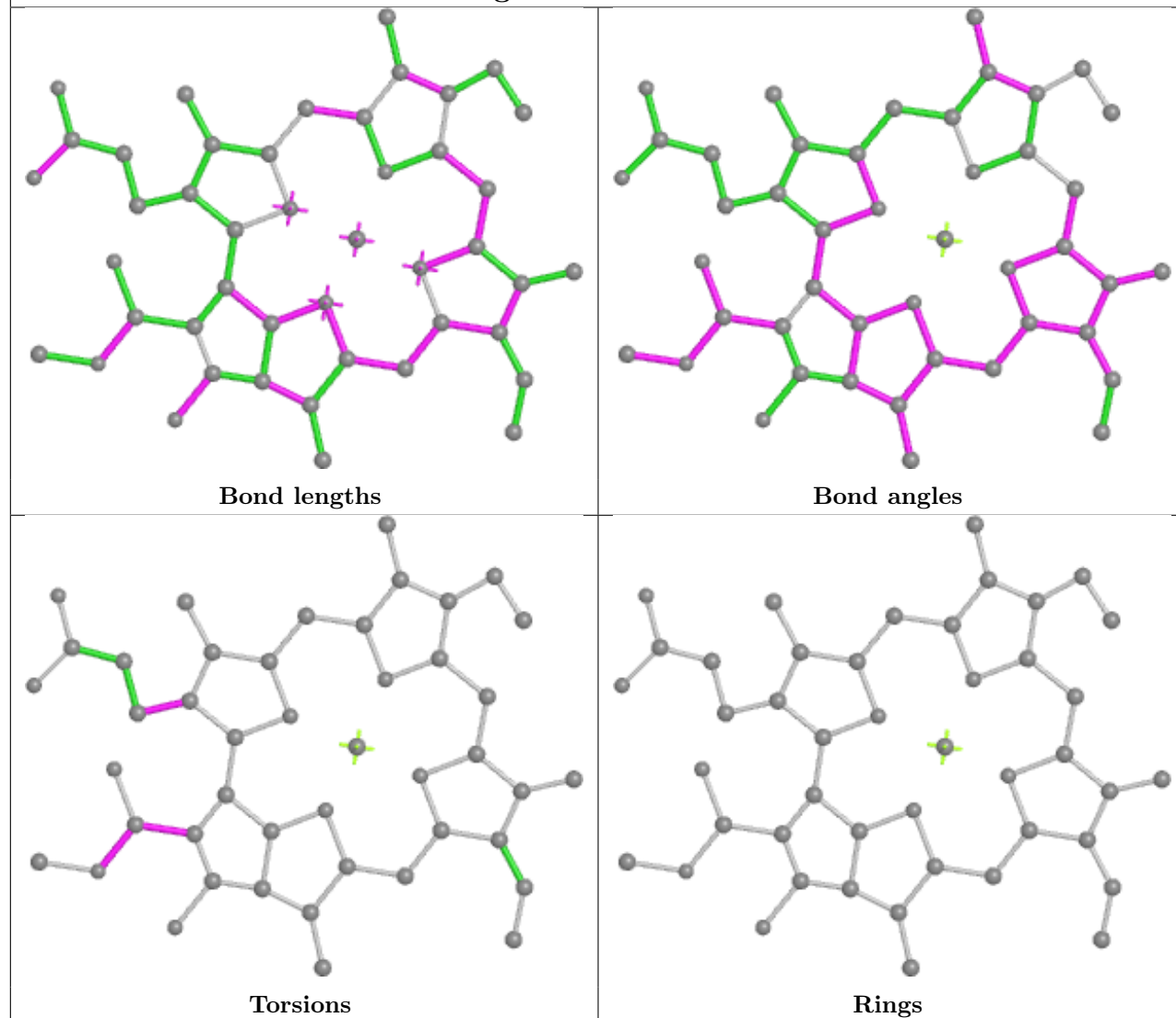
Torsions



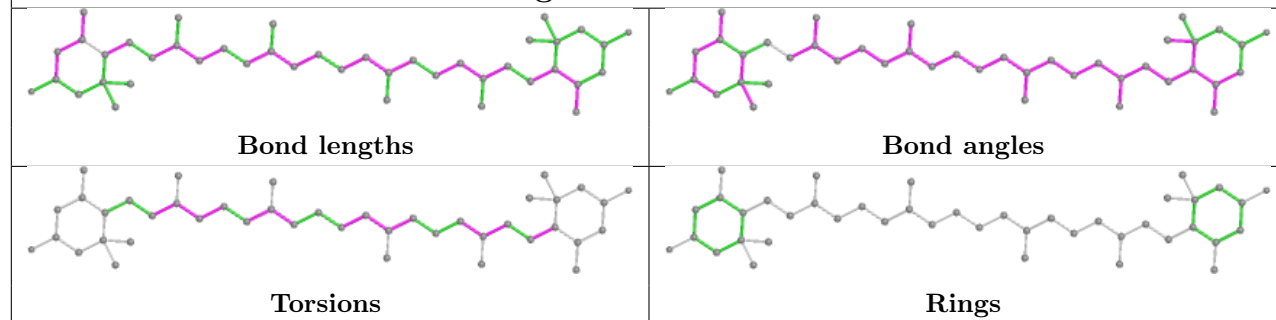
Rings

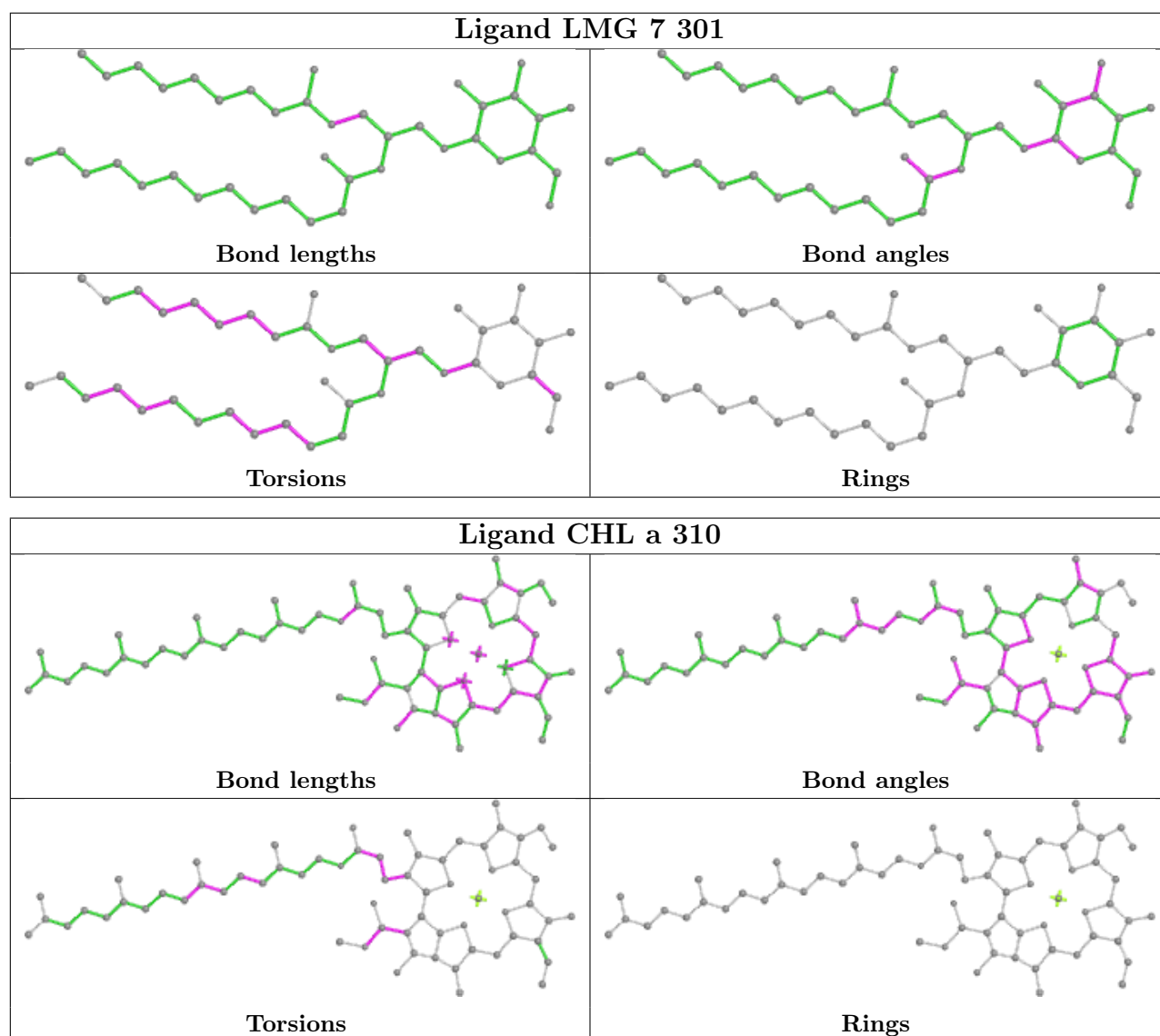


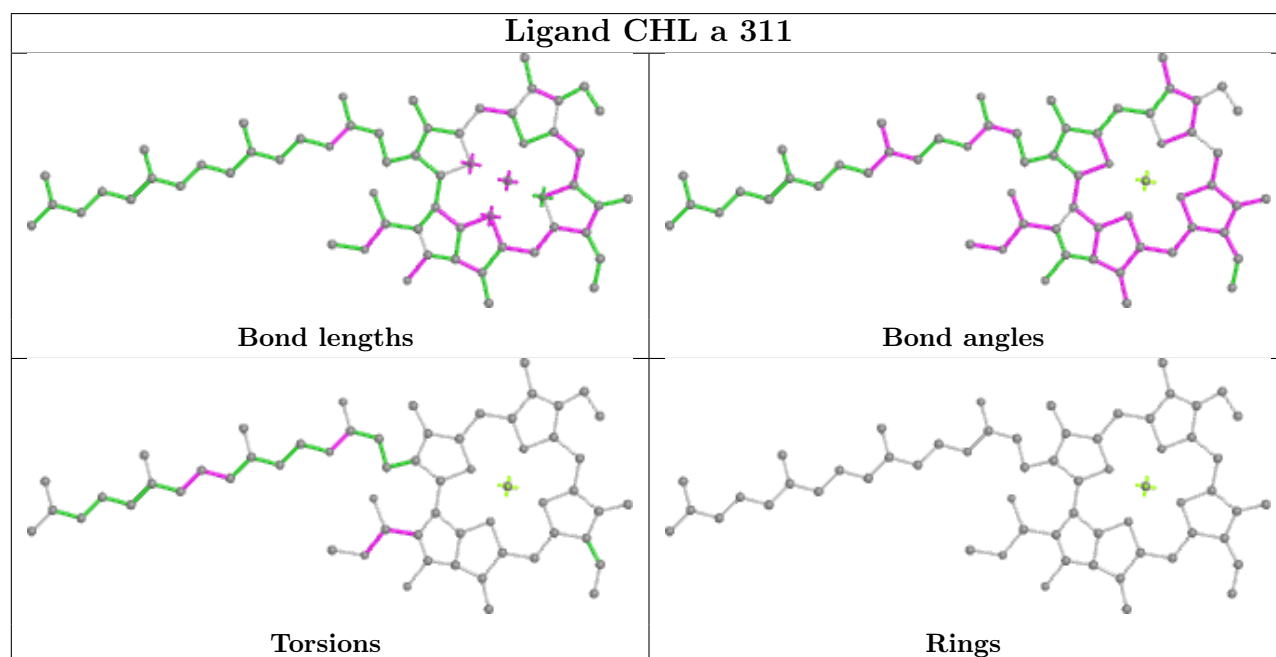
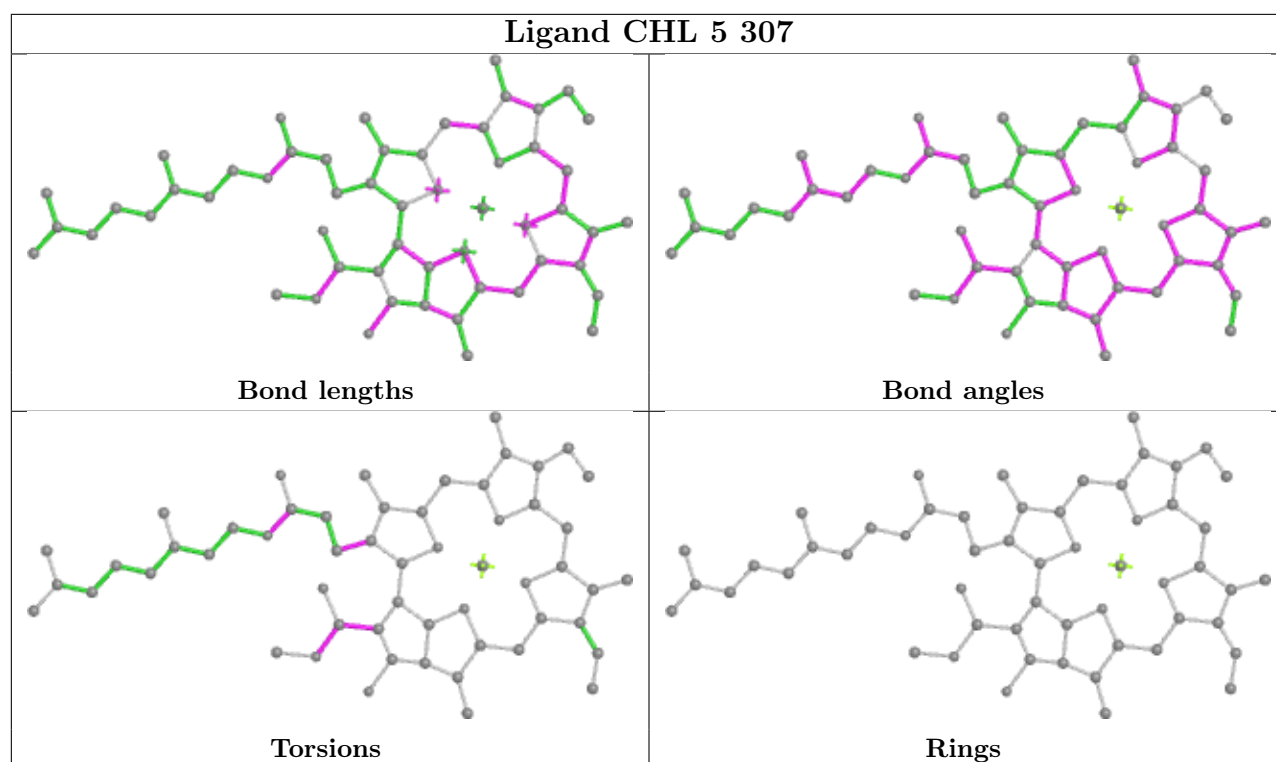
Ligand CHL a 308



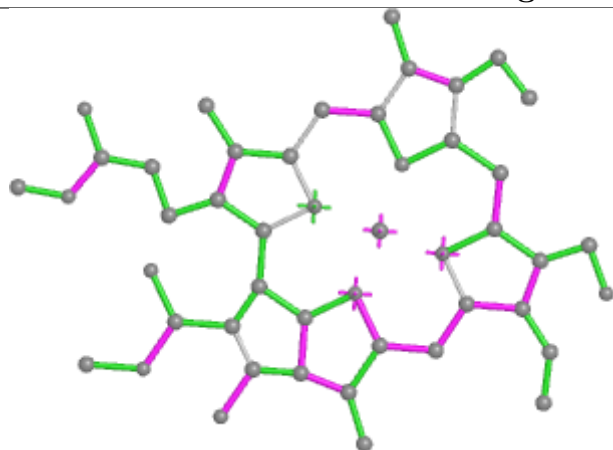
Ligand LUT b 301



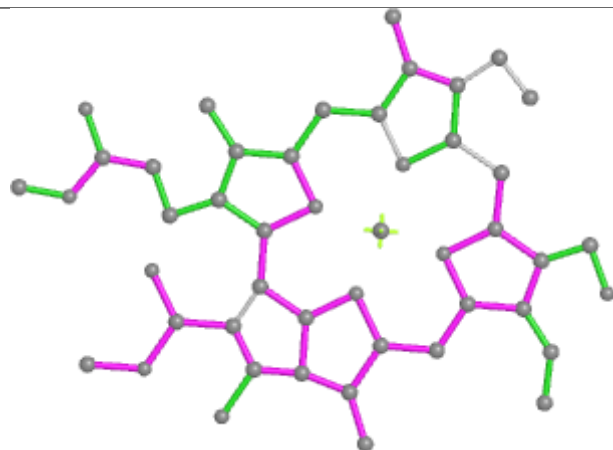




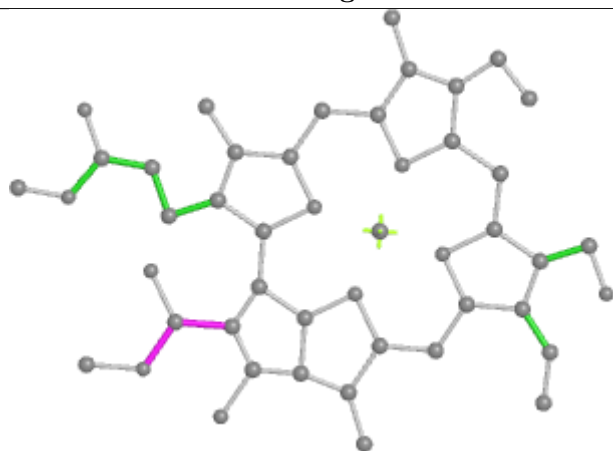
Ligand CHL 5 322



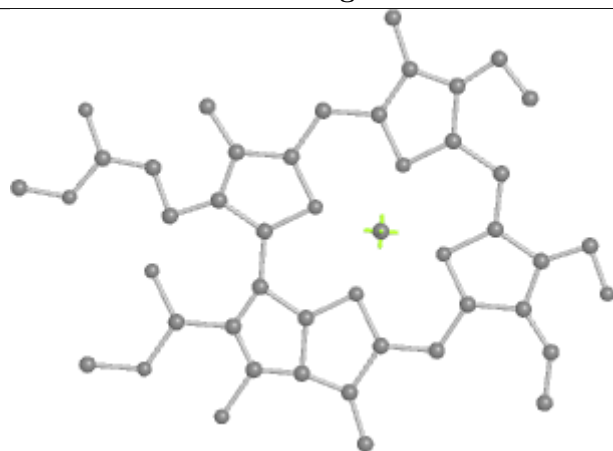
Bond lengths



Bond angles

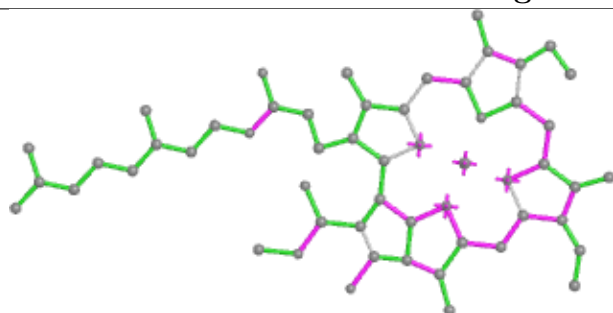


Torsions

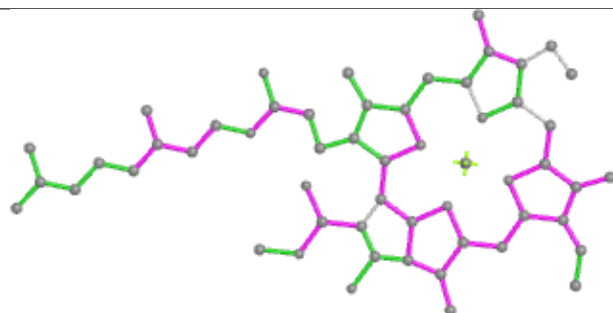


Rings

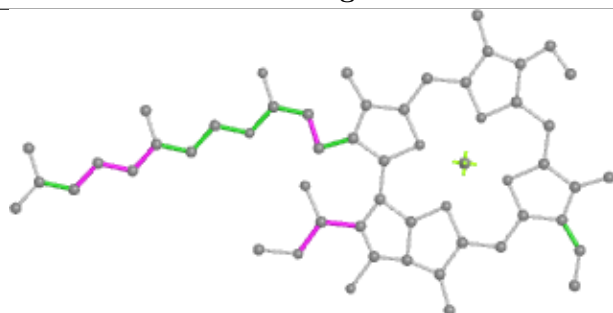
Ligand CHL B 823



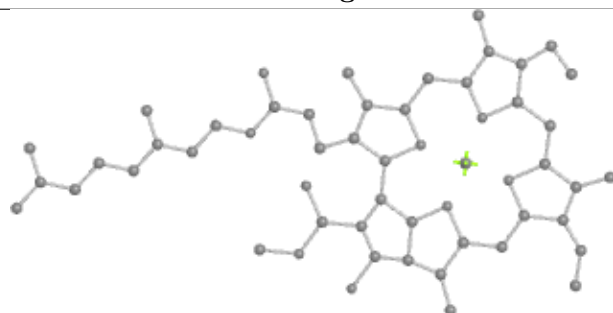
Bond lengths



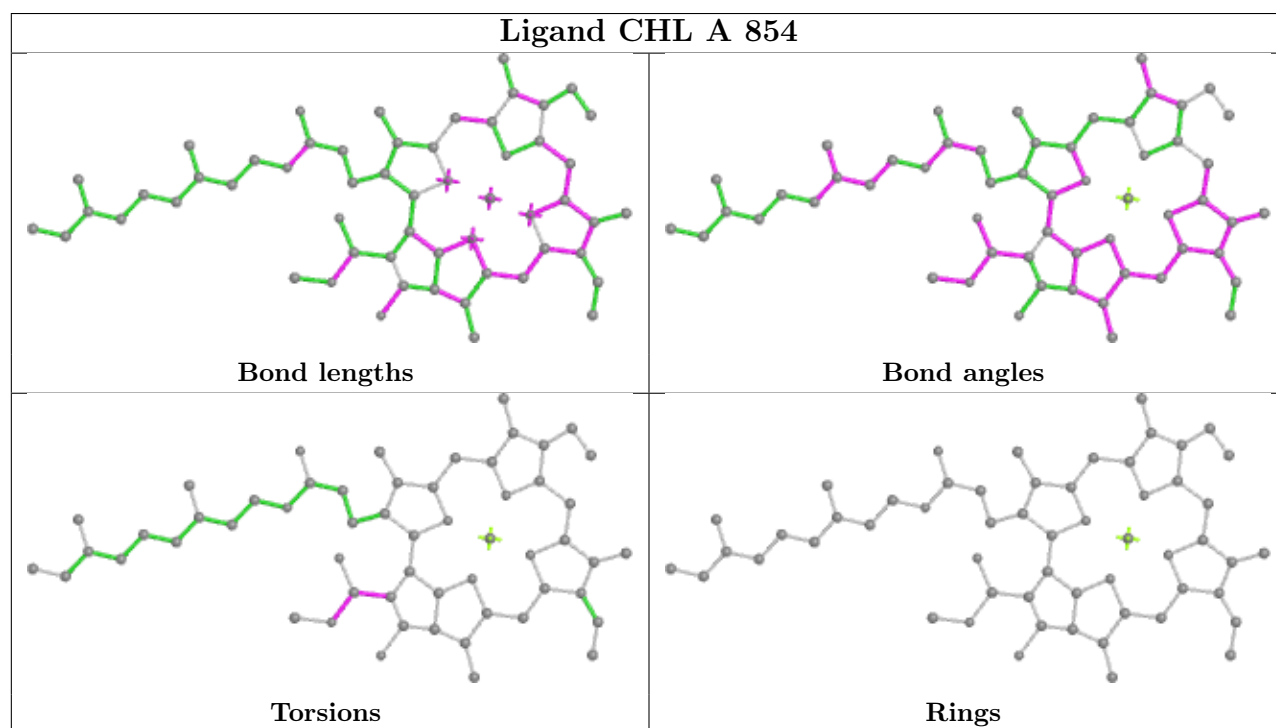
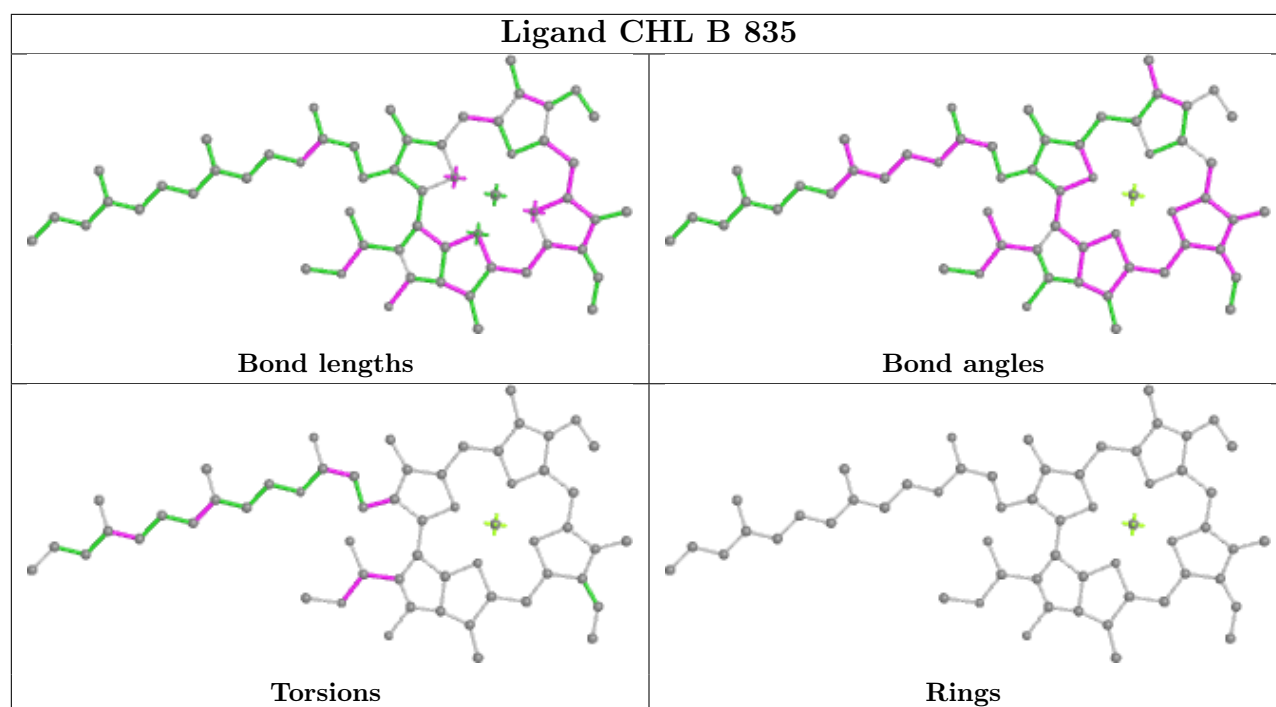
Bond angles

