



Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 12:28 PM JST

PDB ID : 7D1U / pdb_00007d1u
EMDB ID : EMD-30548
Title : Cryo-EM Structure of PSII at 2.08 angstrom resolution
Authors : Kato, K.; Miyazaki, N.; Hamaguchi, T.; Nakajima, Y.; Akita, F.; Yonekura, K.; Shen, J.R.
Deposited on : 2020-09-15
Resolution : 2.08 Å(reported)
Based on initial model : 3WU2

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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

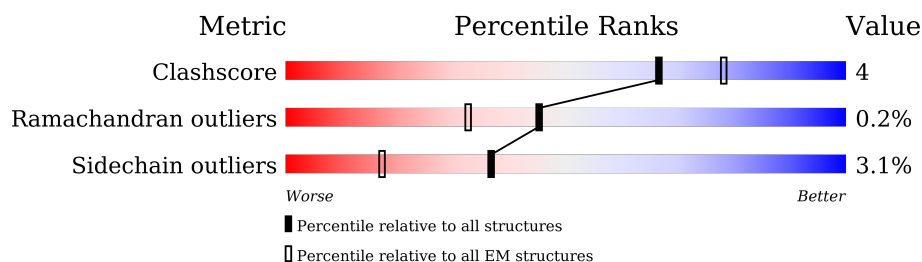
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.08 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)
Clashscore	210492	15764
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	334	93% 7%
1	a	334	93% 7%
2	B	505	91% 8% .
2	b	505	92% 8% .
3	C	451	92% 8%
3	c	451	91% 8%
4	D	342	92% 8%
4	d	342	91% 8%

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Mol	Chain	Length	Quality of chain
5	E	81	
5	e	81	
6	F	34	
6	f	34	
7	H	63	
7	h	63	
8	I	36	
8	i	36	
9	J	37	
9	j	37	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	244	
13	o	244	
14	T	31	
14	t	31	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	

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Mol	Chain	Length	Quality of chain
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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
24	CLA	A	405	X	-	-	-
24	CLA	A	408	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	405	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 52655 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2620	1716	431	458	15		
1	a	334	Total	C	N	O	S	0	0
			2620	1716	431	458	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	0	0
			3969	2605	661	690	13		
2	b	504	Total	C	N	O	S	0	0
			3969	2605	661	690	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3486	2281	584	608	13		
3	c	451	Total	C	N	O	S	0	0
			3486	2281	584	608	13		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2718	1800	444	462	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	341	Total	C	N	O	S	0	0
			2718	1800	444	462	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	81	Total	C	N	O		0	0
			661	432	107	122			
5	e	81	Total	C	N	O		0	0
			661	432	107	122			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	34	Total	C	N	O	S	0	0
			275	187	45	42	1		
6	f	34	Total	C	N	O	S	0	0
			275	187	45	42	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	63	Total	C	N	O	S	0	0
			498	333	80	83	2		
7	h	63	Total	C	N	O	S	0	0
			498	333	80	83	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	36	Total	C	N	O	S	0	0
			296	200	46	49	1		
8	i	36	Total	C	N	O	S	0	0
			296	200	46	49	1		

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	36	Total	C	N	O	S	0	0
			257	174	40	42	1		
9	j	36	Total	C	N	O	S	0	0
			257	174	40	42	1		

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			293	204	43	46		
10	k	37	Total	C	N	O	0	0
			293	204	43	46		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	37	Total	C	N	O	S	0	0
			304	202	48	53	1		
11	l	37	Total	C	N	O	S	0	0
			304	202	48	53	1		

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	33	Total	C	N	O	S	0	0
			260	173	38	48	1		
12	m	33	Total	C	N	O	S	0	0
			260	173	38	48	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	244	Total	C	N	O	S	0	0
			1874	1170	317	383	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	o	244	Total	C	N	O	S	0	0
			1874	1170	317	383	4		

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total	C	N	O	S	0	0
			258	181	36	39	2		
14	t	30	Total	C	N	O	S	0	0
			258	181	36	39	2		

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	97	Total	C	N	O	S	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	S	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	137	Total	C	N	O	S	0	0
			1064	675	177	208	4		
16	v	137	Total	C	N	O	S	0	0
			1064	675	177	208	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0
			200	131	35	31	3		
17	y	27	Total	C	N	O	S	0	0
			200	131	35	31	3		

- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	38	Total	C	N	O	S	0	0
			281	188	45	48			
18	x	38	Total	C	N	O	S	0	0
			281	188	45	48			

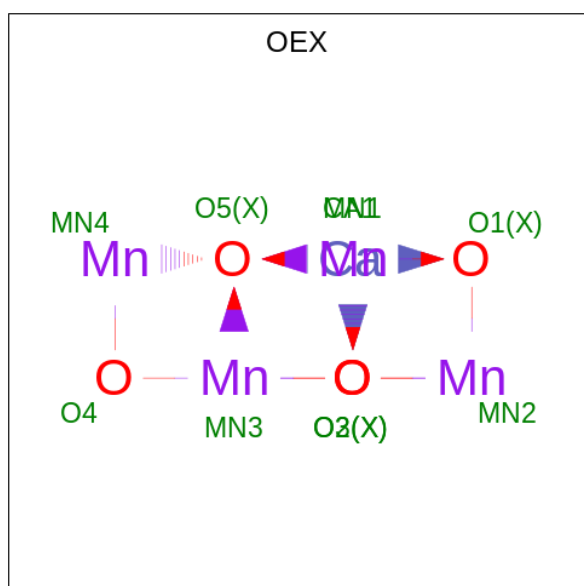
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0
			479	328	72	77	2		
19	z	62	Total	C	N	O	S	0	0
			479	328	72	77	2		

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	34	Total	C	N	O	0	0
			273	186	47	40		
20	r	34	Total	C	N	O	0	0
			273	186	47	40		

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
21	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

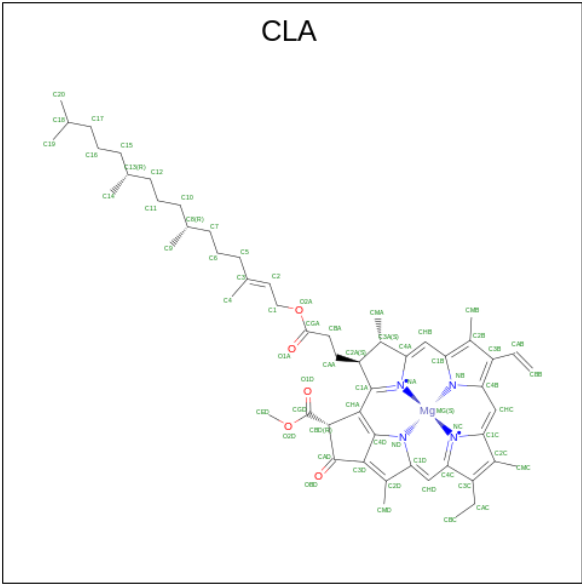
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	Fe	0
			1	1	
22	a	1	Total	Fe	0
			1	1	

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Cl	0
			2	2	
23	a	2	Total	Cl	0
			2	2	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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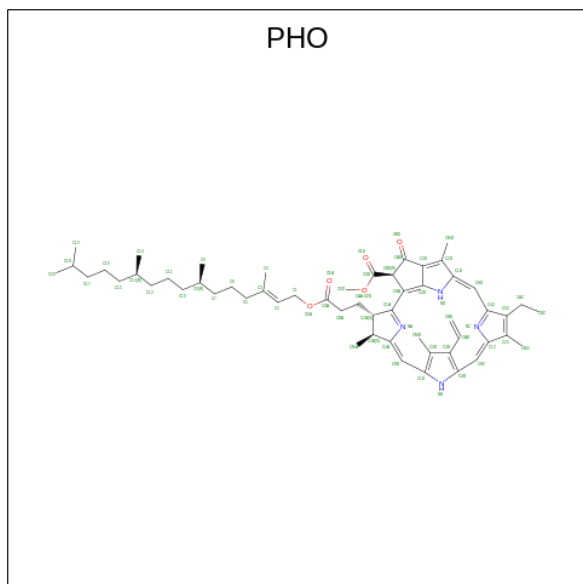
Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0

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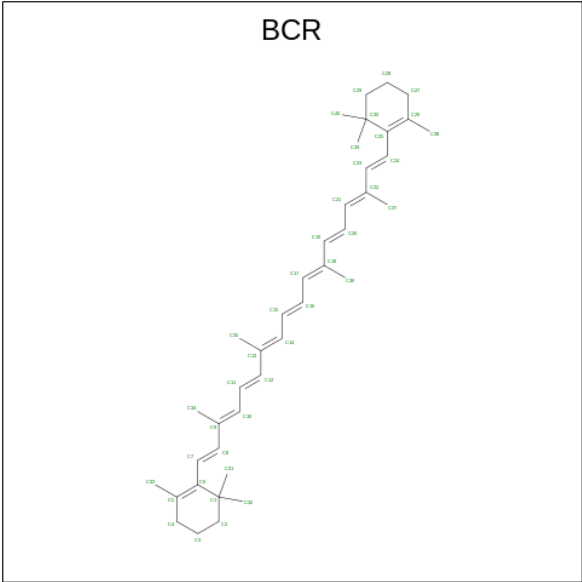
Mol	Chain	Residues	Atoms					AltConf
24	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	N	O	0
			64	55	4	5	
25	D	1	Total	C	N	O	0
			64	55	4	5	
25	a	1	Total	C	N	O	0
			64	55	4	5	
25	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



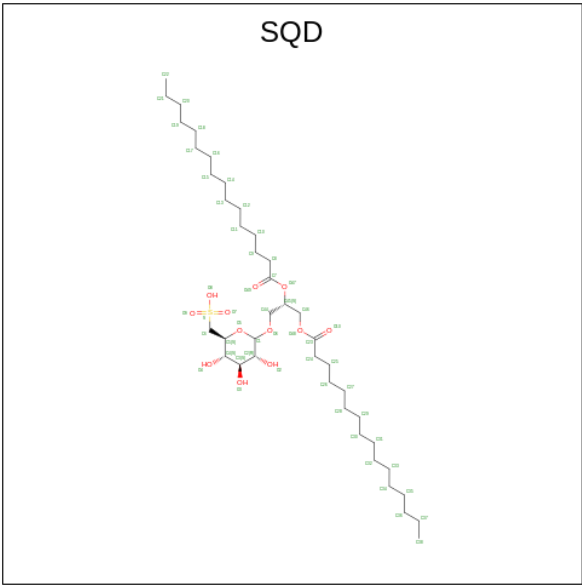
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	D	1	Total C 40 40	0
26	T	1	Total C 40 40	0
26	Y	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	b	1	Total C 40 40	0
26	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
26	b	1	Total C 40 40	0
26	c	1	Total C 40 40	0
26	c	1	Total C 40 40	0
26	c	1	Total C 40 40	0
26	d	1	Total C 40 40	0
26	y	1	Total C 40 40	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



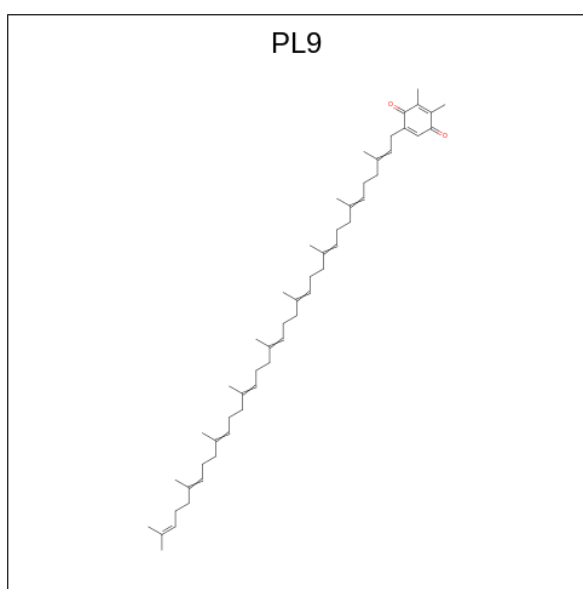
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C O S 54 41 12 1	0
27	A	1	Total C O S 54 41 12 1	0
27	D	1	Total C O S 45 32 12 1	0
27	L	1	Total C O S 54 41 12 1	0
27	a	1	Total C O S 54 41 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	C	O	S	0
			54	41	12	1	
27	d	1	Total	C	O	S	0
			45	32	12	1	
27	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O		0
			55	53	2		
28	D	1	Total	C	O		0
			55	53	2		
28	a	1	Total	C	O		0
			55	53	2		
28	d	1	Total	C	O		0
			55	53	2		

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

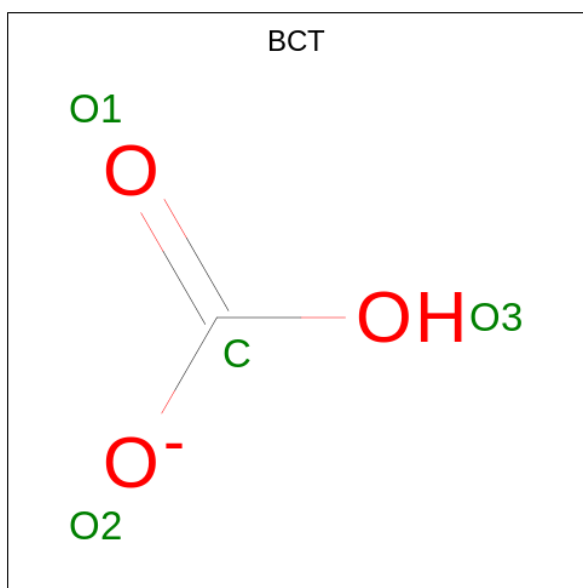
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O		0
			36	31	5		

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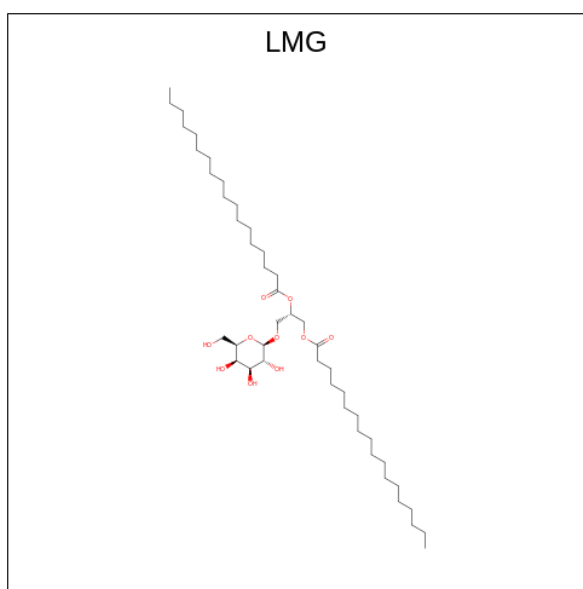
Mol	Chain	Residues	Atoms			AltConf
29	B	6	Total	C	O	0
			85	80	5	
29	C	1	Total	C		0
			10	10		
29	D	1	Total	C	O	0
			40	35	5	
29	E	1	Total	C		0
			10	10		
29	I	2	Total	C		0
			17	17		
29	J	1	Total	C		0
			10	10		
29	K	1	Total	C	O	0
			34	29	5	
29	M	1	Total	C		0
			10	10		
29	T	2	Total	C		0
			26	26		
29	X	1	Total	C		0
			10	10		
29	a	1	Total	C	O	0
			36	31	5	
29	b	6	Total	C	O	0
			85	80	5	
29	c	1	Total	C		0
			10	10		
29	d	1	Total	C	O	0
			40	35	5	
29	e	1	Total	C		0
			10	10		
29	i	2	Total	C		0
			17	17		
29	j	1	Total	C		0
			10	10		
29	k	1	Total	C	O	0
			34	29	5	
29	m	1	Total	C		0
			10	10		
29	t	2	Total	C		0
			26	26		
29	x	1	Total	C		0
			10	10		

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



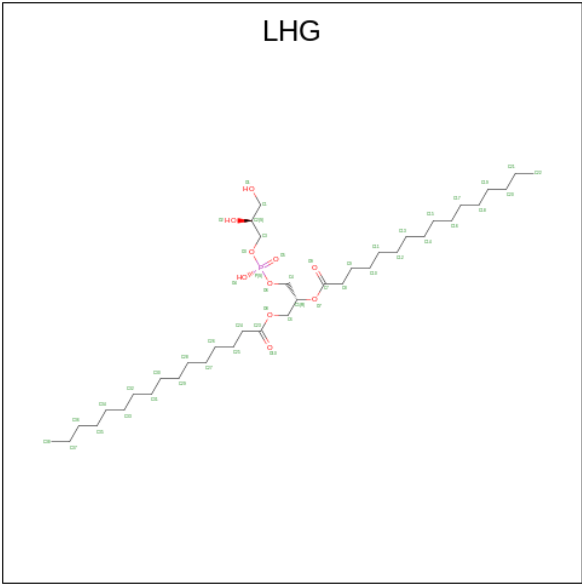
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			4	1	3	
30	a	1	Total	C	O	0
			4	1	3	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			51	41	10	
31	C	1	Total	C	O	0
			51	41	10	
31	C	1	Total	C	O	0
			51	41	10	
31	C	1	Total	C	O	0
			51	41	10	
31	D	1	Total	C	O	0
			51	41	10	
31	b	1	Total	C	O	0
			51	41	10	
31	c	1	Total	C	O	0
			51	41	10	
31	c	1	Total	C	O	0
			51	41	10	
31	c	1	Total	C	O	0
			51	41	10	
31	d	1	Total	C	O	0
			51	41	10	

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



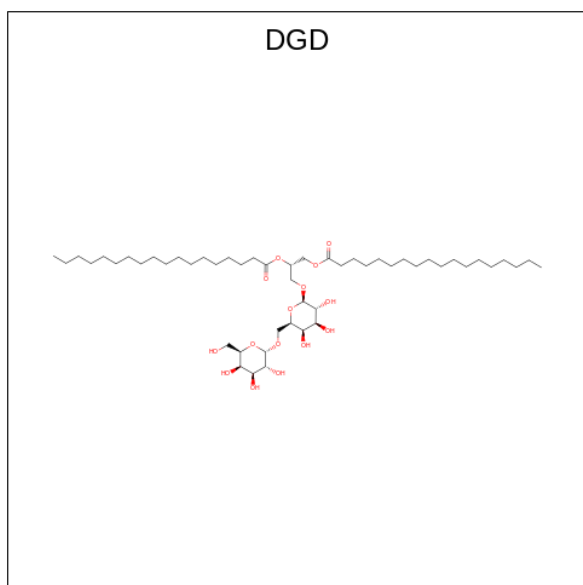
Mol	Chain	Residues	Atoms				AltConf
32	B	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
32	D	1	Total	C	O	P	0
			49	38	10	1	
32	D	1	Total	C	O	P	0
			49	38	10	1	
32	D	1	Total	C	O	P	0
			46	35	10	1	
32	E	1	Total	C	O	P	0
			49	38	10	1	
32	b	1	Total	C	O	P	0
			49	38	10	1	
32	d	1	Total	C	O	P	0
			49	38	10	1	
32	d	1	Total	C	O	P	0
			49	38	10	1	
32	d	1	Total	C	O	P	0
			46	35	10	1	
32	e	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



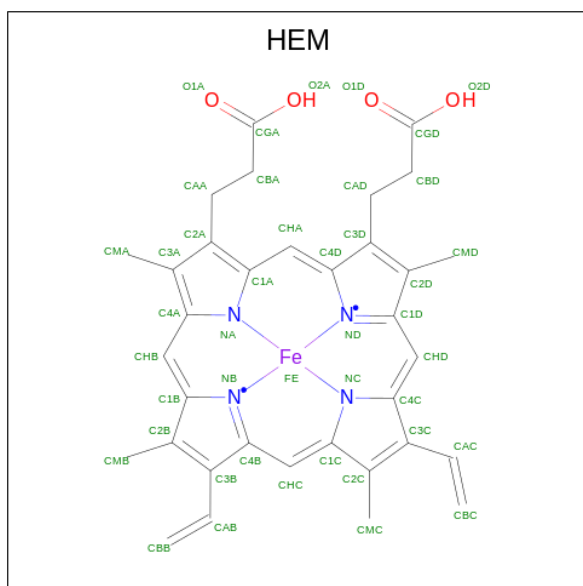
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			62	47	15	
33	C	1	Total	C	O	0
			62	47	15	

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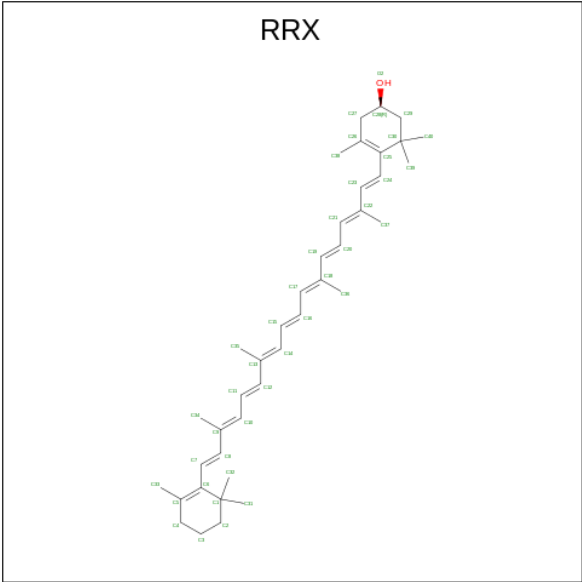
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total 62	C 47	O 15	0
33	H	1	Total 62	C 47	O 15	0
33	c	1	Total 62	C 47	O 15	0
33	c	1	Total 62	C 47	O 15	0
33	c	1	Total 62	C 47	O 15	0
33	h	1	Total 62	C 47	O 15	0

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



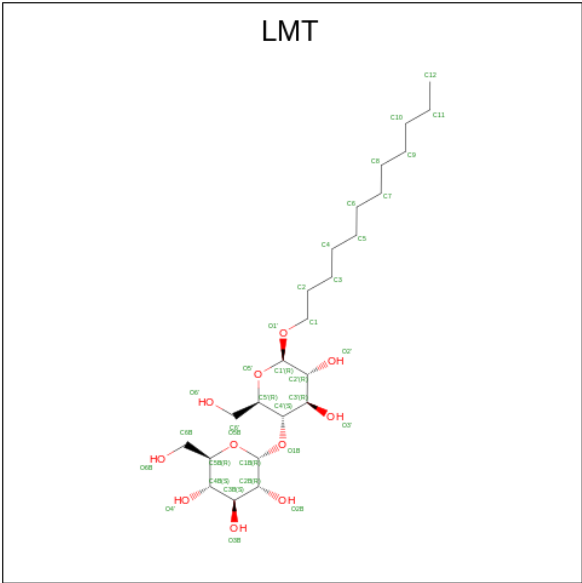
Mol	Chain	Residues	Atoms					AltConf
34	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
34	e	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



Mol	Chain	Residues	Atoms			AltConf
35	H	1	Total	C	O	0
			41	40	1	
35	h	1	Total	C	O	0
			41	40	1	

- Molecule 36 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
36	I	1	Total	C	O	0
			35	24	11	
36	J	1	Total	C	O	0
			24	18	6	

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Mol	Chain	Residues	Atoms			AltConf
36	M	1	Total 35	C 24	O 11	0
36	Z	1	Total 35	C 24	O 11	0
36	i	1	Total 35	C 24	O 11	0
36	j	1	Total 24	C 18	O 6	0
36	m	1	Total 35	C 24	O 11	0
36	z	1	Total 35	C 24	O 11	0

- | Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 37 | J | 1 | Total
1 | Mg
1 | 0 |
| 37 | j | 1 | Total
1 | Mg
1 | 0 |

- [illegible]

Mol	Chain	Residues	Atoms					AltConf
38	V	1	Total 43	C 34	Fe 1	N 4	O 4	0



WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					AltConf
38	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	142	Total	O	0
			142	142	
39	B	252	Total	O	0
			252	252	
39	C	184	Total	O	0
			184	184	
39	D	145	Total	O	0
			145	145	
39	E	21	Total	O	0
			21	21	
39	F	2	Total	O	0
			2	2	
39	H	34	Total	O	0
			34	34	
39	I	13	Total	O	0
			13	13	
39	J	5	Total	O	0
			5	5	
39	K	3	Total	O	0
			3	3	
39	L	15	Total	O	0
			15	15	
39	M	6	Total	O	0
			6	6	
39	O	104	Total	O	0
			104	104	
39	T	9	Total	O	0
			9	9	
39	U	56	Total	O	0
			56	56	
39	V	63	Total	O	0
			63	63	
39	X	6	Total	O	0
			6	6	
39	a	141	Total	O	0
			141	141	

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Mol	Chain	Residues	Atoms		AltConf
39	b	253	Total 253	O 253	0
39	c	184	Total 184	O 184	0
39	d	145	Total 145	O 145	0
39	e	21	Total 21	O 21	0
39	f	2	Total 2	O 2	0
39	h	34	Total 34	O 34	0
39	i	13	Total 13	O 13	0
39	j	5	Total 5	O 5	0
39	k	3	Total 3	O 3	0
39	l	15	Total 15	O 15	0
39	m	6	Total 6	O 6	0
39	o	105	Total 105	O 105	0
39	t	9	Total 9	O 9	0
39	u	56	Total 56	O 56	0
39	v	63	Total 63	O 63	0
39	x	6	Total 6	O 6	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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 II protein D1

Chain A: 




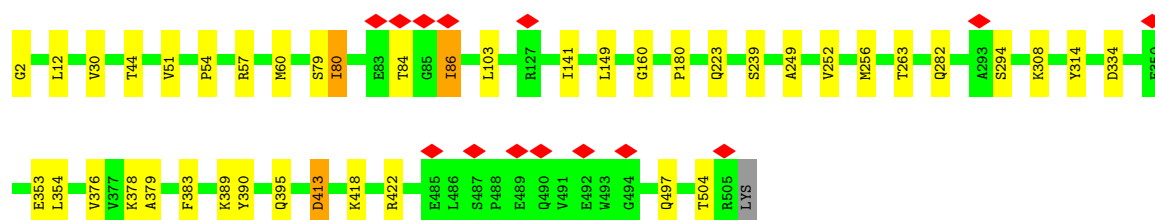
- Molecule 1: Photosystem II protein D1

Chain a: 



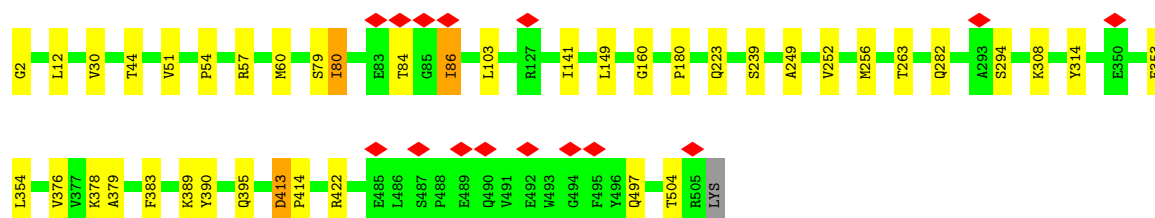
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