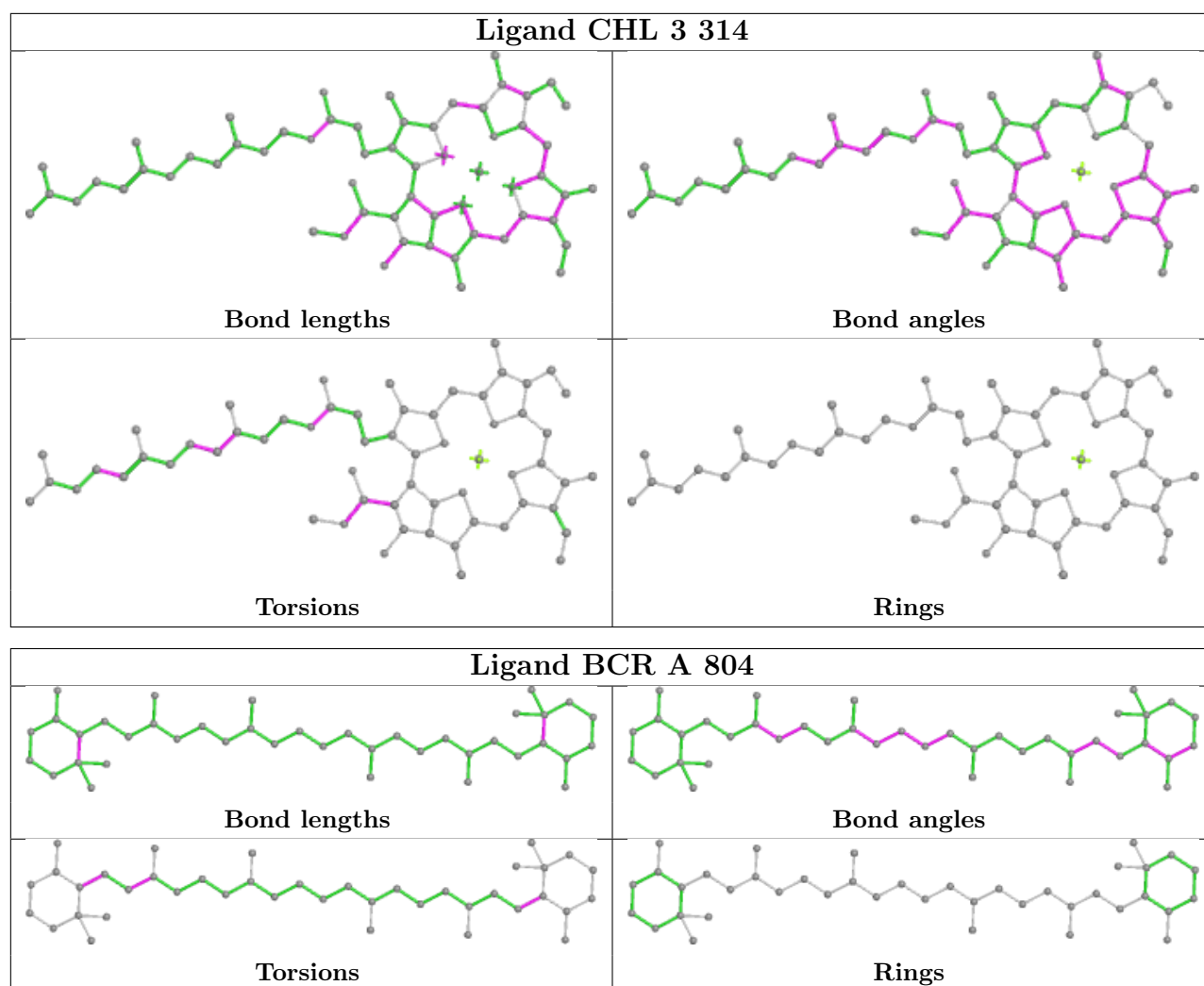


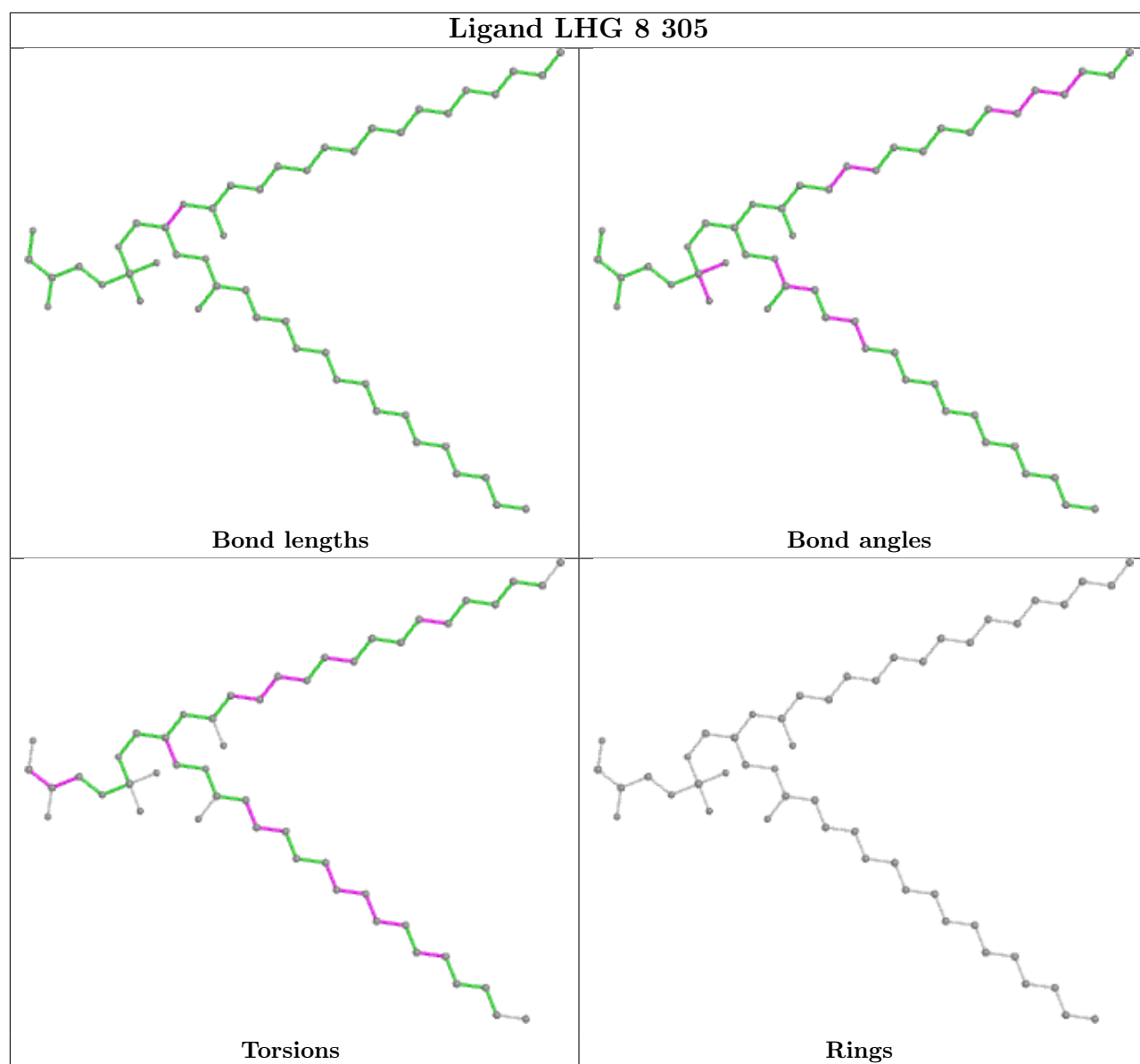
Torsions

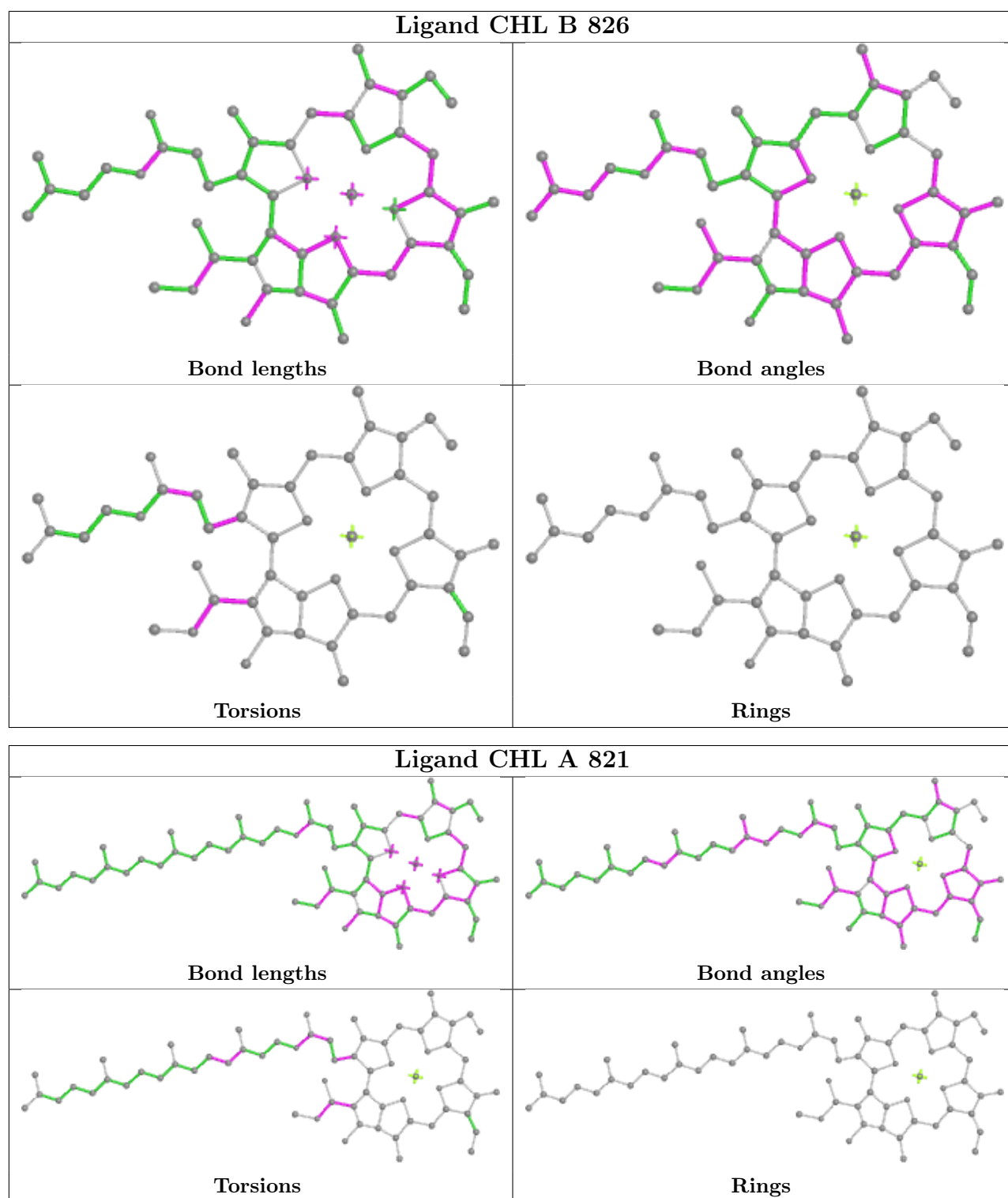


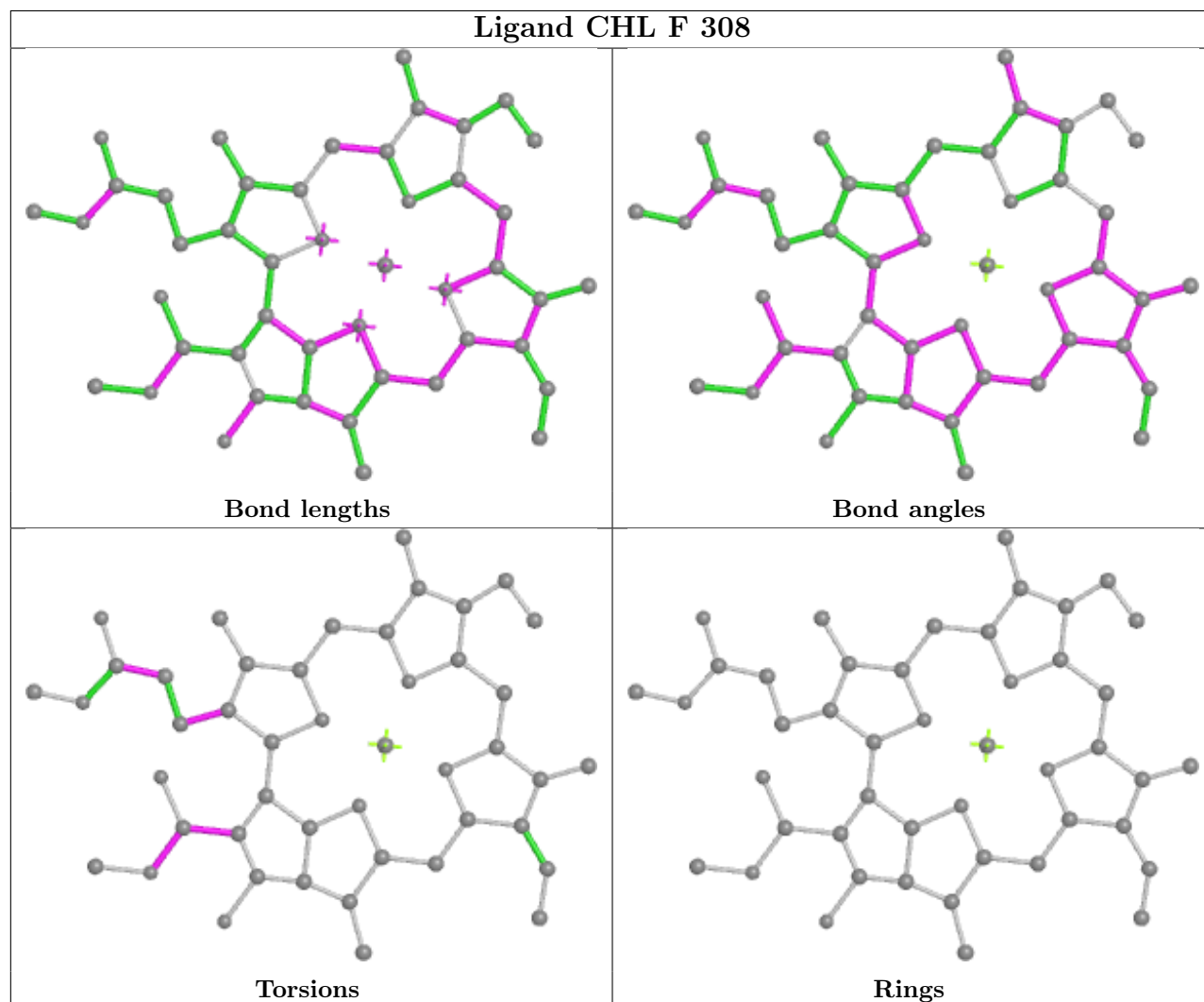
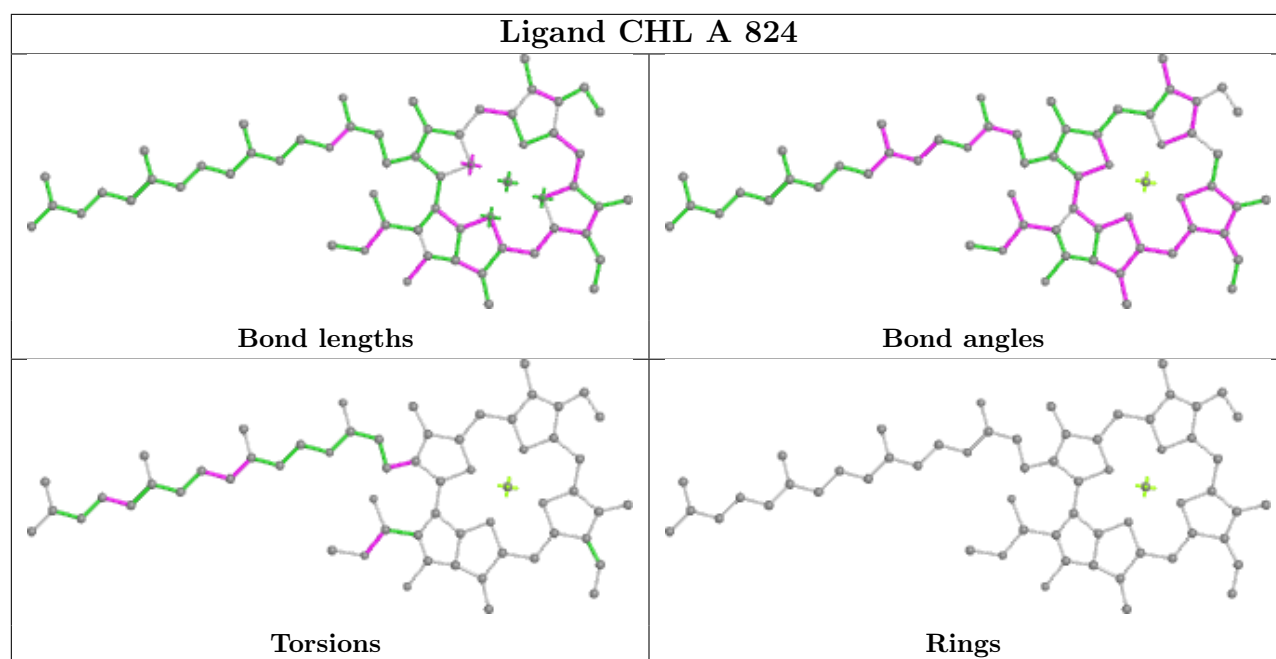
Rings



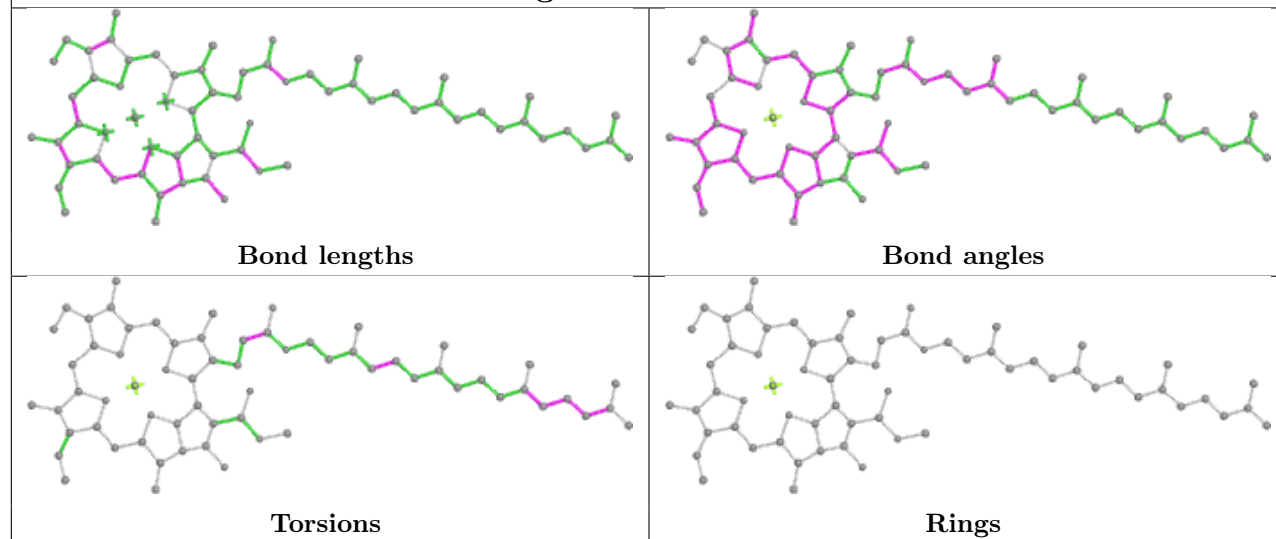




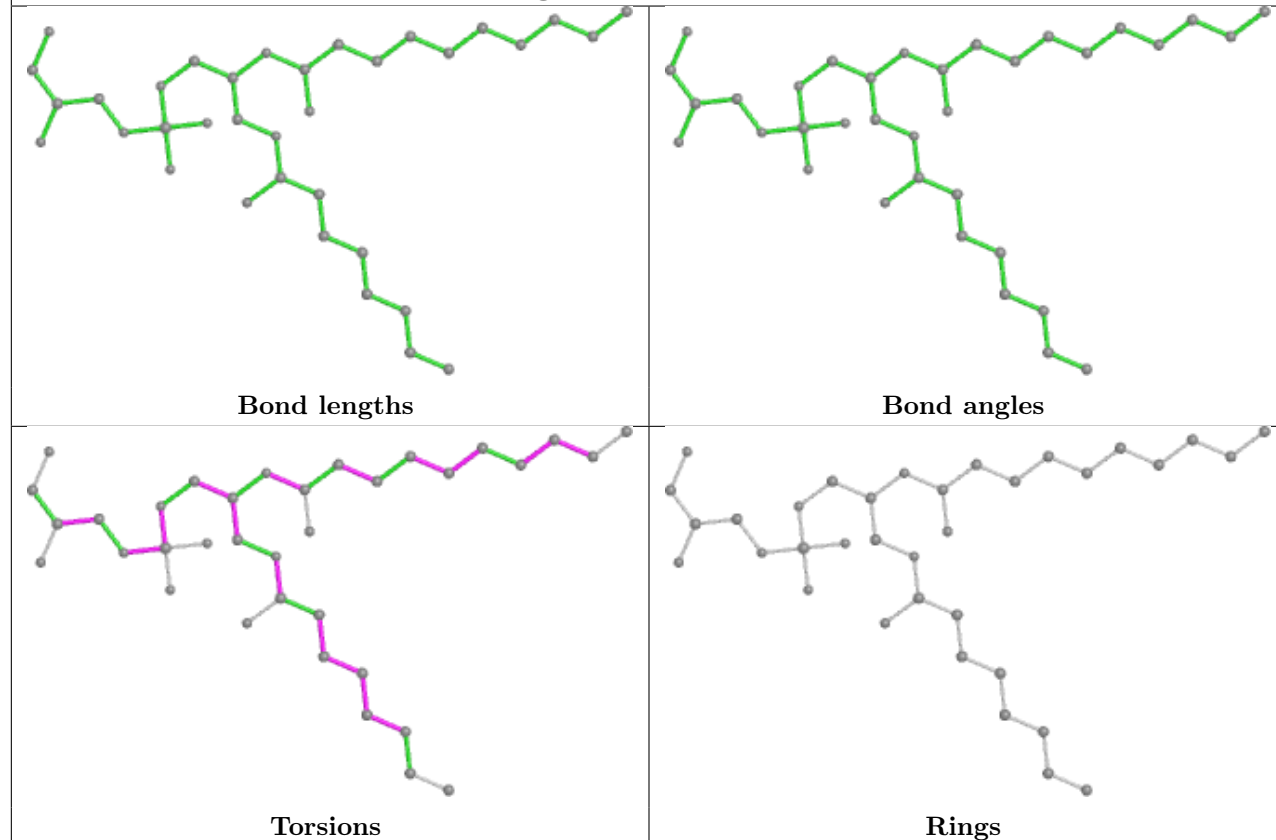


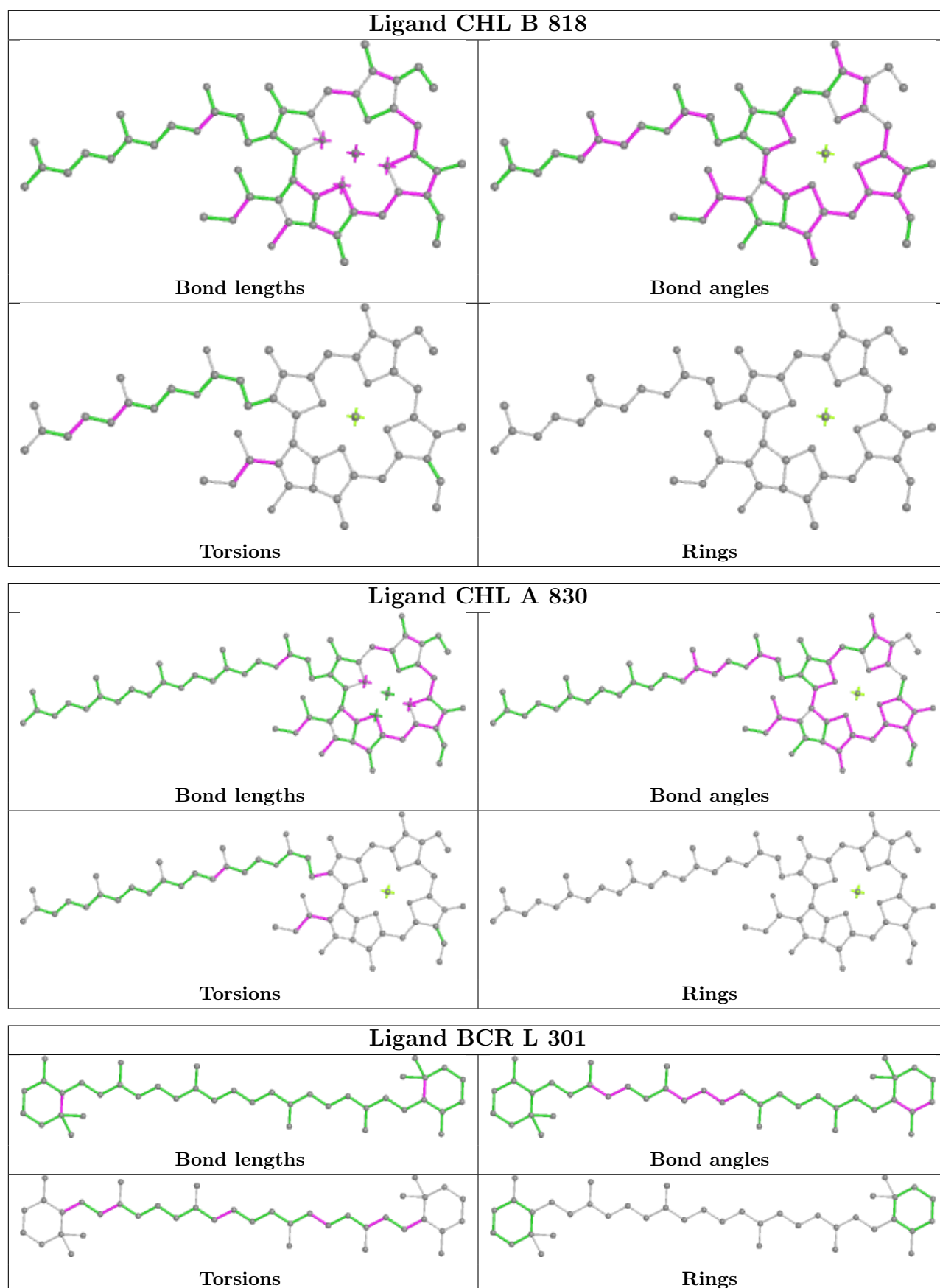


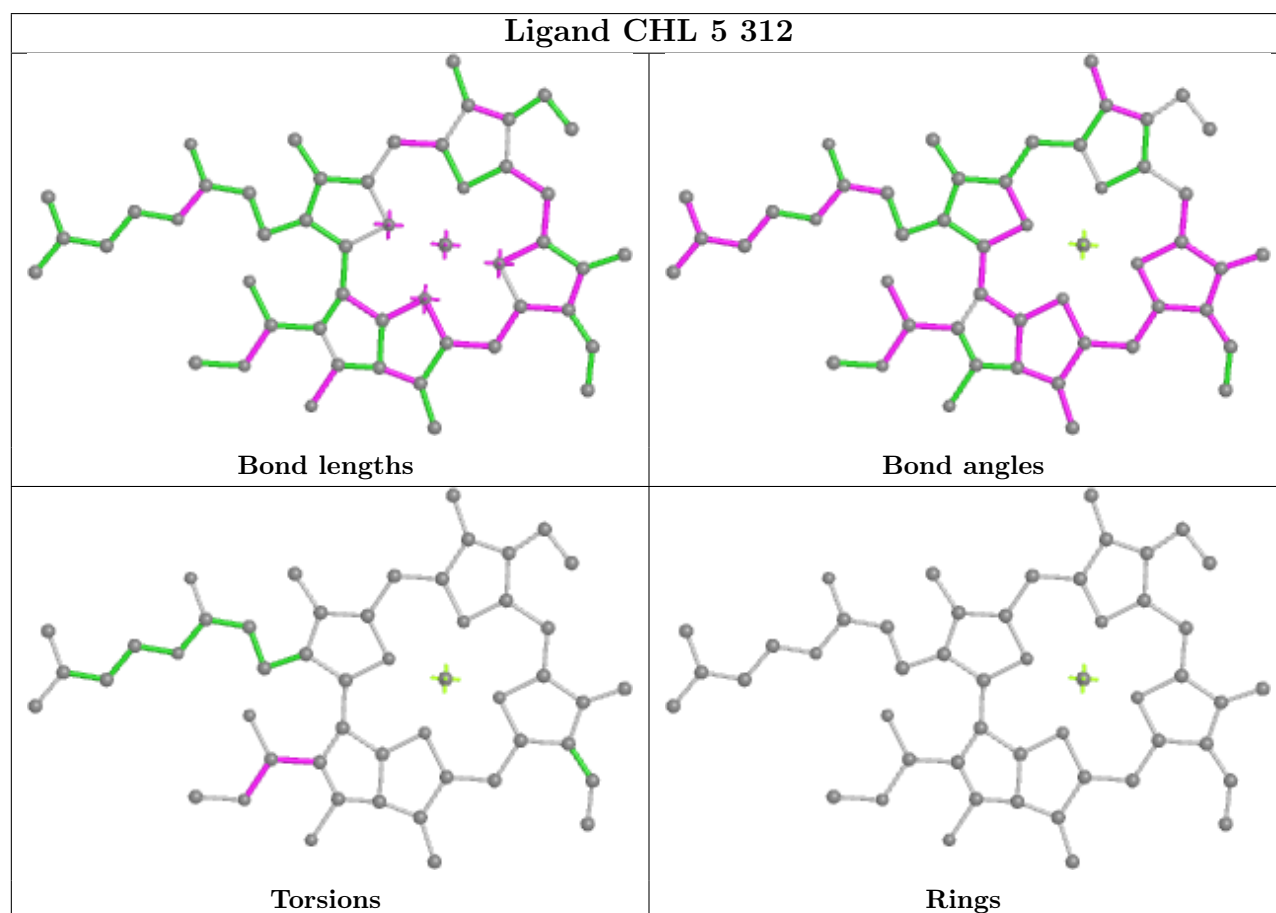
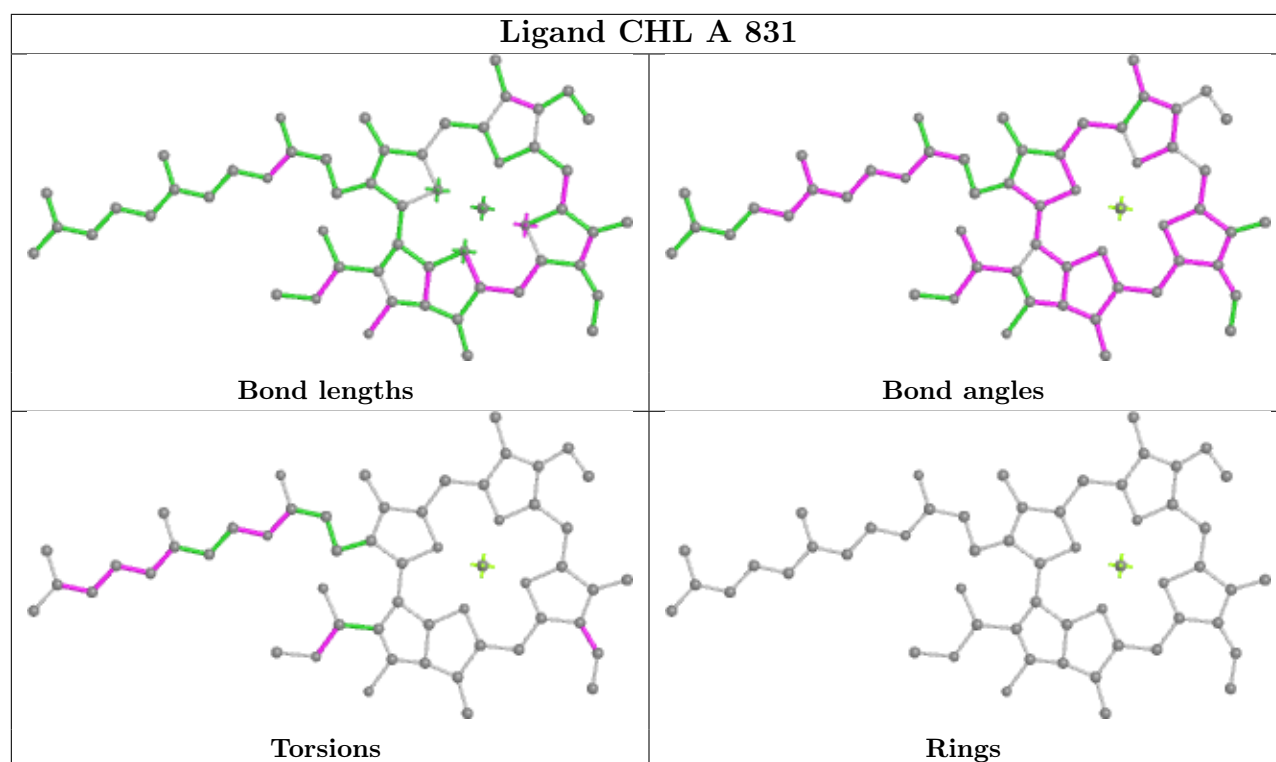
Ligand CL0 A 815