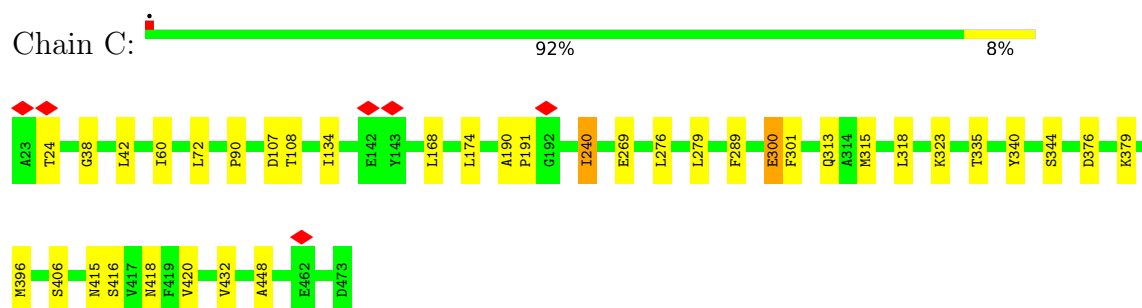


- Molecule 2: Photosystem II CP47 reaction center protein

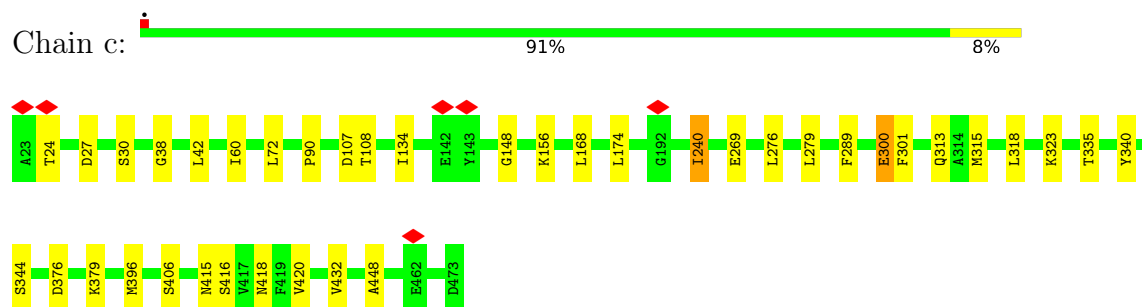
Chain b: 



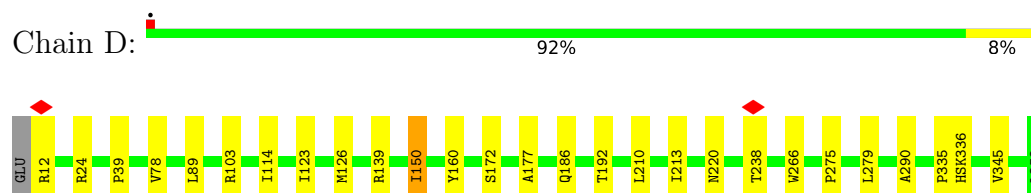
- Molecule 3: Photosystem II CP43 reaction center protein



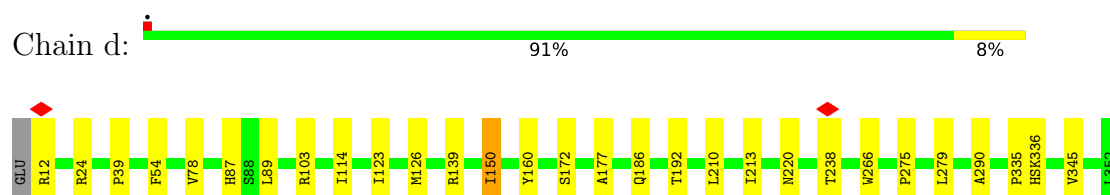
- Molecule 3: Photosystem II CP43 reaction center protein



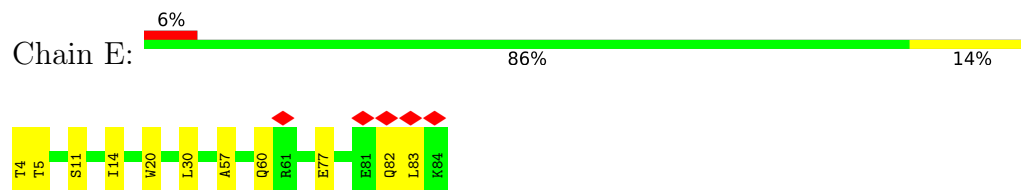
- Molecule 4: Photosystem II D2 protein



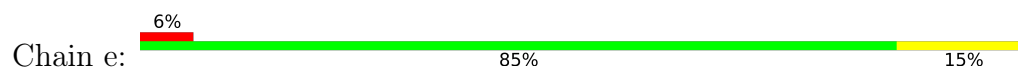
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha

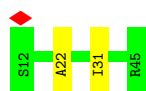


- Molecule 5: Cytochrome b559 subunit alpha

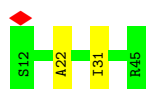




- Molecule 6: Cytochrome b559 subunit beta



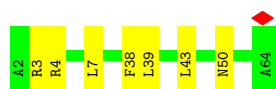
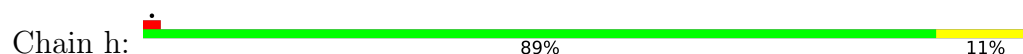
- Molecule 6: Cytochrome b559 subunit beta



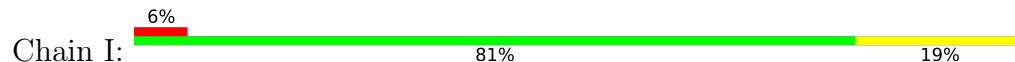
- Molecule 7: Photosystem II reaction center protein H



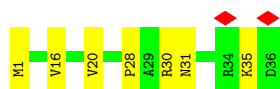
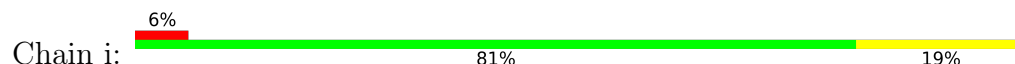
- Molecule 7: Photosystem II reaction center protein H



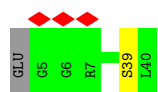
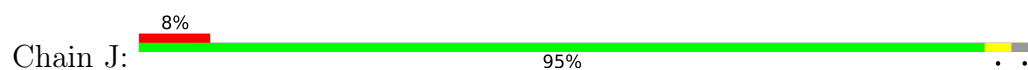
- Molecule 8: Photosystem II reaction center protein I



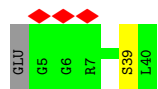
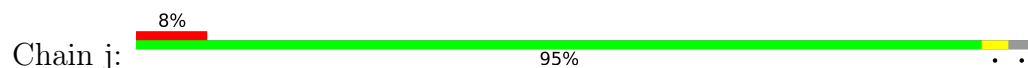
- Molecule 8: Photosystem II reaction center protein I



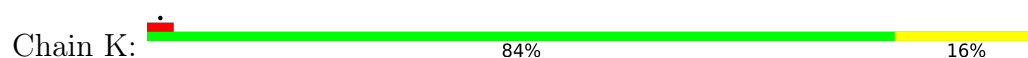
- Molecule 9: Photosystem II reaction center protein J



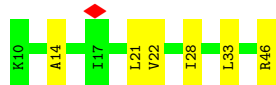
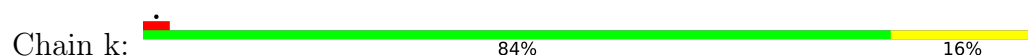
- Molecule 9: Photosystem II reaction center protein J



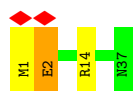
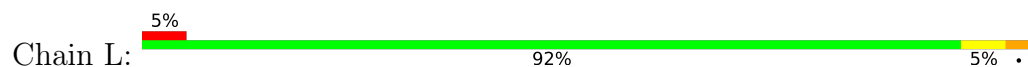
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



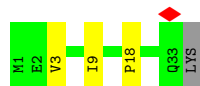
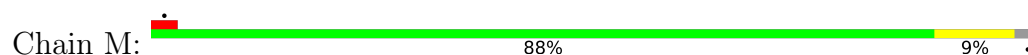
- Molecule 11: Photosystem II reaction center protein L



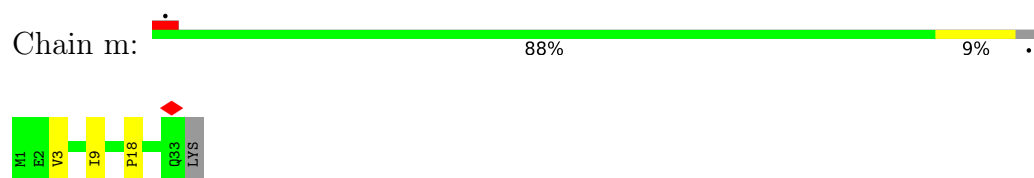
- Molecule 11: Photosystem II reaction center protein L



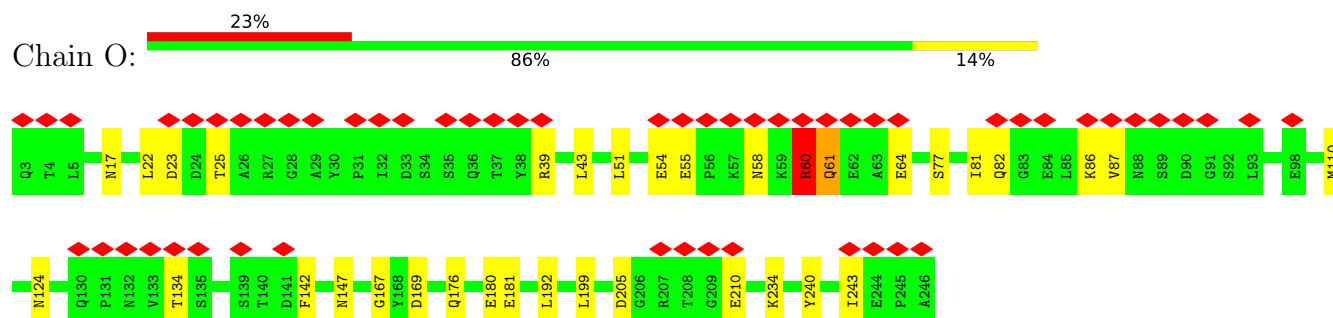
- Molecule 12: Photosystem II reaction center protein M



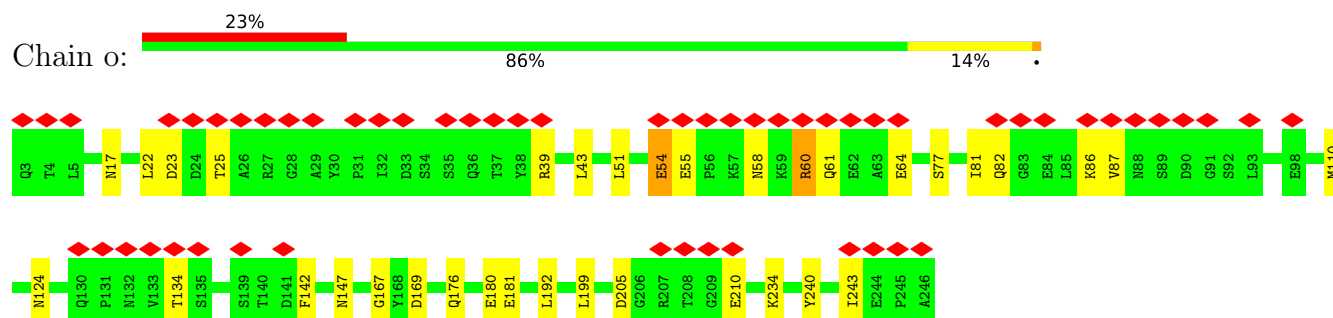
- Molecule 12: Photosystem II reaction center protein M



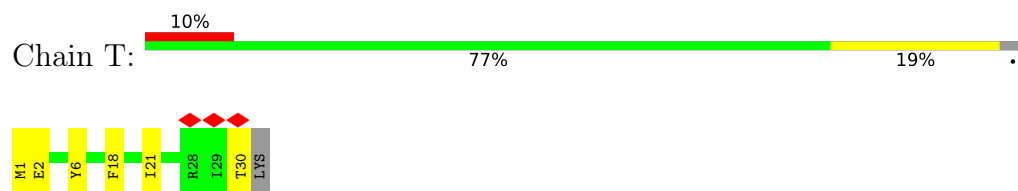
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



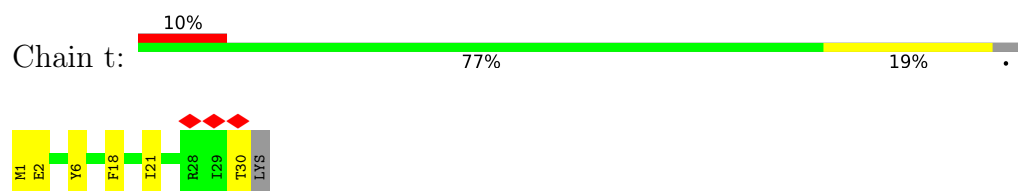
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



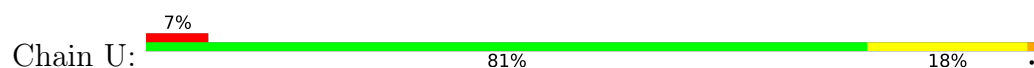
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

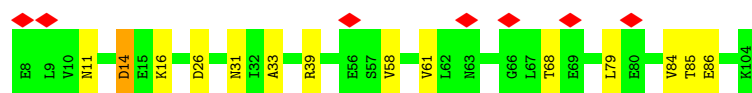
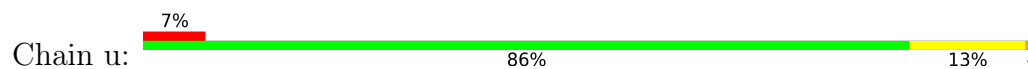


- Molecule 15: Photosystem II 12 kDa extrinsic protein

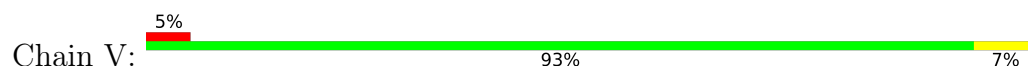




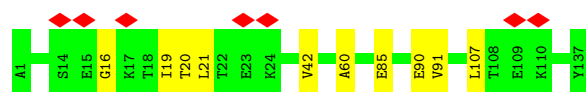
- Molecule 15: Photosystem II 12 kDa extrinsic protein



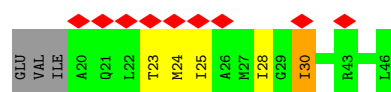
- Molecule 16: Cytochrome c-550



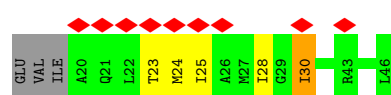
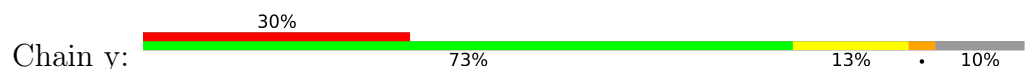
- Molecule 16: Cytochrome c-550



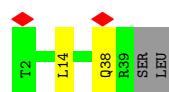
- Molecule 17: Photosystem II reaction center protein Ycf12



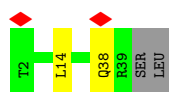
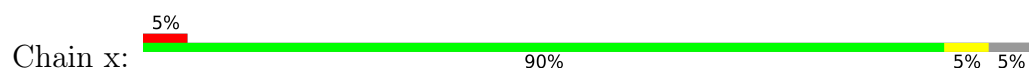
- Molecule 17: Photosystem II reaction center protein Ycf12



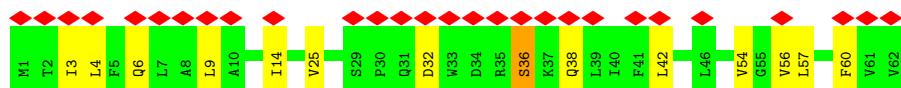
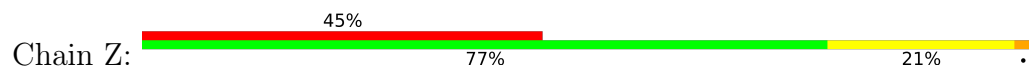
- Molecule 18: Photosystem II reaction center protein X



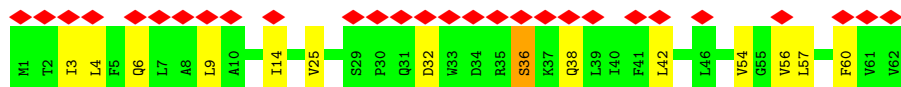
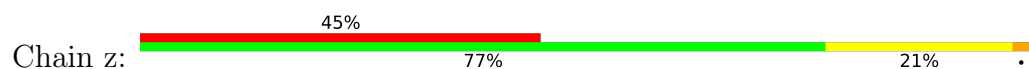
- Molecule 18: Photosystem II reaction center protein X



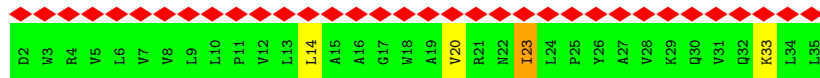
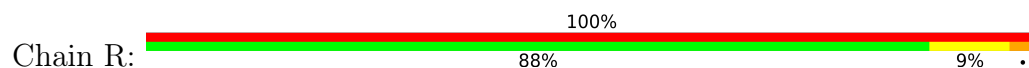
• Molecule 19: Photosystem II reaction center protein Z



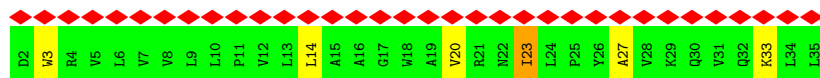
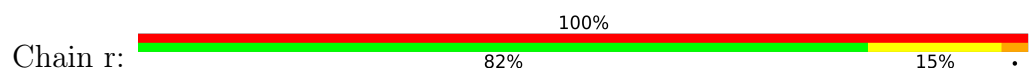
• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



• Molecule 20: Photosystem II protein Y



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	174099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	83	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	328.80002, 328.80002, 328.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, FE2, BCR, CLA, UNL, OEX, PL9, FME, HEM, LMG, MG, HSK, CL, PHO, LHG, SQD, RRX, HEC, DGD, BCT

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	0.39	0/2705	0.60	0/3689
1	a	0.39	0/2705	0.60	0/3689
2	B	0.37	0/4109	0.55	0/5600
2	b	0.37	0/4109	0.55	0/5600
3	C	0.36	0/3599	0.54	0/4900
3	c	0.36	0/3599	0.54	0/4900
4	D	0.39	0/2800	0.59	0/3814
4	d	0.39	0/2800	0.59	0/3814
5	E	0.34	0/680	0.59	0/928
5	e	0.35	0/680	0.59	0/928
6	F	0.35	0/284	0.51	0/387
6	f	0.35	0/284	0.51	0/387
7	H	0.38	0/511	0.55	0/697
7	h	0.38	0/511	0.55	0/697
8	I	0.34	0/293	0.59	0/396
8	i	0.34	0/293	0.59	0/396
9	J	0.29	0/263	0.54	0/356
9	j	0.29	0/263	0.54	0/356
10	K	0.36	0/303	0.64	0/416
10	k	0.36	0/303	0.64	0/416
11	L	0.37	0/311	0.57	0/422
11	l	0.37	0/311	0.57	0/422
12	M	0.40	0/253	0.62	0/346
12	m	0.39	0/253	0.61	0/346
13	O	0.33	0/1905	0.57	0/2583
13	o	0.33	0/1905	0.57	0/2583
14	T	0.36	0/257	0.63	0/349
14	t	0.36	0/257	0.63	0/349
15	U	0.33	0/785	0.55	0/1064
15	u	0.33	0/785	0.55	0/1064
16	V	0.35	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.35	0/1085	0.53	0/1473
17	Y	0.31	0/201	0.58	0/268
17	y	0.31	0/201	0.57	0/268
18	X	0.29	0/284	0.51	0/384
18	x	0.29	0/284	0.51	0/384
19	Z	0.28	0/490	0.55	0/669
19	z	0.28	0/490	0.55	0/669
20	R	0.29	0/279	0.60	0/383
20	r	0.29	0/279	0.59	0/383
All	All	0.36	0/42794	0.57	0/58248