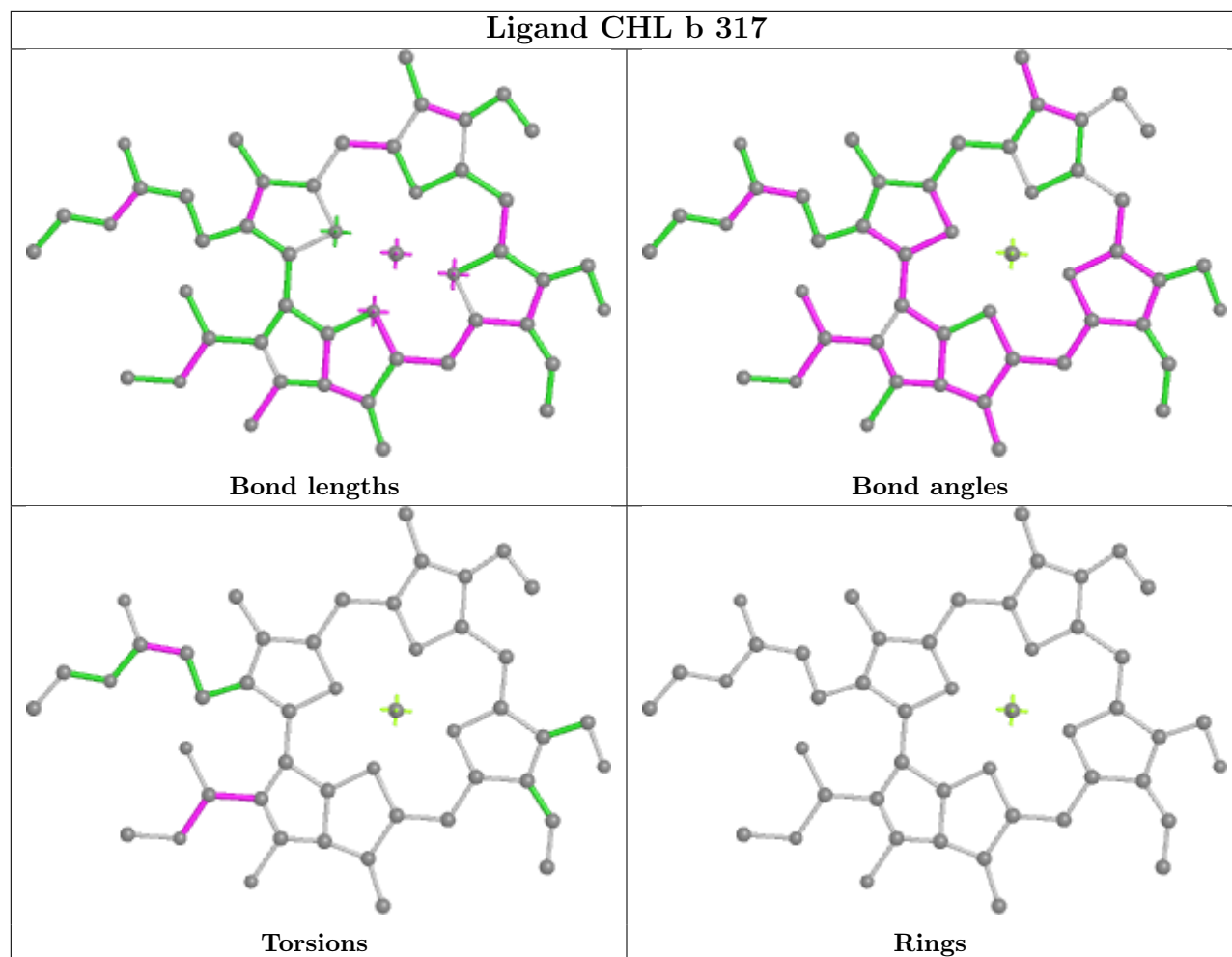
Ligand LHG 5 304



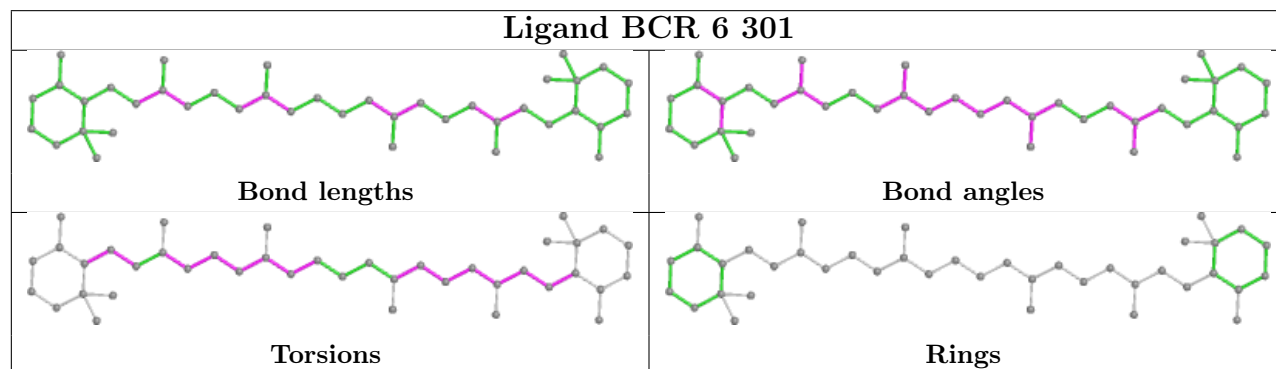


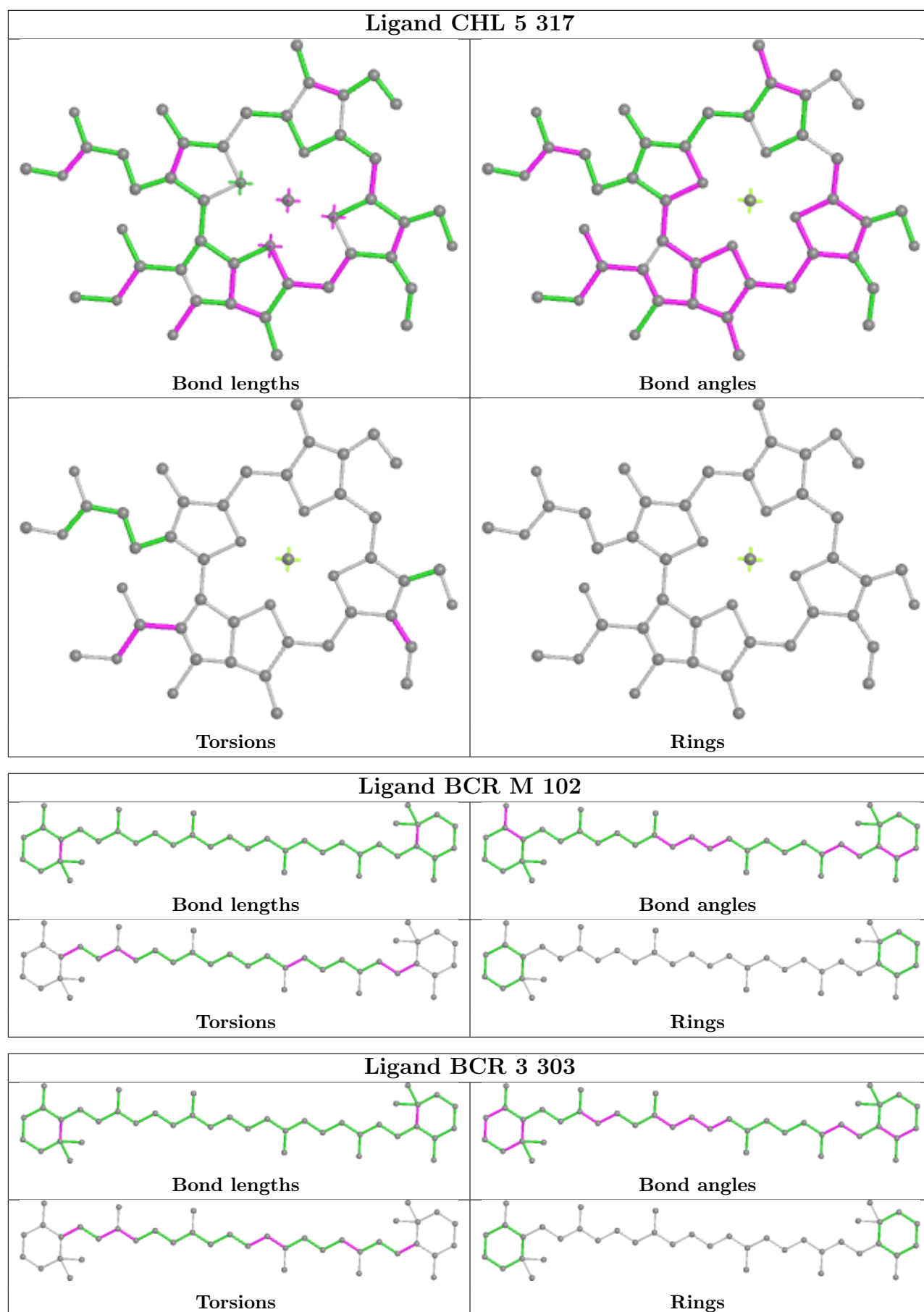


Ligand CHL b 317

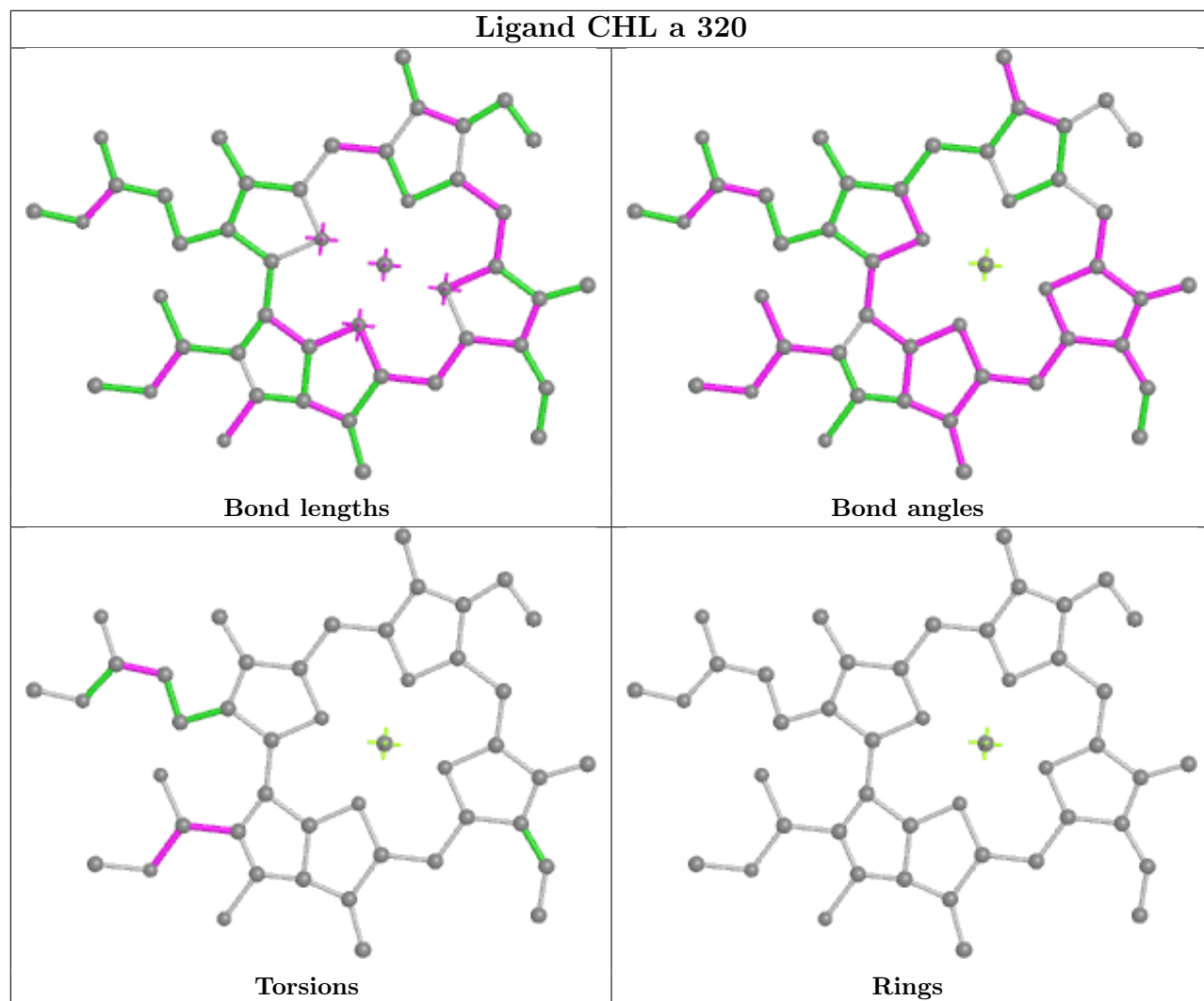


Ligand BCR 6 301

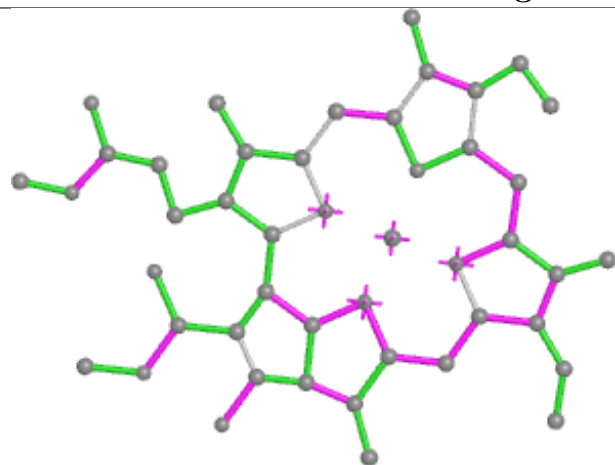




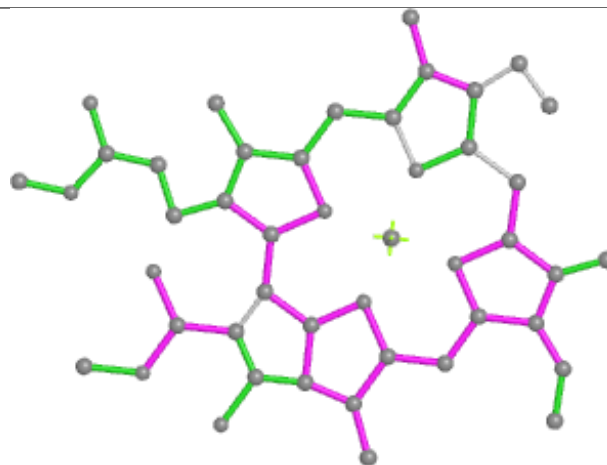
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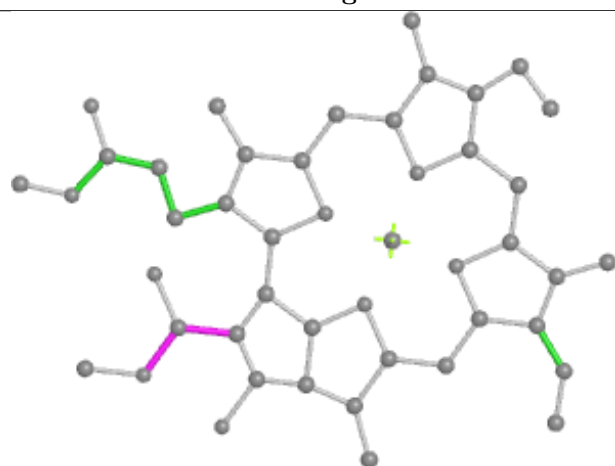
Ligand CHL K 205



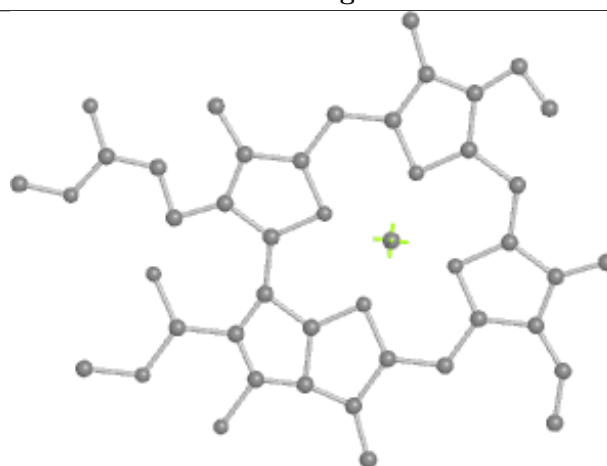
Bond lengths



Bond angles

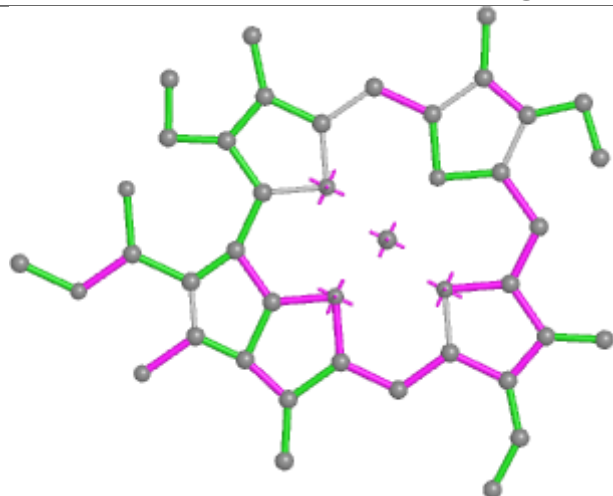


Torsions

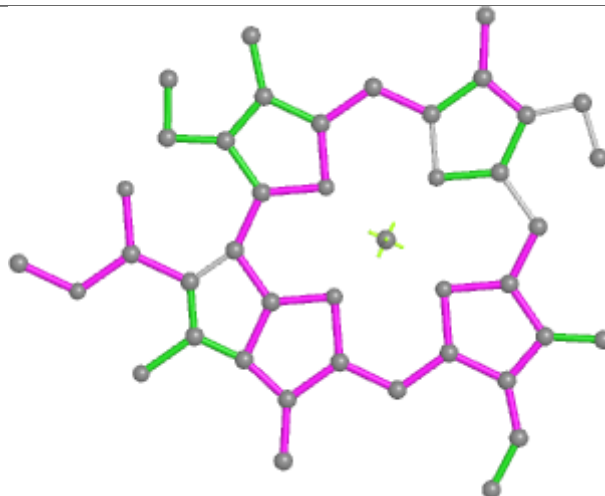


Rings

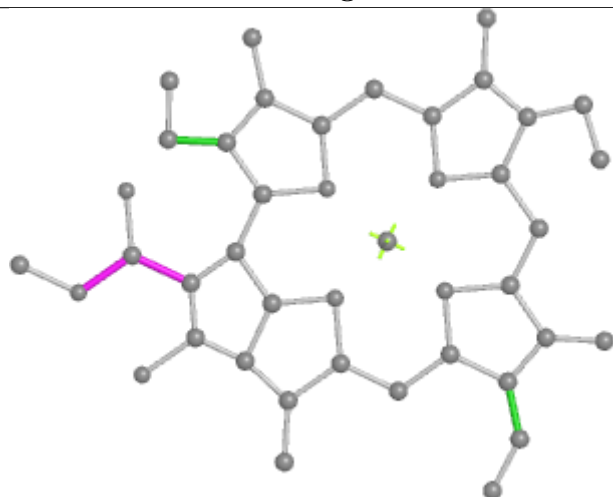
Ligand CHL 4 318



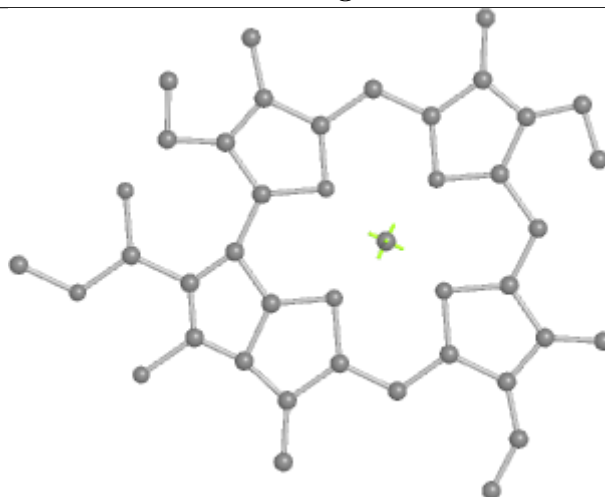
Bond lengths



Bond angles

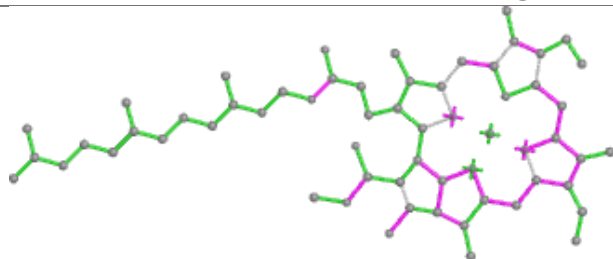


Torsions

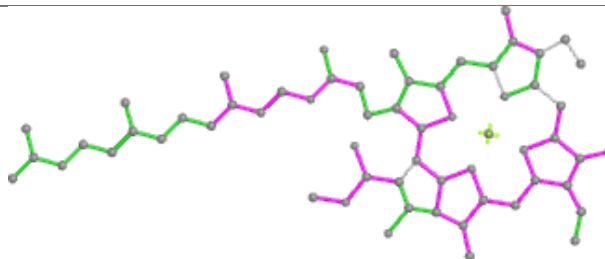


Rings

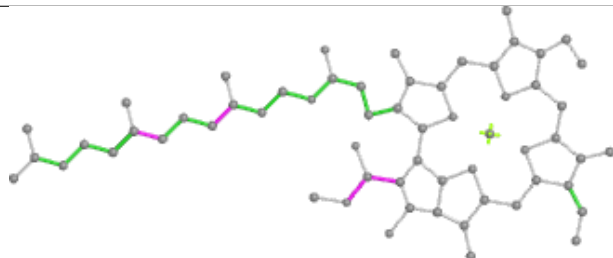
Ligand CHL B 825



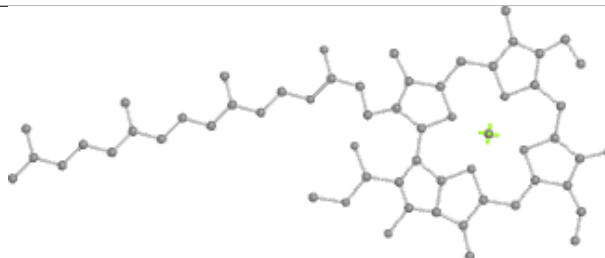
Bond lengths



Bond angles

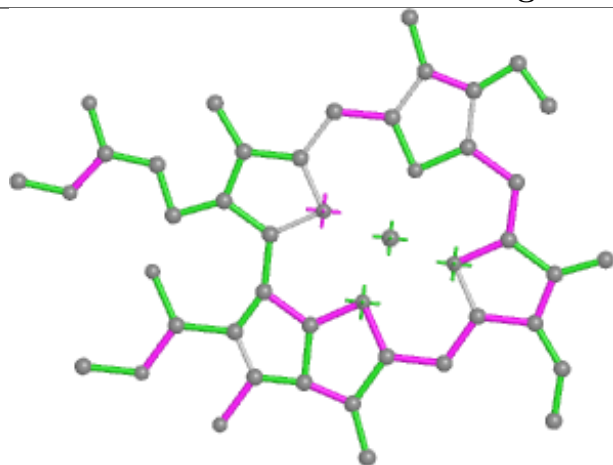


Torsions

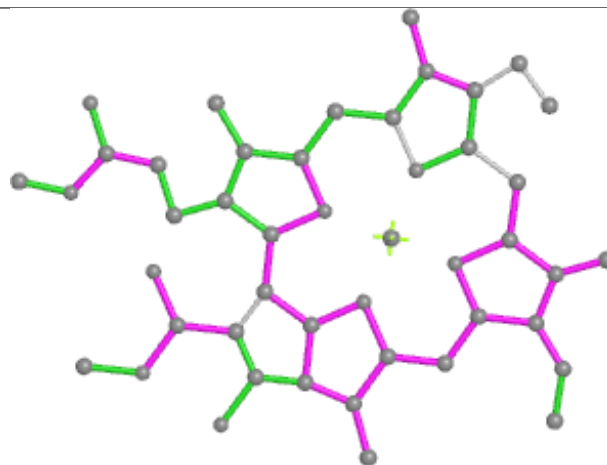


Rings

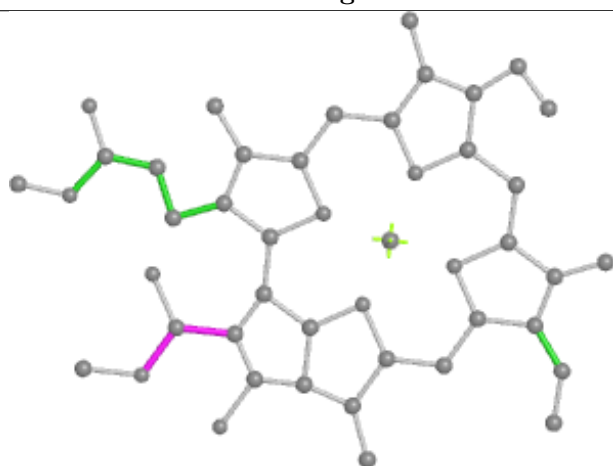
Ligand CHL 6 320



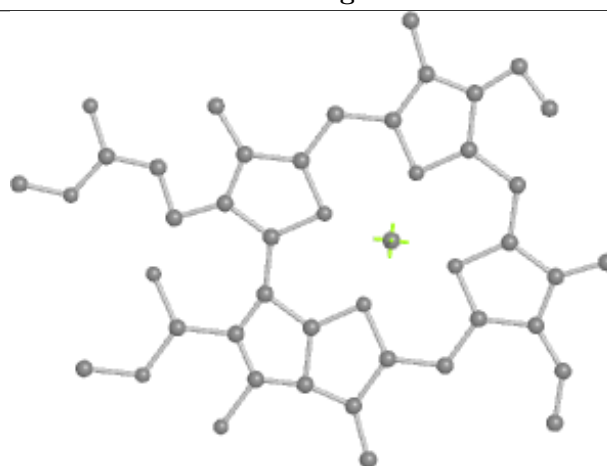
Bond lengths



Bond angles

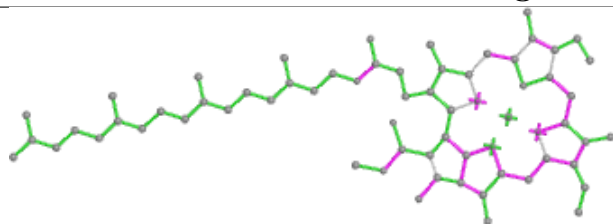


Torsions

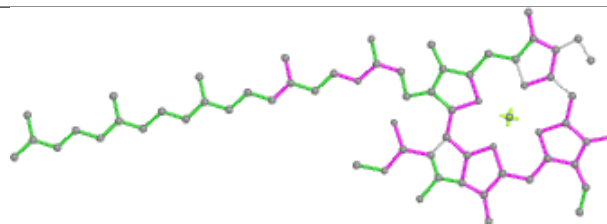


Rings

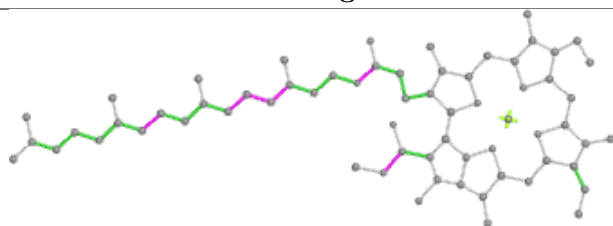
Ligand CHL B 837



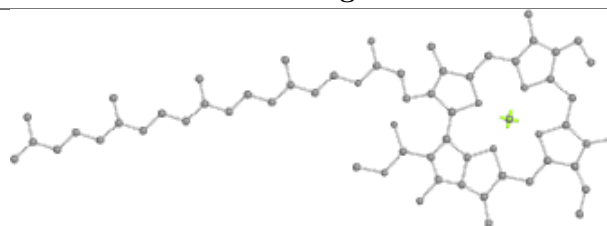
Bond lengths



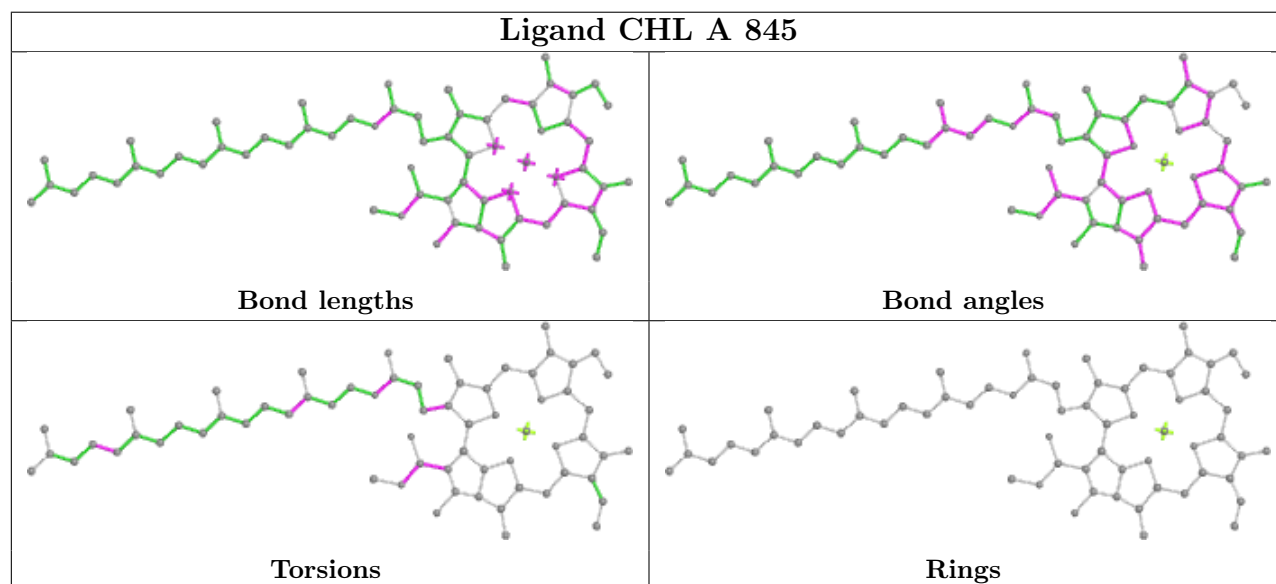
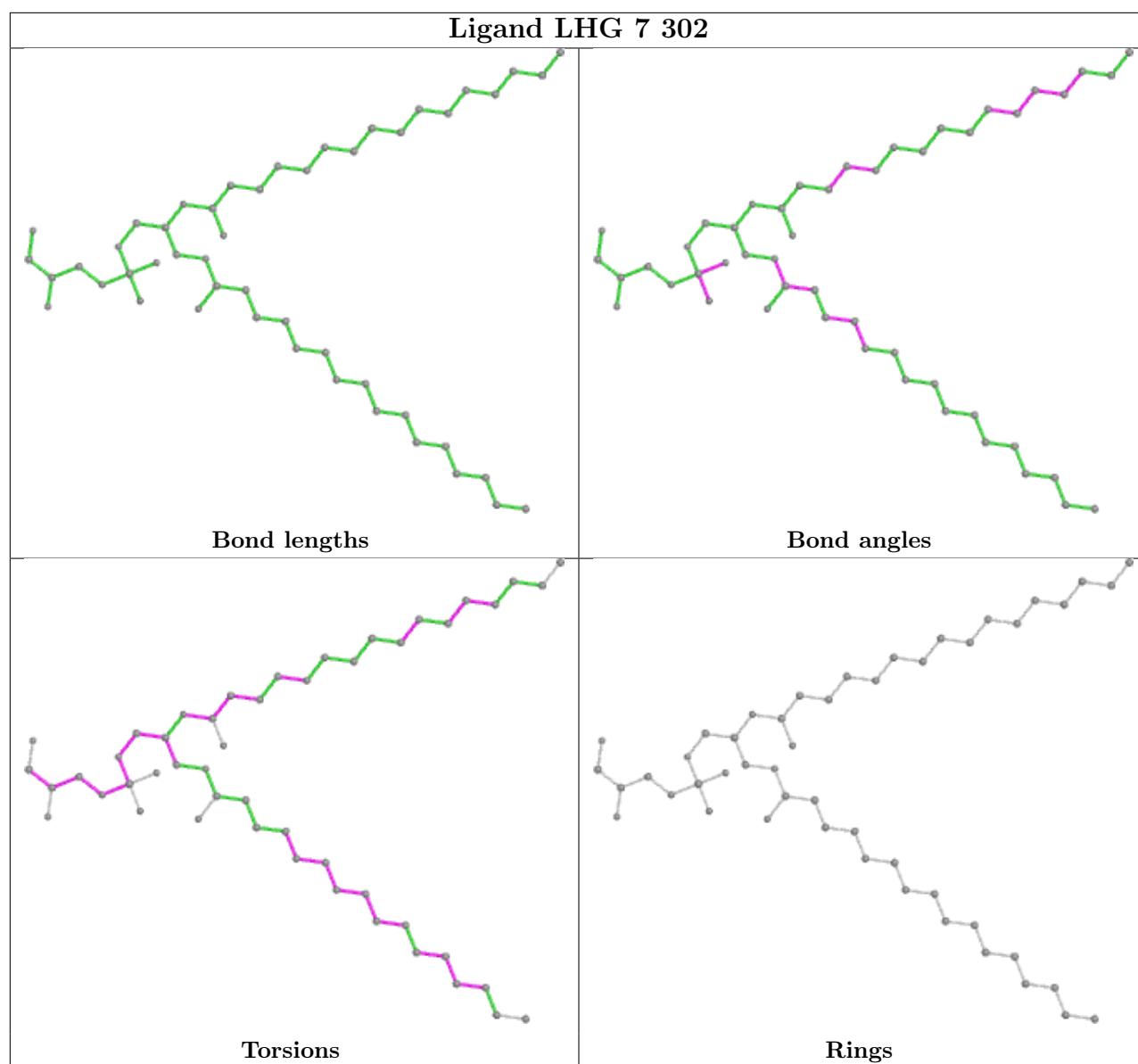
Bond angles