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
4	D	0	1
4	d	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	335	PRO	Mainchain
4	d	335	PRO	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2620	0	2517	18	0
1	a	2620	0	2517	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3969	0	3828	29	0
2	b	3969	0	3828	29	0
3	C	3486	0	3407	26	0
3	c	3486	0	3407	26	0
4	D	2718	0	2620	18	0
4	d	2718	0	2620	20	0
5	E	661	0	648	4	0
5	e	661	0	648	5	0
6	F	275	0	282	2	0
6	f	275	0	282	2	0
7	H	498	0	518	2	0
7	h	498	0	518	3	0
8	I	296	0	311	5	0
8	i	296	0	311	5	0
9	J	257	0	268	1	0
9	j	257	0	268	1	0
10	K	293	0	305	5	0
10	k	293	0	305	5	0
11	L	304	0	316	3	0
11	l	304	0	316	2	0
12	M	260	0	275	2	0
12	m	260	0	275	2	0
13	O	1874	0	1846	13	0
13	o	1874	0	1846	13	0
14	T	258	0	261	4	0
14	t	258	0	261	4	0
15	U	774	0	773	10	0
15	u	774	0	773	6	0
16	V	1064	0	1073	3	0
16	v	1064	0	1073	4	0
17	Y	200	0	226	4	0
17	y	200	0	226	4	0
18	X	281	0	312	2	0
18	x	281	0	312	2	0
19	Z	479	0	516	4	0
19	z	479	0	516	4	0
20	R	273	0	305	1	0
20	r	273	0	305	3	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	195	0	216	5	0
24	B	1040	0	1152	16	0
24	C	845	0	936	23	0
24	D	195	0	216	4	0
24	a	195	0	216	5	0
24	b	1040	0	1152	19	0
24	c	845	0	936	24	0
24	d	195	0	216	4	0
25	A	64	0	74	0	0
25	D	64	0	74	1	0
25	a	64	0	74	0	0
25	d	64	0	74	2	0
26	A	40	0	56	1	0
26	B	160	0	224	8	0
26	C	120	0	168	6	0
26	D	40	0	56	0	0
26	T	40	0	56	1	0
26	Y	40	0	56	1	0
26	a	40	0	56	1	0
26	b	120	0	168	1	0
26	c	120	0	168	4	0
26	d	40	0	56	0	0
26	y	40	0	56	0	0
27	A	108	0	154	2	0
27	D	45	0	56	0	0
27	L	54	0	77	1	0
27	a	108	0	154	3	0
27	d	45	0	56	0	0
27	l	54	0	77	1	0
28	A	55	0	80	2	0
28	D	55	0	80	2	0
28	a	55	0	80	2	0
28	d	55	0	80	1	0
29	A	36	0	0	0	0
29	B	85	0	0	0	0
29	C	10	0	0	0	0
29	D	40	0	0	0	0
29	E	10	0	0	0	0
29	I	17	0	0	0	0
29	J	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	34	0	0	0	0
29	M	10	0	0	0	0
29	T	26	0	0	0	0
29	X	10	0	0	0	0
29	a	36	0	0	0	0
29	b	85	0	0	0	0
29	c	10	0	0	0	0
29	d	40	0	0	0	0
29	e	10	0	0	0	0
29	i	17	0	0	0	0
29	j	10	0	0	0	0
29	k	34	0	0	0	0
29	m	10	0	0	0	0
29	t	26	0	0	0	0
29	x	10	0	0	0	0
30	A	4	0	0	0	0
30	a	4	0	0	0	0
31	B	51	0	72	2	0
31	C	153	0	216	5	0
31	D	51	0	72	1	0
31	b	51	0	72	2	0
31	c	153	0	216	5	0
31	d	51	0	72	1	0
32	B	49	0	74	2	0
32	D	144	0	213	3	0
32	E	49	0	74	1	0
32	b	49	0	74	2	0
32	d	144	0	213	3	0
32	e	49	0	74	1	0
33	C	186	0	242	6	0
33	H	62	0	82	1	0
33	c	186	0	242	6	0
33	h	62	0	82	2	0
34	E	43	0	30	3	0
34	e	43	0	30	3	0
35	H	41	0	56	7	0
35	h	41	0	56	9	0
36	I	35	0	44	2	0
36	J	24	0	35	1	0
36	M	35	0	43	0	0
36	Z	35	0	44	0	0
36	i	35	0	44	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	j	24	0	35	1	0
36	m	35	0	43	0	0
36	z	35	0	44	0	0
37	J	1	0	0	0	0
37	j	1	0	0	0	0
38	V	43	0	30	0	0
38	v	43	0	30	0	0
39	A	142	0	0	3	0
39	B	252	0	0	5	0
39	C	184	0	0	2	0
39	D	145	0	0	2	0
39	E	21	0	0	0	0
39	F	2	0	0	0	0
39	H	34	0	0	0	0
39	I	13	0	0	1	0
39	J	5	0	0	0	0
39	K	3	0	0	1	0
39	L	15	0	0	0	0
39	M	6	0	0	0	0
39	O	104	0	0	0	0
39	T	9	0	0	0	0
39	U	56	0	0	1	0
39	V	63	0	0	0	0
39	X	6	0	0	0	0
39	a	141	0	0	3	0
39	b	253	0	0	5	0
39	c	184	0	0	2	0
39	d	145	0	0	2	0
39	e	21	0	0	0	0
39	f	2	0	0	0	0
39	h	34	0	0	0	0
39	i	13	0	0	1	0
39	j	5	0	0	0	0
39	k	3	0	0	1	0
39	l	15	0	0	0	0
39	m	6	0	0	0	0
39	o	105	0	0	0	0
39	t	9	0	0	0	0
39	u	56	0	0	0	0
39	v	63	0	0	1	0
39	x	6	0	0	0	0
All	All	52655	0	51218	380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (380) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:101:RRX:H55	35:h:101:RRX:H46	1.73	0.70
1:a:341:LEU:H	3:c:313:GLN:HE22	1.38	0.70
24:c:504:CLA:H193	24:c:511:CLA:HAB	1.75	0.69
35:H:101:RRX:H55	35:H:101:RRX:H46	1.73	0.69
24:C:504:CLA:H193	24:C:511:CLA:HAB	1.75	0.68
1:A:341:LEU:H	3:C:313:GLN:HE22	1.38	0.68
4:d:192:THR:HG23	24:d:403:CLA:HBC2	1.77	0.67
35:H:101:RRX:H55	35:H:101:RRX:C8	2.26	0.66
4:D:192:THR:HG23	24:D:403:CLA:HBC2	1.77	0.65
35:h:101:RRX:H55	35:h:101:RRX:C8	2.26	0.65
2:b:282:GLN:NE2	39:b:707:HOH:O	2.33	0.61
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.82	0.61
3:c:418:ASN:HD21	33:c:518:DGD:HD4	1.65	0.61
2:B:413:ASP:N	2:B:413:ASP:OD1	2.33	0.61
2:B:12:LEU:HB2	24:B:612:CLA:HMC2	1.84	0.60
3:C:418:ASN:HD21	33:C:518:DGD:HD4	1.65	0.60
2:B:282:GLN:NE2	39:B:708:HOH:O	2.33	0.60
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.82	0.60
2:b:12:LEU:HB2	24:b:614:CLA:HMC2	1.84	0.60
2:B:149:LEU:HB2	24:B:604:CLA:H171	1.82	0.59
2:b:149:LEU:HB2	24:b:606:CLA:H171	1.83	0.59
15:U:39:ARG:NH1	16:V:60:ALA:O	2.36	0.58
2:B:497:GLN:HB2	2:B:504:THR:HB	1.84	0.58
24:A:406:CLA:H112	31:D:411:LMG:H241	1.86	0.58
2:b:354:LEU:O	39:b:701:HOH:O	2.17	0.58
3:c:300:GLU:OE2	39:c:601:HOH:O	2.17	0.58
24:a:406:CLA:H112	31:d:411:LMG:H241	1.86	0.58
32:b:627:LHG:H322	12:m:18:PRO:HB3	1.86	0.58
3:C:300:GLU:OE2	39:C:601:HOH:O	2.17	0.57
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.87	0.57
2:b:497:GLN:HB2	2:b:504:THR:HB	1.84	0.57
2:B:354:LEU:O	39:B:701:HOH:O	2.17	0.57
2:B:422:ARG:NH1	13:O:169:ASP:OD1	2.38	0.57
32:B:625:LHG:H322	12:M:18:PRO:HB3	1.86	0.57
15:u:39:ARG:NH1	16:v:60:ALA:O	2.36	0.57
10:K:46:ARG:NH1	39:K:1002:HOH:O	2.38	0.56
3:C:60:ILE:HG22	24:C:504:CLA:HHD	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:89:LEU:H	7:H:50:ASN:HD21	1.53	0.56
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.87	0.56
2:b:422:ARG:NH1	13:o:169:ASP:OD1	2.38	0.56
8:i:30:ARG:NH2	39:i:202:HOH:O	2.37	0.56
24:C:509:CLA:H192	10:K:33:LEU:HD23	1.87	0.56
4:d:89:LEU:H	7:h:50:ASN:HD21	1.53	0.56
3:c:60:ILE:HG22	24:c:504:CLA:HHD	1.88	0.56
24:c:509:CLA:H192	10:k:33:LEU:HD23	1.87	0.56
2:B:79:SER:HB3	2:B:86:ILE:HD11	1.88	0.55
10:k:46:ARG:NH1	39:k:1002:HOH:O	2.38	0.55
2:b:79:SER:HB3	2:b:86:ILE:HD11	1.88	0.55
3:C:269:GLU:HG2	3:C:448:ALA:HB2	1.88	0.55
35:H:101:RRX:C23	35:H:101:RRX:H17	2.36	0.55
5:E:30:LEU:HD11	34:E:103:HEM:HAB	1.89	0.55
24:C:505:CLA:H151	24:C:509:CLA:H143	1.88	0.55
3:c:269:GLU:HG2	3:c:448:ALA:HB2	1.88	0.55
2:B:44:THR:HG23	2:B:60:MET:HE1	1.89	0.54
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	1.89	0.54
35:h:101:RRX:C23	35:h:101:RRX:H17	2.36	0.54
15:u:26:ASP:OD2	15:u:85:THR:OG1	2.23	0.54
5:e:30:LEU:HD11	34:e:103:HEM:HAB	1.89	0.54
35:h:101:RRX:C8	35:h:101:RRX:C33	2.85	0.54
8:I:30:ARG:NH2	39:I:202:HOH:O	2.36	0.54
3:c:323:LYS:NZ	39:c:615:HOH:O	2.37	0.54
24:c:505:CLA:H151	24:c:509:CLA:H143	1.88	0.54
2:b:44:THR:HG23	2:b:60:MET:HE1	1.89	0.53
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.89	0.53
24:A:408:CLA:H191	24:C:506:CLA:H52	1.91	0.53
3:c:42:LEU:HD21	24:c:512:CLA:H2A	1.91	0.53
3:C:42:LEU:HD21	24:C:512:CLA:H2A	1.91	0.53
4:D:24:ARG:NH1	39:D:505:HOH:O	2.33	0.53
28:A:411:PL9:H502	4:D:39:PRO:HG3	1.91	0.52
24:C:508:CLA:HMA1	24:C:508:CLA:H2	1.91	0.52
10:k:14:ALA:O	19:z:6:GLN:NE2	2.42	0.52
35:H:101:RRX:C8	35:H:101:RRX:C33	2.86	0.52
15:U:26:ASP:OD2	15:U:85:THR:OG1	2.23	0.52
24:a:408:CLA:H191	24:c:506:CLA:H52	1.91	0.52
2:b:413:ASP:N	2:b:413:ASP:OD1	2.33	0.51
28:a:411:PL9:H502	4:d:39:PRO:HG3	1.91	0.51
24:c:509:CLA:HBC3	24:c:511:CLA:H71	1.92	0.51
3:C:323:LYS:NZ	39:C:615:HOH:O	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:620:BCR:HC31	31:b:622:LMG:H131	1.93	0.51
24:c:508:CLA:HMA1	24:c:508:CLA:H2	1.91	0.51
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.92	0.51
15:u:11:ASN:HB3	15:u:14:ASP:HB2	1.92	0.50
15:U:11:ASN:HB3	15:U:14:ASP:HB2	1.92	0.50
13:o:39:ARG:HH21	13:o:82:GLN:HB3	1.77	0.50
3:C:174:LEU:HD22	24:C:503:CLA:H172	1.93	0.50
4:D:123:ILE:HD11	33:H:102:DGD:HAE1	1.94	0.50
13:O:39:ARG:HH21	13:O:82:GLN:HB3	1.77	0.50
13:O:124:ASN:HB2	13:O:147:ASN:HD22	1.77	0.49
3:c:174:LEU:HD22	24:c:503:CLA:H172	1.93	0.49
26:B:618:BCR:HC31	31:B:620:LMG:H131	1.93	0.49
4:d:126:MET:HE3	4:d:150:ILE:HD12	1.93	0.49
4:d:24:ARG:NH1	39:d:505:HOH:O	2.33	0.49
3:C:376:ASP:HB3	3:C:379:LYS:HB2	1.95	0.49
10:k:28:ILE:HD11	17:y:28:ILE:HD13	1.95	0.49
1:A:200:LEU:HD11	33:C:519:DGD:HBE2	1.95	0.49
13:O:17:ASN:O	13:O:77:SER:OG	2.31	0.49
2:B:314:TYR:OH	13:O:176:GLN:NE2	2.38	0.49
33:C:518:DGD:HA32	36:J:102:LMT:H81	1.95	0.49
13:o:124:ASN:HB2	13:o:147:ASN:HD22	1.77	0.49
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.49
1:a:200:LEU:HD11	33:c:519:DGD:HBE2	1.95	0.49
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.48
3:c:376:ASP:HB3	3:c:379:LYS:HB2	1.95	0.48
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.96	0.48
4:D:126:MET:HE3	4:D:150:ILE:HD12	1.93	0.48
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.96	0.48
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.94	0.48
2:b:314:TYR:OH	13:o:176:GLN:NE2	2.38	0.48
4:d:123:ILE:HD11	33:h:102:DGD:HAE1	1.94	0.48
33:c:518:DGD:HA32	36:j:102:LMT:H81	1.95	0.48
10:K:28:ILE:HD11	17:Y:28:ILE:HD13	1.95	0.48
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.48
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.96	0.48
13:o:17:ASN:O	13:o:77:SER:OG	2.31	0.48
10:K:14:ALA:O	19:Z:6:GLN:NE2	2.42	0.48
15:U:57:SER:OG	15:U:60:ASP:OD1	2.28	0.48
3:c:38:GLY:HA3	24:c:512:CLA:HMD2	1.96	0.48
2:B:389:LYS:O	2:B:395:GLN:NE2	2.46	0.47
11:l:2:GLU:H	11:l:2:GLU:HG3	1.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:ASP:OD2	31:C:522:LMG:O2	2.28	0.47
24:C:506:CLA:H141	8:I:16:VAL:HG22	1.95	0.47
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.49	0.47
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.49	0.47
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.96	0.47
3:c:107:ASP:OD2	31:c:522:LMG:O2	2.28	0.47
15:U:16:LYS:NZ	15:U:86:GLU:OE2	2.44	0.47
24:b:611:CLA:HMB2	35:h:101:RRX:H50	1.97	0.47
1:A:63:ILE:HB	3:C:335:THR:HG21	1.97	0.47
3:C:406:SER:HA	3:C:420:VAL:HG23	1.97	0.47
5:E:57:ALA:HB3	5:E:60:GLN:HB2	1.97	0.47
2:b:30:VAL:HG12	24:b:607:CLA:HHD	1.96	0.47
2:b:389:LYS:O	2:b:395:GLN:NE2	2.46	0.47
24:c:506:CLA:H141	8:i:16:VAL:HG22	1.95	0.47
5:e:57:ALA:HB3	5:e:60:GLN:HB2	1.97	0.47
2:B:353:GLU:O	39:B:702:HOH:O	2.20	0.47
1:A:267:ASN:HB3	1:A:270:SER:HB2	1.97	0.47
8:i:28:PRO:O	8:i:31:ASN:ND2	2.48	0.47
20:r:20:VAL:HA	20:r:23:ILE:HG22	1.97	0.46
24:b:616:CLA:H62	24:b:616:CLA:H41	1.54	0.46
4:d:78:VAL:HG11	4:d:114:ILE:HD12	1.96	0.46
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.97	0.46
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.50	0.46
4:D:186:GLN:HB2	24:D:403:CLA:HBC1	1.97	0.46
5:E:14:ILE:O	5:E:20:TRP:NE1	2.44	0.46
27:a:410:SQD:H122	27:a:410:SQD:H91	1.79	0.46
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.50	0.46
5:e:14:ILE:O	5:e:20:TRP:NE1	2.44	0.46
24:b:611:CLA:NC	35:h:101:RRX:H56	2.31	0.46
15:u:16:LYS:NZ	15:u:86:GLU:OE2	2.44	0.46
1:A:305:SER:HA	9:J:39:SER:HB3	1.98	0.46
2:B:2:GLY:N	39:B:728:HOH:O	2.49	0.46
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.97	0.46
24:b:603:CLA:H52	24:b:603:CLA:H12	1.72	0.46
3:c:406:SER:HA	3:c:420:VAL:HG23	1.97	0.46
3:C:38:GLY:HA3	24:C:512:CLA:HMD2	1.96	0.46
2:B:30:VAL:HG12	24:B:605:CLA:HHD	1.96	0.46
24:B:609:CLA:NC	35:H:101:RRX:H56	2.31	0.46
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.96	0.46
24:a:408:CLA:H41	24:a:408:CLA:H61	1.77	0.46
24:b:604:CLA:H111	24:b:604:CLA:H91	1.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:101:RRX:H26	35:h:101:RRX:H22	1.83	0.46
16:v:90:GLU:HG2	16:v:91:VAL:HG13	1.98	0.46
24:B:611:CLA:H142	32:B:625:LHG:H361	1.98	0.46
14:T:18:PHE:HB2	26:T:101:BCR:HC8	1.97	0.46
1:a:63:ILE:HB	3:c:335:THR:HG21	1.97	0.46
3:C:72:LEU:HD11	3:C:108:THR:HB	1.98	0.46
4:d:186:GLN:HB2	24:d:403:CLA:HBC1	1.97	0.46
16:V:90:GLU:HG2	16:V:91:VAL:HG13	1.98	0.45
20:R:20:VAL:HA	20:R:23:ILE:HG22	1.97	0.45
13:o:54:GLU:H	13:o:54:GLU:HG3	1.51	0.45
2:B:497:GLN:HE22	18:X:38:GLN:HB2	1.82	0.45
2:b:2:GLY:N	39:b:729:HOH:O	2.49	0.45
3:C:415:ASN:ND2	33:C:519:DGD:O2E	2.47	0.45
26:C:521:BCR:H24C	26:C:521:BCR:H371	1.71	0.45
8:I:28:PRO:O	8:I:31:ASN:ND2	2.48	0.45
2:b:353:GLU:O	39:b:702:HOH:O	2.20	0.45
24:b:613:CLA:H142	32:b:627:LHG:H361	1.98	0.45
2:B:389:LYS:HE3	2:B:389:LYS:HB2	1.77	0.45
24:C:506:CLA:HBC2	26:C:516:BCR:H341	1.99	0.45
24:C:511:CLA:H192	24:C:511:CLA:HBC3	1.98	0.45
24:c:508:CLA:H41	24:c:508:CLA:H62	1.72	0.45
3:C:90:PRO:HB3	3:C:301:PHE:HB3	1.97	0.45
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.81	0.45
4:d:266:TRP:CD1	32:d:409:LHG:HC32	2.52	0.45
26:Y:101:BCR:H20C	26:Y:101:BCR:H361	1.85	0.45
1:a:267:ASN:HB3	1:a:270:SER:HB2	1.97	0.45
24:b:606:CLA:H111	24:b:606:CLA:H152	1.70	0.45
3:c:90:PRO:HB3	3:c:301:PHE:HB3	1.97	0.45
4:d:54:PHE:O	5:e:49:THR:OG1	2.30	0.45
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.99	0.45
3:c:134:ILE:HG21	24:c:512:CLA:H43	1.99	0.45
3:c:318:LEU:HD12	3:c:340:TYR:HB3	1.99	0.45
26:B:627:BCR:HC8	14:t:18:PHE:HB2	1.97	0.45
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.99	0.45
2:b:239:SER:OG	24:b:610:CLA:O1D	2.34	0.45
26:c:515:BCR:H20C	26:c:515:BCR:H361	1.86	0.45
27:A:412:SQD:H191	27:A:412:SQD:H162	1.81	0.45
4:D:266:TRP:CD1	32:D:409:LHG:HC32	2.52	0.45
15:U:31:ASN:ND2	15:U:33:ALA:H	2.15	0.45
1:a:305:SER:HA	9:j:39:SER:HB3	1.98	0.45
2:b:497:GLN:HE22	18:x:38:GLN:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:511:CLA:H192	24:c:511:CLA:HBC3	1.98	0.45
24:B:612:CLA:H102	24:B:612:CLA:H61	1.77	0.44
4:D:279:LEU:HD22	25:D:402:PHO:HBC3	1.98	0.44
24:c:506:CLA:HBC2	26:c:516:BCR:H341	1.99	0.44
19:Z:32:ASP:O	19:Z:36:SER:OG	2.34	0.44
19:z:32:ASP:O	19:z:36:SER:OG	2.34	0.44
24:B:609:CLA:HMB2	35:H:101:RRX:H50	1.99	0.44
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.99	0.44
36:I:102:LMT:H11	36:I:102:LMT:H42	1.84	0.44
15:u:31:ASN:ND2	15:u:33:ALA:H	2.15	0.44
13:O:147:ASN:HB3	13:O:192:LEU:HD11	2.00	0.44
16:V:55:ARG:NH2	16:V:128:ASP:O	2.46	0.44
24:b:609:CLA:H42	31:b:622:LMG:H301	1.99	0.44
24:c:502:CLA:C4D	24:c:504:CLA:H2	2.48	0.44
4:d:279:LEU:HD22	25:d:402:PHO:HBC3	1.98	0.44
24:B:607:CLA:H42	31:B:620:LMG:H301	1.99	0.44
17:Y:30:ILE:HD13	17:Y:30:ILE:HA	1.78	0.44
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.99	0.44
3:c:72:LEU:HD11	3:c:108:THR:HB	1.98	0.44
3:c:148:GLY:O	3:c:156:LYS:NZ	2.42	0.44
3:c:432:VAL:HG11	24:c:505:CLA:H122	2.00	0.44
24:C:502:CLA:H202	24:C:508:CLA:HBB1	2.00	0.44
26:a:409:BCR:H24C	26:a:409:BCR:H371	1.75	0.44
4:d:210:LEU:HA	4:d:213:ILE:HG22	1.99	0.44
24:c:514:CLA:H111	26:c:515:BCR:H23C	2.00	0.44
1:A:238:LYS:NZ	39:A:509:HOH:O	2.40	0.44
24:A:408:CLA:H41	24:A:408:CLA:H61	1.77	0.44
2:B:239:SER:OG	24:B:608:CLA:O1D	2.34	0.44
2:B:256:MET:HA	2:B:263:THR:HG21	2.00	0.44
3:C:318:LEU:HD12	3:C:340:TYR:HB3	1.99	0.44
24:C:502:CLA:C4D	24:C:504:CLA:H2	2.48	0.44
26:B:618:BCR:H20C	26:B:618:BCR:H361	1.87	0.43
27:a:410:SQD:H251	32:d:410:LHG:H141	2.00	0.43
11:l:14:ARG:HD3	27:l:101:SQD:H241	2.00	0.43
32:e:101:LHG:H302	32:e:101:LHG:H272	1.85	0.43
3:C:134:ILE:HG21	24:C:512:CLA:H43	1.99	0.43
11:L:2:GLU:H	11:L:2:GLU:HG3	1.46	0.43
27:a:412:SQD:H191	27:a:412:SQD:H162	1.81	0.43
27:A:410:SQD:H251	32:D:410:LHG:H141	2.00	0.43
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.99	0.43
2:B:334:ASP:OD1	2:B:334:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.82	0.43
26:C:521:BCR:H20C	26:C:521:BCR:H361	1.86	0.43
11:L:14:ARG:HD3	27:L:101:SQD:H241	2.00	0.43
26:B:627:BCR:H20C	26:B:627:BCR:H361	1.88	0.43
3:c:168:LEU:HD13	24:c:508:CLA:H43	1.99	0.43
3:C:276:LEU:HD23	24:C:510:CLA:HED1	2.01	0.43
35:H:101:RRX:H32	35:H:101:RRX:H28	1.77	0.43
1:a:334:ARG:NH2	39:a:522:HOH:O	2.51	0.43
24:b:617:CLA:H2	24:b:618:CLA:HBB2	2.01	0.43
13:O:60:ARG:HB3	13:O:61:GLN:H	1.59	0.43
3:c:415:ASN:ND2	33:c:519:DGD:O2E	2.47	0.43
1:A:341:LEU:N	3:C:313:GLN:HE22	2.12	0.43
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.00	0.43
3:C:168:LEU:HD13	24:C:508:CLA:H43	1.99	0.43
31:C:520:LMG:H172	17:Y:25:ILE:HG12	2.01	0.43
24:D:401:CLA:H101	24:D:401:CLA:H3A	2.01	0.43
8:I:20:VAL:HG11	36:I:102:LMT:H122	2.01	0.43
3:c:27:ASP:OD1	3:c:30:SER:OG	2.33	0.43
31:c:522:LMG:H402	31:c:522:LMG:H242	2.00	0.43
1:A:334:ARG:NH2	39:A:522:HOH:O	2.52	0.43
4:D:12:ARG:HA	4:D:12:ARG:HD3	1.82	0.42
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.00	0.42
28:D:406:PL9:H43	28:D:406:PL9:H472	1.70	0.42
2:b:103:LEU:HD21	24:b:607:CLA:HMC2	2.01	0.42
24:C:514:CLA:H111	26:C:515:BCR:H23C	2.00	0.42
13:o:147:ASN:HB3	13:o:192:LEU:HD11	2.00	0.42
3:C:432:VAL:HG11	24:C:505:CLA:H122	2.00	0.42
31:C:522:LMG:H402	31:C:522:LMG:H242	2.01	0.42
34:E:103:HEM:HMC2	6:F:31:ILE:HG13	2.01	0.42
24:c:502:CLA:H202	24:c:508:CLA:HBB1	2.00	0.42
2:B:103:LEU:HD21	24:B:605:CLA:HMC2	2.01	0.42
2:b:256:MET:HA	2:b:263:THR:HG21	2.00	0.42
2:b:389:LYS:HB2	2:b:389:LYS:HE3	1.77	0.42
31:c:520:LMG:H172	17:y:25:ILE:HG12	2.01	0.42
3:c:276:LEU:HD23	24:c:510:CLA:HED1	2.01	0.42
33:c:518:DGD:HB61	31:c:520:LMG:H402	2.01	0.42
4:d:12:ARG:HA	4:d:12:ARG:HD3	1.82	0.42
25:d:402:PHO:H41	25:d:402:PHO:H62	1.88	0.42
35:h:101:RRX:H32	35:h:101:RRX:H28	1.76	0.42
24:B:614:CLA:H62	24:B:614:CLA:H41	1.54	0.42
17:y:30:ILE:HD13	17:y:30:ILE:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:408:CLA:H8	8:I:16:VAL:HG11	2.02	0.42
33:C:518:DGD:HB61	31:C:520:LMG:H402	2.01	0.42
1:a:238:LYS:NZ	39:a:509:HOH:O	2.40	0.42
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.81	0.42
4:D:139:ARG:NH2	39:D:515:HOH:O	2.45	0.42
26:B:618:BCR:H15C	26:B:618:BCR:H351	1.86	0.42
13:O:51:LEU:HD12	13:O:234:LYS:HD2	2.02	0.42
24:b:613:CLA:H72	24:b:613:CLA:H112	1.83	0.42
4:d:103:ARG:HE	5:e:77:GLU:HG3	1.84	0.42
2:b:413:ASP:HA	2:b:414:PRO:HD3	1.91	0.42
4:d:87:HIS:ND1	33:h:102:DGD:O2D	2.48	0.42
24:B:612:CLA:H162	24:B:612:CLA:H122	1.91	0.41
4:D:103:ARG:HE	5:E:77:GLU:HG3	1.85	0.41
1:a:201:GLY:HA3	1:a:286:ALA:HB2	2.02	0.41
24:b:614:CLA:H61	24:b:614:CLA:H102	1.76	0.41
2:B:80:ILE:HA	39:B:733:HOH:O	2.19	0.41
11:L:1:MET:HE3	11:L:1:MET:HB2	1.89	0.41
28:D:406:PL9:H371	28:D:406:PL9:H351	1.87	0.41
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.01	0.41
1:a:244:GLU:HB3	39:a:622:HOH:O	2.21	0.41
24:a:406:CLA:HED1	33:c:519:DGD:HAE2	2.01	0.41
4:d:139:ARG:NH2	39:d:515:HOH:O	2.45	0.41
8:i:20:VAL:HG11	36:i:102:LMT:H122	2.01	0.41
13:o:142:PHE:HB2	13:o:199:LEU:HB2	2.02	0.41
10:K:21:LEU:HD13	17:Y:24:MET:HE2	2.02	0.41
24:d:401:CLA:H101	24:d:401:CLA:H3A	2.01	0.41
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.01	0.41
28:A:411:PL9:H372	6:F:22:ALA:HA	2.03	0.41
24:B:615:CLA:H2	24:B:616:CLA:HBB2	2.01	0.41
24:C:508:CLA:H41	24:C:508:CLA:H62	1.72	0.41
28:a:411:PL9:H372	6:f:22:ALA:HA	2.03	0.41
2:b:141:ILE:HG21	24:b:617:CLA:HBB1	2.02	0.41
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.03	0.41
26:c:516:BCR:H20C	26:c:516:BCR:H361	1.97	0.41
24:d:404:CLA:H152	18:x:14:LEU:HG	2.03	0.41
16:v:107:LEU:HD23	16:v:107:LEU:HA	1.87	0.41
2:B:141:ILE:HG21	24:B:615:CLA:HBB1	2.02	0.41
2:B:418:LYS:NZ	15:U:14:ASP:OD2	2.51	0.41
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.88	0.41
2:B:249:ALA:HA	2:B:252:VAL:HG22	2.03	0.41
26:B:618:BCR:H363	26:B:627:BCR:H19C	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.03	0.41
2:b:80:ILE:HA	39:b:733:HOH:O	2.20	0.41
36:i:102:LMT:H11	36:i:102:LMT:H42	1.84	0.41
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.91	0.41
26:B:617:BCR:H20C	26:B:617:BCR:H361	1.82	0.41
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.02	0.41
10:k:21:LEU:HD13	17:y:24:MET:HE2	2.02	0.41
1:A:244:GLU:HB3	39:A:623:HOH:O	2.21	0.41
26:A:409:BCR:H371	26:A:409:BCR:H24C	1.75	0.41
26:C:515:BCR:H20C	26:C:515:BCR:H361	1.86	0.41
19:Z:57:LEU:HD23	19:Z:60:PHE:HD2	1.86	0.41
24:a:408:CLA:H8	8:i:16:VAL:HG11	2.02	0.41
2:b:80:ILE:H	2:b:80:ILE:HG13	1.75	0.41
24:b:617:CLA:H161	7:h:7:LEU:HD21	2.02	0.41
3:c:279:LEU:HD22	24:c:510:CLA:HED2	2.02	0.41
32:d:409:LHG:H331	14:t:21:ILE:HD11	2.03	0.41
20:r:23:ILE:O	20:r:27:ALA:N	2.52	0.41
24:A:406:CLA:HED1	33:C:519:DGD:HAE2	2.01	0.41
24:B:613:CLA:H72	24:B:613:CLA:H112	1.91	0.41
24:B:615:CLA:H161	7:H:7:LEU:HD21	2.02	0.41
3:C:313:GLN:HB2	3:C:396:MET:HG3	2.03	0.41
24:C:506:CLA:H61	24:C:506:CLA:H2	1.86	0.41
34:E:103:HEM:HBC2	34:E:103:HEM:HHD	2.02	0.41
1:a:85:SER:HA	1:a:109:GLY:HA3	2.03	0.41
24:c:514:CLA:H18	24:c:514:CLA:H151	1.90	0.41
34:e:103:HEM:HMC2	6:f:31:ILE:HG13	2.01	0.41
13:o:22:LEU:HD21	13:o:240:TYR:HE1	1.86	0.41
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.03	0.41
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.04	0.40
3:C:279:LEU:HD22	24:C:510:CLA:HED2	2.02	0.40
24:D:404:CLA:H152	18:X:14:LEU:HG	2.03	0.40
32:E:101:LHG:H302	32:E:101:LHG:H272	1.85	0.40
15:U:95:GLY:HA2	39:U:250:HOH:O	2.21	0.40
1:a:213:ALA:HB2	4:d:275:PRO:HG2	2.03	0.40
2:b:249:ALA:HA	2:b:252:VAL:HG22	2.03	0.40
3:c:313:GLN:HB2	3:c:396:MET:HG3	2.04	0.40
20:r:3:TRP:CD1	20:r:3:TRP:H	2.40	0.40
1:A:85:SER:HA	1:A:109:GLY:HA3	2.03	0.40
31:C:522:LMG:H222	31:C:522:LMG:H391	2.03	0.40
31:c:522:LMG:H391	31:c:522:LMG:H222	2.03	0.40
34:e:103:HEM:HBC2	34:e:103:HEM:HHD	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:51:LEU:HD12	13:o:234:LYS:HD2	2.02	0.40
16:v:85:GLU:OE1	39:v:301:HOH:O	2.22	0.40
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.03	0.40
32:D:409:LHG:H331	14:T:21:ILE:HD11	2.03	0.40
15:U:104:LYS:HD3	15:U:104:LYS:HA	1.94	0.40
28:d:406:PL9:H401	28:d:406:PL9:H422	1.84	0.40
19:z:57:LEU:HD23	19:z:60:PHE:HD2	1.86	0.40
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.97	0.40
13:O:205:ASP:HB3	13:O:210:GLU:H	1.86	0.40
24:b:618:CLA:H41	24:b:618:CLA:H61	1.93	0.40
24:c:506:CLA:H111	24:c:506:CLA:H152	1.94	0.40
1:A:201:GLY:HA3	1:A:286:ALA:HB2	2.02	0.40
13:O:22:LEU:HD21	13:O:240:TYR:HE1	1.86	0.40
7:h:38:PHE:HB2	35:h:101:RRX:C10	2.52	0.40
13:o:205:ASP:HB3	13:o:210:GLU:H	1.86	0.40

There are no symmetry-related clashes.

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	332/334 (99%)	326 (98%)	5 (2%)	1 (0%)	37	36
1	a	332/334 (99%)	326 (98%)	5 (2%)	1 (0%)	37	36
2	B	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
2	b	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
3	C	449/451 (100%)	439 (98%)	9 (2%)	1 (0%)	44	44
3	c	449/451 (100%)	439 (98%)	9 (2%)	1 (0%)	44	44
4	D	338/342 (99%)	329 (97%)	9 (3%)	0	100	100
4	d	338/342 (99%)	329 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	79/81 (98%)	79 (100%)	0	0	100	100
5	e	79/81 (98%)	79 (100%)	0	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
9	j	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	31/34 (91%)	31 (100%)	0	0	100	100
12	m	31/34 (91%)	31 (100%)	0	0	100	100
13	O	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	16	12
13	o	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	16	12
14	T	28/31 (90%)	28 (100%)	0	0	100	100
14	t	28/31 (90%)	28 (100%)	0	0	100	100
15	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
15	u	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	19	15
16	v	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	19	15
17	Y	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
17	y	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
19	z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	R	32/34 (94%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	r	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5230/5332 (98%)	5102 (98%)	118 (2%)	10 (0%)	45	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	58	ASN
3	c	416	SER
13	o	58	ASN
13	O	60	ARG
13	o	60	ARG
16	V	16	GLY
16	v	16	GLY
1	A	30	VAL
1	a	30	VAL

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	269/269 (100%)	268 (100%)	1 (0%)	89	92
1	a	269/269 (100%)	268 (100%)	1 (0%)	89	92
2	B	402/403 (100%)	394 (98%)	8 (2%)	50	55
2	b	402/403 (100%)	394 (98%)	8 (2%)	50	55
3	C	352/352 (100%)	346 (98%)	6 (2%)	56	62
3	c	352/352 (100%)	346 (98%)	6 (2%)	56	62
4	D	275/276 (100%)	272 (99%)	3 (1%)	70	76
4	d	275/276 (100%)	272 (99%)	3 (1%)	70	76
5	E	72/72 (100%)	67 (93%)	5 (7%)	13	10
5	e	72/72 (100%)	67 (93%)	5 (7%)	13	10
6	F	28/28 (100%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	28/28 (100%)	28 (100%)	0	100	100
7	H	53/53 (100%)	49 (92%)	4 (8%)	11	8
7	h	53/53 (100%)	49 (92%)	4 (8%)	11	8
8	I	32/32 (100%)	31 (97%)	1 (3%)	35	37
8	i	32/32 (100%)	31 (97%)	1 (3%)	35	37
9	J	24/25 (96%)	24 (100%)	0	100	100
9	j	24/25 (96%)	24 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	34
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	34
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	40
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	40
12	M	29/30 (97%)	28 (97%)	1 (3%)	32	33
12	m	29/30 (97%)	28 (97%)	1 (3%)	32	33
13	O	207/207 (100%)	193 (93%)	14 (7%)	13	10
13	o	207/207 (100%)	193 (93%)	14 (7%)	13	10
14	T	26/27 (96%)	25 (96%)	1 (4%)	28	29
14	t	26/27 (96%)	25 (96%)	1 (4%)	28	29
15	U	84/84 (100%)	80 (95%)	4 (5%)	21	20
15	u	84/84 (100%)	80 (95%)	4 (5%)	21	20
16	V	117/117 (100%)	113 (97%)	4 (3%)	32	33
16	v	117/117 (100%)	113 (97%)	4 (3%)	32	33
17	Y	20/23 (87%)	18 (90%)	2 (10%)	6	3
17	y	20/23 (87%)	18 (90%)	2 (10%)	6	3
18	X	31/33 (94%)	31 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	44 (85%)	8 (15%)	2	1
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	1
20	R	29/29 (100%)	26 (90%)	3 (10%)	6	3
20	r	29/29 (100%)	26 (90%)	3 (10%)	6	3
All	All	4334/4354 (100%)	4200 (97%)	134 (3%)	37	37

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
2	B	80	ILE
2	B	84	THR
2	B	86	ILE
2	B	223	GLN
2	B	294	SER
2	B	376	VAL
2	B	378	LYS
2	B	413	ASP
3	C	24	THR
3	C	240	ILE
3	C	289	PHE
3	C	300	GLU
3	C	315	MET
3	C	344	SER
4	D	150	ILE
4	D	238	THR
4	D	345	VAL
5	E	4	THR
5	E	5	THR
5	E	11	SER
5	E	82	GLN
5	E	83	LEU
7	H	3	ARG
7	H	4	ARG
7	H	39	LEU
7	H	43	LEU
8	I	35	LYS
10	K	22	VAL
11	L	2	GLU
12	M	9	ILE
13	O	23	ASP
13	O	25	THR
13	O	54	GLU
13	O	55	GLU
13	O	60	ARG
13	O	61	GLN
13	O	64	GLU
13	O	86	LYS
13	O	87	VAL
13	O	110	MET
13	O	134	THR
13	O	180	GLU

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Mol	Chain	Res	Type
13	O	181	GLU
13	O	243	ILE
14	T	30	THR
15	U	14	ASP
15	U	61	VAL
15	U	68	THR
15	U	84	VAL
16	V	19	ILE
16	V	20	THR
16	V	21	LEU
16	V	42	VAL
17	Y	23	THR
17	Y	30	ILE
19	Z	3	ILE
19	Z	4	LEU
19	Z	14	ILE
19	Z	25	VAL
19	Z	36	SER
19	Z	38	GLN
19	Z	42	LEU
19	Z	56	VAL
20	R	14	LEU
20	R	23	ILE
20	R	33	LYS
1	a	60	ILE
2	b	80	ILE
2	b	84	THR
2	b	86	ILE
2	b	223	GLN
2	b	294	SER
2	b	376	VAL
2	b	378	LYS
2	b	413	ASP
3	c	24	THR
3	c	240	ILE
3	c	289	PHE
3	c	300	GLU
3	c	315	MET
3	c	344	SER
4	d	150	ILE
4	d	238	THR
4	d	345	VAL

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Mol	Chain	Res	Type
5	e	4	THR
5	e	5	THR
5	e	11	SER
5	e	82	GLN
5	e	83	LEU
7	h	3	ARG
7	h	4	ARG
7	h	39	LEU
7	h	43	LEU
8	i	35	LYS
10	k	22	VAL
11	l	2	GLU
12	m	9	ILE
13	o	23	ASP
13	o	25	THR
13	o	54	GLU
13	o	55	GLU
13	o	60	ARG
13	o	61	GLN
13	o	64	GLU
13	o	86	LYS
13	o	87	VAL
13	o	110	MET
13	o	134	THR
13	o	180	GLU
13	o	181	GLU
13	o	243	ILE
14	t	30	THR
15	u	14	ASP
15	u	61	VAL
15	u	68	THR
15	u	84	VAL
16	v	19	ILE
16	v	20	THR
16	v	21	LEU
16	v	42	VAL
17	y	23	THR
17	y	30	ILE
19	z	3	ILE
19	z	4	LEU
19	z	14	ILE
19	z	25	VAL

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Mol	Chain	Res	Type
19	z	36	SER
19	z	38	GLN
19	z	42	LEU
19	z	56	VAL
20	r	14	LEU
20	r	23	ILE
20	r	33	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	181	ASN
1	A	315	ASN
2	B	179	GLN
2	B	331	ASN
3	C	201	ASN
3	C	311	GLN
3	C	313	GLN
3	C	382	ASN
3	C	415	ASN
3	C	418	ASN
4	D	98	GLN
4	D	186	GLN
6	F	44	GLN
7	H	50	ASN
13	O	36	GLN
13	O	58	ASN
13	O	88	ASN
13	O	124	ASN
13	O	132	ASN
13	O	147	ASN
13	O	196	GLN
15	U	31	ASN
15	U	63	ASN
15	U	78	ASN
15	U	81	HIS
16	V	25	GLN
16	V	34	GLN
20	R	22	ASN
1	a	75	ASN

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Mol	Chain	Res	Type
1	a	165	GLN
1	a	181	ASN
1	a	315	ASN
2	b	179	GLN
2	b	331	ASN
3	c	201	ASN
3	c	229	ASN
3	c	311	GLN
3	c	313	GLN
3	c	382	ASN
3	c	415	ASN
3	c	418	ASN
4	d	98	GLN
4	d	186	GLN
6	f	44	GLN
7	h	50	ASN
12	m	5	GLN
13	o	36	GLN
13	o	58	ASN
13	o	88	ASN
13	o	124	ASN
13	o	132	ASN
13	o	147	ASN
13	o	196	GLN
15	u	31	ASN
15	u	63	ASN
15	u	78	ASN
15	u	81	HIS
16	v	25	GLN
16	v	34	GLN
20	r	22	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HSK	d	336	4	7,11,12	1.43	1 (14%)	3,14,16	1.47	1 (33%)
14	FME	t	1	14	8,9,10	0.99	0	7,9,11	1.32	1 (14%)
14	FME	T	1	14	8,9,10	1.00	0	7,9,11	1.32	1 (14%)
4	HSK	D	336	4	7,11,12	1.42	1 (14%)	3,14,16	1.47	1 (33%)
8	FME	i	1	8	8,9,10	0.82	0	7,9,11	1.03	1 (14%)
8	FME	I	1	8	8,9,10	0.85	0	7,9,11	1.03	1 (14%)
12	FME	m	1	12	8,9,10	1.01	0	7,9,11	0.66	0
12	FME	M	1	12	8,9,10	1.02	0	7,9,11	0.66	0

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
4	HSK	d	336	4	-	1/5/6/8	0/1/1/1
14	FME	t	1	14	-	3/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
4	HSK	D	336	4	-	1/5/6/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	HSK	CE1-ND1	2.71	1.40	1.36
4	D	336	HSK	CE1-ND1	2.61	1.39	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	2.94	115.04	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	C-CA-N	2.93	115.01	109.73
4	D	336	HSK	CB-CA-C	-2.30	107.16	111.47
4	d	336	HSK	CB-CA-C	-2.30	107.17	111.47
8	I	1	FME	C-CA-N	2.27	113.83	109.73
8	i	1	FME	C-CA-N	2.24	113.78	109.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	336	HSK	O-C-CA-CB
12	M	1	FME	CB-CA-N-CN
4	d	336	HSK	O-C-CA-CB
12	m	1	FME	CB-CA-N-CN
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	N-CA-CB-CG
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 196 ligands modelled in this entry, 8 are monoatomic and 36 are unknown - leaving 152 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
24	CLA	b	604	2	65,73,73	1.99	15 (23%)	76,113,113	2.85	29 (38%)
24	CLA	C	508	39	65,73,73	1.95	17 (26%)	76,113,113	2.73	27 (35%)
26	BCR	b	621	-	41,41,41	1.05	2 (4%)	56,56,56	1.06	2 (3%)
24	CLA	b	609	39	65,73,73	1.91	16 (24%)	76,113,113	2.80	28 (36%)
24	CLA	b	612	39	65,73,73	1.96	17 (26%)	76,113,113	2.75	26 (34%)
32	LHG	E	101	-	48,48,48	0.68	0	51,54,54	1.20	6 (11%)
27	SQD	a	412	-	53,54,54	0.94	4 (7%)	62,65,65	1.72	12 (19%)
24	CLA	a	406	39	65,73,73	2.00	17 (26%)	76,113,113	2.67	28 (36%)
34	HEM	e	103	5,6	41,50,50	1.54	4 (9%)	45,82,82	1.53	6 (13%)
33	DGD	H	102	-	63,63,67	1.08	5 (7%)	77,77,81	1.16	5 (6%)
24	CLA	c	512	3	65,73,73	1.95	17 (26%)	76,113,113	2.74	27 (35%)
36	LMT	j	102	-	24,24,36	1.09	3 (12%)	29,29,47	1.15	2 (6%)
24	CLA	C	506	3	65,73,73	1.94	20 (30%)	76,113,113	2.58	26 (34%)
36	LMT	m	102	-	36,36,36	1.28	6 (16%)	47,47,47	0.95	1 (2%)
31	LMG	D	411	37	51,51,55	0.97	5 (9%)	59,59,63	1.33	6 (10%)
24	CLA	c	504	3	65,73,73	2.03	19 (29%)	76,113,113	2.64	23 (30%)
38	HEC	v	201	16	32,50,50	2.12	4 (12%)	24,82,82	1.69	4 (16%)
27	SQD	A	410	-	53,54,54	0.95	6 (11%)	62,65,65	1.92	10 (16%)
24	CLA	D	403	4	65,73,73	1.86	18 (27%)	76,113,113	2.59	30 (39%)
24	CLA	C	513	3	65,73,73	1.99	18 (27%)	76,113,113	2.61	24 (31%)
24	CLA	b	611	2	65,73,73	1.96	15 (23%)	76,113,113	2.72	28 (36%)
33	DGD	c	518	-	63,63,67	1.21	9 (14%)	77,77,81	1.39	9 (11%)
31	LMG	c	501	-	51,51,55	0.94	3 (5%)	59,59,63	1.35	6 (10%)
24	CLA	b	606	2	65,73,73	1.91	16 (24%)	76,113,113	2.60	30 (39%)
26	BCR	b	619	-	41,41,41	1.00	1 (2%)	56,56,56	1.11	4 (7%)
26	BCR	B	617	-	41,41,41	1.00	1 (2%)	56,56,56	1.11	4 (7%)
26	BCR	b	620	-	41,41,41	1.03	2 (4%)	56,56,56	1.25	7 (12%)
24	CLA	d	401	39	65,73,73	2.07	16 (24%)	76,113,113	2.77	29 (38%)
27	SQD	A	412	-	53,54,54	0.95	5 (9%)	62,65,65	1.72	12 (19%)
24	CLA	B	601	39	65,73,73	2.03	19 (29%)	76,113,113	2.70	27 (35%)
24	CLA	A	408	1	65,73,73	1.93	16 (24%)	76,113,113	2.69	27 (35%)
26	BCR	B	627	-	41,41,41	0.98	1 (2%)	56,56,56	1.29	8 (14%)
28	PL9	D	406	-	55,55,55	1.44	7 (12%)	68,69,69	1.51	13 (19%)
25	PHO	d	402	-	51,69,69	1.06	5 (9%)	47,99,99	1.39	8 (17%)
24	CLA	C	503	3	65,73,73	1.92	19 (29%)	76,113,113	2.59	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	d	411	37	51,51,55	0.98	5 (9%)	59,59,63	1.33	6 (10%)
24	CLA	B	610	39	65,73,73	1.98	17 (26%)	76,113,113	2.66	28 (36%)
24	CLA	b	603	39	65,73,73	2.03	19 (29%)	76,113,113	2.70	27 (35%)
24	CLA	b	610	2	65,73,73	1.94	17 (26%)	76,113,113	2.47	31 (40%)
26	BCR	a	409	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	7 (12%)
24	CLA	b	614	2	65,73,73	1.85	17 (26%)	76,113,113	2.61	32 (42%)
31	LMG	c	522	-	51,51,55	0.89	4 (7%)	59,59,63	1.46	7 (11%)
24	CLA	b	605	2	65,73,73	1.94	15 (23%)	76,113,113	2.73	28 (36%)
30	BCT	a	414	22	2,3,3	1.32	0	2,3,3	4.48	2 (100%)
24	CLA	c	510	3	65,73,73	2.04	16 (24%)	76,113,113	2.76	32 (42%)
24	CLA	B	613	2	65,73,73	1.97	19 (29%)	76,113,113	2.75	26 (34%)
24	CLA	C	507	3	65,73,73	1.98	18 (27%)	76,113,113	2.65	27 (35%)
24	CLA	A	405	1	65,73,73	1.98	18 (27%)	76,113,113	2.51	26 (34%)
24	CLA	c	505	39	65,73,73	2.01	19 (29%)	76,113,113	2.84	29 (38%)
24	CLA	b	613	2	65,73,73	1.93	17 (26%)	76,113,113	2.56	24 (31%)
36	LMT	i	102	-	36,36,36	1.31	6 (16%)	47,47,47	1.25	3 (6%)
35	RRX	h	101	-	42,42,42	1.94	11 (26%)	57,58,58	1.99	15 (26%)
24	CLA	D	404	4	65,73,73	2.04	16 (24%)	76,113,113	2.84	28 (36%)
27	SQD	D	407	-	44,45,54	1.10	5 (11%)	53,56,65	1.96	13 (24%)
32	LHG	d	408	-	48,48,48	0.80	1 (2%)	51,54,54	1.31	6 (11%)
24	CLA	C	511	3	65,73,73	2.00	17 (26%)	76,113,113	2.59	28 (36%)
26	BCR	T	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.30	8 (14%)
24	CLA	c	508	39	65,73,73	1.96	17 (26%)	76,113,113	2.73	27 (35%)
24	CLA	B	609	2	65,73,73	1.97	14 (21%)	76,113,113	2.72	28 (36%)
32	LHG	d	410	-	45,45,48	0.77	1 (2%)	48,51,54	1.14	5 (10%)
31	LMG	c	520	-	51,51,55	1.00	6 (11%)	59,59,63	1.41	8 (13%)
25	PHO	A	407	-	51,69,69	1.00	5 (9%)	47,99,99	1.30	7 (14%)
33	DGD	C	518	-	63,63,67	1.22	9 (14%)	77,77,81	1.39	9 (11%)
26	BCR	C	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	6 (10%)
34	HEM	E	103	5,6	41,50,50	1.54	4 (9%)	45,82,82	1.53	6 (13%)
24	CLA	C	512	3	65,73,73	1.95	17 (26%)	76,113,113	2.74	27 (35%)
24	CLA	A	406	39	65,73,73	1.99	17 (26%)	76,113,113	2.66	28 (36%)
36	LMT	J	102	-	24,24,36	1.09	3 (12%)	29,29,47	1.15	2 (6%)
24	CLA	a	405	1	65,73,73	1.97	18 (27%)	76,113,113	2.51	26 (34%)
24	CLA	b	618	2	65,73,73	1.95	16 (24%)	76,113,113	2.70	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	D	408	-	48,48,48	0.80	1 (2%)	51,54,54	1.31	6 (11%)
27	SQD	L	101	-	53,54,54	0.93	5 (9%)	62,65,65	2.00	12 (19%)
28	PL9	d	406	-	55,55,55	1.45	7 (12%)	68,69,69	1.51	13 (19%)
24	CLA	b	617	2	65,73,73	1.90	17 (26%)	76,113,113	2.67	26 (34%)
24	CLA	B	602	2	65,73,73	2.00	15 (23%)	76,113,113	2.85	29 (38%)
24	CLA	C	502	3	65,73,73	1.94	17 (26%)	76,113,113	2.70	24 (31%)
26	BCR	D	405	-	41,41,41	1.12	3 (7%)	56,56,56	1.15	7 (12%)
26	BCR	C	516	-	41,41,41	1.02	2 (4%)	56,56,56	1.17	5 (8%)
27	SQD	d	407	-	44,45,54	1.10	5 (11%)	53,56,65	1.96	13 (24%)
24	CLA	c	511	3	65,73,73	2.00	17 (26%)	76,113,113	2.59	28 (36%)
33	DGD	C	519	-	63,63,67	1.15	7 (11%)	77,77,81	1.26	7 (9%)
36	LMT	I	102	-	36,36,36	1.31	5 (13%)	47,47,47	1.24	3 (6%)
28	PL9	A	411	-	55,55,55	1.47	9 (16%)	68,69,69	1.52	13 (19%)
33	DGD	c	517	-	63,63,67	1.17	7 (11%)	77,77,81	1.38	7 (9%)
24	CLA	C	505	39	65,73,73	2.01	19 (29%)	76,113,113	2.84	29 (38%)
32	LHG	D	410	-	45,45,48	0.77	1 (2%)	48,51,54	1.14	5 (10%)
24	CLA	c	502	3	65,73,73	1.94	17 (26%)	76,113,113	2.70	24 (31%)
31	LMG	b	622	-	51,51,55	0.92	2 (3%)	59,59,63	1.27	7 (11%)
24	CLA	B	615	2	65,73,73	1.90	17 (26%)	76,113,113	2.67	26 (34%)
24	CLA	D	401	39	65,73,73	2.06	15 (23%)	76,113,113	2.76	29 (38%)
24	CLA	c	514	3	65,73,73	2.07	19 (29%)	76,113,113	2.84	32 (42%)
24	CLA	C	514	3	65,73,73	2.08	19 (29%)	76,113,113	2.84	32 (42%)
24	CLA	C	510	3	65,73,73	2.04	15 (23%)	76,113,113	2.76	31 (40%)
24	CLA	b	608	2	65,73,73	1.99	18 (27%)	76,113,113	2.84	27 (35%)
24	CLA	d	403	4	65,73,73	1.86	18 (27%)	76,113,113	2.59	30 (39%)
24	CLA	B	605	2	65,73,73	1.85	15 (23%)	76,113,113	2.73	26 (34%)
24	CLA	b	616	2	65,73,73	1.95	17 (26%)	76,113,113	2.62	29 (38%)
26	BCR	B	618	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	7 (12%)
31	LMG	C	522	-	51,51,55	0.89	4 (7%)	59,59,63	1.46	7 (11%)
26	BCR	Y	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.21	7 (12%)
24	CLA	C	509	3	65,73,73	1.96	17 (26%)	76,113,113	2.70	24 (31%)
26	BCR	c	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	6 (10%)
24	CLA	d	404	4	65,73,73	2.04	16 (24%)	76,113,113	2.84	28 (36%)
21	OEX	A	401	3,1,39	0,15,15	-	-	-	-	-
36	LMT	Z	101	-	36,36,36	1.19	5 (13%)	47,47,47	1.01	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	OEX	a	401	3,1,39	0,15,15	-	-	-		
27	SQD	l	101	-	53,54,54	0.92	5 (9%)	62,65,65	2.00	12 (19%)
25	PHO	a	407	-	51,69,69	1.01	5 (9%)	47,99,99	1.30	7 (14%)
26	BCR	c	516	-	41,41,41	1.03	2 (4%)	56,56,56	1.18	5 (8%)
26	BCR	B	619	-	41,41,41	1.05	2 (4%)	56,56,56	1.06	2 (3%)
24	CLA	B	608	2	65,73,73	1.94	17 (26%)	76,113,113	2.47	31 (40%)
32	LHG	B	625	-	48,48,48	0.76	1 (2%)	51,54,54	1.21	5 (9%)
24	CLA	C	504	3	65,73,73	2.02	19 (29%)	76,113,113	2.64	23 (30%)
33	DGD	c	519	-	63,63,67	1.15	7 (11%)	77,77,81	1.26	7 (9%)
30	BCT	A	414	22	2,3,3	1.32	0	2,3,3	4.47	2 (100%)
24	CLA	c	503	3	65,73,73	1.92	19 (29%)	76,113,113	2.59	23 (30%)
24	CLA	a	408	1	65,73,73	1.93	16 (24%)	76,113,113	2.69	27 (35%)
24	CLA	B	612	2	65,73,73	1.86	17 (26%)	76,113,113	2.61	32 (42%)
31	LMG	C	501	-	51,51,55	0.93	3 (5%)	59,59,63	1.35	6 (10%)
31	LMG	C	520	-	51,51,55	1.00	6 (11%)	59,59,63	1.41	6 (10%)
26	BCR	C	515	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	8 (14%)
24	CLA	B	611	2	65,73,73	1.93	16 (24%)	76,113,113	2.56	24 (31%)
35	RRX	H	101	-	42,42,42	1.94	11 (26%)	57,58,58	1.99	15 (26%)
24	CLA	B	607	39	65,73,73	1.91	16 (24%)	76,113,113	2.80	28 (36%)
26	BCR	A	409	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	7 (12%)
26	BCR	c	515	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	8 (14%)
32	LHG	d	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.16	6 (11%)
24	CLA	c	506	3	65,73,73	1.94	20 (30%)	76,113,113	2.58	26 (34%)
28	PL9	a	411	-	55,55,55	1.46	9 (16%)	68,69,69	1.53	13 (19%)
36	LMT	M	101	-	36,36,36	1.28	6 (16%)	47,47,47	0.95	1 (2%)
31	LMG	B	620	-	51,51,55	0.92	2 (3%)	59,59,63	1.27	7 (11%)
33	DGD	h	102	-	63,63,67	1.08	5 (7%)	77,77,81	1.17	5 (6%)
38	HEC	V	201	16	32,50,50	2.13	4 (12%)	24,82,82	1.69	4 (16%)
24	CLA	B	606	2	65,73,73	1.99	18 (27%)	76,113,113	2.84	27 (35%)
24	CLA	b	615	2	65,73,73	1.97	19 (29%)	76,113,113	2.75	26 (34%)
24	CLA	c	507	3	65,73,73	1.98	18 (27%)	76,113,113	2.65	27 (35%)
24	CLA	c	509	3	65,73,73	1.96	17 (26%)	76,113,113	2.70	24 (31%)
36	LMT	z	101	-	36,36,36	1.19	6 (16%)	47,47,47	1.01	3 (6%)
32	LHG	b	627	-	48,48,48	0.76	1 (2%)	51,54,54	1.21	5 (9%)
24	CLA	B	603	2	65,73,73	1.94	15 (23%)	76,113,113	2.73	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	e	101	-	48,48,48	0.68	0	51,54,54	1.20	6 (11%)
26	BCR	y	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.21	7 (12%)
33	DGD	C	517	-	63,63,67	1.17	7 (11%)	77,77,81	1.38	7 (9%)
25	PHO	D	402	-	51,69,69	1.06	5 (9%)	47,99,99	1.38	8 (17%)
32	LHG	D	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.16	6 (11%)
26	BCR	d	405	-	41,41,41	1.12	3 (7%)	56,56,56	1.15	7 (12%)
24	CLA	B	604	2	65,73,73	1.91	16 (24%)	76,113,113	2.60	31 (40%)
24	CLA	c	513	3	65,73,73	1.98	18 (27%)	76,113,113	2.60	24 (31%)
24	CLA	B	616	2	65,73,73	1.95	16 (24%)	76,113,113	2.70	28 (36%)
24	CLA	b	607	2	65,73,73	1.86	15 (23%)	76,113,113	2.73	26 (34%)
27	SQD	a	410	-	53,54,54	0.95	6 (11%)	62,65,65	1.92	10 (16%)
24	CLA	B	614	2	65,73,73	1.95	17 (26%)	76,113,113	2.62	29 (38%)