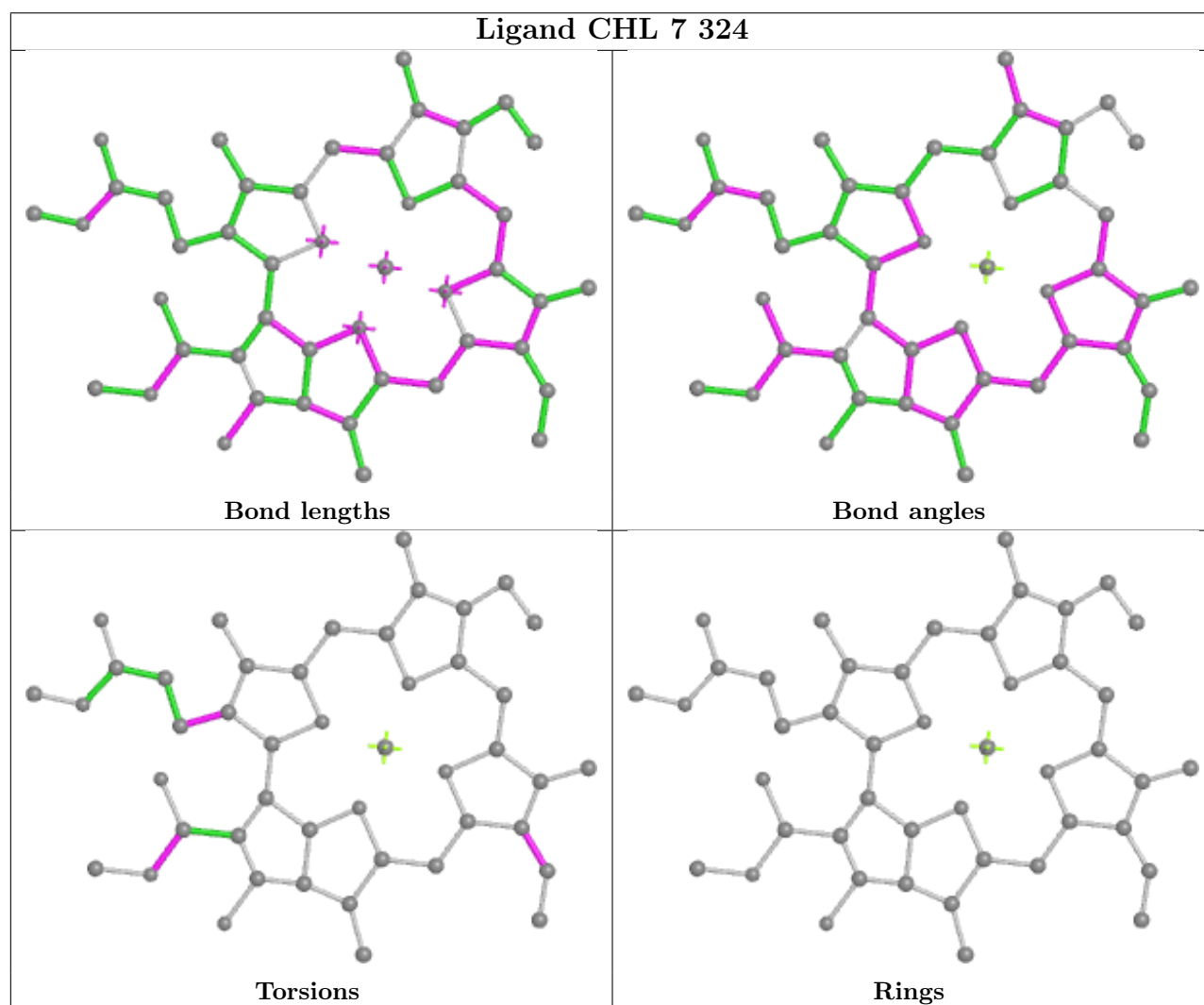
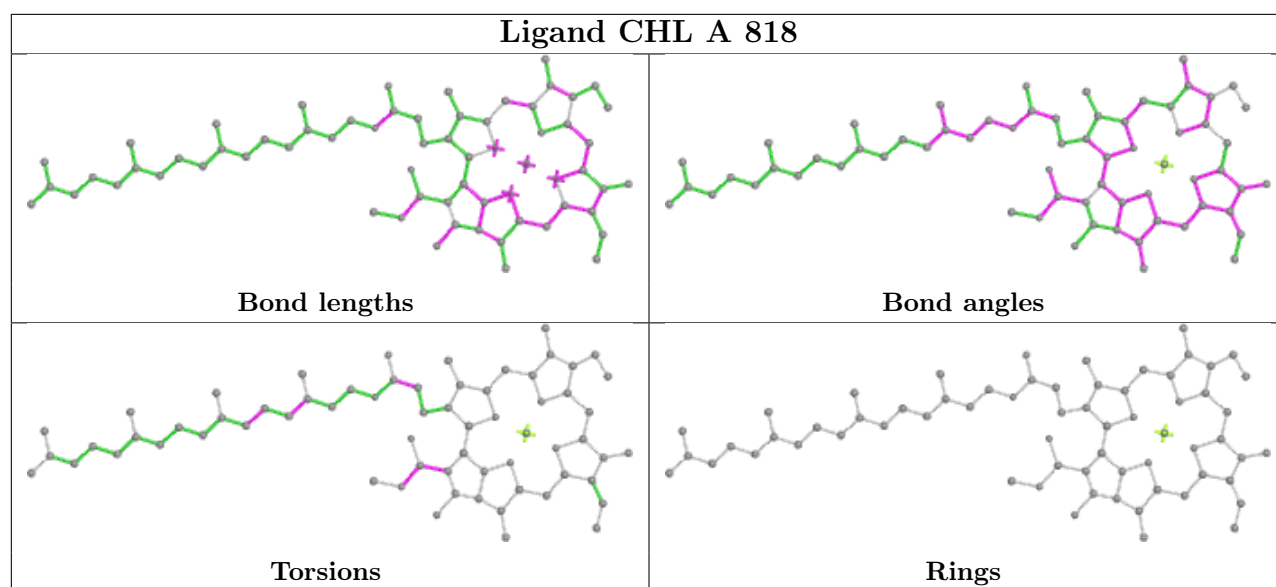


Torsions

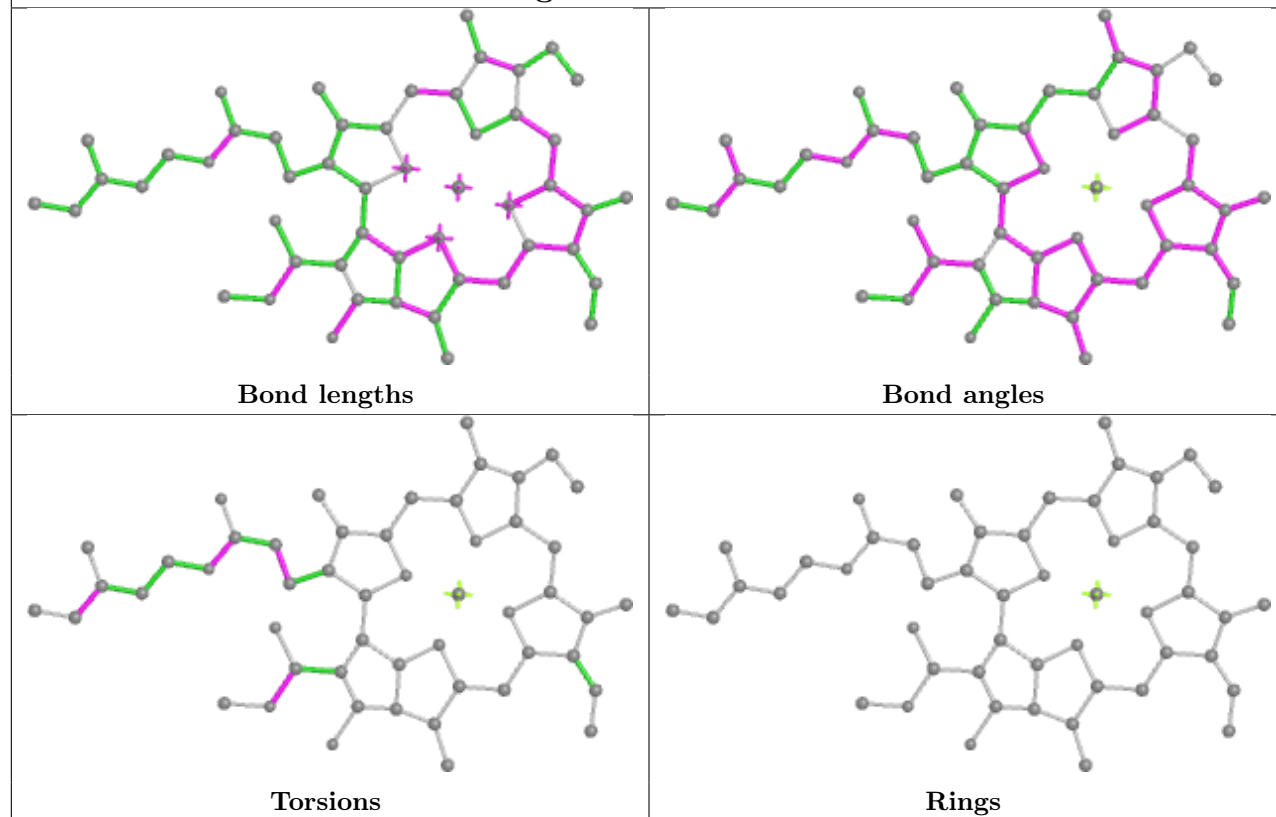


Rings

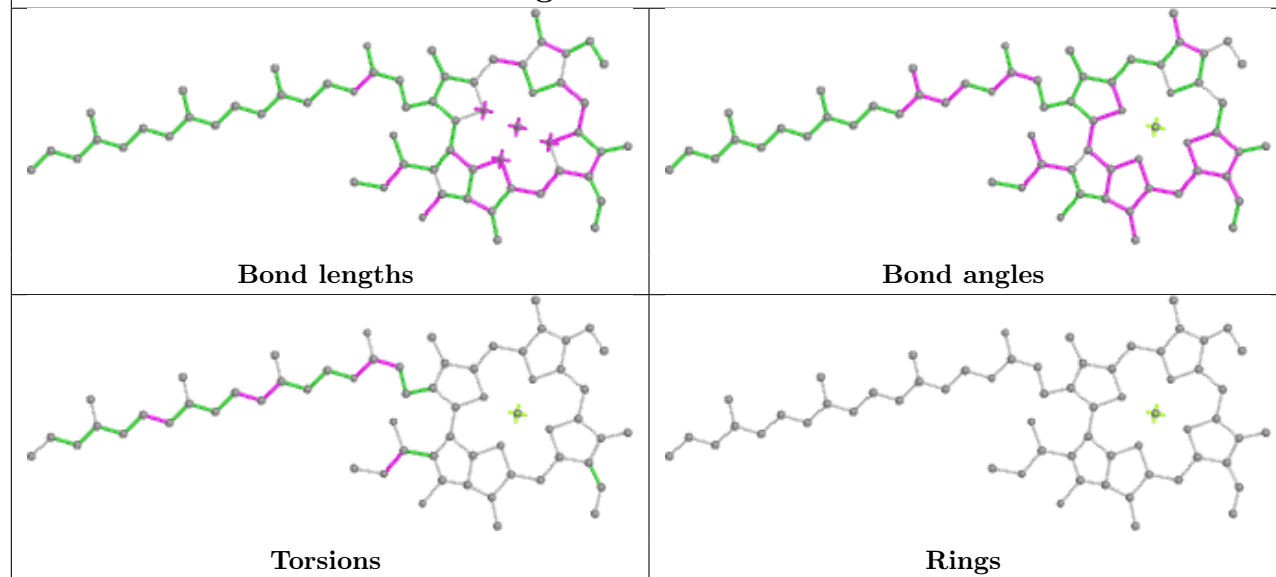


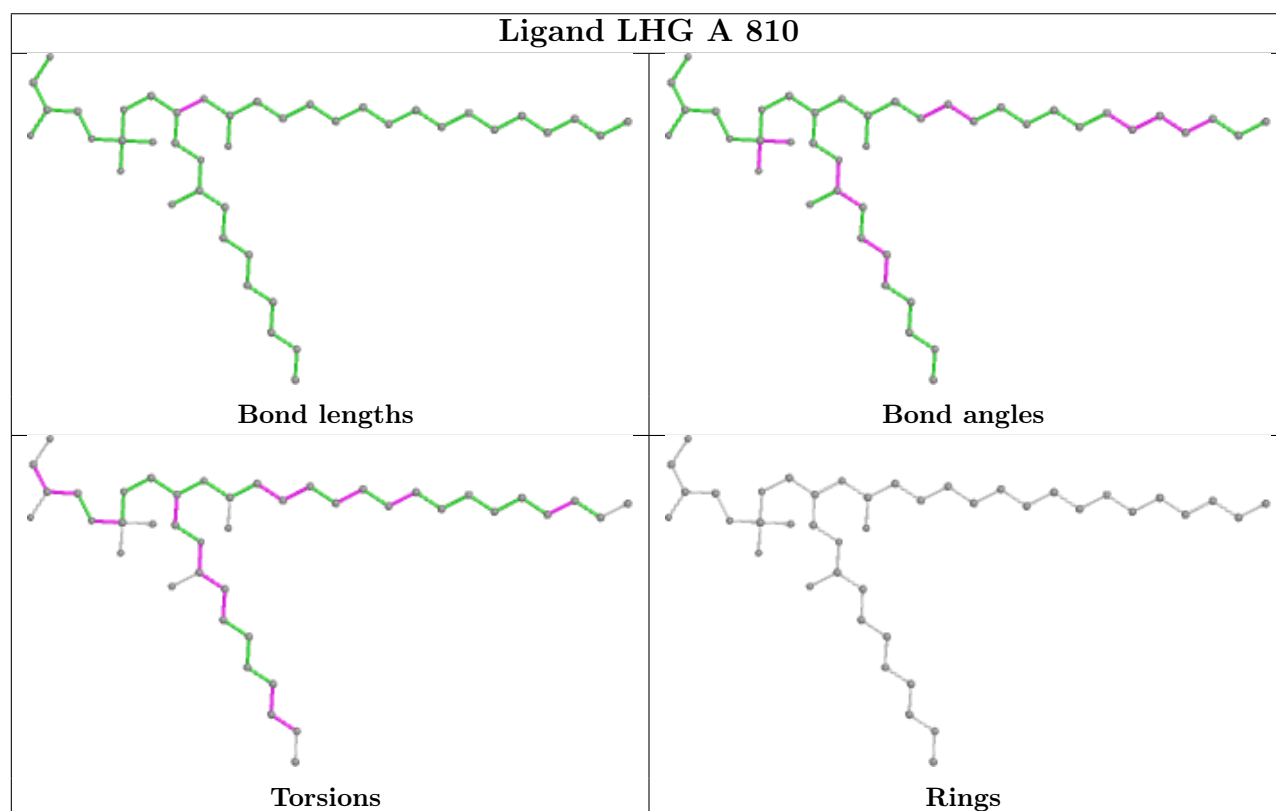
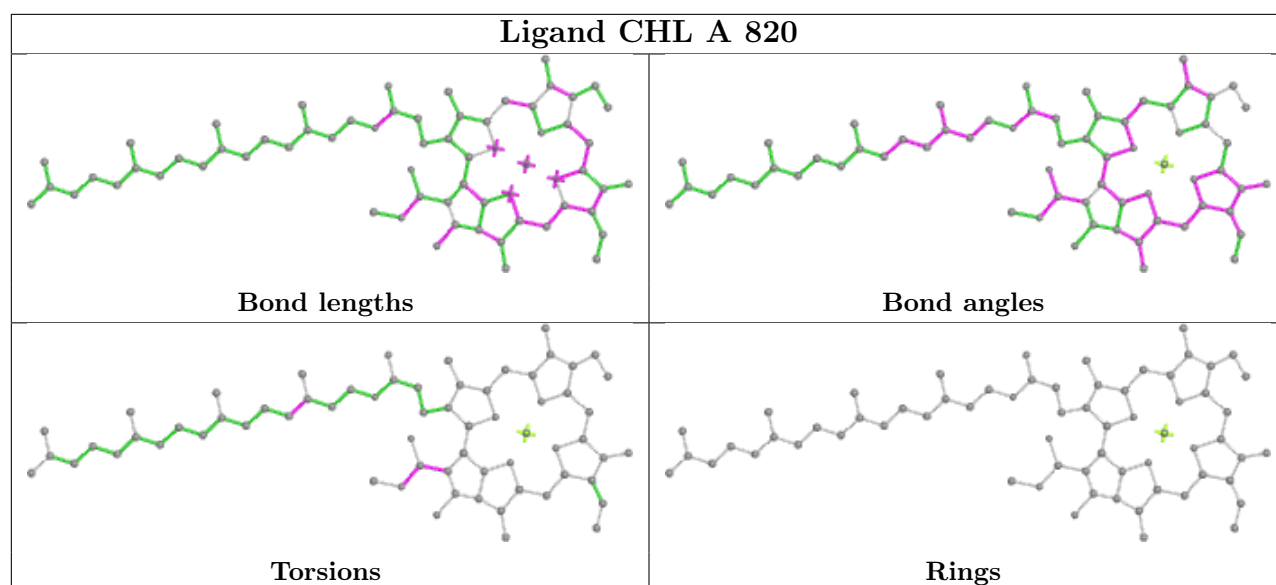


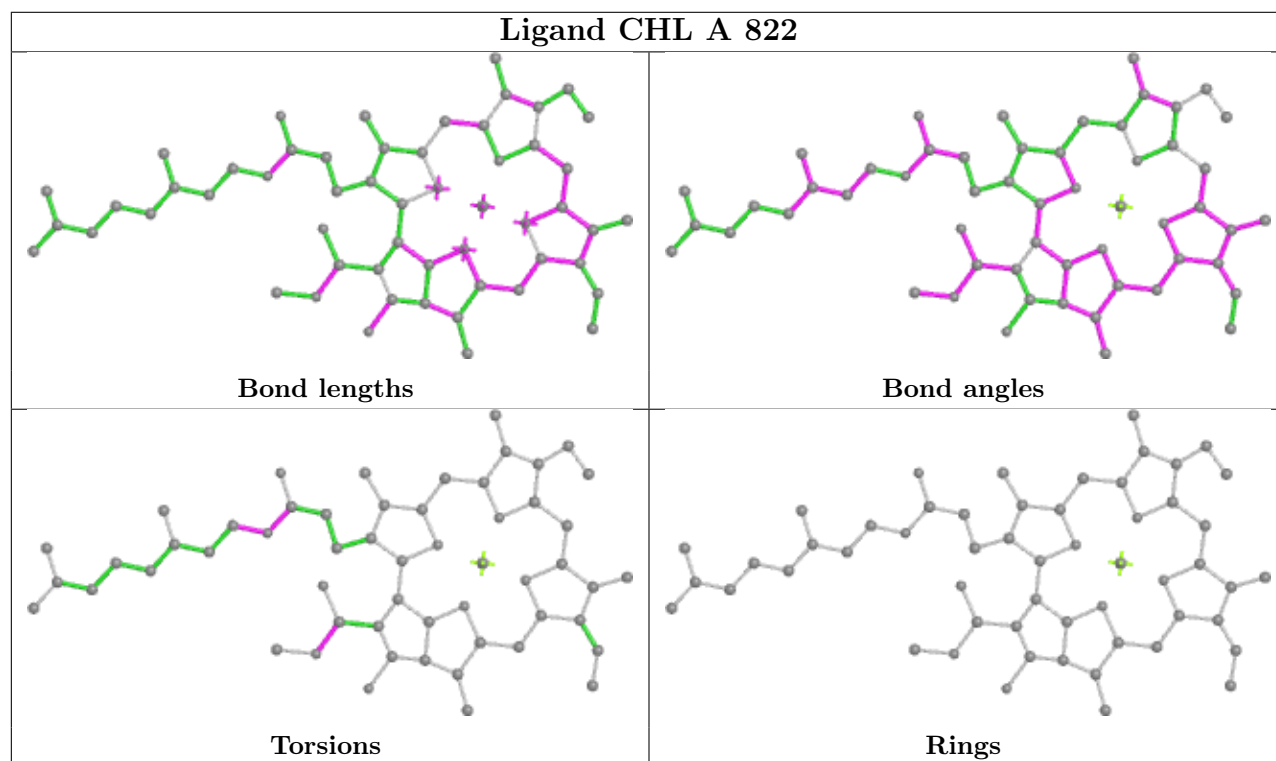
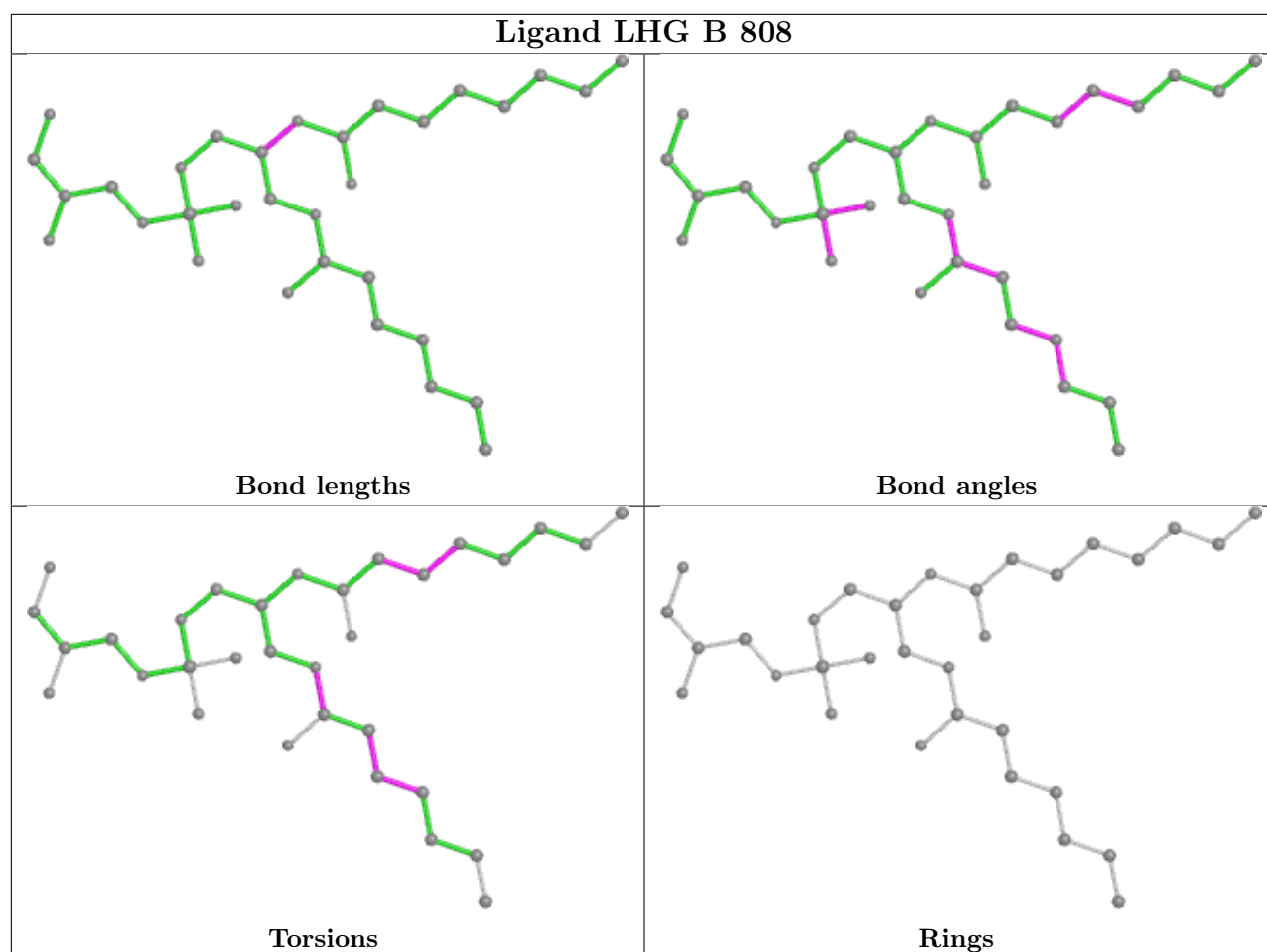
Ligand CHL 3 318