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
24	CLA	b	604	2	1/1/15/20	2/37/115/115	-
24	CLA	C	508	39	1/1/15/20	10/37/115/115	-
26	BCR	b	621	-	-	11/29/63/63	0/2/2/2
24	CLA	b	609	39	1/1/15/20	3/37/115/115	-
24	CLA	b	612	39	-	8/37/115/115	-
32	LHG	E	101	-	-	24/53/53/53	-
27	SQD	a	412	-	-	17/49/69/69	0/1/1/1
24	CLA	a	406	39	-	6/37/115/115	-
34	HEM	e	103	5,6	-	2/12/54/54	-
33	DGD	H	102	-	-	14/51/91/95	0/2/2/2
24	CLA	c	512	3	1/1/15/20	5/37/115/115	-
36	LMT	j	102	-	-	5/15/35/61	0/1/1/2
24	CLA	C	506	3	1/1/15/20	9/37/115/115	-
36	LMT	m	102	-	-	4/21/61/61	0/2/2/2
31	LMG	D	411	37	-	16/46/66/70	0/1/1/1
24	CLA	c	504	3	1/1/15/20	7/37/115/115	-
38	HEC	v	201	16	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	410	-	-	21/49/69/69	0/1/1/1
24	CLA	D	403	4	1/1/15/20	4/37/115/115	-
24	CLA	C	513	3	1/1/15/20	13/37/115/115	-
24	CLA	b	611	2	1/1/15/20	3/37/115/115	-
33	DGD	c	518	-	-	23/51/91/95	0/2/2/2
31	LMG	c	501	-	-	22/46/66/70	0/1/1/1
24	CLA	b	606	2	1/1/15/20	5/37/115/115	-
26	BCR	b	619	-	-	7/29/63/63	0/2/2/2
26	BCR	B	617	-	-	6/29/63/63	0/2/2/2
26	BCR	b	620	-	-	4/29/63/63	0/2/2/2
24	CLA	d	401	39	1/1/15/20	8/37/115/115	-
27	SQD	A	412	-	-	17/49/69/69	0/1/1/1
24	CLA	B	601	39	1/1/15/20	9/37/115/115	-
24	CLA	A	408	1	1/1/15/20	12/37/115/115	-
26	BCR	B	627	-	-	8/29/63/63	0/2/2/2
28	PL9	D	406	-	-	10/53/73/73	0/1/1/1
25	PHO	d	402	-	-	3/37/103/103	0/5/6/6
24	CLA	C	503	3	-	8/37/115/115	-
31	LMG	d	411	37	-	16/46/66/70	0/1/1/1
24	CLA	B	610	39	1/1/15/20	8/37/115/115	-
24	CLA	b	603	39	1/1/15/20	9/37/115/115	-
24	CLA	b	610	2	-	2/37/115/115	-
26	BCR	a	409	-	-	8/29/63/63	0/2/2/2
24	CLA	b	614	2	1/1/15/20	6/37/115/115	-
31	LMG	c	522	-	-	25/46/66/70	0/1/1/1
24	CLA	b	605	2	1/1/15/20	10/37/115/115	-
24	CLA	c	510	3	1/1/15/20	6/37/115/115	-
24	CLA	B	613	2	1/1/15/20	8/37/115/115	-
24	CLA	C	507	3	1/1/15/20	14/37/115/115	-
24	CLA	A	405	1	1/1/15/20	5/37/115/115	-
24	CLA	c	505	39	1/1/15/20	6/37/115/115	-
24	CLA	b	613	2	1/1/15/20	6/37/115/115	-
36	LMT	i	102	-	-	10/21/61/61	0/2/2/2
35	RRX	h	101	-	-	2/29/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	404	4	1/1/15/20	11/37/115/115	-
27	SQD	D	407	-	-	18/40/60/69	0/1/1/1
32	LHG	d	408	-	-	12/53/53/53	-
24	CLA	C	511	3	1/1/15/20	8/37/115/115	-
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2
24	CLA	c	508	39	1/1/15/20	10/37/115/115	-
24	CLA	B	609	2	1/1/15/20	3/37/115/115	-
32	LHG	d	410	-	-	15/50/50/53	-
31	LMG	c	520	-	-	22/46/66/70	0/1/1/1
25	PHO	A	407	-	-	3/37/103/103	0/5/6/6
33	DGD	C	518	-	-	23/51/91/95	0/2/2/2
26	BCR	C	521	-	-	9/29/63/63	0/2/2/2
34	HEM	E	103	5,6	-	2/12/54/54	-
24	CLA	C	512	3	1/1/15/20	5/37/115/115	-
24	CLA	A	406	39	-	6/37/115/115	-
36	LMT	J	102	-	-	5/15/35/61	0/1/1/2
24	CLA	a	405	1	1/1/15/20	5/37/115/115	-
24	CLA	b	618	2	1/1/15/20	10/37/115/115	-
32	LHG	D	408	-	-	12/53/53/53	-
27	SQD	L	101	-	-	20/49/69/69	0/1/1/1
28	PL9	d	406	-	-	10/53/73/73	0/1/1/1
24	CLA	b	617	2	1/1/15/20	5/37/115/115	-
24	CLA	B	602	2	1/1/15/20	2/37/115/115	-
24	CLA	C	502	3	1/1/15/20	5/37/115/115	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
26	BCR	C	516	-	-	11/29/63/63	0/2/2/2
27	SQD	d	407	-	-	18/40/60/69	0/1/1/1
24	CLA	c	511	3	1/1/15/20	8/37/115/115	-
33	DGD	C	519	-	-	16/51/91/95	0/2/2/2
36	LMT	I	102	-	-	10/21/61/61	0/2/2/2
28	PL9	A	411	-	-	12/53/73/73	0/1/1/1
33	DGD	c	517	-	-	17/51/91/95	0/2/2/2
24	CLA	C	505	39	1/1/15/20	6/37/115/115	-
32	LHG	D	410	-	-	15/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	502	3	1/1/15/20	5/37/115/115	-
31	LMG	b	622	-	-	17/46/66/70	0/1/1/1
24	CLA	B	615	2	1/1/15/20	6/37/115/115	-
24	CLA	D	401	39	1/1/15/20	8/37/115/115	-
24	CLA	c	514	3	-	12/37/115/115	-
24	CLA	C	514	3	-	12/37/115/115	-
24	CLA	C	510	3	1/1/15/20	6/37/115/115	-
24	CLA	b	608	2	1/1/15/20	5/37/115/115	-
24	CLA	d	403	4	1/1/15/20	4/37/115/115	-
24	CLA	B	605	2	1/1/15/20	9/37/115/115	-
24	CLA	b	616	2	1/1/15/20	13/37/115/115	-
26	BCR	B	618	-	-	4/29/63/63	0/2/2/2
31	LMG	C	522	-	-	25/46/66/70	0/1/1/1
26	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
24	CLA	C	509	3	1/1/15/20	3/37/115/115	-
26	BCR	c	521	-	-	9/29/63/63	0/2/2/2
24	CLA	d	404	4	1/1/15/20	11/37/115/115	-
36	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
27	SQD	l	101	-	-	21/49/69/69	0/1/1/1
25	PHO	a	407	-	-	3/37/103/103	0/5/6/6
26	BCR	c	516	-	-	11/29/63/63	0/2/2/2
26	BCR	B	619	-	-	11/29/63/63	0/2/2/2
24	CLA	B	608	2	-	2/37/115/115	-
32	LHG	B	625	-	-	19/53/53/53	-
24	CLA	C	504	3	1/1/15/20	7/37/115/115	-
33	DGD	c	519	-	-	16/51/91/95	0/2/2/2
24	CLA	c	503	3	-	8/37/115/115	-
24	CLA	a	408	1	1/1/15/20	12/37/115/115	-
24	CLA	B	612	2	1/1/15/20	6/37/115/115	-
31	LMG	C	501	-	-	22/46/66/70	0/1/1/1
31	LMG	C	520	-	-	22/46/66/70	0/1/1/1
26	BCR	C	515	-	-	8/29/63/63	0/2/2/2
24	CLA	B	611	2	1/1/15/20	6/37/115/115	-
35	RRX	H	101	-	-	2/29/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	607	39	1/1/15/20	3/37/115/115	-
26	BCR	A	409	-	-	8/29/63/63	0/2/2/2
26	BCR	c	515	-	-	8/29/63/63	0/2/2/2
32	LHG	d	409	-	-	18/53/53/53	-
24	CLA	c	506	3	1/1/15/20	9/37/115/115	-
28	PL9	a	411	-	-	12/53/73/73	0/1/1/1
36	LMT	M	101	-	-	4/21/61/61	0/2/2/2
31	LMG	B	620	-	-	17/46/66/70	0/1/1/1
33	DGD	h	102	-	-	14/51/91/95	0/2/2/2
38	HEC	V	201	16	-	2/10/54/54	-
24	CLA	B	606	2	1/1/15/20	5/37/115/115	-
24	CLA	b	615	2	1/1/15/20	8/37/115/115	-
24	CLA	c	507	3	1/1/15/20	14/37/115/115	-
24	CLA	c	509	3	1/1/15/20	3/37/115/115	-
36	LMT	z	101	-	-	11/21/61/61	0/2/2/2
32	LHG	b	627	-	-	19/53/53/53	-
24	CLA	B	603	2	1/1/15/20	9/37/115/115	-
32	LHG	e	101	-	-	24/53/53/53	-
26	BCR	y	101	-	-	5/29/63/63	0/2/2/2
33	DGD	C	517	-	-	17/51/91/95	0/2/2/2
25	PHO	D	402	-	-	3/37/103/103	0/5/6/6
32	LHG	D	409	-	-	18/53/53/53	-
26	BCR	d	405	-	-	5/29/63/63	0/2/2/2
24	CLA	B	604	2	1/1/15/20	5/37/115/115	-
24	CLA	c	513	3	1/1/15/20	13/37/115/115	-
24	CLA	B	616	2	1/1/15/20	10/37/115/115	-
24	CLA	b	607	2	1/1/15/20	9/37/115/115	-
27	SQD	a	410	-	-	21/49/69/69	0/1/1/1
24	CLA	B	614	2	1/1/15/20	13/37/115/115	-