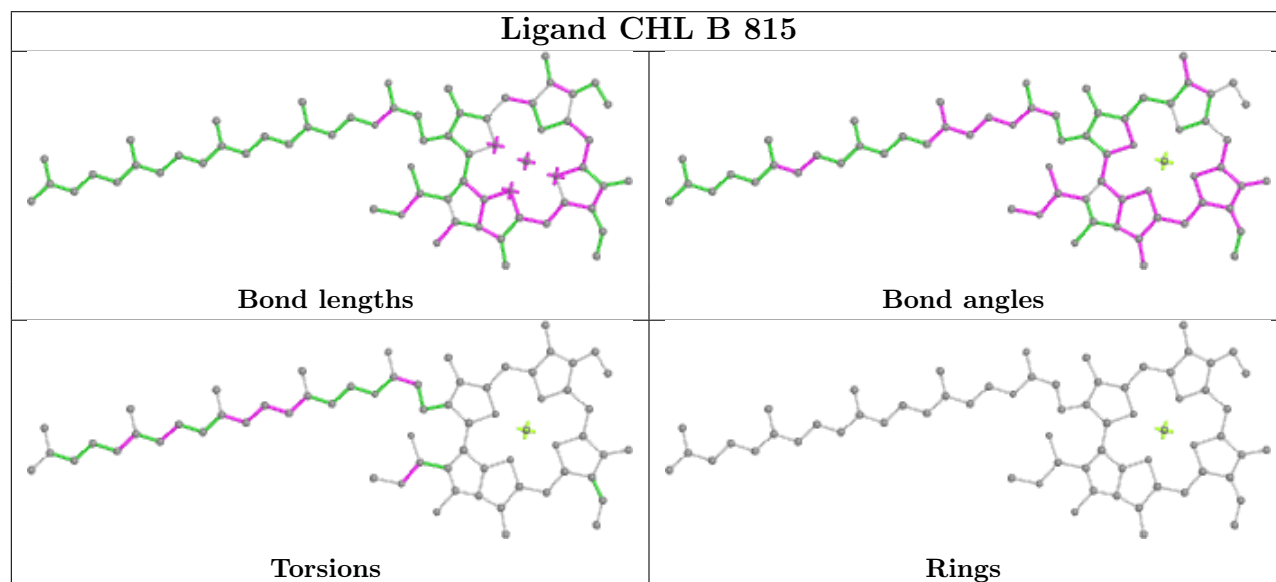
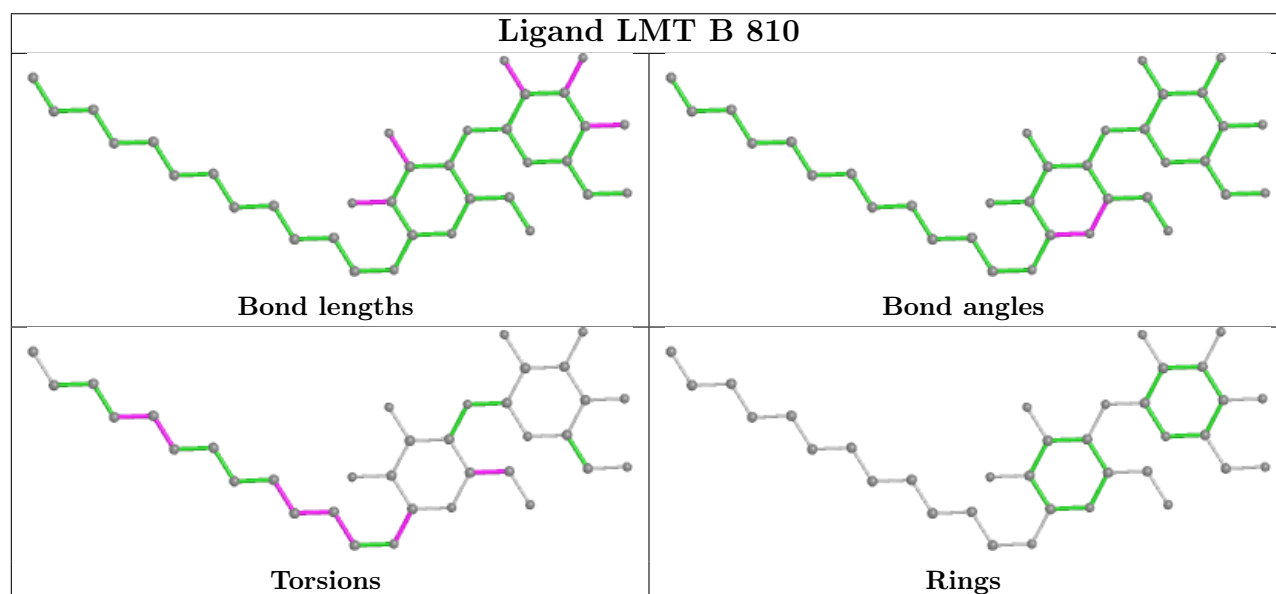
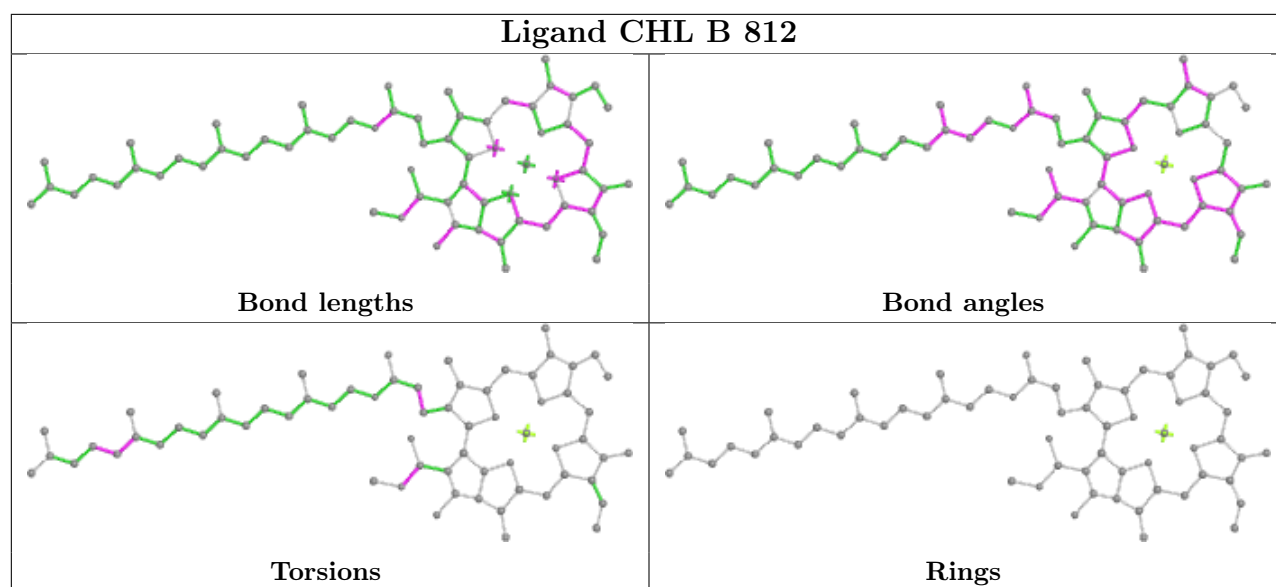


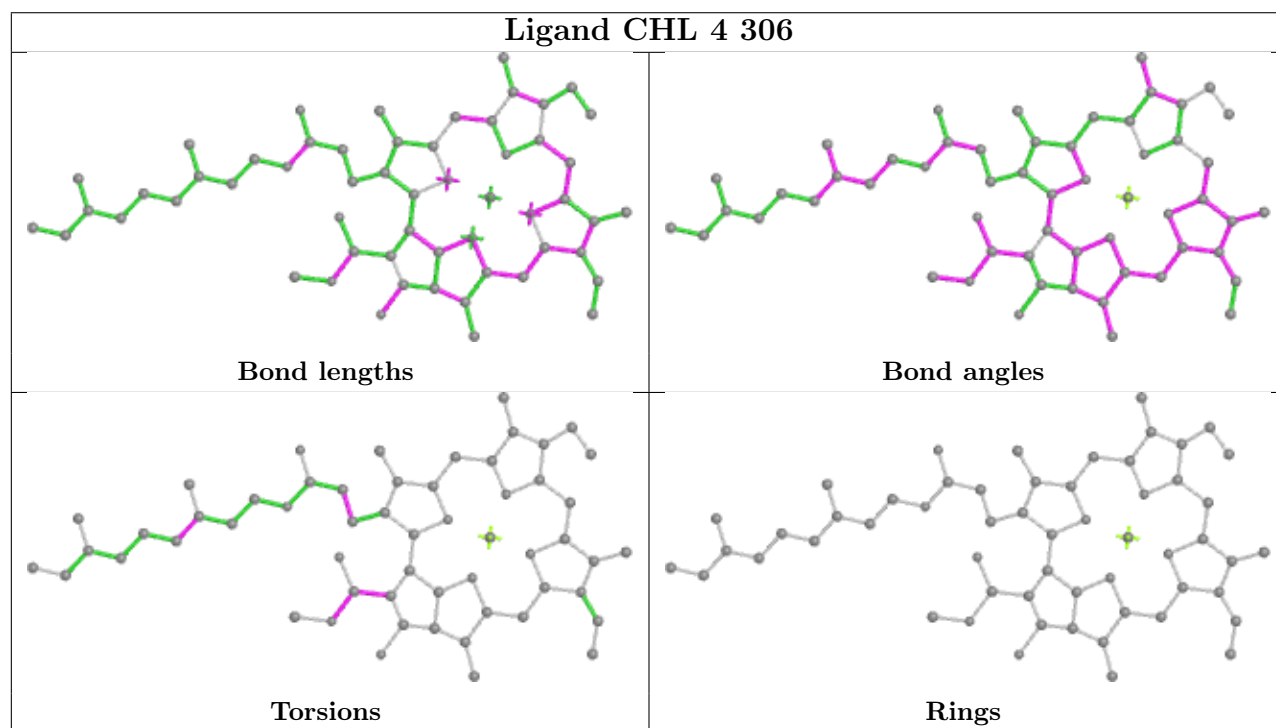
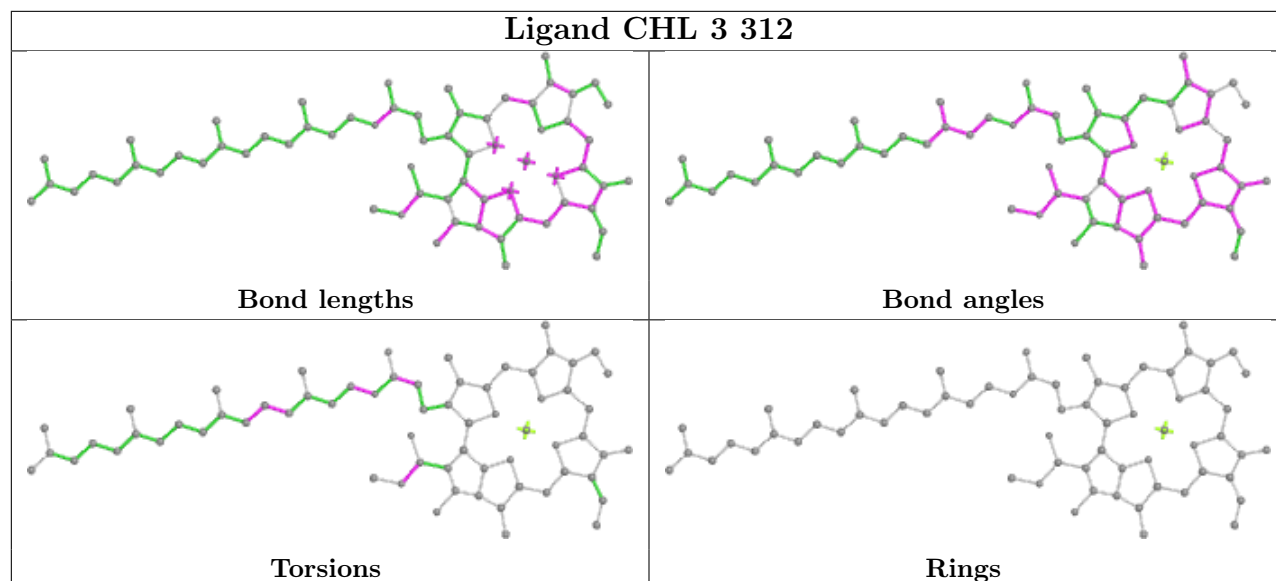
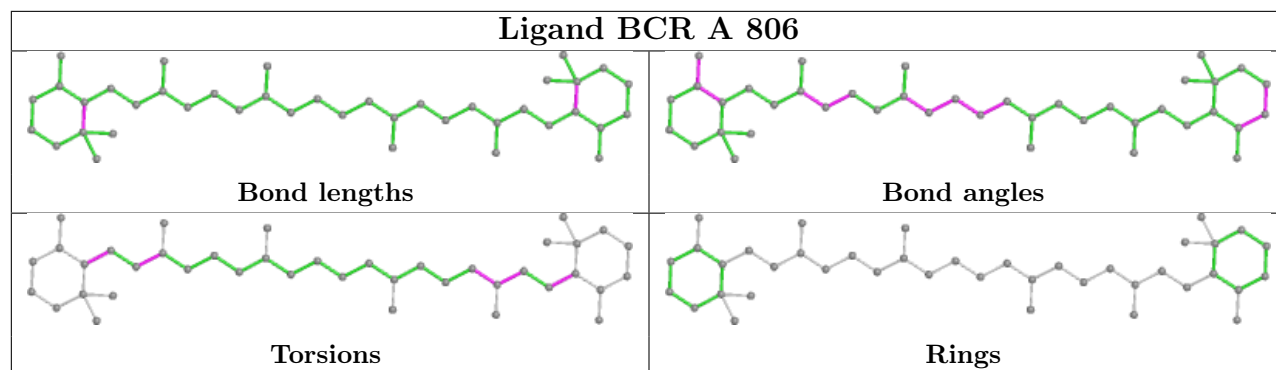
Ligand CHL 3 317