All (1515) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	V	201	HEC	C2B-C3B	-7.12	1.33	1.40
38	v	201	HEC	C2B-C3B	-7.12	1.33	1.40
24	C	513	CLA	C3B-C2B	6.49	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	C3B-C2B	6.48	1.49	1.40
24	D	404	CLA	C3B-C2B	6.45	1.49	1.40
24	d	404	CLA	C3B-C2B	6.45	1.49	1.40
24	b	618	CLA	C3B-C2B	6.33	1.49	1.40
24	c	510	CLA	C3B-C2B	6.32	1.49	1.40
24	C	510	CLA	C3B-C2B	6.31	1.49	1.40
24	C	502	CLA	C3B-C2B	6.29	1.49	1.40
24	c	502	CLA	C3B-C2B	6.29	1.49	1.40
24	C	514	CLA	C3B-C2B	6.27	1.49	1.40
24	B	613	CLA	C3B-C2B	6.25	1.49	1.40
24	b	615	CLA	C3B-C2B	6.25	1.49	1.40
24	B	616	CLA	C3B-C2B	6.24	1.49	1.40
24	C	508	CLA	C3B-C2B	6.24	1.49	1.40
24	c	508	CLA	C3B-C2B	6.24	1.49	1.40
24	B	610	CLA	C3B-C2B	6.22	1.49	1.40
24	c	514	CLA	C3B-C2B	6.21	1.49	1.40
24	C	504	CLA	C3B-C2B	6.18	1.48	1.40
24	c	504	CLA	C3B-C2B	6.18	1.48	1.40
24	b	612	CLA	C3B-C2B	6.15	1.48	1.40
24	C	506	CLA	C3B-C2B	6.08	1.48	1.40
24	c	506	CLA	C3B-C2B	6.08	1.48	1.40
24	c	505	CLA	C3B-C2B	6.07	1.48	1.40
24	C	505	CLA	C3B-C2B	6.05	1.48	1.40
24	B	606	CLA	C3B-C2B	5.96	1.48	1.40
24	b	608	CLA	C3B-C2B	5.96	1.48	1.40
24	D	401	CLA	C3B-C2B	5.95	1.48	1.40
24	d	401	CLA	C3B-C2B	5.95	1.48	1.40
24	B	601	CLA	C3B-C2B	5.93	1.48	1.40
24	b	603	CLA	C3B-C2B	5.93	1.48	1.40
24	D	401	CLA	C3C-C2C	5.93	1.49	1.36
24	d	401	CLA	C3C-C2C	5.93	1.49	1.36
24	B	614	CLA	C3B-C2B	5.90	1.48	1.40
24	b	616	CLA	C3B-C2B	5.90	1.48	1.40
24	C	511	CLA	C3B-C2B	5.89	1.48	1.40
24	c	511	CLA	C3B-C2B	5.89	1.48	1.40
24	C	512	CLA	C3B-C2B	5.88	1.48	1.40
24	c	512	CLA	C3B-C2B	5.88	1.48	1.40
24	C	509	CLA	C3B-C2B	5.78	1.48	1.40
24	c	509	CLA	C3B-C2B	5.78	1.48	1.40
24	B	602	CLA	C3B-C2B	5.68	1.48	1.40
24	b	604	CLA	C3B-C2B	5.68	1.48	1.40
24	B	612	CLA	C3B-C2B	5.61	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	C3B-C2B	5.53	1.48	1.40
24	a	405	CLA	C3B-C2B	5.53	1.48	1.40
24	b	614	CLA	C3B-C2B	5.51	1.48	1.40
24	B	604	CLA	C3B-C2B	5.49	1.48	1.40
24	b	606	CLA	C3B-C2B	5.49	1.48	1.40
24	C	505	CLA	C3C-C2C	5.49	1.48	1.36
24	c	505	CLA	C3C-C2C	5.46	1.48	1.36
24	D	403	CLA	C3B-C2B	5.39	1.47	1.40
24	B	603	CLA	C3B-C2B	5.37	1.47	1.40
24	b	605	CLA	C3B-C2B	5.37	1.47	1.40
24	d	403	CLA	C3B-C2B	5.35	1.47	1.40
24	B	602	CLA	C3C-C2C	5.33	1.48	1.36
24	b	604	CLA	C3C-C2C	5.33	1.48	1.36
24	b	613	CLA	C3B-C2B	5.30	1.47	1.40
24	B	611	CLA	C3B-C2B	5.30	1.47	1.40
24	B	606	CLA	C3C-C2C	5.29	1.48	1.36
24	b	608	CLA	C3C-C2C	5.29	1.48	1.36
24	B	608	CLA	C3B-C2B	5.29	1.47	1.40
24	b	610	CLA	C3B-C2B	5.29	1.47	1.40
24	C	503	CLA	C3B-C2B	5.23	1.47	1.40
24	c	503	CLA	C3B-C2B	5.23	1.47	1.40
38	V	201	HEC	C3C-C2C	-5.23	1.35	1.40
24	d	404	CLA	C3C-C2C	5.23	1.47	1.36
24	D	404	CLA	C3C-C2C	5.22	1.47	1.36
24	B	601	CLA	C3C-C2C	5.21	1.47	1.36
24	b	603	CLA	C3C-C2C	5.21	1.47	1.36
28	D	406	PL9	C7-C3	-5.20	1.46	1.51
28	d	406	PL9	C7-C3	-5.20	1.46	1.51
24	C	514	CLA	C3C-C2C	5.18	1.47	1.36
24	c	514	CLA	C3C-C2C	5.18	1.47	1.36
24	B	605	CLA	C3B-C2B	5.17	1.47	1.40
24	b	607	CLA	C3B-C2B	5.17	1.47	1.40
24	c	504	CLA	C3C-C2C	5.16	1.47	1.36
24	B	615	CLA	C3B-C2B	5.15	1.47	1.40
24	b	617	CLA	C3B-C2B	5.15	1.47	1.40
24	C	513	CLA	C3C-C2C	5.14	1.47	1.36
24	C	504	CLA	C3C-C2C	5.14	1.47	1.36
34	E	103	HEM	C3C-C2C	-5.13	1.33	1.40
34	e	103	HEM	C3C-C2C	-5.13	1.33	1.40
24	A	408	CLA	C3B-C2B	5.12	1.47	1.40
24	a	408	CLA	C3B-C2B	5.12	1.47	1.40
24	b	612	CLA	C3C-C2C	5.11	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C3C-C2C	5.10	1.47	1.36
24	c	513	CLA	C3C-C2C	5.10	1.47	1.36
38	v	201	HEC	C3C-C2C	-5.09	1.35	1.40
24	c	514	CLA	CHC-C1C	5.08	1.48	1.35
24	C	514	CLA	CHC-C1C	5.07	1.48	1.35
24	A	408	CLA	C3C-C2C	5.07	1.47	1.36
24	a	408	CLA	C3C-C2C	5.07	1.47	1.36
24	B	602	CLA	CHC-C1C	5.07	1.48	1.35
24	b	604	CLA	CHC-C1C	5.07	1.48	1.35
24	C	512	CLA	C3C-C2C	5.04	1.47	1.36
24	c	512	CLA	C3C-C2C	5.04	1.47	1.36
24	c	507	CLA	C3B-C2B	5.04	1.47	1.40
24	B	607	CLA	C3C-C2C	5.03	1.47	1.36
24	b	609	CLA	C3C-C2C	5.03	1.47	1.36
24	a	406	CLA	C1D-ND	5.01	1.43	1.37
24	C	507	CLA	C3B-C2B	5.01	1.47	1.40
35	H	101	RRX	C8-C9	4.99	1.56	1.45
24	C	510	CLA	C3C-C2C	4.99	1.47	1.36
24	c	510	CLA	C3C-C2C	4.99	1.47	1.36
24	A	406	CLA	C3C-C2C	4.99	1.47	1.36
24	a	406	CLA	C3C-C2C	4.99	1.47	1.36
24	C	512	CLA	CHC-C1C	4.98	1.47	1.35
24	c	512	CLA	CHC-C1C	4.98	1.47	1.35
24	B	609	CLA	O2D-CGD	4.97	1.45	1.33
24	B	608	CLA	C3C-C2C	4.97	1.47	1.36
35	h	101	RRX	C8-C9	4.97	1.56	1.45
24	C	504	CLA	CHC-C1C	4.96	1.47	1.35
24	b	607	CLA	CHC-C1C	4.96	1.47	1.35
24	B	605	CLA	CHC-C1C	4.96	1.47	1.35
24	c	504	CLA	CHC-C1C	4.95	1.47	1.35
24	B	609	CLA	C3B-C2B	4.95	1.47	1.40
24	B	613	CLA	CHC-C1C	4.94	1.47	1.35
24	b	615	CLA	CHC-C1C	4.94	1.47	1.35
24	b	611	CLA	O2D-CGD	4.94	1.45	1.33
24	A	406	CLA	O2D-CGD	4.94	1.45	1.33
24	a	406	CLA	O2D-CGD	4.94	1.45	1.33
24	A	406	CLA	C1D-ND	4.93	1.43	1.37
24	c	506	CLA	CHC-C1C	4.92	1.47	1.35
24	B	603	CLA	C3C-C2C	4.92	1.47	1.36
24	B	601	CLA	O2D-CGD	4.92	1.45	1.33
24	b	603	CLA	O2D-CGD	4.92	1.45	1.33
24	b	617	CLA	C3C-C2C	4.91	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	C3C-C2C	4.91	1.47	1.36
24	C	510	CLA	O2D-CGD	4.91	1.45	1.33
24	c	510	CLA	O2D-CGD	4.91	1.45	1.33
24	C	506	CLA	CHC-C1C	4.90	1.47	1.35
24	C	507	CLA	C3C-C2C	4.88	1.47	1.36
24	c	507	CLA	C3C-C2C	4.88	1.47	1.36
24	A	406	CLA	CHC-C1C	4.88	1.47	1.35
24	a	406	CLA	CHC-C1C	4.88	1.47	1.35
24	b	605	CLA	C3C-C2C	4.88	1.47	1.36
24	A	408	CLA	CHC-C1C	4.87	1.47	1.35
24	a	408	CLA	CHC-C1C	4.87	1.47	1.35
24	B	615	CLA	C3C-C2C	4.87	1.47	1.36
24	A	408	CLA	O2D-CGD	4.86	1.45	1.33
24	a	408	CLA	O2D-CGD	4.86	1.45	1.33
24	B	614	CLA	CHC-C1C	4.86	1.47	1.35
24	b	616	CLA	CHC-C1C	4.86	1.47	1.35
24	C	509	CLA	C3C-C2C	4.86	1.47	1.36
24	c	509	CLA	C3C-C2C	4.86	1.47	1.36
24	B	613	CLA	C1D-ND	4.85	1.43	1.37
24	C	513	CLA	CHC-C1C	4.84	1.47	1.35
24	c	513	CLA	CHC-C1C	4.84	1.47	1.35
24	C	506	CLA	C3C-C2C	4.82	1.47	1.36
24	c	506	CLA	C3C-C2C	4.82	1.47	1.36
24	B	611	CLA	O2D-CGD	4.82	1.45	1.33
24	b	613	CLA	O2D-CGD	4.82	1.45	1.33
24	D	401	CLA	O2D-CGD	4.81	1.44	1.33
24	d	401	CLA	O2D-CGD	4.81	1.44	1.33
24	C	504	CLA	C1D-ND	4.81	1.43	1.37
24	c	504	CLA	C1D-ND	4.81	1.43	1.37
24	C	507	CLA	O2D-CGD	4.80	1.44	1.33
24	c	507	CLA	O2D-CGD	4.80	1.44	1.33
24	B	606	CLA	CHC-C1C	4.79	1.47	1.35
24	B	610	CLA	CHC-C1C	4.79	1.47	1.35
24	b	608	CLA	CHC-C1C	4.79	1.47	1.35
24	A	406	CLA	C3B-C2B	4.79	1.47	1.40
24	a	406	CLA	C3B-C2B	4.79	1.47	1.40
24	b	615	CLA	C1D-ND	4.78	1.43	1.37
24	b	609	CLA	O2D-CGD	4.78	1.44	1.33
24	b	611	CLA	C3B-C2B	4.78	1.47	1.40
24	B	605	CLA	O2D-CGD	4.78	1.44	1.33
24	b	607	CLA	O2D-CGD	4.78	1.44	1.33
24	B	607	CLA	O2D-CGD	4.78	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	O2D-CGD	4.76	1.44	1.33
24	c	511	CLA	O2D-CGD	4.76	1.44	1.33
24	C	503	CLA	C3C-C2C	4.76	1.46	1.36
24	B	603	CLA	CHC-C1C	4.76	1.47	1.35
24	b	605	CLA	CHC-C1C	4.76	1.47	1.35
24	C	511	CLA	C3C-C2C	4.74	1.46	1.36
24	c	511	CLA	C3C-C2C	4.74	1.46	1.36
24	C	505	CLA	CHC-C1C	4.73	1.47	1.35
24	c	508	CLA	C3C-C2C	4.73	1.46	1.36
24	b	614	CLA	CHC-C1C	4.73	1.47	1.35
24	C	508	CLA	C3C-C2C	4.73	1.46	1.36
24	B	606	CLA	O2D-CGD	4.73	1.44	1.33
24	b	608	CLA	O2D-CGD	4.73	1.44	1.33
24	B	612	CLA	CHC-C1C	4.72	1.47	1.35
24	B	601	CLA	CHC-C1C	4.72	1.47	1.35
24	b	612	CLA	CHC-C1C	4.72	1.47	1.35
24	c	503	CLA	C3C-C2C	4.72	1.46	1.36
24	B	614	CLA	C3C-C2C	4.72	1.46	1.36
24	b	616	CLA	C3C-C2C	4.72	1.46	1.36
24	C	503	CLA	O2D-CGD	4.72	1.44	1.33
24	c	503	CLA	O2D-CGD	4.72	1.44	1.33
24	C	506	CLA	O2D-CGD	4.72	1.44	1.33
24	c	506	CLA	O2D-CGD	4.72	1.44	1.33
24	c	505	CLA	CHC-C1C	4.70	1.47	1.35
24	B	615	CLA	CHC-C1C	4.69	1.47	1.35
24	B	611	CLA	C3C-C2C	4.69	1.46	1.36
24	b	613	CLA	C3C-C2C	4.69	1.46	1.36
24	C	509	CLA	CHC-C1C	4.68	1.47	1.35
24	c	509	CLA	CHC-C1C	4.68	1.47	1.35
24	B	609	CLA	CHC-C1C	4.68	1.47	1.35
24	b	603	CLA	CHC-C1C	4.67	1.46	1.35
24	B	616	CLA	O2D-CGD	4.66	1.44	1.33
24	D	401	CLA	CHC-C1C	4.66	1.46	1.35
24	b	617	CLA	CHC-C1C	4.66	1.46	1.35
24	c	505	CLA	O2D-CGD	4.66	1.44	1.33
24	d	404	CLA	C1D-ND	4.66	1.43	1.37
24	C	514	CLA	O2D-CGD	4.64	1.44	1.33
24	C	502	CLA	CHC-C1C	4.64	1.46	1.35
24	D	404	CLA	CHC-C1C	4.64	1.46	1.35
24	d	404	CLA	CHC-C1C	4.64	1.46	1.35
24	c	502	CLA	CHC-C1C	4.64	1.46	1.35
24	C	505	CLA	O2D-CGD	4.63	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	O2D-CGD	4.63	1.44	1.33
24	d	401	CLA	CHC-C1C	4.63	1.46	1.35
24	D	404	CLA	C1D-ND	4.63	1.43	1.37
24	C	502	CLA	C3C-C2C	4.63	1.46	1.36
24	c	502	CLA	C3C-C2C	4.63	1.46	1.36
24	C	509	CLA	O2D-CGD	4.63	1.44	1.33
24	c	509	CLA	O2D-CGD	4.63	1.44	1.33
24	C	512	CLA	O2D-CGD	4.63	1.44	1.33
24	c	512	CLA	O2D-CGD	4.63	1.44	1.33
24	c	514	CLA	O2D-CGD	4.62	1.44	1.33
24	B	601	CLA	C1D-ND	4.62	1.43	1.37
24	b	603	CLA	C1D-ND	4.62	1.43	1.37
24	b	611	CLA	CHC-C1C	4.61	1.46	1.35
24	b	617	CLA	O2D-CGD	4.61	1.44	1.33
24	B	607	CLA	C3B-C2B	4.60	1.46	1.40
24	b	609	CLA	C3B-C2B	4.60	1.46	1.40
24	B	615	CLA	O2D-CGD	4.59	1.44	1.33
24	B	607	CLA	CHC-C1C	4.59	1.46	1.35
24	b	609	CLA	CHC-C1C	4.59	1.46	1.35
24	D	403	CLA	CHC-C1C	4.58	1.46	1.35
24	d	403	CLA	CHC-C1C	4.58	1.46	1.35
24	C	502	CLA	O2D-CGD	4.57	1.44	1.33
24	c	502	CLA	O2D-CGD	4.57	1.44	1.33
24	C	511	CLA	CHC-C1C	4.56	1.46	1.35
24	c	511	CLA	CHC-C1C	4.56	1.46	1.35
24	B	616	CLA	CHC-C1C	4.56	1.46	1.35
24	b	618	CLA	CHC-C1C	4.56	1.46	1.35
24	B	614	CLA	O2D-CGD	4.56	1.44	1.33
24	b	616	CLA	O2D-CGD	4.56	1.44	1.33
24	B	603	CLA	O2D-CGD	4.55	1.44	1.33
24	b	605	CLA	O2D-CGD	4.55	1.44	1.33
24	A	405	CLA	CHC-C1C	4.55	1.46	1.35
24	B	613	CLA	O2D-CGD	4.55	1.44	1.33
24	b	615	CLA	O2D-CGD	4.55	1.44	1.33
24	b	607	CLA	C3C-C2C	4.55	1.46	1.36
24	C	503	CLA	CHC-C1C	4.54	1.46	1.35
24	b	610	CLA	CHC-C1C	4.54	1.46	1.35
24	c	503	CLA	CHC-C1C	4.54	1.46	1.35
24	B	612	CLA	O2D-CGD	4.54	1.44	1.33
24	B	605	CLA	C3C-C2C	4.53	1.46	1.36
24	a	405	CLA	CHC-C1C	4.52	1.46	1.35
24	b	615	CLA	C3C-C2C	4.52	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	O2D-CGD	4.52	1.44	1.33
24	C	513	CLA	O2D-CGD	4.51	1.44	1.33
24	c	513	CLA	O2D-CGD	4.51	1.44	1.33
24	C	507	CLA	C1D-ND	4.51	1.43	1.37
24	c	507	CLA	C1D-ND	4.51	1.43	1.37
24	B	608	CLA	CHC-C1C	4.51	1.46	1.35
24	B	602	CLA	C1D-ND	4.51	1.43	1.37
24	C	514	CLA	O2A-CGA	4.50	1.46	1.33
24	c	514	CLA	O2A-CGA	4.50	1.46	1.33
24	b	604	CLA	C1D-ND	4.50	1.43	1.37
24	C	507	CLA	CHC-C1C	4.50	1.46	1.35
24	c	507	CLA	CHC-C1C	4.50	1.46	1.35
24	B	613	CLA	C3C-C2C	4.49	1.46	1.36
24	C	510	CLA	CHC-C1C	4.48	1.46	1.35
24	c	510	CLA	CHC-C1C	4.48	1.46	1.35
24	B	602	CLA	O2D-CGD	4.48	1.44	1.33
24	B	604	CLA	O2D-CGD	4.47	1.44	1.33
24	b	606	CLA	O2D-CGD	4.47	1.44	1.33
24	B	609	CLA	C3C-C2C	4.47	1.46	1.36
24	b	611	CLA	C3C-C2C	4.46	1.46	1.36
24	b	618	CLA	C3C-C2C	4.46	1.46	1.36
24	C	508	CLA	O2D-CGD	4.46	1.44	1.33
24	c	508	CLA	O2D-CGD	4.46	1.44	1.33
24	B	616	CLA	C3C-C2C	4.45	1.46	1.36
24	B	604	CLA	C3C-C2C	4.45	1.46	1.36
24	b	606	CLA	C3C-C2C	4.45	1.46	1.36
24	b	604	CLA	O2D-CGD	4.44	1.44	1.33
24	B	611	CLA	CHC-C1C	4.43	1.46	1.35
24	D	403	CLA	C3C-C2C	4.42	1.46	1.36
24	d	403	CLA	C3C-C2C	4.42	1.46	1.36
24	b	613	CLA	CHC-C1C	4.42	1.46	1.35
24	A	405	CLA	C3C-C2C	4.41	1.46	1.36
24	a	405	CLA	C3C-C2C	4.41	1.46	1.36
24	B	601	CLA	O2A-CGA	4.41	1.46	1.33
24	D	404	CLA	O2D-CGD	4.41	1.44	1.33
24	d	404	CLA	O2D-CGD	4.41	1.44	1.33
24	D	401	CLA	O2A-CGA	4.41	1.46	1.33
24	d	401	CLA	O2A-CGA	4.41	1.46	1.33
24	B	610	CLA	C1B-NB	-4.40	1.31	1.35
24	C	510	CLA	O2A-CGA	4.39	1.46	1.33
24	c	510	CLA	O2A-CGA	4.39	1.46	1.33
24	c	508	CLA	CHC-C1C	4.37	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	O2A-CGA	4.37	1.46	1.33
24	C	508	CLA	CHC-C1C	4.37	1.46	1.35
24	B	610	CLA	O2D-CGD	4.36	1.43	1.33
24	C	514	CLA	C1D-ND	4.35	1.43	1.37
24	D	401	CLA	C1D-ND	4.34	1.43	1.37
24	d	401	CLA	C1D-ND	4.34	1.43	1.37
24	D	404	CLA	O2A-CGA	4.33	1.46	1.33
24	d	404	CLA	O2A-CGA	4.33	1.46	1.33
24	b	612	CLA	O2D-CGD	4.32	1.43	1.33
24	C	513	CLA	O2A-CGA	4.30	1.45	1.33
24	c	513	CLA	O2A-CGA	4.30	1.45	1.33
24	c	510	CLA	C1D-ND	4.30	1.43	1.37
24	b	611	CLA	CHD-C1D	4.29	1.46	1.38
24	b	617	CLA	O2A-CGA	4.28	1.45	1.33
24	c	514	CLA	C1D-ND	4.28	1.43	1.37
24	B	609	CLA	CHD-C1D	4.28	1.46	1.38
24	B	615	CLA	O2A-CGA	4.27	1.45	1.33
24	C	511	CLA	CHD-C1D	4.27	1.46	1.38
24	c	511	CLA	CHD-C1D	4.27	1.46	1.38
24	C	510	CLA	C1D-ND	4.25	1.43	1.37
24	B	609	CLA	C1D-ND	4.25	1.43	1.37
24	b	611	CLA	C1D-ND	4.25	1.43	1.37
24	C	504	CLA	O2D-CGD	4.25	1.43	1.33
24	b	610	CLA	O2D-CGD	4.24	1.43	1.33
24	B	604	CLA	CHC-C1C	4.23	1.45	1.35
24	b	606	CLA	CHC-C1C	4.23	1.45	1.35
24	B	608	CLA	O2D-CGD	4.23	1.43	1.33
24	c	504	CLA	O2D-CGD	4.23	1.43	1.33
24	B	606	CLA	C1B-NB	-4.23	1.31	1.35
24	b	608	CLA	C1B-NB	-4.23	1.31	1.35
24	D	403	CLA	O2D-CGD	4.21	1.43	1.33
24	d	403	CLA	O2D-CGD	4.21	1.43	1.33
24	a	406	CLA	O2A-CGA	4.21	1.45	1.33
24	c	508	CLA	C1D-ND	4.20	1.42	1.37
24	B	608	CLA	CHD-C1D	4.20	1.46	1.38
24	b	610	CLA	CHD-C1D	4.19	1.46	1.38
24	B	612	CLA	C3C-C2C	4.19	1.45	1.36
35	H	101	RRX	C12-C13	4.19	1.55	1.45
35	h	101	RRX	C12-C13	4.19	1.55	1.45
24	D	401	CLA	CHD-C1D	4.19	1.46	1.38
24	d	401	CLA	CHD-C1D	4.19	1.46	1.38
28	A	411	PL9	C3-C4	-4.19	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	411	PL9	C3-C4	-4.19	1.42	1.49
38	V	201	HEC	CBC-CAC	-4.18	1.33	1.49
24	c	502	CLA	C1D-ND	4.18	1.42	1.37
24	C	508	CLA	C1D-ND	4.17	1.42	1.37
24	b	614	CLA	C3C-C2C	4.17	1.45	1.36
24	C	507	CLA	CHD-C1D	4.17	1.46	1.38
24	c	507	CLA	CHD-C1D	4.17	1.46	1.38
38	v	201	HEC	CBC-CAC	-4.17	1.33	1.49
24	b	610	CLA	C1B-NB	-4.16	1.31	1.35
24	C	510	CLA	CHD-C1D	4.16	1.46	1.38
24	A	406	CLA	O2A-CGA	4.15	1.45	1.33
24	B	604	CLA	C1D-ND	4.15	1.42	1.37
24	A	405	CLA	C1D-ND	4.13	1.42	1.37
24	a	405	CLA	C1D-ND	4.13	1.42	1.37
24	C	502	CLA	C1D-ND	4.12	1.42	1.37
24	A	405	CLA	O2D-CGD	4.11	1.43	1.33
24	b	612	CLA	C1B-NB	-4.11	1.31	1.35
24	b	606	CLA	C1D-ND	4.10	1.42	1.37
24	C	505	CLA	O2A-CGA	4.10	1.45	1.33
24	c	505	CLA	O2A-CGA	4.10	1.45	1.33
24	C	503	CLA	C1D-ND	4.10	1.42	1.37
24	c	503	CLA	C1D-ND	4.10	1.42	1.37
35	H	101	RRX	C19-C18	4.10	1.54	1.45
24	c	510	CLA	CHD-C1D	4.09	1.46	1.38
38	v	201	HEC	CBB-CAB	-4.09	1.34	1.49
24	B	608	CLA	C1B-NB	-4.09	1.31	1.35
24	a	405	CLA	O2D-CGD	4.08	1.43	1.33
38	V	201	HEC	CBB-CAB	-4.07	1.34	1.49
24	B	602	CLA	CHD-C1D	4.07	1.46	1.38
35	h	101	RRX	C19-C18	4.06	1.54	1.45
24	a	406	CLA	CHD-C1D	4.06	1.46	1.38
24	B	605	CLA	C1D-ND	4.06	1.42	1.37
24	b	607	CLA	C1D-ND	4.06	1.42	1.37
24	D	401	CLA	CHD-C4C	4.06	1.48	1.39
24	d	401	CLA	CHD-C4C	4.06	1.48	1.39
24	c	512	CLA	O2A-CGA	4.06	1.45	1.33
24	A	406	CLA	CHD-C1D	4.04	1.46	1.38
24	B	603	CLA	O2A-CGA	4.04	1.45	1.33
24	C	512	CLA	O2A-CGA	4.04	1.45	1.33
24	b	605	CLA	O2A-CGA	4.04	1.45	1.33
24	B	604	CLA	CHD-C1D	4.04	1.46	1.38
24	b	606	CLA	CHD-C1D	4.04	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	O2A-CGA	4.03	1.45	1.33
24	b	609	CLA	O2A-CGA	4.03	1.45	1.33
24	b	604	CLA	CHD-C1D	4.03	1.46	1.38
24	B	609	CLA	O2A-CGA	4.03	1.45	1.33
24	b	611	CLA	O2A-CGA	4.03	1.45	1.33
24	C	511	CLA	O2A-CGA	4.01	1.45	1.33
24	c	511	CLA	O2A-CGA	4.01	1.45	1.33
24	A	405	CLA	CHD-C1D	4.01	1.46	1.38
24	a	405	CLA	CHD-C1D	4.01	1.46	1.38
24	C	511	CLA	C1D-ND	4.00	1.42	1.37
24	c	511	CLA	C1D-ND	4.00	1.42	1.37
24	c	514	CLA	CHD-C1D	3.99	1.46	1.38
24	C	514	CLA	CHD-C1D	3.99	1.46	1.38
24	B	602	CLA	CHD-C4C	3.99	1.48	1.39
24	C	514	CLA	CHD-C4C	3.99	1.48	1.39
24	c	514	CLA	CHD-C4C	3.99	1.48	1.39
24	C	509	CLA	C1B-NB	-3.98	1.31	1.35
24	c	509	CLA	C1B-NB	-3.98	1.31	1.35
24	B	603	CLA	C1B-NB	-3.98	1.31	1.35
24	b	605	CLA	C1B-NB	-3.98	1.31	1.35
24	b	604	CLA	CHD-C4C	3.97	1.48	1.39
24	b	612	CLA	O2A-CGA	3.95	1.44	1.33
24	B	610	CLA	O2A-CGA	3.95	1.44	1.33
24	C	509	CLA	O2A-CGA	3.93	1.44	1.33
24	c	509	CLA	O2A-CGA	3.93	1.44	1.33
24	C	507	CLA	C1B-NB	-3.93	1.31	1.35
24	c	507	CLA	C1B-NB	-3.93	1.31	1.35
24	C	502	CLA	O2A-CGA	3.92	1.44	1.33
24	c	502	CLA	O2A-CGA	3.92	1.44	1.33
24	B	615	CLA	C1D-ND	3.92	1.42	1.37
24	b	617	CLA	C1D-ND	3.92	1.42	1.37
35	h	101	RRX	C23-C22	3.92	1.54	1.45
24	b	613	CLA	CHD-C1D	3.91	1.46	1.38
24	B	609	CLA	C3D-C2D	3.90	1.49	1.39
24	b	613	CLA	C1D-ND	3.90	1.42	1.37
24	B	611	CLA	CHD-C1D	3.90	1.46	1.38
24	b	613	CLA	C3D-C2D	3.89	1.49	1.39
24	B	606	CLA	O2A-CGA	3.89	1.44	1.33
24	b	608	CLA	O2A-CGA	3.89	1.44	1.33
24	b	611	CLA	C3D-C2D	3.88	1.49	1.39
24	b	618	CLA	O2A-CGA	3.88	1.44	1.33
24	B	616	CLA	O2A-CGA	3.88	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	O2A-CGA	3.88	1.44	1.33
35	H	101	RRX	C23-C22	3.88	1.54	1.45
24	D	404	CLA	CHD-C4C	3.87	1.48	1.39
24	d	404	CLA	CHD-C4C	3.87	1.48	1.39
24	a	408	CLA	O2A-CGA	3.87	1.44	1.33
24	A	408	CLA	O2A-CGA	3.87	1.44	1.33
24	B	611	CLA	C3D-C2D	3.86	1.49	1.39
24	C	503	CLA	O2A-CGA	3.86	1.44	1.33
24	c	503	CLA	O2A-CGA	3.86	1.44	1.33
24	B	604	CLA	O2A-CGA	3.86	1.44	1.33
24	C	508	CLA	O2A-CGA	3.86	1.44	1.33
24	D	403	CLA	O2A-CGA	3.85	1.44	1.33
24	A	405	CLA	CHD-C4C	3.84	1.48	1.39
24	a	405	CLA	CHD-C4C	3.84	1.48	1.39
24	C	510	CLA	C1B-NB	-3.84	1.31	1.35
24	C	505	CLA	C1D-ND	3.84	1.42	1.37
24	c	505	CLA	C1D-ND	3.84	1.42	1.37
24	C	513	CLA	C3D-C2D	3.84	1.49	1.39
24	c	513	CLA	C3D-C2D	3.84	1.49	1.39
24	B	602	CLA	O2A-CGA	3.83	1.44	1.33
24	b	604	CLA	O2A-CGA	3.83	1.44	1.33
24	c	504	CLA	O2A-CGA	3.82	1.44	1.33
24	d	403	CLA	O2A-CGA	3.82	1.44	1.33
24	B	611	CLA	C1D-ND	3.82	1.42	1.37
24	c	508	CLA	O2A-CGA	3.81	1.44	1.33
24	a	408	CLA	C1D-ND	3.81	1.42	1.37
24	A	408	CLA	C1D-ND	3.81	1.42	1.37
24	a	406	CLA	CHD-C4C	3.80	1.47	1.39
24	A	406	CLA	CHD-C4C	3.80	1.47	1.39
24	C	509	CLA	C3D-C2D	3.79	1.49	1.39
24	c	509	CLA	C3D-C2D	3.79	1.49	1.39
24	C	504	CLA	O2A-CGA	3.79	1.44	1.33
24	D	404	CLA	CHD-C1D	3.79	1.45	1.38
24	d	404	CLA	CHD-C1D	3.79	1.45	1.38
24	B	615	CLA	CHD-C1D	3.77	1.45	1.38
24	b	617	CLA	CHD-C1D	3.77	1.45	1.38
24	B	614	CLA	O2A-CGA	3.77	1.44	1.33
24	b	616	CLA	O2A-CGA	3.77	1.44	1.33
24	c	510	CLA	C1B-NB	-3.76	1.31	1.35
28	A	411	PL9	C7-C8	-3.76	1.45	1.50
28	a	411	PL9	C7-C8	-3.76	1.45	1.50
24	B	601	CLA	CHD-C1D	3.74	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C1D-ND	3.74	1.42	1.37
24	b	618	CLA	C1D-ND	3.74	1.42	1.37
24	b	611	CLA	CHD-C4C	3.74	1.47	1.39
24	B	607	CLA	C1D-ND	3.74	1.42	1.37
24	b	609	CLA	C1D-ND	3.74	1.42	1.37
24	B	609	CLA	CHD-C4C	3.73	1.47	1.39
24	b	603	CLA	CHD-C4C	3.72	1.47	1.39
24	C	507	CLA	O2A-CGA	3.72	1.44	1.33
24	c	507	CLA	O2A-CGA	3.72	1.44	1.33
24	c	513	CLA	C1D-ND	3.72	1.42	1.37
24	B	612	CLA	C1B-NB	-3.71	1.31	1.35
24	b	614	CLA	C1B-NB	-3.71	1.31	1.35
24	C	505	CLA	CHD-C4C	3.71	1.47	1.39
24	B	615	CLA	C3D-C2D	3.70	1.49	1.39
24	b	617	CLA	C3D-C2D	3.70	1.49	1.39
24	B	601	CLA	CHD-C4C	3.70	1.47	1.39
24	C	504	CLA	CHD-C1D	3.70	1.45	1.38
24	c	504	CLA	CHD-C1D	3.70	1.45	1.38
24	C	513	CLA	C1D-ND	3.70	1.42	1.37
24	b	603	CLA	CHD-C1D	3.70	1.45	1.38
24	A	405	CLA	C1B-NB	-3.68	1.31	1.35
24	a	405	CLA	C1B-NB	-3.68	1.31	1.35
24	c	505	CLA	CHD-C4C	3.67	1.47	1.39
24	C	512	CLA	C1D-ND	3.67	1.42	1.37
24	c	512	CLA	C1D-ND	3.67	1.42	1.37
24	C	509	CLA	CHD-C1D	3.67	1.45	1.38
24	c	509	CLA	CHD-C1D	3.67	1.45	1.38
24	C	506	CLA	O2A-CGA	3.66	1.44	1.33
24	c	506	CLA	O2A-CGA	3.66	1.44	1.33
24	B	614	CLA	C3D-C2D	3.66	1.49	1.39
24	b	616	CLA	C3D-C2D	3.66	1.49	1.39
24	B	610	CLA	C1D-ND	3.66	1.42	1.37
24	b	613	CLA	O2A-CGA	3.65	1.44	1.33
24	a	408	CLA	CHD-C1D	3.65	1.45	1.38
24	A	408	CLA	CHD-C1D	3.65	1.45	1.38
24	B	607	CLA	CHD-C4C	3.64	1.47	1.39
24	b	609	CLA	CHD-C4C	3.64	1.47	1.39
24	B	614	CLA	C1D-ND	3.64	1.42	1.37
24	b	616	CLA	C1D-ND	3.64	1.42	1.37
24	B	614	CLA	CHD-C1D	3.64	1.45	1.38
24	b	616	CLA	CHD-C1D	3.64	1.45	1.38
24	B	611	CLA	O2A-CGA	3.63	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	C1B-NB	-3.63	1.32	1.35
24	B	608	CLA	O2A-CGA	3.62	1.43	1.33
28	D	406	PL9	C3-C4	-3.62	1.43	1.49
28	d	406	PL9	C3-C4	-3.62	1.43	1.49
24	b	611	CLA	C1B-NB	-3.62	1.32	1.35
24	d	401	CLA	C3D-C2D	3.61	1.49	1.39
24	B	606	CLA	C3D-C2D	3.61	1.49	1.39
24	b	608	CLA	C3D-C2D	3.61	1.49	1.39
24	C	503	CLA	CHD-C1D	3.61	1.45	1.38
24	c	503	CLA	CHD-C1D	3.61	1.45	1.38
34	E	103	HEM	C3C-CAC	3.61	1.55	1.47
34	e	103	HEM	C3C-CAC	3.61	1.55	1.47
24	B	608	CLA	CHD-C4C	3.60	1.47	1.39
35	H	101	RRX	C15-C14	3.60	1.54	1.43
35	h	101	RRX	C15-C14	3.60	1.54	1.43
24	b	610	CLA	O2A-CGA	3.60	1.43	1.33
24	b	614	CLA	O2A-CGA	3.60	1.43	1.33
24	b	612	CLA	C1D-ND	3.59	1.42	1.37
24	C	507	CLA	CHD-C4C	3.59	1.47	1.39
24	B	612	CLA	O2A-CGA	3.59	1.43	1.33
24	D	401	CLA	C3D-C2D	3.59	1.48	1.39
24	C	505	CLA	CHD-C1D	3.58	1.45	1.38
24	c	505	CLA	CHD-C1D	3.58	1.45	1.38
24	C	505	CLA	C3D-C2D	3.58	1.48	1.39
24	B	603	CLA	CHD-C1D	3.58	1.45	1.38
24	b	605	CLA	CHD-C1D	3.58	1.45	1.38
24	B	602	CLA	C3D-C2D	3.58	1.48	1.39
24	b	604	CLA	C3D-C2D	3.58	1.48	1.39
24	c	507	CLA	CHD-C4C	3.57	1.47	1.39
24	C	514	CLA	C3D-C2D	3.57	1.48	1.39
24	c	514	CLA	C3D-C2D	3.57	1.48	1.39
24	b	610	CLA	CHD-C4C	3.57	1.47	1.39
24	C	513	CLA	CHD-C1D	3.57	1.45	1.38
24	c	513	CLA	CHD-C1D	3.57	1.45	1.38
24	B	603	CLA	C1D-ND	3.57	1.42	1.37
24	b	605	CLA	C1D-ND	3.57	1.42	1.37
24	C	507	CLA	C3D-C2D	3.57	1.48	1.39
24	c	507	CLA	C3D-C2D	3.57	1.48	1.39
24	B	605	CLA	CHD-C1D	3.57	1.45	1.38
24	b	607	CLA	CHD-C1D	3.57	1.45	1.38
24	c	505	CLA	C3D-C2D	3.57	1.48	1.39
24	A	406	CLA	C3D-C2D	3.55	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	CLA	C3D-C2D	3.55	1.48	1.39
24	B	616	CLA	CHD-C1D	3.55	1.45	1.38
24	b	618	CLA	CHD-C1D	3.55	1.45	1.38
24	A	408	CLA	C3D-C2D	3.55	1.48	1.39
24	a	408	CLA	C3D-C2D	3.55	1.48	1.39
24	C	511	CLA	CHD-C4C	3.55	1.47	1.39
24	c	511	CLA	CHD-C4C	3.55	1.47	1.39
24	C	512	CLA	CHD-C1D	3.54	1.45	1.38
24	c	512	CLA	CHD-C1D	3.54	1.45	1.38
24	C	502	CLA	CHD-C1D	3.54	1.45	1.38
24	c	502	CLA	CHD-C1D	3.54	1.45	1.38
32	D	408	LHG	O7-C5	-3.53	1.37	1.46
24	b	609	CLA	C3D-C2D	3.52	1.48	1.39
32	d	408	LHG	O7-C5	-3.52	1.37	1.46
24	c	508	CLA	OBD-CAD	3.51	1.28	1.22
35	H	101	RRX	C11-C10	3.51	1.54	1.43
35	h	101	RRX	C11-C10	3.51	1.54	1.43
24	b	616	CLA	C1B-NB	-3.51	1.32	1.35
24	C	504	CLA	C3D-C2D	3.51	1.48	1.39
24	c	504	CLA	C3D-C2D	3.51	1.48	1.39
24	B	606	CLA	C1D-ND	3.50	1.42	1.37
24	b	608	CLA	C1D-ND	3.50	1.42	1.37
24	B	611	CLA	C1B-NB	-3.50	1.32	1.35
24	b	613	CLA	C1B-NB	-3.50	1.32	1.35
26	D	405	BCR	C1-C6	-3.49	1.49	1.53
26	d	405	BCR	C1-C6	-3.49	1.49	1.53
24	B	607	CLA	C3D-C2D	3.49	1.48	1.39
24	c	503	CLA	C3D-C2D	3.49	1.48	1.39
24	C	503	CLA	C3D-C2D	3.49	1.48	1.39
24	B	601	CLA	C3D-C2D	3.48	1.48	1.39
24	b	603	CLA	C3D-C2D	3.48	1.48	1.39
24	B	616	CLA	C1B-NB	-3.47	1.32	1.35
24	b	618	CLA	C1B-NB	-3.47	1.32	1.35
35	H	101	RRX	C16-C17	3.47	1.54	1.43
35	h	101	RRX	C16-C17	3.46	1.54	1.43
24	C	508	CLA	OBD-CAD	3.46	1.28	1.22
24	C	504	CLA	CHD-C4C	3.46	1.47	1.39
24	c	504	CLA	CHD-C4C	3.46	1.47	1.39
24	B	616	CLA	C1C-NC	-3.46	1.32	1.37
24	b	618	CLA	C1C-NC	-3.46	1.32	1.37
24	C	512	CLA	C1B-NB	-3.45	1.32	1.35
24	c	512	CLA	C1B-NB	-3.45	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C3D-C2D	3.45	1.48	1.39
24	A	405	CLA	O2A-CGA	3.45	1.43	1.33
24	C	502	CLA	C3D-C2D	3.44	1.48	1.39
24	c	502	CLA	C3D-C2D	3.44	1.48	1.39
24	C	511	CLA	OBD-CAD	3.44	1.28	1.22
24	c	511	CLA	OBD-CAD	3.44	1.28	1.22
24	B	613	CLA	O2A-CGA	3.44	1.43	1.33
24	b	615	CLA	O2A-CGA	3.44	1.43	1.33
24	a	405	CLA	O2A-CGA	3.43	1.43	1.33
24	C	503	CLA	CHD-C4C	3.43	1.47	1.39
24	c	503	CLA	CHD-C4C	3.43	1.47	1.39
24	C	508	CLA	CHD-C1D	3.43	1.45	1.38
24	C	513	CLA	CHD-C4C	3.43	1.47	1.39
24	c	513	CLA	CHD-C4C	3.43	1.47	1.39
24	c	508	CLA	CHD-C1D	3.42	1.45	1.38
24	B	611	CLA	CHD-C4C	3.42	1.47	1.39
24	b	613	CLA	CHD-C4C	3.42	1.47	1.39
24	B	604	CLA	C1B-NB	-3.42	1.32	1.35
24	b	606	CLA	C1B-NB	-3.42	1.32	1.35
24	B	610	CLA	CHD-C1D	3.41	1.45	1.38
24	B	614	CLA	C1B-NB	-3.41	1.32	1.35
24	C	508	CLA	C3D-C2D	3.41	1.48	1.39
24	b	612	CLA	C3D-C2D	3.40	1.48	1.39
24	C	509	CLA	C1D-ND	3.40	1.42	1.37
24	c	509	CLA	C1D-ND	3.40	1.42	1.37
24	c	508	CLA	C3D-C2D	3.40	1.48	1.39
24	A	408	CLA	CHD-C4C	3.39	1.47	1.39
24	a	408	CLA	CHD-C4C	3.39	1.47	1.39
24	b	612	CLA	CHD-C1D	3.39	1.45	1.38
32	D	409	LHG	O7-C5	-3.39	1.38	1.46
32	d	409	LHG	O7-C5	-3.39	1.38	1.46
26	c	515	BCR	C1-C6	-3.39	1.49	1.53
24	B	605	CLA	C3D-C2D	3.39	1.48	1.39
24	b	607	CLA	C3D-C2D	3.39	1.48	1.39
24	B	605	CLA	CHD-C4C	3.38	1.47	1.39
24	b	607	CLA	CHD-C4C	3.38	1.47	1.39
24	B	603	CLA	CHD-C4C	3.38	1.47	1.39
24	C	508	CLA	CHD-C4C	3.38	1.47	1.39
24	c	508	CLA	CHD-C4C	3.38	1.47	1.39
24	B	606	CLA	CHD-C1D	3.38	1.44	1.38
24	b	608	CLA	CHD-C1D	3.38	1.44	1.38
24	D	404	CLA	C4B-NB	-3.37	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	C4B-NB	-3.37	1.32	1.35
24	B	604	CLA	CHD-C4C	3.36	1.46	1.39
24	b	606	CLA	CHD-C4C	3.36	1.46	1.39
24	B	605	CLA	O2A-CGA	3.36	1.43	1.33
24	b	607	CLA	O2A-CGA	3.36	1.43	1.33
24	C	510	CLA	CHD-C4C	3.36	1.46	1.39
24	c	510	CLA	CHD-C4C	3.36	1.46	1.39
24	C	511	CLA	C1B-NB	-3.36	1.32	1.35
24	c	511	CLA	C1B-NB	-3.36	1.32	1.35
24	b	605	CLA	CHD-C4C	3.35	1.46	1.39
24	B	615	CLA	CHD-C4C	3.35	1.46	1.39
24	b	617	CLA	CHD-C4C	3.35	1.46	1.39
24	C	502	CLA	CHD-C4C	3.35	1.46	1.39
24	c	502	CLA	CHD-C4C	3.35	1.46	1.39
24	B	612	CLA	C3D-C2D	3.34	1.48	1.39
35	H	101	RRX	C20-C21	3.34	1.53	1.43
35	h	101	RRX	C20-C21	3.34	1.53	1.43
31	C	522	LMG	C4-C5	3.33	1.60	1.53
24	B	614	CLA	CHD-C4C	3.33	1.46	1.39
24	b	616	CLA	CHD-C4C	3.33	1.46	1.39
24	B	616	CLA	C3D-C2D	3.33	1.48	1.39
24	b	618	CLA	C3D-C2D	3.33	1.48	1.39
24	c	509	CLA	OBD-CAD	3.33	1.28	1.22
24	b	614	CLA	CHD-C1D	3.33	1.44	1.38
26	C	515	BCR	C1-C6	-3.33	1.49	1.53
24	B	612	CLA	CHD-C1D	3.32	1.44	1.38
24	B	613	CLA	CHD-C1D	3.32	1.44	1.38
24	b	615	CLA	CHD-C1D	3.32	1.44	1.38
31	c	522	LMG	C4-C5	3.32	1.60	1.53
24	b	609	CLA	C1B-NB	-3.31	1.32	1.35
24	C	512	CLA	C3D-C2D	3.31	1.48	1.39
24	c	512	CLA	C3D-C2D	3.31	1.48	1.39
24	B	607	CLA	CHD-C1D	3.30	1.44	1.38
24	B	613	CLA	C1B-NB	-3.30	1.32	1.35
24	b	615	CLA	C1B-NB	-3.30	1.32	1.35
24	C	509	CLA	OBD-CAD	3.30	1.28	1.22
24	B	601	CLA	OBD-CAD	3.30	1.28	1.22
24	b	603	CLA	OBD-CAD	3.30	1.28	1.22
24	C	513	CLA	OBD-CAD	3.29	1.28	1.22
24	c	513	CLA	OBD-CAD	3.29	1.28	1.22
24	b	609	CLA	CHD-C1D	3.29	1.44	1.38
24	d	404	CLA	C3D-C2D	3.29	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C3D-C2D	3.29	1.48	1.39
24	B	607	CLA	C1B-NB	-3.29	1.32	1.35
24	c	508	CLA	C1B-NB	-3.29	1.32	1.35
24	C	510	CLA	C3D-C2D	3.29	1.48	1.39
24	c	510	CLA	C3D-C2D	3.29	1.48	1.39
24	D	404	CLA	C1B-NB	-3.29	1.32	1.35
24	d	404	CLA	C1B-NB	-3.29	1.32	1.35
24	B	608	CLA	C3D-C2D	3.29	1.48	1.39
24	B	613	CLA	CHD-C4C	3.28	1.46	1.39
24	D	404	CLA	C3D-C2D	3.28	1.48	1.39
31	c	520	LMG	O7-C8	-3.28	1.38	1.46
24	B	616	CLA	CHD-C4C	3.28	1.46	1.39
24	b	618	CLA	CHD-C4C	3.28	1.46	1.39
24	C	514	CLA	OBD-CAD	3.28	1.28	1.22
24	B	602	CLA	C1B-NB	-3.27	1.32	1.35
24	b	604	CLA	C1B-NB	-3.27	1.32	1.35
24	C	508	CLA	C1B-NB	-3.26	1.32	1.35
24	b	609	CLA	OBD-CAD	3.26	1.28	1.22
24	D	403	CLA	C1B-NB	-3.26	1.32	1.35
24	d	403	CLA	C1B-NB	-3.25	1.32	1.35
24	b	615	CLA	CHD-C4C	3.25	1.46	1.39
24	B	613	CLA	C3D-C2D	3.25	1.48	1.39
24	b	615	CLA	C3D-C2D	3.25	1.48	1.39
24	B	607	CLA	OBD-CAD	3.25	1.28	1.22
27	D	407	SQD	O47-C7	3.25	1.43	1.34
27	d	407	SQD	O47-C7	3.25	1.43	1.34
24	c	514	CLA	OBD-CAD	3.24	1.28	1.22
31	C	520	LMG	O7-C8	-3.24	1.38	1.46
24	b	610	CLA	C3D-C2D	3.24	1.48	1.39
24	c	505	CLA	OBD-CAD	3.23	1.28	1.22
24	B	609	CLA	OBD-CAD	3.23	1.28	1.22
24	b	611	CLA	OBD-CAD	3.23	1.28	1.22
24	C	512	CLA	CHD-C4C	3.22	1.46	1.39
24	c	512	CLA	CHD-C4C	3.22	1.46	1.39
24	a	408	CLA	OBD-CAD	3.21	1.28	1.22
24	B	606	CLA	CHD-C4C	3.21	1.46	1.39
24	b	608	CLA	CHD-C4C	3.21	1.46	1.39
24	A	408	CLA	OBD-CAD	3.19	1.28	1.22
24	C	506	CLA	CHD-C1D	3.19	1.44	1.38
24	c	506	CLA	CHD-C1D	3.19	1.44	1.38
24	B	615	CLA	OBD-CAD	3.19	1.28	1.22
24	b	617	CLA	OBD-CAD	3.19	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	C1B-NB	-3.18	1.32	1.35
24	d	401	CLA	C1B-NB	-3.18	1.32	1.35
24	D	403	CLA	CHD-C4C	3.17	1.46	1.39
24	B	610	CLA	CHD-C4C	3.17	1.46	1.39
24	C	505	CLA	C1B-NB	-3.17	1.32	1.35
24	c	505	CLA	C1B-NB	-3.17	1.32	1.35
24	C	506	CLA	C1D-ND	3.17	1.41	1.37
24	c	506	CLA	C1D-ND	3.17	1.41	1.37
24	d	403	CLA	CHD-C4C	3.17	1.46	1.39
24	D	403	CLA	CHD-C1D	3.17	1.44	1.38
24	d	403	CLA	CHD-C1D	3.17	1.44	1.38
27	D	407	SQD	O48-C23	3.16	1.42	1.33
27	d	407	SQD	O48-C23	3.15	1.42	1.33
24	B	601	CLA	C1B-NB	-3.14	1.32	1.35
24	b	603	CLA	C1B-NB	-3.14	1.32	1.35
24	C	505	CLA	OBD-CAD	3.14	1.27	1.22
24	b	612	CLA	CHD-C4C	3.14	1.46	1.39
24	A	408	CLA	C1B-NB	-3.11	1.32	1.35
24	C	514	CLA	C4B-NB	-3.11	1.32	1.35
33	C	519	DGD	O3G-C3G	-3.10	1.38	1.43
33	c	519	DGD	O3G-C3G	-3.10	1.38	1.43
24	a	408	CLA	C1B-NB	-3.10	1.32	1.35
24	D	403	CLA	C3D-C4D	-3.10	1.37	1.44
24	d	403	CLA	C3D-C4D	-3.10	1.37	1.44
33	C	517	DGD	O5D-C6D	-3.10	1.38	1.43
33	c	517	DGD	O5D-C6D	-3.10	1.38	1.43
24	c	510	CLA	C3D-C4D	-3.08	1.37	1.44
24	C	509	CLA	CHD-C4C	3.07	1.46	1.39
24	c	509	CLA	CHD-C4C	3.07	1.46	1.39
24	C	503	CLA	OBD-CAD	3.06	1.27	1.22
24	c	503	CLA	OBD-CAD	3.06	1.27	1.22
28	a	411	PL9	C53-C6	-3.06	1.44	1.50
24	A	406	CLA	OBD-CAD	3.06	1.27	1.22
24	C	510	CLA	C3D-C4D	-3.05	1.37	1.44
24	B	614	CLA	OBD-CAD	3.05	1.27	1.22
24	b	616	CLA	OBD-CAD	3.05	1.27	1.22
24	a	406	CLA	OBD-CAD	3.04	1.27	1.22
24	C	511	CLA	C3D-C4D	-3.04	1.37	1.44
24	c	511	CLA	C3D-C4D	-3.04	1.37	1.44
24	b	606	CLA	C3D-C2D	3.03	1.47	1.39
24	B	608	CLA	C3D-C4D	-3.02	1.37	1.44
24	b	610	CLA	C3D-C4D	-3.02	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	411	PL9	C53-C6	-3.02	1.44	1.50
34	E	103	HEM	CAB-C3B	3.02	1.55	1.47
34	e	103	HEM	CAB-C3B	3.02	1.55	1.47
24	b	614	CLA	CHD-C4C	3.01	1.46	1.39
24	c	514	CLA	C4B-NB	-3.01	1.32	1.35
24	B	612	CLA	CHD-C4C	3.01	1.46	1.39
24	B	604	CLA	C3D-C2D	3.01	1.47	1.39
24	D	403	CLA	C1D-ND	3.00	1.41	1.37
24	d	403	CLA	C1D-ND	3.00	1.41	1.37
24	c	503	CLA	C4B-NB	-3.00	1.32	1.35
24	C	511	CLA	C3D-C2D	2.99	1.47	1.39
24	c	511	CLA	C3D-C2D	2.99	1.47	1.39
24	b	605	CLA	OBD-CAD	2.99	1.27	1.22
28	D	406	PL9	C6-C1	-2.98	1.43	1.48
28	d	406	PL9	C6-C1	-2.98	1.43	1.48
24	c	511	CLA	C4B-NB	-2.98	1.32	1.35
24	C	514	CLA	C1B-NB	-2.97	1.32	1.35
24	c	514	CLA	C1B-NB	-2.97	1.32	1.35
24	B	603	CLA	OBD-CAD	2.96	1.27	1.22
24	B	608	CLA	C1D-ND	2.96	1.41	1.37
24	B	603	CLA	C3D-C2D	2.95	1.47	1.39
24	b	605	CLA	C3D-C2D	2.95	1.47	1.39
33	C	517	DGD	O2G-C2G	-2.95	1.39	1.46
28	A	411	PL9	C16-C14	-2.95	1.45	1.51
28	a	411	PL9	C16-C14	-2.95	1.45	1.51
31	c	501	LMG	O7-C8	-2.95	1.39	1.46
33	C	517	DGD	O1G-C1G	-2.94	1.38	1.45
33	c	517	DGD	O1G-C1G	-2.94	1.38	1.45
28	A	411	PL9	C7-C3	-2.94	1.48	1.51
24	B	606	CLA	OBD-CAD	2.94	1.27	1.22
33	C	518	DGD	O1G-C1G	-2.93	1.38	1.45
33	c	518	DGD	O1G-C1G	-2.93	1.38	1.45
33	c	517	DGD	O2G-C2G	-2.93	1.39	1.46
24	C	506	CLA	CHD-C4C	2.92	1.45	1.39
24	c	506	CLA	CHD-C4C	2.92	1.45	1.39
27	A	412	SQD	O48-C23	2.92	1.41	1.33
24	C	511	CLA	C4B-NB	-2.92	1.32	1.35
26	C	521	BCR	C1-C6	-2.91	1.49	1.53
27	a	412	SQD	O48-C23	2.91	1.41	1.33
24	C	512	CLA	OBD-CAD	2.91	1.27	1.22
24	c	512	CLA	OBD-CAD	2.91	1.27	1.22
24	C	503	CLA	C4B-NB	-2.91	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	608	CLA	OBD-CAD	2.91	1.27	1.22
24	A	405	CLA	C3D-C2D	2.90	1.47	1.39
24	a	405	CLA	C3D-C2D	2.90	1.47	1.39
31	C	501	LMG	O7-C8	-2.90	1.39	1.46
24	C	506	CLA	C4B-NB	-2.90	1.32	1.35
24	c	506	CLA	C4B-NB	-2.90	1.32	1.35
26	y	101	BCR	C1-C6	-2.90	1.49	1.53
26	c	521	BCR	C1-C6	-2.89	1.49	1.53
24	b	610	CLA	C1D-ND	2.89	1.41	1.37
36	z	101	LMT	O3'-C3'	-2.88	1.36	1.43
24	c	510	CLA	C4B-NB	-2.88	1.32	1.35
24	b	614	CLA	C1D-ND	2.88	1.41	1.37
24	B	603	CLA	C3D-C4D	-2.88	1.37	1.44
24	b	605	CLA	C3D-C4D	-2.88	1.37	1.44
36	i	102	LMT	O3'-C3'	-2.87	1.36	1.43
24	c	506	CLA	C1B-NB	-2.87	1.32	1.35
26	B	619	BCR	C30-C25	-2.87	1.49	1.53
26	b	621	BCR	C30-C25	-2.87	1.49	1.53
24	B	605	CLA	OBD-CAD	2.87	1.27	1.22
24	b	607	CLA	OBD-CAD	2.87	1.27	1.22
36	I	102	LMT	O3'-C3'	-2.86	1.36	1.43
24	B	602	CLA	OBD-CAD	2.86	1.27	1.22
36	Z	101	LMT	O3'-C3'	-2.85	1.36	1.43
24	A	405	CLA	C4B-NB	-2.85	1.32	1.35
24	a	405	CLA	C4B-NB	-2.85	1.32	1.35
28	a	411	PL9	C7-C3	-2.85	1.48	1.51
24	B	616	CLA	C4B-NB	-2.85	1.32	1.35
24	b	618	CLA	C4B-NB	-2.85	1.32	1.35
24	b	604	CLA	OBD-CAD	2.84	1.27	1.22
36	z	101	LMT	O2'-C2'	-2.84	1.36	1.43
26	Y	101	BCR	C1-C6	-2.83	1.49	1.53
24	d	403	CLA	OBD-CAD	2.83	1.27	1.22
36	M	101	LMT	O2B-C2B	-2.83	1.36	1.43
36	m	102	LMT	O2B-C2B	-2.83	1.36	1.43
36	Z	101	LMT	O2'-C2'	-2.83	1.36	1.43
24	d	403	CLA	C3D-C2D	2.83	1.46	1.39
24	A	406	CLA	C1B-NB	-2.82	1.32	1.35
24	a	406	CLA	C1B-NB	-2.82	1.32	1.35
24	C	506	CLA	C3D-C2D	2.82	1.46	1.39
33	C	519	DGD	O3E-C3E	-2.82	1.36	1.43
33	c	519	DGD	O3E-C3E	-2.82	1.36	1.43
26	B	617	BCR	C1-C6	-2.81	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	619	BCR	C1-C6	-2.81	1.49	1.53
24	C	507	CLA	OBD-CAD	2.81	1.27	1.22
24	c	507	CLA	OBD-CAD	2.81	1.27	1.22
27	A	410	SQD	O48-C23	2.81	1.41	1.33
27	a	410	SQD	O48-C23	2.81	1.41	1.33
24	D	403	CLA	OBD-CAD	2.81	1.27	1.22
24	C	510	CLA	OBD-CAD	2.81	1.27	1.22
24	c	510	CLA	OBD-CAD	2.81	1.27	1.22
26	B	618	BCR	C30-C25	-2.80	1.49	1.53
26	b	620	BCR	C30-C25	-2.80	1.49	1.53
24	b	610	CLA	C4B-NB	-2.80	1.32	1.35
24	a	405	CLA	C1C-NC	-2.80	1.33	1.37
24	A	405	CLA	C1C-NC	-2.80	1.33	1.37
27	A	412	SQD	O47-C7	2.79	1.42	1.34
27	a	412	SQD	O47-C7	2.79	1.42	1.34
24	c	502	CLA	C1B-NB	-2.79	1.32	1.35
24	D	403	CLA	C3D-C2D	2.79	1.46	1.39
26	B	619	BCR	C1-C6	-2.79	1.49	1.53
24	C	506	CLA	C1B-NB	-2.79	1.32	1.35
24	C	510	CLA	C4B-NB	-2.79	1.32	1.35
26	b	621	BCR	C1-C6	-2.79	1.49	1.53
24	C	509	CLA	C1C-NC	-2.78	1.33	1.37
24	c	509	CLA	C1C-NC	-2.78	1.33	1.37
33	C	518	DGD	O3D-C3D	-2.77	1.36	1.43
24	B	606	CLA	C1C-NC	-2.77	1.33	1.37
24	b	608	CLA	C1C-NC	-2.77	1.33	1.37
24	B	611	CLA	C4C-C3C	2.77	1.49	1.45
24	b	613	CLA	C4C-C3C	2.77	1.49	1.45
24	C	508	CLA	C4B-NB	-2.77	1.32	1.35
24	c	508	CLA	C4B-NB	-2.77	1.32	1.35
24	c	506	CLA	C3D-C2D	2.77	1.46	1.39
24	C	506	CLA	C3D-C4D	-2.77	1.37	1.44
24	C	502	CLA	C1B-NB	-2.76	1.32	1.35
36	m	102	LMT	O3'-C3'	-2.76	1.36	1.43
24	c	506	CLA	C3D-C4D	-2.75	1.38	1.44
31	B	620	LMG	O1-C7	-2.75	1.38	1.43
31	b	622	LMG	O1-C7	-2.75	1.38	1.43
24	B	612	CLA	C1D-ND	2.75	1.41	1.37
24	B	608	CLA	C4B-NB	-2.74	1.32	1.35
24	C	506	CLA	OBD-CAD	2.74	1.27	1.22
24	c	506	CLA	OBD-CAD	2.74	1.27	1.22
36	M	101	LMT	O3'-C3'	-2.74	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3D-C4D	-2.73	1.38	1.44
24	c	502	CLA	C3D-C4D	-2.73	1.38	1.44
26	Y	101	BCR	C33-C5	-2.72	1.46	1.50
26	y	101	BCR	C33-C5	-2.72	1.46	1.50
24	B	605	CLA	C3D-C4D	-2.72	1.38	1.44
24	b	607	CLA	C3D-C4D	-2.72	1.38	1.44
24	b	615	CLA	C1C-NC	-2.72	1.33	1.37
24	B	614	CLA	C3D-C4D	-2.72	1.38	1.44
24	b	616	CLA	C3D-C4D	-2.72	1.38	1.44
33	C	517	DGD	O3D-C3D	-2.71	1.36	1.43
33	c	517	DGD	O3D-C3D	-2.71	1.36	1.43
33	c	518	DGD	O3D-C3D	-2.71	1.36	1.43
24	c	506	CLA	C1C-NC	-2.71	1.33	1.37
24	C	506	CLA	C1C-NC	-2.71	1.33	1.37
24	B	602	CLA	C3D-C4D	-2.71	1.38	1.44
24	b	604	CLA	C3D-C4D	-2.71	1.38	1.44
24	C	505	CLA	C3D-C4D	-2.71	1.38	1.44
24	c	505	CLA	C3D-C4D	-2.71	1.38	1.44
33	C	519	DGD	O5D-C6D	-2.71	1.38	1.43
33	c	519	DGD	O5D-C6D	-2.71	1.38	1.43
33	c	517	DGD	O3G-C3G	-2.70	1.38	1.43
24	b	607	CLA	C4B-CHC	2.68	1.48	1.41
25	d	402	PHO	CAC-C3C	-2.68	1.47	1.52
33	C	517	DGD	O3G-C3G	-2.67	1.38	1.43
24	B	613	CLA	C1C-NC	-2.67	1.33	1.37
24	B	609	CLA	C4D-CHA	2.67	1.47	1.38
24	b	611	CLA	C4D-CHA	2.67	1.47	1.38
24	C	504	CLA	C1B-NB	-2.67	1.32	1.35
24	c	504	CLA	C1B-NB	-2.67	1.32	1.35
24	c	504	CLA	C4C-C3C	2.67	1.49	1.45
25	D	402	PHO	CAC-C3C	-2.66	1.47	1.52
24	C	504	CLA	C4C-C3C	2.66	1.49	1.45
24	C	502	CLA	OBD-CAD	2.66	1.27	1.22
24	c	502	CLA	OBD-CAD	2.66	1.27	1.22
24	C	514	CLA	C3D-C4D	-2.65	1.38	1.44
24	c	514	CLA	C3D-C4D	-2.65	1.38	1.44
24	C	504	CLA	C4D-CHA	2.65	1.47	1.38
24	c	504	CLA	C4D-CHA	2.65	1.47	1.38
24	B	605	CLA	C4B-CHC	2.65	1.48	1.41
24	C	506	CLA	C1C-C2C	2.64	1.49	1.44
24	D	403	CLA	C1C-NC	-2.64	1.33	1.37
33	C	518	DGD	O3E-C3E	-2.64	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	C4B-NB	-2.64	1.32	1.35
24	d	401	CLA	C4B-NB	-2.64	1.32	1.35
24	C	513	CLA	C4B-NB	-2.63	1.32	1.35
24	d	403	CLA	C1C-NC	-2.63	1.33	1.37
28	d	406	PL9	C7-C8	-2.63	1.46	1.50
24	B	615	CLA	C1B-NB	-2.63	1.32	1.35
24	b	617	CLA	C1B-NB	-2.63	1.32	1.35
24	b	610	CLA	OBD-CAD	2.62	1.27	1.22
24	B	604	CLA	C4D-CHA	2.62	1.47	1.38
24	b	606	CLA	C4D-CHA	2.62	1.47	1.38
24	D	401	CLA	OBD-CAD	2.62	1.27	1.22
24	d	401	CLA	OBD-CAD	2.62	1.27	1.22
28	D	406	PL9	C7-C8	-2.62	1.46	1.50
28	D	406	PL9	C31-C29	-2.62	1.45	1.51
28	d	406	PL9	C31-C29	-2.62	1.45	1.51
33	c	518	DGD	O3E-C3E	-2.62	1.36	1.43
24	b	612	CLA	OBD-CAD	2.61	1.27	1.22
24	A	405	CLA	C4C-C3C	2.61	1.49	1.45
24	a	405	CLA	C4C-C3C	2.61	1.49	1.45
24	c	506	CLA	C1C-C2C	2.61	1.49	1.44
32	b	627	LHG	O7-C5	-2.61	1.40	1.46
24	A	408	CLA	C1C-NC	-2.60	1.33	1.37
24	a	408	CLA	C1C-NC	-2.60	1.33	1.37
24	C	504	CLA	C1C-C2C	2.60	1.49	1.44
24	c	504	CLA	C1C-C2C	2.60	1.49	1.44
24	A	405	CLA	OBD-CAD	2.60	1.27	1.22
24	a	405	CLA	OBD-CAD	2.60	1.27	1.22
24	C	504	CLA	C3D-C4D	-2.60	1.38	1.44
24	c	504	CLA	C3D-C4D	-2.60	1.38	1.44
24	C	502	CLA	C1C-NC	-2.60	1.33	1.37
27	L	101	SQD	O4-C4	-2.59	1.36	1.43
24	B	610	CLA	OBD-CAD	2.59	1.26	1.22
36	Z	101	LMT	O3B-C3B	-2.59	1.36	1.43
25	A	407	PHO	CAC-C3C	-2.58	1.47	1.52
32	B	625	LHG	O7-C5	-2.58	1.40	1.46
24	B	601	CLA	C4D-CHA	2.58	1.47	1.38
24	b	603	CLA	C4D-CHA	2.58	1.47	1.38
24	B	611	CLA	C4D-CHA	2.58	1.47	1.38
24	B	610	CLA	C1C-NC	-2.58	1.34	1.37
26	d	405	BCR	C30-C25	-2.58	1.50	1.53
24	C	508	CLA	C4D-CHA	2.58	1.47	1.38
24	c	508	CLA	C4D-CHA	2.58	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	OBD-CAD	2.58	1.26	1.22
27	l	101	SQD	O4-C4	-2.58	1.36	1.43
24	A	405	CLA	C3D-C4D	-2.58	1.38	1.44
24	a	405	CLA	C3D-C4D	-2.58	1.38	1.44
25	a	407	PHO	CAC-C3C	-2.57	1.47	1.52
36	z	101	LMT	O3B-C3B	-2.57	1.36	1.43
24	A	406	CLA	C4D-CHA	2.57	1.47	1.38
26	B	618	BCR	C1-C6	-2.56	1.50	1.53
24	C	503	CLA	C1B-CHB	2.56	1.48	1.41
24	c	503	CLA	C1B-CHB	2.56	1.48	1.41
24	B	611	CLA	OBD-CAD	2.56	1.26	1.22
24	b	613	CLA	OBD-CAD	2.56	1.26	1.22
24	C	510	CLA	C1C-NC	-2.56	1.34	1.37
24	c	510	CLA	C1C-NC	-2.56	1.34	1.37
24	b	612	CLA	C1C-NC	-2.56	1.34	1.37