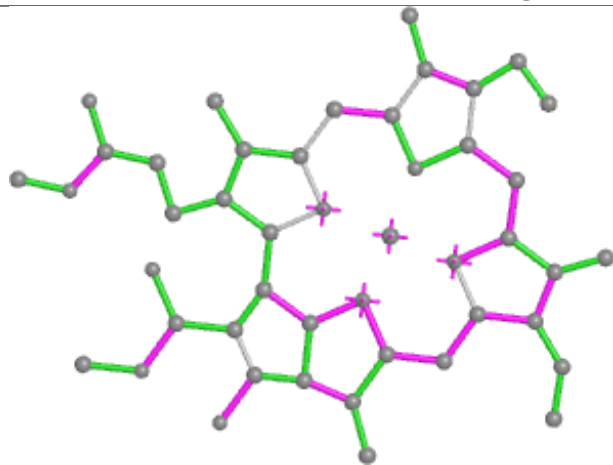




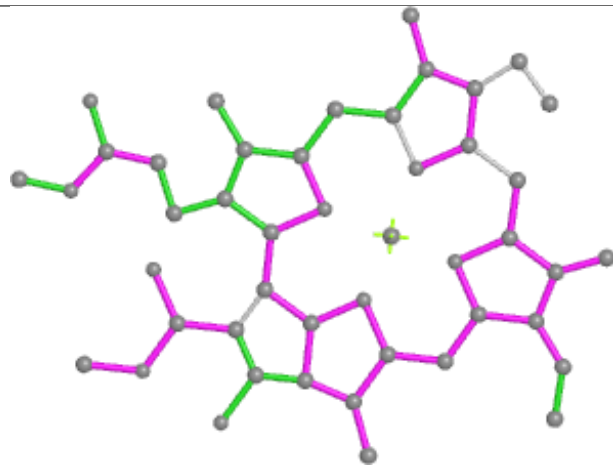




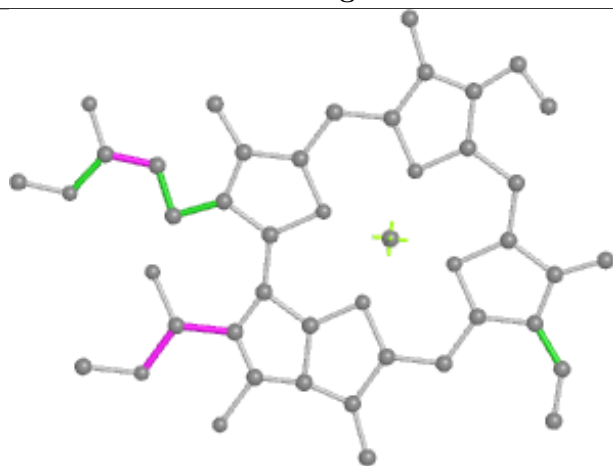
Ligand CHL 6 312



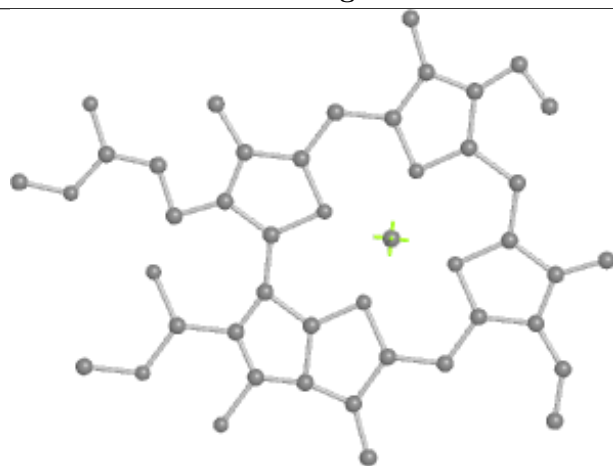
Bond lengths



Bond angles

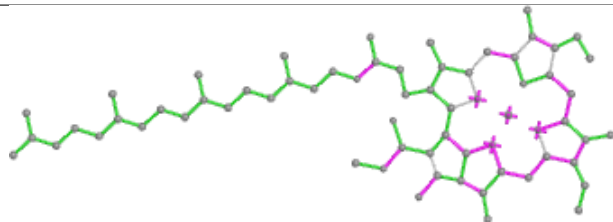


Torsions

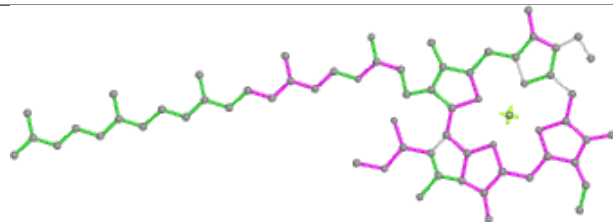


Rings

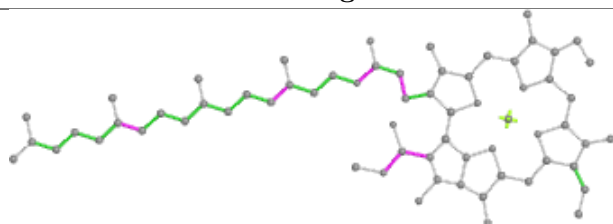
Ligand CHL 6 311



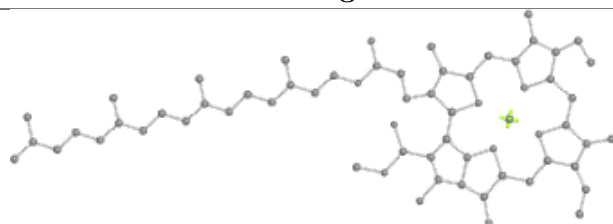
Bond lengths



Bond angles

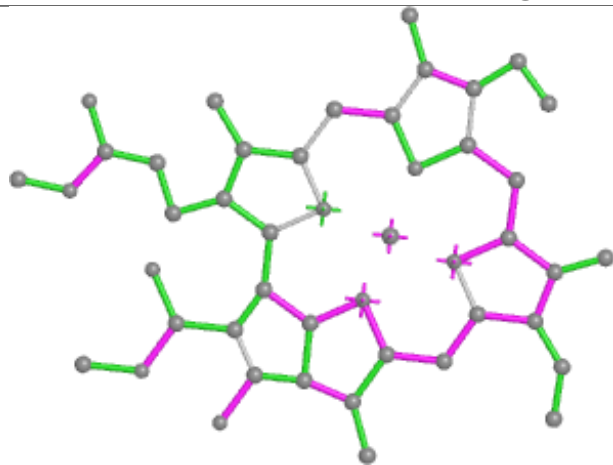


Torsions

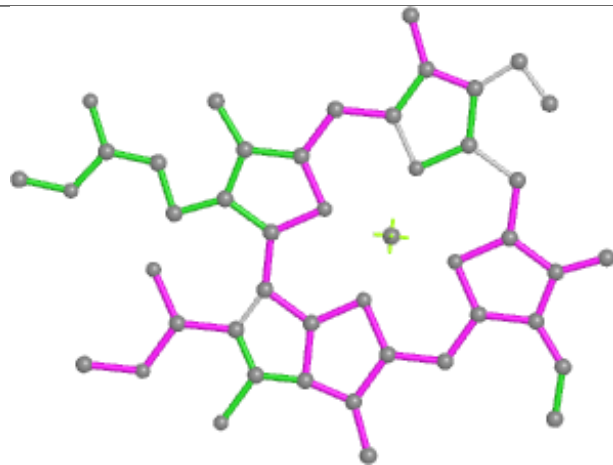


Rings

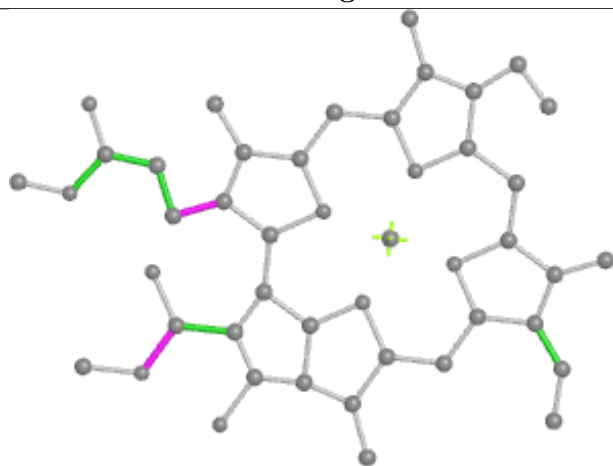
Ligand CHL b 304



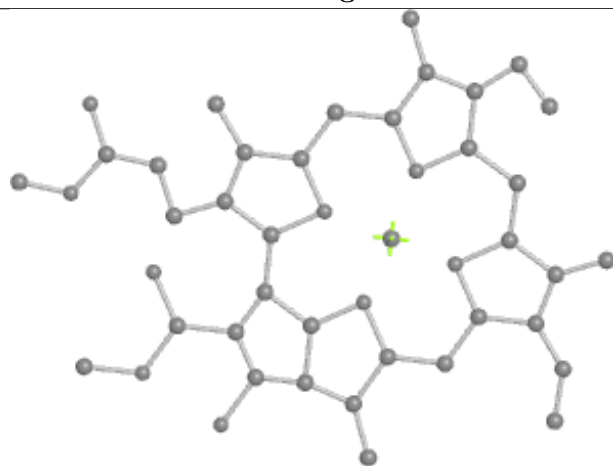
Bond lengths



Bond angles

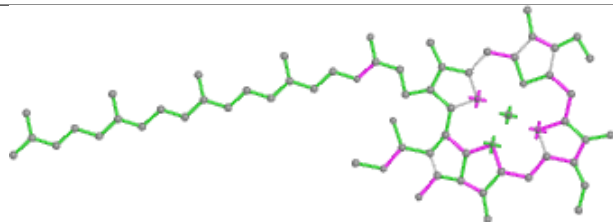


Torsions

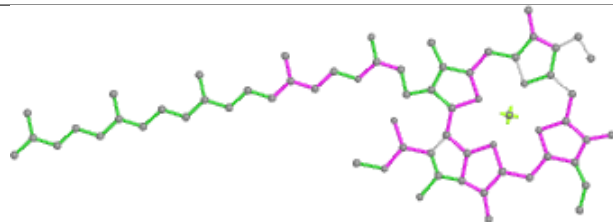


Rings

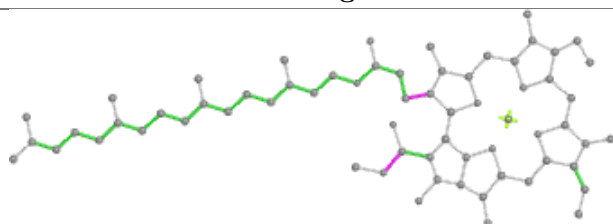
Ligand CHL A 848



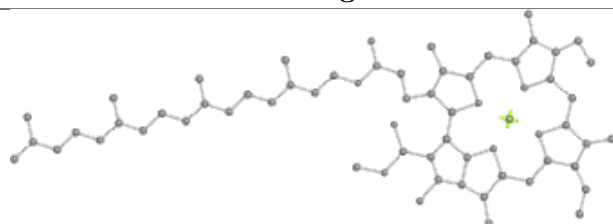
Bond lengths



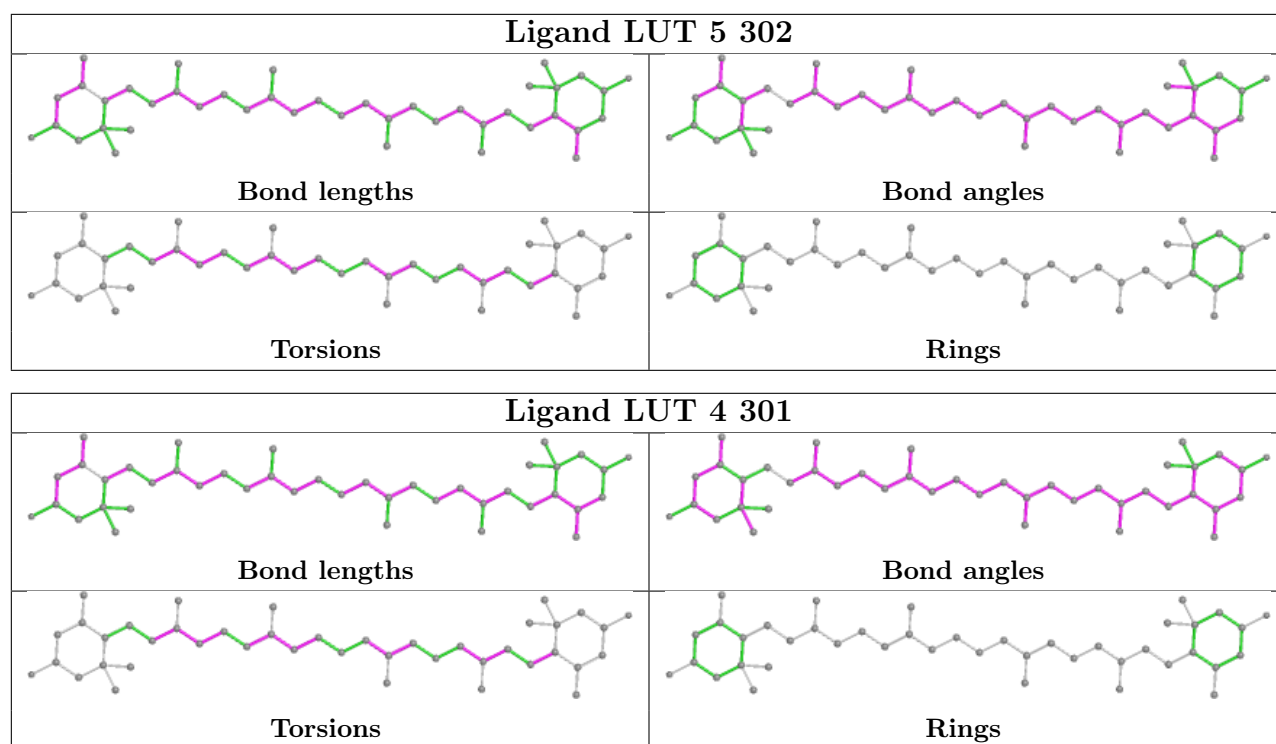
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

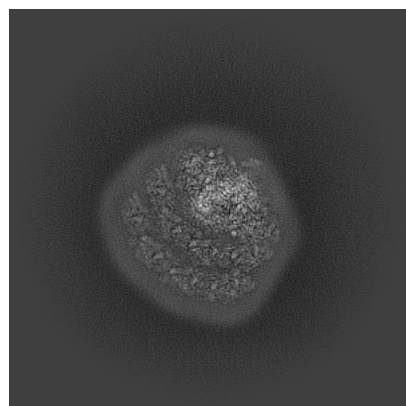
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62512. These allow visual inspection of the internal detail of the map and identification of artifacts.

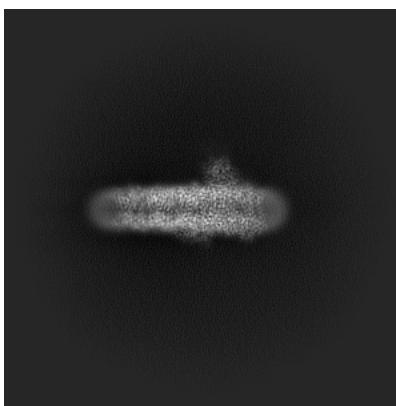
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

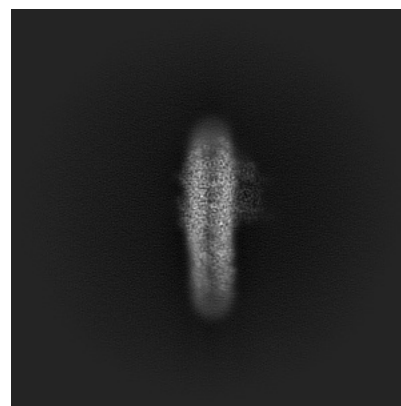
6.1.1 Primary map



X

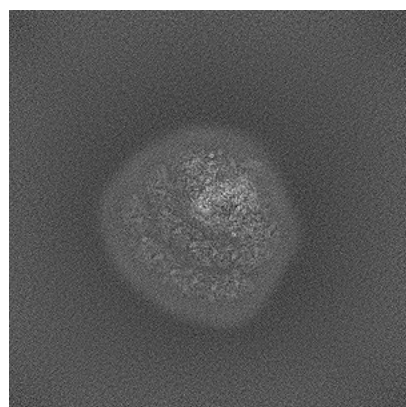


Y

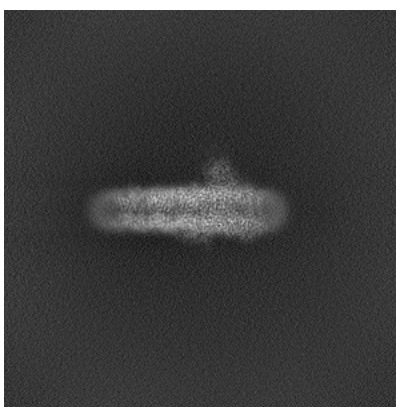


Z

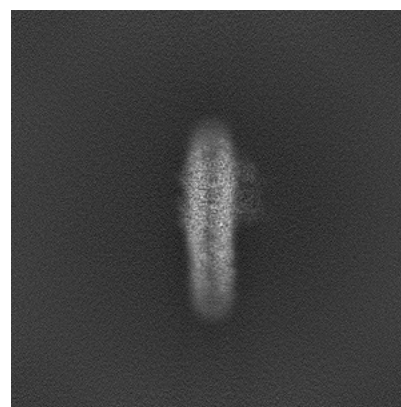
6.1.2 Raw map



X



Y

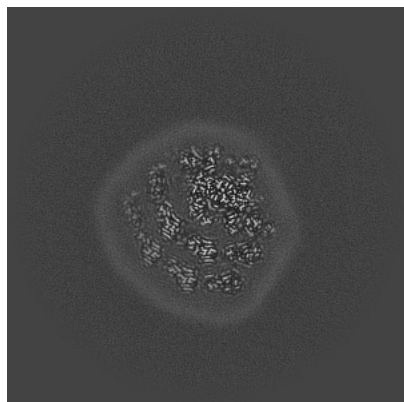


Z

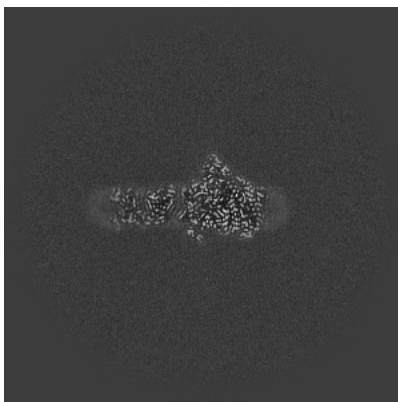
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

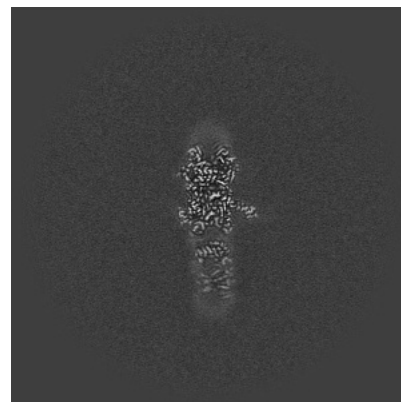
6.2.1 Primary map



X Index: 300

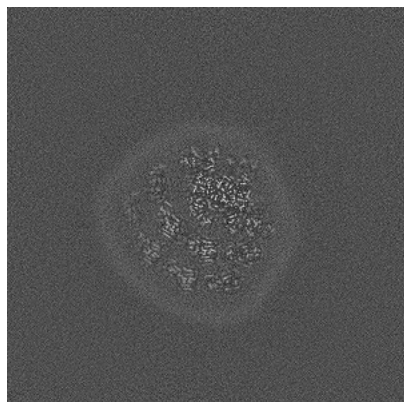


Y Index: 300

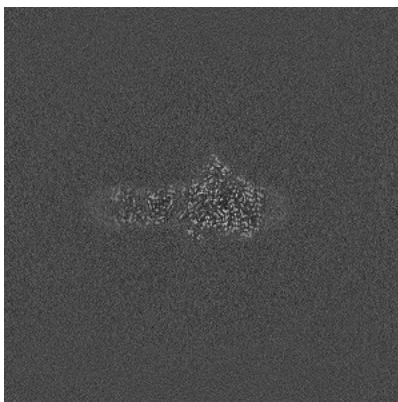


Z Index: 300

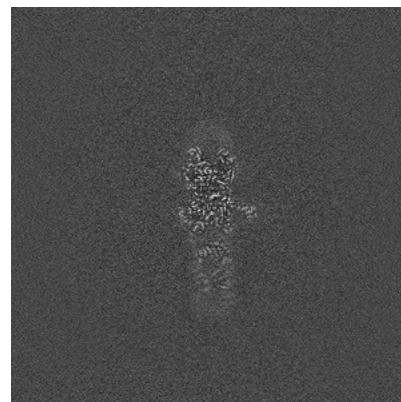
6.2.2 Raw map



X Index: 300



Y Index: 300

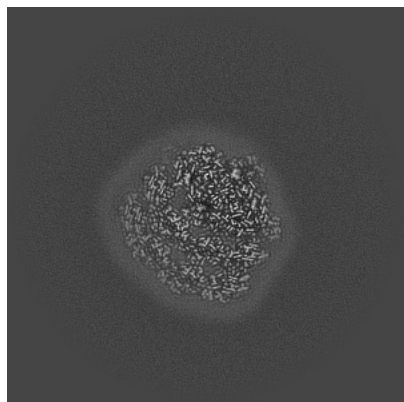


Z Index: 300

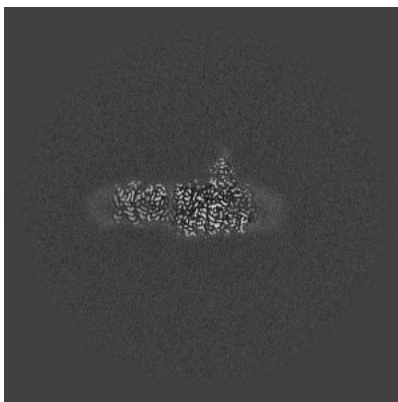
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

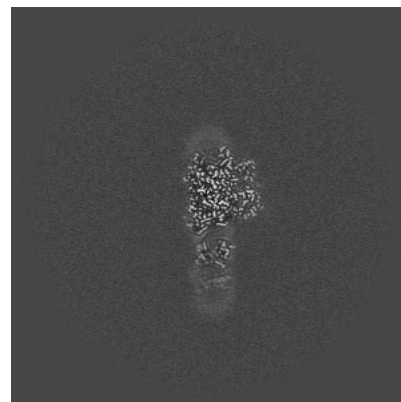
6.3.1 Primary map



X Index: 317

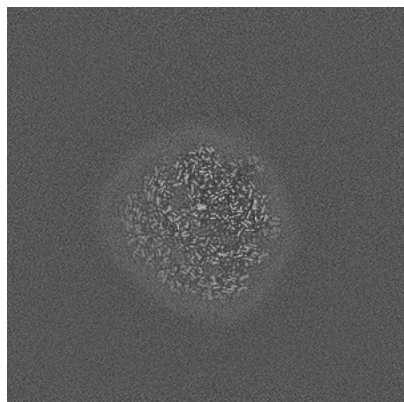


Y Index: 340

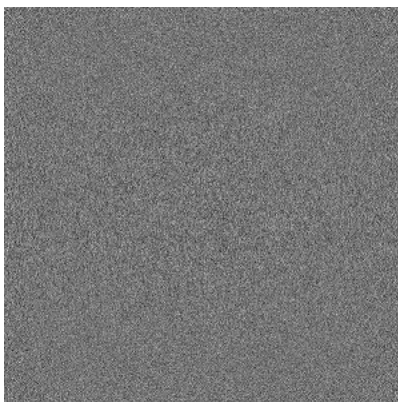


Z Index: 316

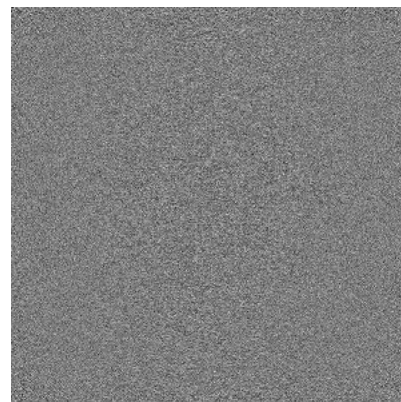
6.3.2 Raw map



X Index: 316



Y Index: 0

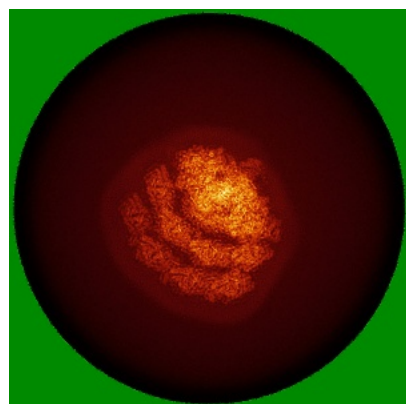


Z Index: 0

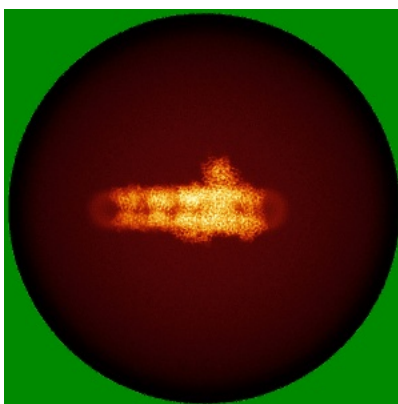
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

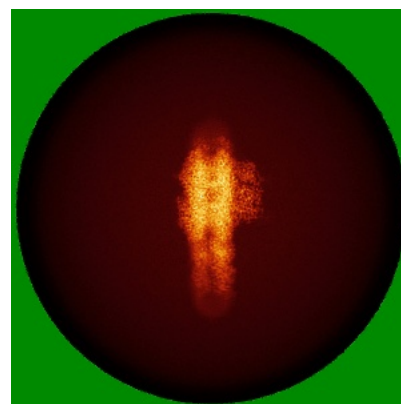
6.4.1 Primary map



X

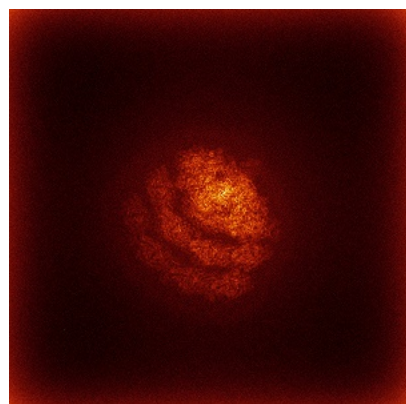


Y

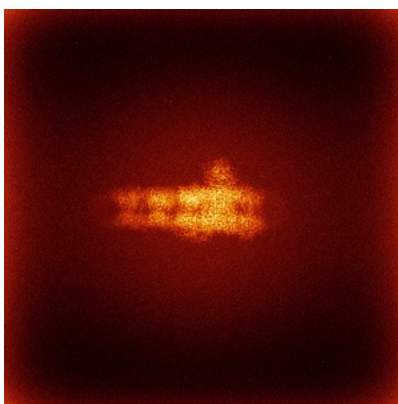


Z

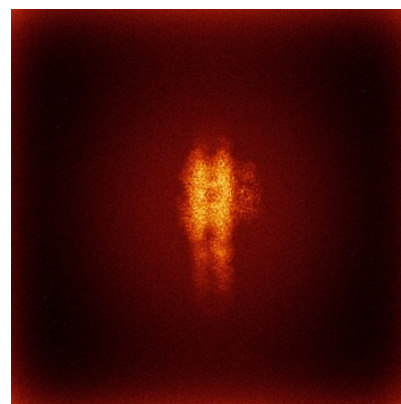
6.4.2 Raw map



X



Y

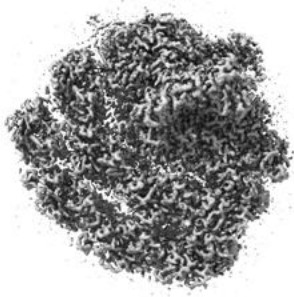


Z

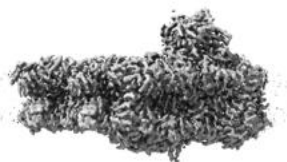
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



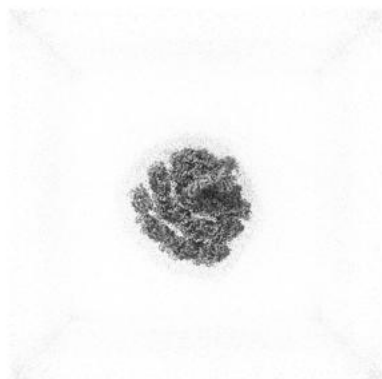
Y



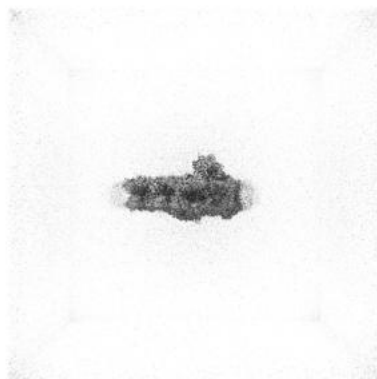
Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

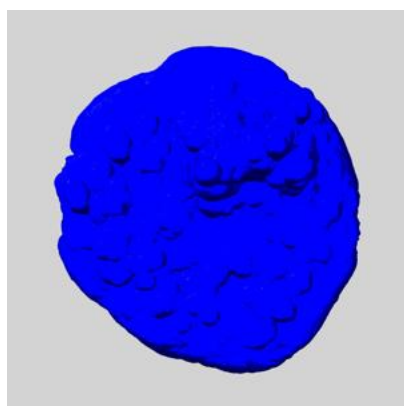
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

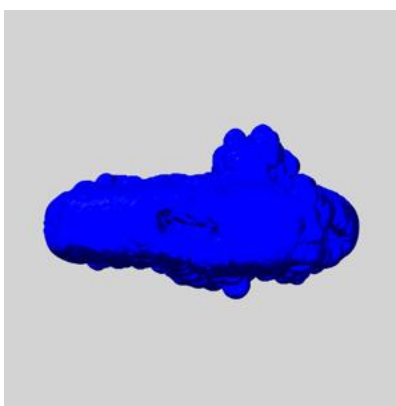
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

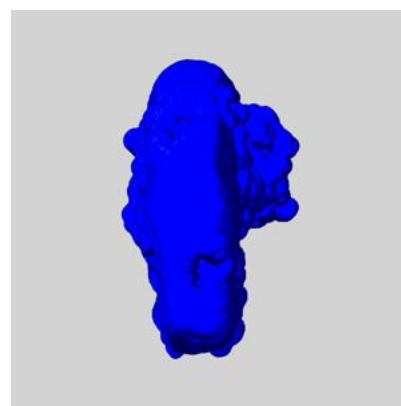
6.6.1 emd_62512_msk_1.map [i](#)



X



Y

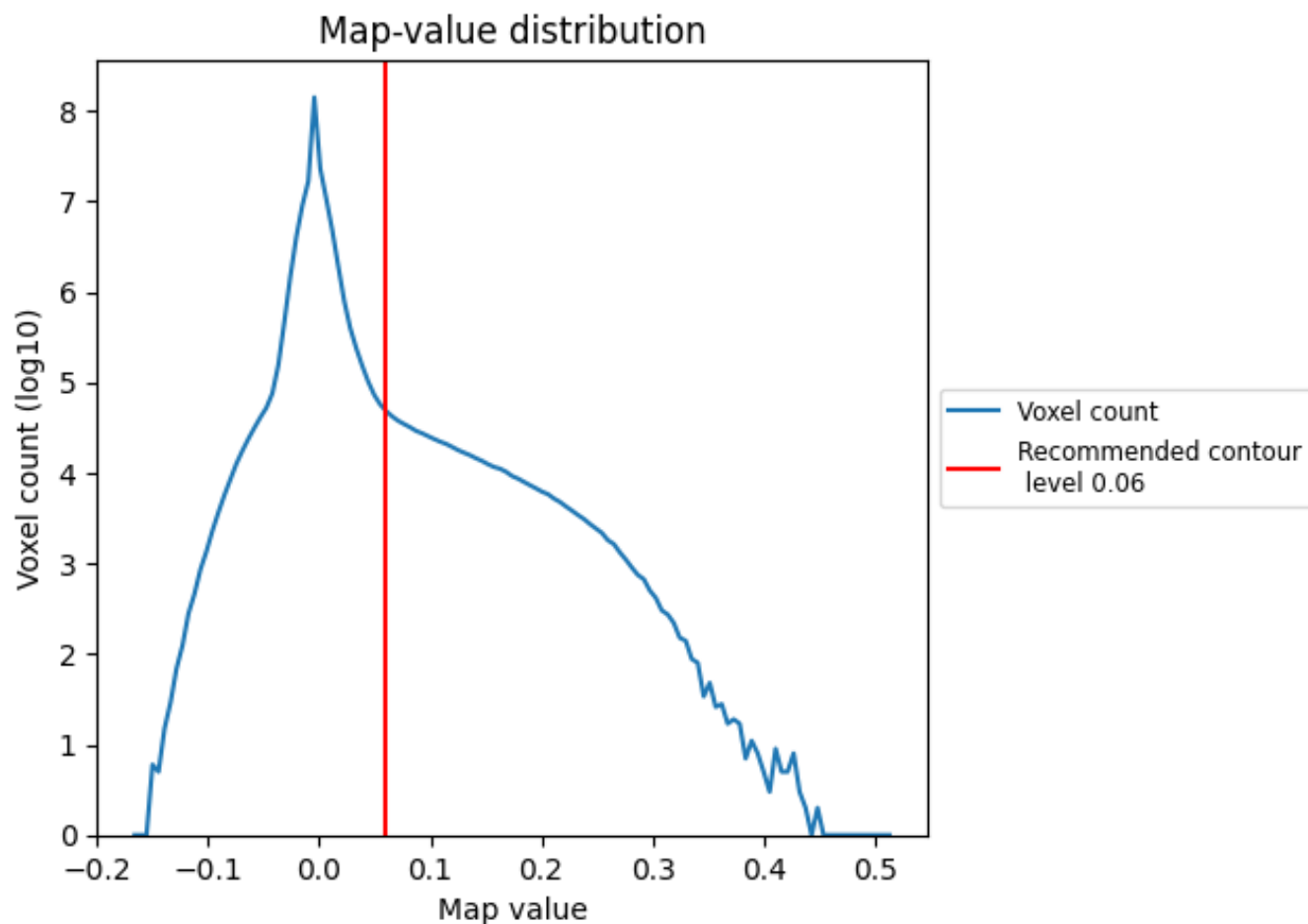


Z

7 Map analysis [i](#)

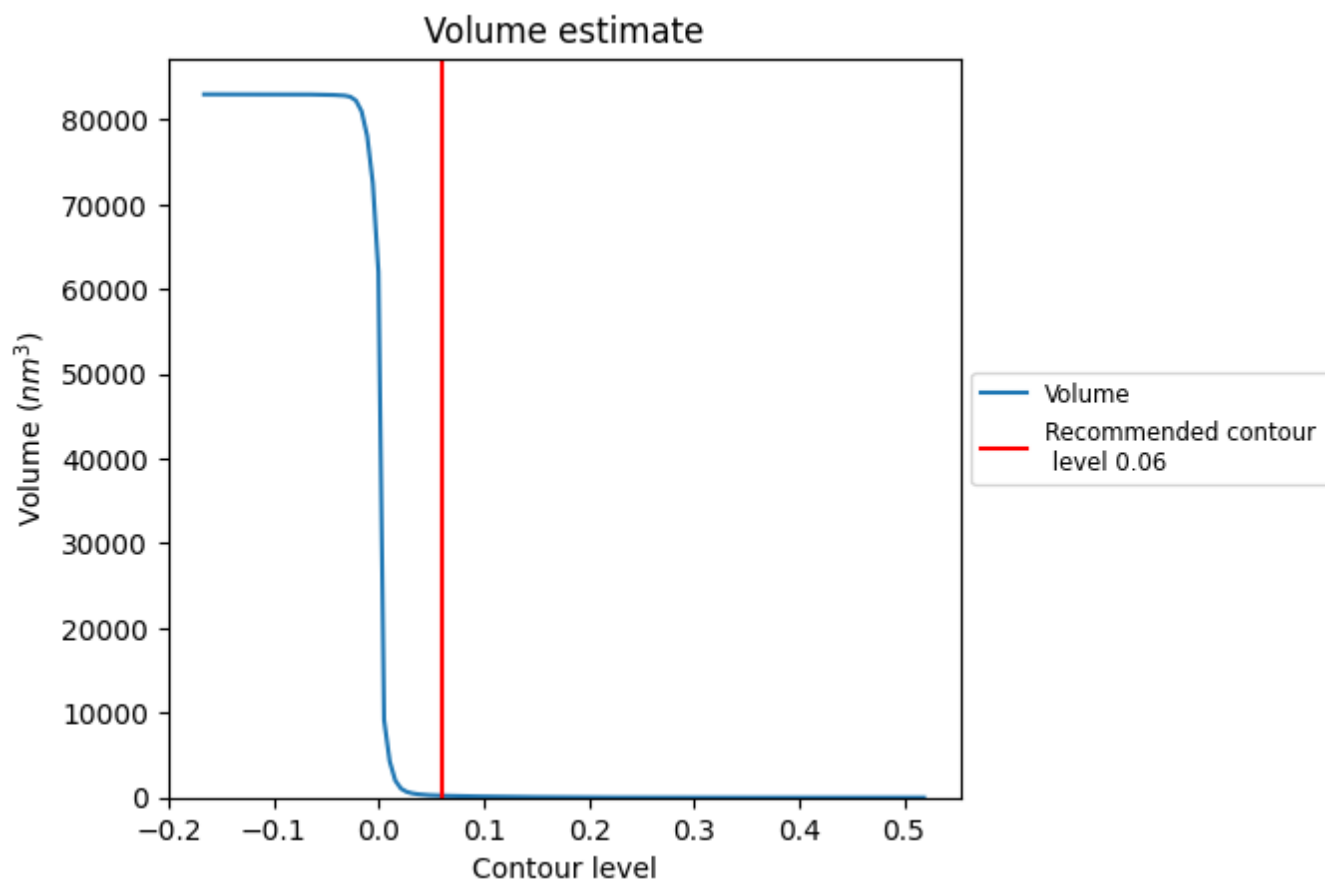
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

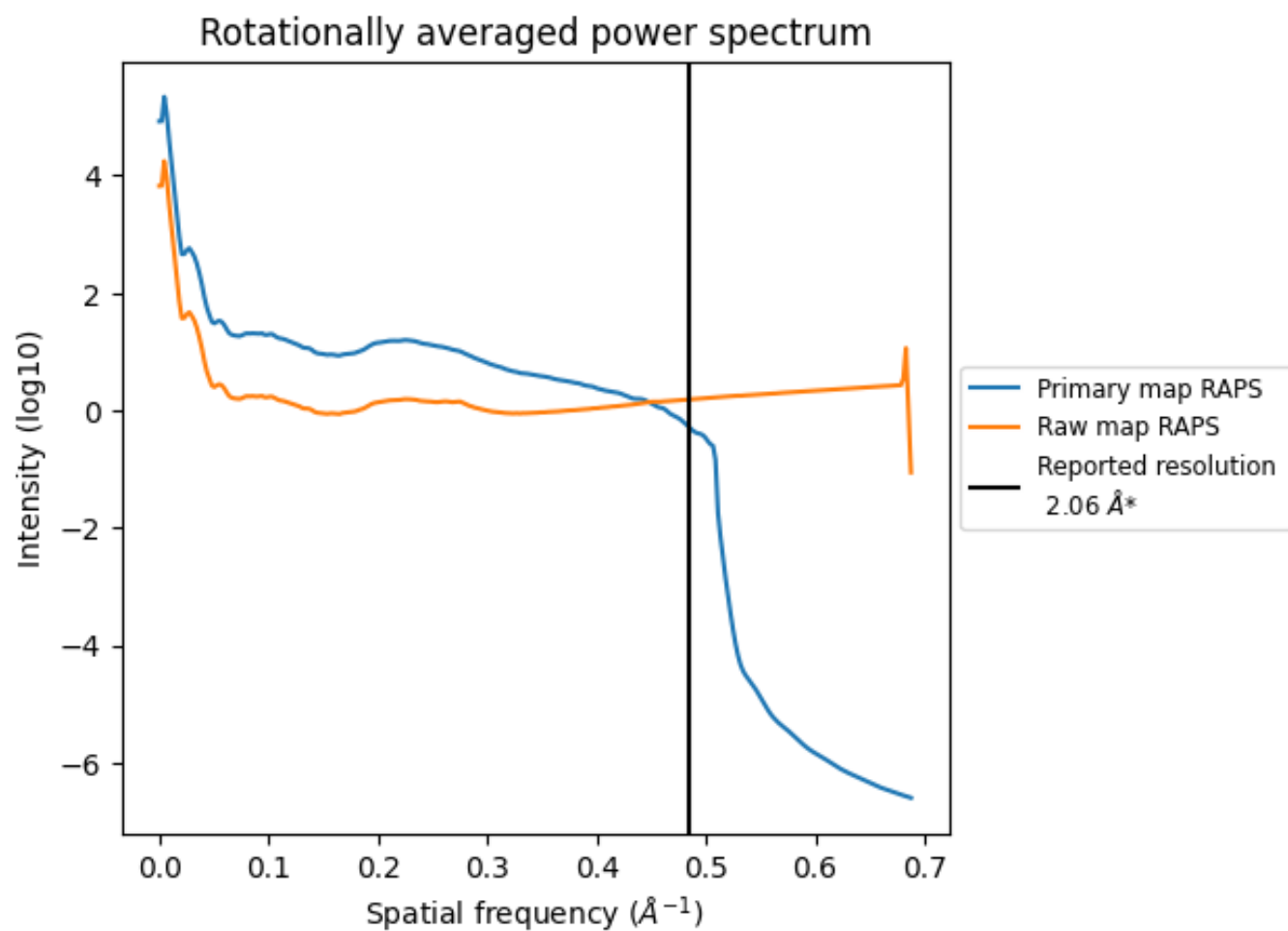
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 225 nm^3 ; this corresponds to an approximate mass of 203 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

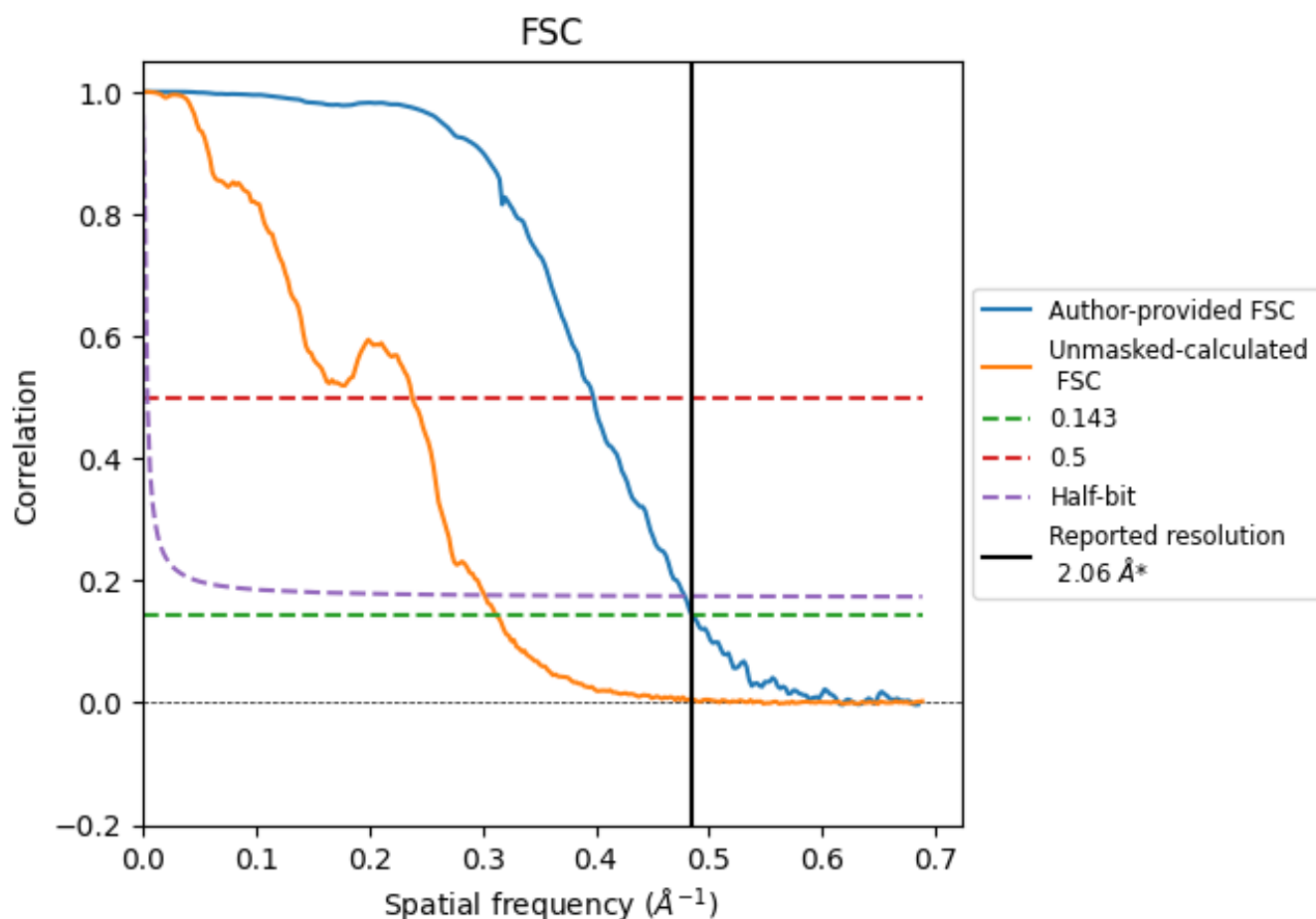


*Reported resolution corresponds to spatial frequency of 0.485 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.485 \AA^{-1}

8.2 Resolution estimates [i](#)

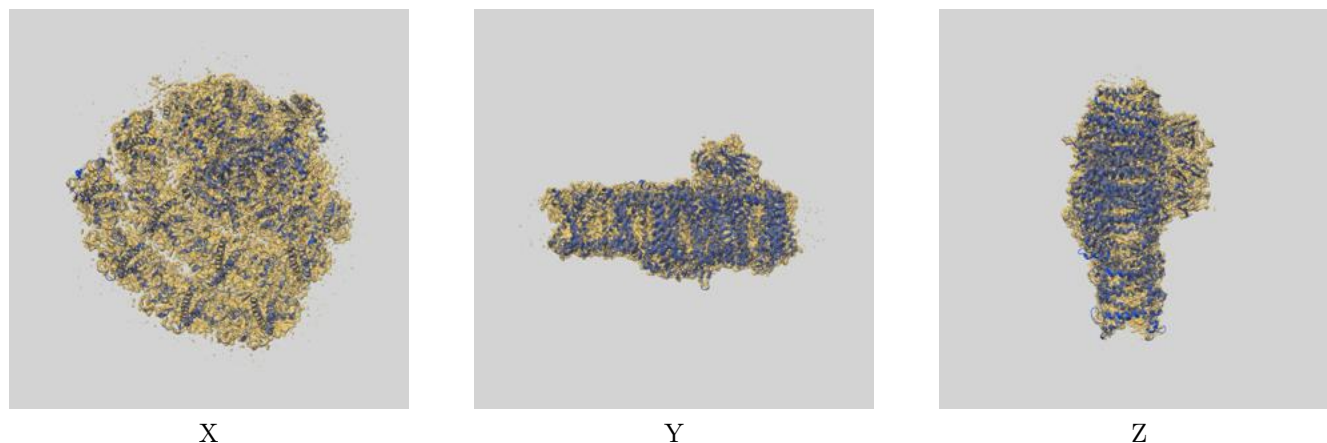
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.51	2.09
Unmasked-calculated*	3.20	4.20	3.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.06 by more than 10 %

9 Map-model fit [i](#)

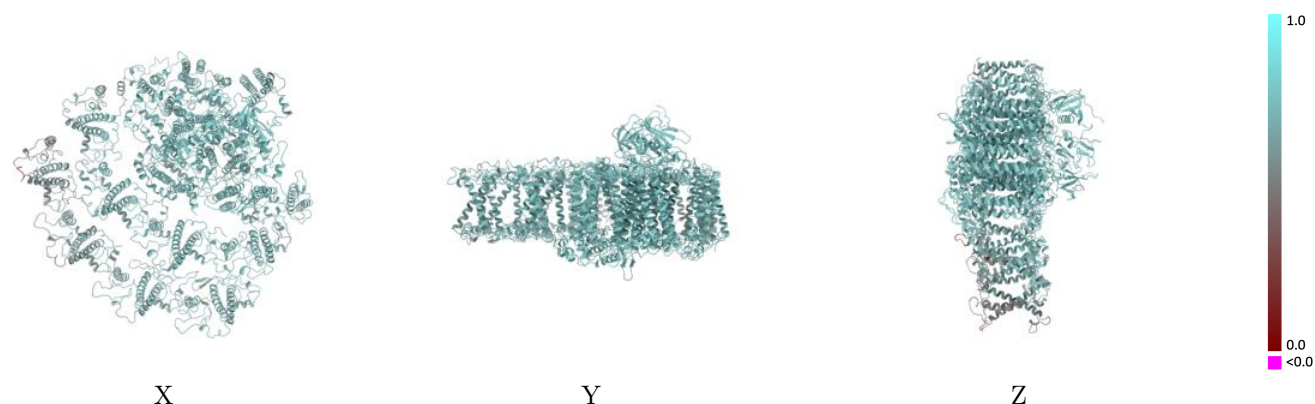
This section contains information regarding the fit between EMDB map EMD-62512 and PDB model 9KQQ. Per-residue inclusion information can be found in [section 3](#) on [page 36](#).

9.1 Map-model overlay [i](#)



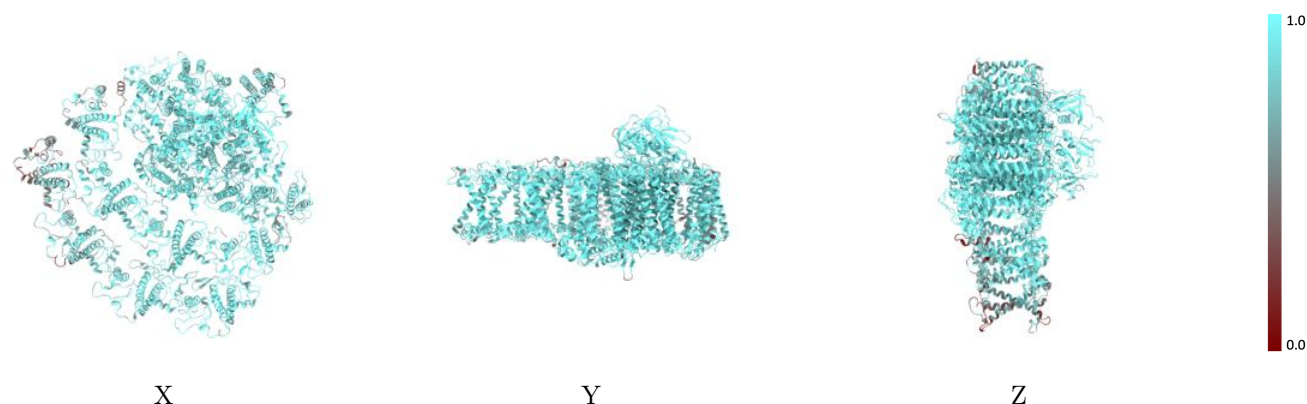
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



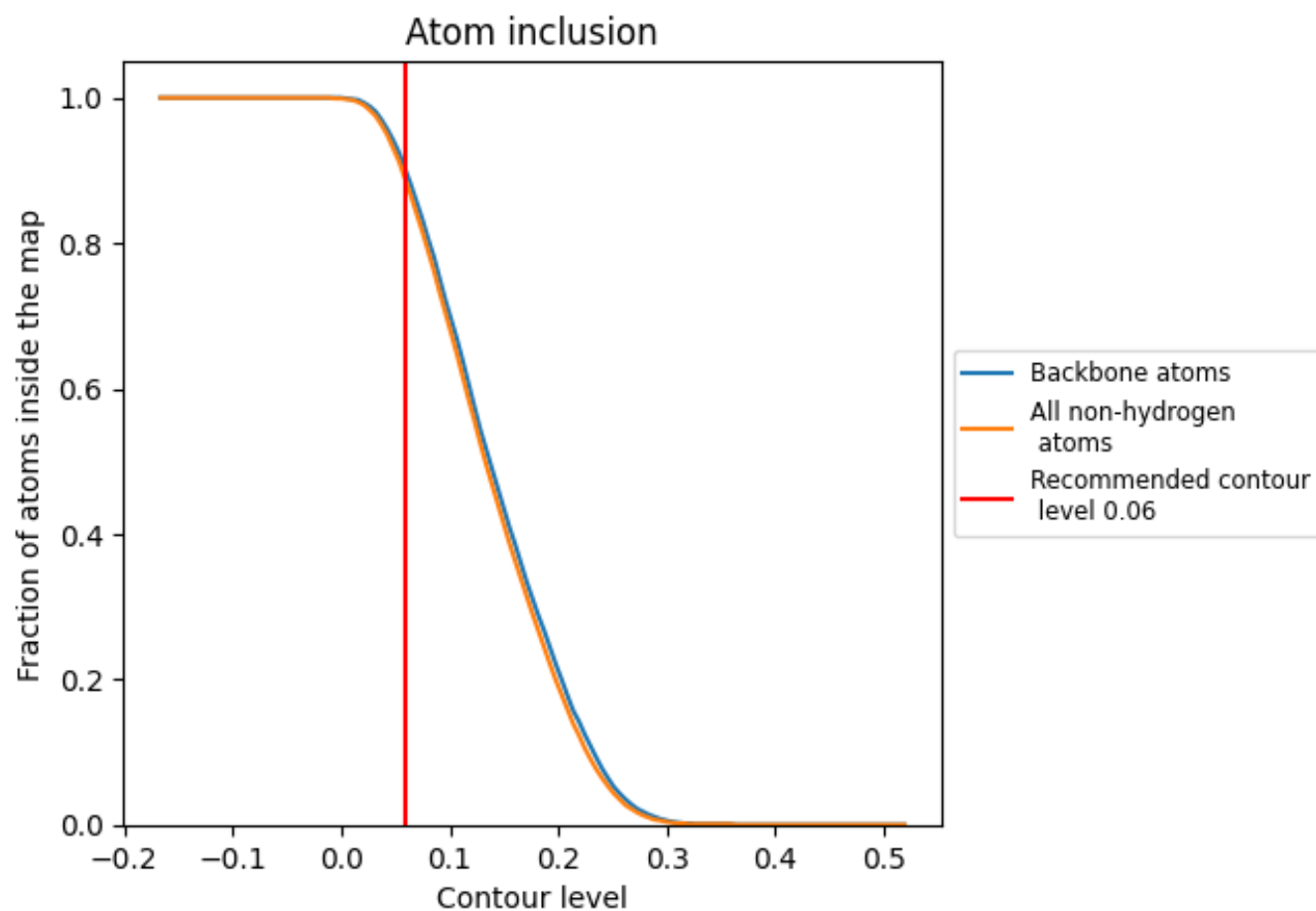
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).











































9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.6680
3	 0.8930	 0.6640
4	 0.7630	 0.5820
5	 0.8680	 0.6390
6	 0.8360	 0.6240
7	 0.9100	 0.6740
8	 0.8850	 0.6680
A	 0.9530	 0.7160
B	 0.9420	 0.7060
C	 0.9880	 0.7270
D	 0.9490	 0.7040
E	 0.9240	 0.6890
F	 0.9120	 0.6940
G	 0.4050	 0.5050
I	 0.9020	 0.6870
J	 0.9300	 0.6950
K	 0.8180	 0.6410
L	 0.8030	 0.6480
M	 0.8490	 0.6630
a	 0.8080	 0.6200
b	 0.6100	 0.5250