24	A	408	CLA	C3D-C4D	-2.56	1.38	1.44
24	a	408	CLA	C3D-C4D	-2.56	1.38	1.44
24	b	613	CLA	C4D-CHA	2.56	1.47	1.38
24	B	612	CLA	C3D-C4D	-2.56	1.38	1.44
36	I	102	LMT	O2B-C2B	-2.56	1.37	1.43
33	C	518	DGD	O2G-C2G	-2.56	1.40	1.46
36	i	102	LMT	O2B-C2B	-2.55	1.37	1.43
24	a	406	CLA	C4D-CHA	2.55	1.47	1.38
24	B	601	CLA	C1C-NC	-2.55	1.34	1.37
26	D	405	BCR	C30-C25	-2.55	1.50	1.53
24	A	406	CLA	C1C-NC	-2.54	1.34	1.37
24	a	406	CLA	C1C-NC	-2.54	1.34	1.37
24	B	604	CLA	OBD-CAD	2.54	1.26	1.22
24	b	606	CLA	OBD-CAD	2.54	1.26	1.22
24	c	502	CLA	C1C-NC	-2.54	1.34	1.37
26	b	620	BCR	C1-C6	-2.54	1.50	1.53
33	H	102	DGD	O5D-C6D	-2.54	1.39	1.43
33	h	102	DGD	O5D-C6D	-2.54	1.39	1.43
24	c	506	CLA	C1B-CHB	2.54	1.48	1.41
24	B	604	CLA	C3D-C4D	-2.54	1.38	1.44
24	b	606	CLA	C3D-C4D	-2.54	1.38	1.44
33	c	518	DGD	O2G-C2G	-2.53	1.40	1.46
24	B	604	CLA	C4B-NB	-2.53	1.32	1.35
24	b	606	CLA	C4B-NB	-2.53	1.32	1.35
24	C	506	CLA	C1B-CHB	2.53	1.48	1.41
24	b	614	CLA	C3D-C4D	-2.53	1.38	1.44
33	C	517	DGD	O3E-C3E	-2.53	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	517	DGD	O3E-C3E	-2.53	1.37	1.43
24	c	505	CLA	C4D-CHA	2.53	1.47	1.38
24	C	507	CLA	C3D-C4D	-2.52	1.38	1.44
24	c	507	CLA	C3D-C4D	-2.52	1.38	1.44
24	b	610	CLA	C1C-NC	-2.52	1.34	1.37
24	B	614	CLA	C4D-CHA	2.52	1.47	1.38
24	b	616	CLA	C4D-CHA	2.52	1.47	1.38
24	B	616	CLA	C4D-CHA	2.51	1.47	1.38
24	b	618	CLA	C4D-CHA	2.51	1.47	1.38
24	B	608	CLA	C1C-NC	-2.51	1.34	1.37
36	J	102	LMT	O3'-C3'	-2.51	1.37	1.43
36	j	102	LMT	O3'-C3'	-2.51	1.37	1.43
36	I	102	LMT	O1'-C1'	-2.51	1.35	1.40
26	C	521	BCR	C30-C25	-2.50	1.50	1.53
26	c	521	BCR	C30-C25	-2.50	1.50	1.53
24	C	505	CLA	C4D-CHA	2.50	1.47	1.38
27	D	407	SQD	O3-C3	-2.50	1.37	1.43
27	d	407	SQD	O3-C3	-2.50	1.37	1.43
24	A	406	CLA	C3D-C4D	-2.50	1.38	1.44
24	a	406	CLA	C3D-C4D	-2.50	1.38	1.44
24	D	404	CLA	C3D-C4D	-2.50	1.38	1.44
24	d	404	CLA	C3D-C4D	-2.50	1.38	1.44
24	d	401	CLA	C1C-NC	-2.50	1.34	1.37
24	C	504	CLA	C4B-NB	-2.50	1.33	1.35
24	c	504	CLA	C4B-NB	-2.50	1.33	1.35
24	b	603	CLA	C1C-NC	-2.49	1.34	1.37
36	i	102	LMT	O1'-C1'	-2.49	1.35	1.40
24	C	513	CLA	C4D-CHA	2.49	1.47	1.38
24	c	513	CLA	C4D-CHA	2.49	1.47	1.38
27	L	101	SQD	O47-C7	2.49	1.41	1.34
27	l	101	SQD	O47-C7	2.49	1.41	1.34
24	B	616	CLA	C3D-C4D	-2.49	1.38	1.44
24	b	618	CLA	C3D-C4D	-2.49	1.38	1.44
24	D	401	CLA	C1C-NC	-2.49	1.34	1.37
28	A	411	PL9	C31-C29	-2.49	1.46	1.51
24	B	613	CLA	C4B-NB	-2.49	1.33	1.35
24	b	615	CLA	C4B-NB	-2.49	1.33	1.35
24	b	616	CLA	C1C-C2C	2.49	1.49	1.44
31	c	520	LMG	O1-C7	-2.49	1.39	1.43
24	B	615	CLA	C1C-NC	-2.48	1.34	1.37
28	a	411	PL9	C31-C29	-2.48	1.46	1.51
31	C	520	LMG	O1-C7	-2.48	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C1C-C2C	2.48	1.49	1.44
27	L	101	SQD	O48-C23	2.48	1.40	1.33
24	B	615	CLA	C4D-CHA	2.48	1.47	1.38
24	b	617	CLA	C4D-CHA	2.48	1.47	1.38
27	a	412	SQD	O2-C2	-2.48	1.37	1.43
24	c	513	CLA	C4B-NB	-2.48	1.33	1.35
27	A	412	SQD	O2-C2	-2.48	1.37	1.43
24	C	504	CLA	OBD-CAD	2.48	1.26	1.22
24	c	504	CLA	OBD-CAD	2.48	1.26	1.22
24	B	602	CLA	C4D-CHA	2.47	1.47	1.38
24	b	604	CLA	C4D-CHA	2.47	1.47	1.38
26	a	409	BCR	C30-C25	-2.47	1.50	1.53
33	c	518	DGD	O6D-C5D	-2.47	1.38	1.44
24	D	404	CLA	OBD-CAD	2.47	1.26	1.22
24	d	404	CLA	OBD-CAD	2.47	1.26	1.22
24	B	606	CLA	C1C-C2C	2.47	1.49	1.44
24	b	608	CLA	C1C-C2C	2.47	1.49	1.44
27	l	101	SQD	O48-C23	2.46	1.40	1.33
24	A	405	CLA	C4D-CHA	2.46	1.47	1.38
24	a	405	CLA	C4D-CHA	2.46	1.47	1.38
33	C	519	DGD	O2G-C2G	-2.46	1.40	1.46
33	c	519	DGD	O2G-C2G	-2.46	1.40	1.46
24	B	605	CLA	C1C-C2C	2.46	1.49	1.44
24	C	507	CLA	C4C-C3C	2.45	1.49	1.45
24	c	507	CLA	C4C-C3C	2.45	1.49	1.45
24	C	507	CLA	C4D-CHA	2.45	1.47	1.38
24	c	507	CLA	C4D-CHA	2.45	1.47	1.38
24	B	606	CLA	C4D-CHA	2.45	1.47	1.38
24	b	608	CLA	C4D-CHA	2.45	1.47	1.38
24	B	612	CLA	C1C-C2C	2.45	1.49	1.44
36	I	102	LMT	O4'-C4B	-2.45	1.37	1.43
36	i	102	LMT	O4'-C4B	-2.45	1.37	1.43
24	C	506	CLA	CMD-C2D	-2.45	1.45	1.50
24	c	506	CLA	CMD-C2D	-2.45	1.45	1.50
27	A	410	SQD	O2-C2	-2.45	1.37	1.43
33	C	518	DGD	O6D-C5D	-2.44	1.38	1.44
27	L	101	SQD	O2-C2	-2.44	1.37	1.43
31	d	411	LMG	C4-C5	2.43	1.58	1.53
31	D	411	LMG	C4-C5	2.43	1.58	1.53
24	A	408	CLA	C4D-CHA	2.43	1.47	1.38
24	a	408	CLA	C4D-CHA	2.43	1.47	1.38
24	C	512	CLA	C3D-C4D	-2.43	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	C3D-C4D	-2.43	1.38	1.44
26	A	409	BCR	C30-C25	-2.43	1.50	1.53
24	D	403	CLA	C1C-C2C	2.43	1.49	1.44
24	d	403	CLA	C1C-C2C	2.43	1.49	1.44
26	D	405	BCR	C33-C5	-2.43	1.46	1.50
26	d	405	BCR	C33-C5	-2.43	1.46	1.50
24	A	405	CLA	O2D-CED	-2.43	1.39	1.45
24	a	405	CLA	O2D-CED	-2.43	1.39	1.45
36	M	101	LMT	O3B-C3B	-2.43	1.37	1.43
36	m	102	LMT	O3B-C3B	-2.43	1.37	1.43
24	C	502	CLA	C4D-CHA	2.43	1.47	1.38
24	c	502	CLA	C4D-CHA	2.43	1.47	1.38
24	b	617	CLA	C1C-NC	-2.43	1.34	1.37
24	b	614	CLA	C1C-C2C	2.42	1.49	1.44
36	z	101	LMT	O4'-C4B	-2.42	1.37	1.43
24	B	610	CLA	C1B-CHB	2.42	1.47	1.41
31	D	411	LMG	O4-C4	-2.42	1.37	1.43
31	d	411	LMG	O4-C4	-2.42	1.37	1.43
24	A	406	CLA	C1C-C2C	2.42	1.49	1.44
24	a	406	CLA	C1C-C2C	2.42	1.49	1.44
31	C	501	LMG	C4-C5	2.42	1.58	1.53
24	d	401	CLA	C4D-CHA	2.41	1.47	1.38
24	b	607	CLA	C1C-C2C	2.41	1.49	1.44
27	l	101	SQD	O2-C2	-2.41	1.37	1.43
24	D	401	CLA	C4D-CHA	2.41	1.47	1.38
36	M	101	LMT	O2'-C2'	-2.41	1.37	1.43
36	m	102	LMT	O2'-C2'	-2.41	1.37	1.43
24	b	612	CLA	C3D-C4D	-2.41	1.38	1.44
24	a	408	CLA	C4B-NB	-2.41	1.33	1.35
31	c	501	LMG	C4-C5	2.40	1.58	1.53
24	B	603	CLA	C1C-C2C	2.40	1.49	1.44
24	b	605	CLA	C1C-C2C	2.40	1.49	1.44
24	B	601	CLA	C4C-C3C	2.40	1.49	1.45
24	b	603	CLA	C4C-C3C	2.40	1.49	1.45
36	I	102	LMT	O2'-C2'	-2.40	1.37	1.43
36	i	102	LMT	O2'-C2'	-2.40	1.37	1.43
26	a	409	BCR	C1-C6	-2.40	1.50	1.53
24	B	612	CLA	C1C-NC	-2.40	1.34	1.37
24	c	505	CLA	C4B-NB	-2.40	1.33	1.35
24	C	509	CLA	C4D-CHA	2.40	1.46	1.38
33	H	102	DGD	O2G-C2G	-2.40	1.40	1.46
24	d	401	CLA	C3D-C4D	-2.40	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	409	BCR	C1-C6	-2.39	1.50	1.53
36	Z	101	LMT	O4'-C4B	-2.39	1.37	1.43
24	b	606	CLA	C1C-NC	-2.39	1.34	1.37
24	B	610	CLA	C3D-C4D	-2.39	1.38	1.44
24	B	605	CLA	C4D-CHA	2.39	1.46	1.38
24	b	607	CLA	C4D-CHA	2.39	1.46	1.38
33	C	518	DGD	O4E-C4E	-2.38	1.37	1.43
33	c	518	DGD	O4E-C4E	-2.38	1.37	1.43
24	C	513	CLA	C3D-C4D	-2.38	1.38	1.44
24	c	513	CLA	C3D-C4D	-2.38	1.38	1.44
24	C	503	CLA	C3D-C4D	-2.38	1.38	1.44
24	C	509	CLA	C3D-C4D	-2.38	1.38	1.44
24	c	509	CLA	C3D-C4D	-2.38	1.38	1.44
24	D	401	CLA	C3D-C4D	-2.38	1.38	1.44
25	D	402	PHO	CMD-C2D	-2.38	1.45	1.51
25	d	402	PHO	CMD-C2D	-2.38	1.45	1.51
24	C	508	CLA	C3D-C4D	-2.38	1.38	1.44
24	c	508	CLA	C3D-C4D	-2.38	1.38	1.44
24	c	509	CLA	C4D-CHA	2.38	1.46	1.38
24	c	510	CLA	C4D-CHA	2.38	1.46	1.38
24	B	607	CLA	C4D-CHA	2.38	1.46	1.38
24	C	514	CLA	C4D-CHA	2.38	1.46	1.38
24	c	514	CLA	C4D-CHA	2.38	1.46	1.38
24	b	615	CLA	C1B-CHB	2.38	1.47	1.41
24	B	610	CLA	C4D-CHA	2.38	1.46	1.38
27	a	410	SQD	O2-C2	-2.38	1.37	1.43
24	D	404	CLA	C1C-NC	-2.37	1.34	1.37
24	d	404	CLA	C1C-NC	-2.37	1.34	1.37
24	B	613	CLA	C1B-CHB	2.37	1.47	1.41
31	c	522	LMG	O2-C2	-2.37	1.37	1.43
24	B	604	CLA	C1C-NC	-2.37	1.34	1.37
24	b	614	CLA	C1C-NC	-2.37	1.34	1.37
24	C	512	CLA	C1B-CHB	2.37	1.47	1.41
24	c	512	CLA	C1B-CHB	2.37	1.47	1.41
27	a	410	SQD	O4-C4	-2.37	1.37	1.43
24	C	510	CLA	C4D-CHA	2.37	1.46	1.38
24	B	603	CLA	C4D-CHA	2.37	1.46	1.38
24	b	605	CLA	C4D-CHA	2.37	1.46	1.38
33	H	102	DGD	C4D-C5D	2.37	1.58	1.53
33	h	102	DGD	C4D-C5D	2.37	1.58	1.53
24	B	601	CLA	C3D-C4D	-2.36	1.38	1.44
24	b	603	CLA	C3D-C4D	-2.36	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C4D-CHA	2.36	1.46	1.38
24	b	612	CLA	C1B-CHB	2.36	1.47	1.41
24	C	503	CLA	C4D-CHA	2.36	1.46	1.38
24	c	503	CLA	C4D-CHA	2.36	1.46	1.38
27	A	410	SQD	O4-C4	-2.36	1.37	1.43
24	C	505	CLA	C1C-NC	-2.36	1.34	1.37
24	c	505	CLA	C1C-NC	-2.36	1.34	1.37
24	b	609	CLA	C4D-CHA	2.36	1.46	1.38
33	h	102	DGD	O2G-C2G	-2.36	1.40	1.46
31	d	411	LMG	O7-C8	-2.35	1.40	1.46
27	D	407	SQD	O4-C4	-2.35	1.37	1.43
27	d	407	SQD	O4-C4	-2.35	1.37	1.43
24	c	503	CLA	C3D-C4D	-2.35	1.38	1.44
33	C	519	DGD	O3D-C3D	-2.35	1.37	1.43
33	c	519	DGD	O3D-C3D	-2.35	1.37	1.43
24	C	503	CLA	C1C-NC	-2.35	1.34	1.37
24	c	503	CLA	C1C-NC	-2.35	1.34	1.37
24	B	615	CLA	C3D-C4D	-2.35	1.38	1.44
24	b	617	CLA	C3D-C4D	-2.35	1.38	1.44
27	A	410	SQD	O47-C45	-2.35	1.40	1.46
27	a	410	SQD	O47-C45	-2.35	1.40	1.46
24	B	610	CLA	C1C-C2C	2.35	1.49	1.44
24	B	612	CLA	C4B-NB	-2.34	1.33	1.35
31	C	522	LMG	O2-C2	-2.34	1.37	1.43
28	d	406	PL9	C16-C14	-2.34	1.46	1.51
24	C	512	CLA	C4D-CHA	2.34	1.46	1.38
24	c	512	CLA	C4D-CHA	2.34	1.46	1.38
24	C	511	CLA	C4D-CHA	2.34	1.46	1.38
24	c	511	CLA	C4D-CHA	2.34	1.46	1.38
24	b	614	CLA	C4D-CHA	2.34	1.46	1.38
24	B	611	CLA	C3D-C4D	-2.34	1.38	1.44
24	b	613	CLA	C3D-C4D	-2.34	1.38	1.44
24	B	606	CLA	C3D-C4D	-2.33	1.38	1.44
24	b	608	CLA	C3D-C4D	-2.33	1.38	1.44
24	c	504	CLA	O2D-CED	-2.33	1.39	1.45
24	B	611	CLA	C1C-NC	-2.33	1.34	1.37
24	b	613	CLA	C1C-NC	-2.33	1.34	1.37
24	b	612	CLA	C4D-CHA	2.33	1.46	1.38
24	B	613	CLA	C3D-C4D	-2.32	1.38	1.44
24	b	615	CLA	C3D-C4D	-2.32	1.38	1.44
24	C	504	CLA	O2D-CED	-2.32	1.39	1.45
31	D	411	LMG	O7-C8	-2.32	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Z	101	LMT	O2B-C2B	-2.32	1.37	1.43
26	c	516	BCR	C1-C6	-2.32	1.50	1.53
33	c	519	DGD	C3E-C2E	2.31	1.58	1.52
24	C	512	CLA	C1C-C2C	2.31	1.49	1.44
24	c	512	CLA	C1C-C2C	2.31	1.49	1.44
24	b	611	CLA	C3D-C4D	-2.31	1.39	1.44
24	b	612	CLA	C1C-C2C	2.31	1.49	1.44
24	A	408	CLA	C4B-NB	-2.31	1.33	1.35
24	b	611	CLA	C1B-CHB	2.31	1.47	1.41
24	b	614	CLA	C4B-NB	-2.31	1.33	1.35
24	B	613	CLA	C4C-C3C	2.31	1.49	1.45
24	b	615	CLA	C4C-C3C	2.31	1.49	1.45
24	c	508	CLA	C1C-NC	-2.31	1.34	1.37
36	m	102	LMT	O1'-C1'	-2.30	1.36	1.40
24	D	404	CLA	C4D-CHA	2.30	1.46	1.38
24	d	404	CLA	C4D-CHA	2.30	1.46	1.38
26	C	516	BCR	C1-C6	-2.30	1.50	1.53
24	C	505	CLA	C4B-NB	-2.30	1.33	1.35
28	D	406	PL9	C16-C14	-2.30	1.46	1.51
24	b	610	CLA	C4D-CHA	2.30	1.46	1.38
36	z	101	LMT	O2B-C2B	-2.30	1.37	1.43
27	D	407	SQD	O2-C2	-2.29	1.37	1.43
27	d	407	SQD	O2-C2	-2.29	1.37	1.43
33	C	519	DGD	C3E-C2E	2.29	1.58	1.52
24	B	609	CLA	C1B-CHB	2.29	1.47	1.41
24	B	608	CLA	C4D-CHA	2.29	1.46	1.38
24	C	511	CLA	C1C-NC	-2.29	1.34	1.37
24	c	511	CLA	C1C-NC	-2.29	1.34	1.37
24	A	406	CLA	C4B-CHC	2.29	1.47	1.41
24	a	406	CLA	C4B-CHC	2.29	1.47	1.41
24	D	403	CLA	C1B-CHB	2.28	1.47	1.41
24	C	502	CLA	C1B-CHB	2.28	1.47	1.41
24	d	403	CLA	C1B-CHB	2.28	1.47	1.41
24	B	609	CLA	C3D-C4D	-2.28	1.39	1.44
24	B	613	CLA	C4D-CHA	2.28	1.46	1.38
24	b	615	CLA	C4D-CHA	2.28	1.46	1.38
31	D	411	LMG	O2-C2	-2.28	1.37	1.43
31	d	411	LMG	O2-C2	-2.28	1.37	1.43
31	C	520	LMG	O2-C2	-2.27	1.37	1.43
31	c	520	LMG	O2-C2	-2.27	1.37	1.43
24	c	504	CLA	C4B-CHC	2.27	1.47	1.41
24	B	607	CLA	C1C-NC	-2.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C4B-NB	-2.27	1.33	1.35
36	J	102	LMT	C3'-C2'	2.27	1.58	1.52
36	j	102	LMT	C3'-C2'	2.27	1.58	1.52
24	b	615	CLA	C1C-C2C	2.27	1.49	1.44
24	c	502	CLA	C1B-CHB	2.27	1.47	1.41
24	B	614	CLA	C4B-NB	-2.27	1.33	1.35
24	C	513	CLA	C4B-CHC	2.26	1.47	1.41
24	b	609	CLA	C1C-NC	-2.26	1.34	1.37
36	M	101	LMT	O1'-C1'	-2.25	1.36	1.40
24	C	508	CLA	C1C-NC	-2.25	1.34	1.37
24	B	607	CLA	C1B-CHB	2.25	1.47	1.41
24	C	512	CLA	C4B-CHC	2.25	1.47	1.41
24	c	512	CLA	C4B-CHC	2.25	1.47	1.41
24	c	513	CLA	C1C-C2C	2.25	1.48	1.44
24	B	604	CLA	C1B-CHB	2.25	1.47	1.41
24	b	606	CLA	C1B-CHB	2.25	1.47	1.41
24	b	609	CLA	C1B-CHB	2.25	1.47	1.41
27	l	101	SQD	O3-C3	-2.25	1.37	1.43
24	C	513	CLA	C1C-C2C	2.25	1.48	1.44
24	C	507	CLA	C4B-NB	-2.24	1.33	1.35
27	L	101	SQD	O3-C3	-2.24	1.37	1.43
24	C	504	CLA	C4B-CHC	2.24	1.47	1.41
28	A	411	PL9	C25-C24	-2.24	1.44	1.50
24	b	617	CLA	C4B-CHC	2.24	1.47	1.41
24	B	615	CLA	C4B-CHC	2.23	1.47	1.41
24	C	514	CLA	C4B-CHC	2.23	1.47	1.41
24	c	514	CLA	C4B-CHC	2.23	1.47	1.41
35	h	101	RRX	C24-C25	2.23	1.53	1.45
26	c	516	BCR	C30-C25	-2.23	1.50	1.53
24	C	509	CLA	C4B-NB	-2.23	1.33	1.35
24	c	509	CLA	C4B-NB	-2.23	1.33	1.35
24	B	614	CLA	C4B-CHC	2.23	1.47	1.41
24	b	616	CLA	C4B-CHC	2.23	1.47	1.41
24	c	505	CLA	C4B-CHC	2.23	1.47	1.41
24	C	512	CLA	C1C-NC	-2.23	1.34	1.37
24	c	512	CLA	C1C-NC	-2.23	1.34	1.37
24	b	615	CLA	OBD-CAD	2.23	1.26	1.22
24	C	514	CLA	C1C-C2C	2.23	1.48	1.44
24	c	514	CLA	C1C-C2C	2.23	1.48	1.44
24	c	513	CLA	C4B-CHC	2.23	1.47	1.41
24	B	613	CLA	C1C-C2C	2.22	1.48	1.44
24	C	509	CLA	C1B-CHB	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	OBD-CAD	2.21	1.26	1.22
24	B	602	CLA	C4B-CHC	2.21	1.47	1.41
24	b	604	CLA	C4B-CHC	2.21	1.47	1.41
24	B	606	CLA	C4B-NB	-2.21	1.33	1.35
24	b	608	CLA	C4B-NB	-2.21	1.33	1.35
24	B	616	CLA	OBD-CAD	2.20	1.26	1.22
24	C	503	CLA	C1B-NB	-2.20	1.33	1.35
24	c	503	CLA	C1B-NB	-2.20	1.33	1.35
28	a	411	PL9	C25-C24	-2.20	1.45	1.50
31	D	411	LMG	O3-C3	-2.19	1.37	1.43
31	d	411	LMG	O3-C3	-2.19	1.37	1.43
24	B	615	CLA	C1C-C2C	2.19	1.48	1.44
24	b	617	CLA	C1C-C2C	2.19	1.48	1.44
35	H	101	RRX	C24-C25	2.19	1.52	1.45
24	D	403	CLA	C4D-CHA	2.19	1.46	1.38
24	d	403	CLA	C4D-CHA	2.19	1.46	1.38
26	C	515	BCR	C30-C25	-2.19	1.50	1.53
26	C	516	BCR	C30-C25	-2.19	1.50	1.53
26	c	515	BCR	C30-C25	-2.19	1.50	1.53
31	c	501	LMG	C4-C3	2.19	1.57	1.52
33	C	518	DGD	C4D-C3D	2.19	1.57	1.52
33	c	518	DGD	C4D-C3D	2.19	1.57	1.52
24	c	503	CLA	C4C-C3C	2.19	1.48	1.45
24	C	506	CLA	C4B-CHC	2.18	1.47	1.41
24	c	506	CLA	C4B-CHC	2.18	1.47	1.41
24	c	509	CLA	C1B-CHB	2.18	1.47	1.41
24	c	507	CLA	C4B-NB	-2.18	1.33	1.35
31	c	522	LMG	O8-C9	-2.18	1.40	1.45
24	C	505	CLA	C4B-CHC	2.18	1.47	1.41
24	B	615	CLA	C1B-CHB	2.18	1.47	1.41
24	b	617	CLA	C1B-CHB	2.18	1.47	1.41
24	C	507	CLA	C1C-NC	-2.17	1.34	1.37
24	c	507	CLA	C1C-NC	-2.17	1.34	1.37
27	A	410	SQD	O47-C7	2.17	1.40	1.34
31	C	522	LMG	O7-C8	-2.17	1.41	1.46
24	B	608	CLA	C1C-C2C	2.17	1.48	1.44
24	C	506	CLA	C4D-CHA	2.16	1.46	1.38
24	c	506	CLA	C4D-CHA	2.16	1.46	1.38
24	A	408	CLA	C1C-C2C	2.16	1.48	1.44
24	a	408	CLA	C1C-C2C	2.16	1.48	1.44
24	C	503	CLA	C4C-C3C	2.16	1.48	1.45
25	a	407	PHO	CMC-C2C	-2.16	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	OBD-CAD	2.16	1.26	1.22
31	C	501	LMG	C4-C3	2.16	1.57	1.52
36	M	101	LMT	O4'-C4B	-2.16	1.37	1.43
24	B	602	CLA	C1B-CHB	2.16	1.47	1.41
24	b	604	CLA	C1B-CHB	2.16	1.47	1.41
27	A	412	SQD	O3-C3	-2.15	1.37	1.43
27	a	412	SQD	O3-C3	-2.15	1.37	1.43
24	b	610	CLA	C1C-C2C	2.15	1.48	1.44
31	C	522	LMG	O8-C9	-2.15	1.40	1.45
33	C	517	DGD	O4D-C4D	-2.15	1.37	1.43
33	c	517	DGD	O4D-C4D	-2.15	1.37	1.43
28	A	411	PL9	C6-C1	-2.15	1.44	1.48
28	a	411	PL9	C6-C1	-2.15	1.44	1.48
24	C	511	CLA	C1B-CHB	2.14	1.47	1.41
24	c	511	CLA	C1B-CHB	2.14	1.47	1.41
28	D	406	PL9	C53-C6	-2.14	1.46	1.50
28	d	406	PL9	C53-C6	-2.14	1.46	1.50
27	a	410	SQD	O47-C7	2.14	1.40	1.34
24	b	610	CLA	C4C-C3C	2.14	1.48	1.45
24	b	612	CLA	C4B-CHC	2.14	1.46	1.41
31	c	522	LMG	O7-C8	-2.14	1.41	1.46
24	B	613	CLA	C4B-CHC	2.13	1.46	1.41
24	b	615	CLA	C4B-CHC	2.13	1.46	1.41
26	B	627	BCR	C30-C25	-2.13	1.50	1.53
24	C	502	CLA	C4B-CHC	2.13	1.46	1.41
24	c	502	CLA	C4B-CHC	2.13	1.46	1.41
24	B	612	CLA	OBD-CAD	2.12	1.26	1.22
36	m	102	LMT	O4'-C4B	-2.12	1.38	1.43
32	d	409	LHG	P-O6	2.12	1.67	1.59
27	A	410	SQD	O3-C3	-2.12	1.38	1.43
27	a	410	SQD	O3-C3	-2.12	1.38	1.43
24	b	614	CLA	OBD-CAD	2.12	1.26	1.22
24	A	406	CLA	C4B-NB	-2.12	1.33	1.35
24	a	406	CLA	C4B-NB	-2.12	1.33	1.35
24	C	514	CLA	C4C-C3C	2.12	1.48	1.45
24	c	514	CLA	C4C-C3C	2.12	1.48	1.45
28	A	411	PL9	C10-C9	-2.12	1.45	1.50
28	a	411	PL9	C10-C9	-2.12	1.45	1.50
24	b	603	CLA	C1B-CHB	2.11	1.46	1.41
24	C	507	CLA	CMB-C2B	-2.11	1.47	1.51
24	c	507	CLA	CMB-C2B	-2.11	1.47	1.51
24	D	403	CLA	O2D-CED	-2.11	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C1C-NC	-2.11	1.34	1.37
24	b	605	CLA	C1C-NC	-2.11	1.34	1.37
32	D	410	LHG	O8-C6	-2.11	1.40	1.45
32	d	410	LHG	O8-C6	-2.11	1.40	1.45
25	A	407	PHO	CMC-C2C	-2.11	1.46	1.51
24	B	610	CLA	C4B-CHC	2.11	1.46	1.41
31	B	620	LMG	C4-C5	2.11	1.57	1.53
31	b	622	LMG	C4-C5	2.11	1.57	1.53
31	c	520	LMG	O6-C5	-2.10	1.39	1.44
31	C	520	LMG	C4-C3	2.10	1.57	1.52
31	c	520	LMG	C4-C3	2.10	1.57	1.52
32	D	409	LHG	P-O6	2.10	1.67	1.59
24	C	509	CLA	C4C-C3C	2.10	1.48	1.45
24	c	509	CLA	C4C-C3C	2.10	1.48	1.45
33	H	102	DGD	O3D-C3D	-2.10	1.38	1.43
33	h	102	DGD	O3D-C3D	-2.10	1.38	1.43
36	j	102	LMT	O2'-C2'	-2.10	1.38	1.43
33	H	102	DGD	C3G-C2G	2.09	1.57	1.50
24	d	403	CLA	O2D-CED	-2.09	1.40	1.45
24	B	608	CLA	C4C-C3C	2.09	1.48	1.45
24	C	504	CLA	C1C-NC	-2.09	1.34	1.37
24	C	513	CLA	C1C-NC	-2.09	1.34	1.37
24	c	504	CLA	C1C-NC	-2.09	1.34	1.37
24	c	513	CLA	C1C-NC	-2.09	1.34	1.37
24	B	601	CLA	C4B-NB	-2.09	1.33	1.35
24	b	603	CLA	C4B-NB	-2.09	1.33	1.35
25	D	402	PHO	CMB-C2B	-2.09	1.46	1.51
24	B	611	CLA	C1B-CHB	2.09	1.46	1.41
24	b	613	CLA	C1B-CHB	2.09	1.46	1.41
35	H	101	RRX	C7-C6	2.09	1.52	1.45
35	h	101	RRX	C7-C6	2.09	1.52	1.45
24	B	606	CLA	C4C-C3C	2.09	1.48	1.45
24	b	608	CLA	C4C-C3C	2.09	1.48	1.45
24	A	405	CLA	C1C-C2C	2.09	1.48	1.44
24	a	405	CLA	C1C-C2C	2.09	1.48	1.44
24	C	508	CLA	C1B-CHB	2.09	1.46	1.41
24	B	607	CLA	C1C-C2C	2.09	1.48	1.44
24	b	609	CLA	C1C-C2C	2.09	1.48	1.44
33	h	102	DGD	C3G-C2G	2.08	1.57	1.50
24	C	513	CLA	C4C-C3C	2.08	1.48	1.45
24	c	513	CLA	C4C-C3C	2.08	1.48	1.45
24	C	506	CLA	MG-ND	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	MG-ND	-2.08	2.01	2.05
24	B	601	CLA	C1B-CHB	2.08	1.46	1.41
25	A	407	PHO	CMB-C2B	-2.08	1.46	1.51
25	a	407	PHO	CMB-C2B	-2.08	1.46	1.51
24	B	616	CLA	C1B-CHB	2.08	1.46	1.41
24	c	508	CLA	C1B-CHB	2.07	1.46	1.41
24	C	508	CLA	C1A-CHA	2.07	1.51	1.43
24	c	508	CLA	C1A-CHA	2.07	1.51	1.43
31	C	520	LMG	O3-C3	-2.07	1.38	1.43
25	A	407	PHO	C1C-NC	-2.07	1.32	1.38
31	C	520	LMG	O6-C5	-2.07	1.39	1.44
24	c	505	CLA	C4C-C3C	2.07	1.48	1.45
24	b	607	CLA	C1B-CHB	2.06	1.46	1.41
24	C	505	CLA	C4C-C3C	2.06	1.48	1.45
24	B	606	CLA	C4B-CHC	2.06	1.46	1.41
24	b	608	CLA	C4B-CHC	2.06	1.46	1.41
24	C	503	CLA	O2A-C1	-2.06	1.40	1.46
24	C	505	CLA	C1B-CHB	2.06	1.46	1.41
24	c	505	CLA	C1B-CHB	2.06	1.46	1.41
24	C	502	CLA	C4C-C3C	2.06	1.48	1.45
24	c	502	CLA	C4C-C3C	2.06	1.48	1.45
24	C	513	CLA	C1B-CHB	2.06	1.46	1.41
24	c	503	CLA	C4B-CHC	2.06	1.46	1.41
24	c	513	CLA	C1B-CHB	2.06	1.46	1.41
35	H	101	RRX	C10-C9	-2.06	1.33	1.35
35	h	101	RRX	C10-C9	-2.06	1.33	1.35
24	C	511	CLA	C4B-CHC	2.06	1.46	1.41
26	T	101	BCR	C30-C25	-2.06	1.50	1.53
33	C	518	DGD	C3E-C2E	2.06	1.57	1.52
33	c	518	DGD	C3E-C2E	2.06	1.57	1.52
36	J	102	LMT	O2'-C2'	-2.06	1.38	1.43
24	c	503	CLA	O2A-C1	-2.06	1.40	1.46
24	c	511	CLA	C4B-CHC	2.05	1.46	1.41
26	C	515	BCR	C33-C5	-2.05	1.47	1.50
26	c	515	BCR	C33-C5	-2.05	1.47	1.50
26	Y	101	BCR	C30-C25	-2.05	1.50	1.53
26	y	101	BCR	C30-C25	-2.05	1.50	1.53
33	C	519	DGD	C4D-C5D	2.05	1.57	1.53
33	c	519	DGD	C4D-C5D	2.05	1.57	1.53
25	d	402	PHO	CMB-C2B	-2.05	1.46	1.51
24	C	505	CLA	C1C-C2C	2.05	1.48	1.44
24	c	505	CLA	C1C-C2C	2.05	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	407	PHO	C1C-NC	-2.05	1.32	1.38
24	C	514	CLA	C1C-NC	-2.04	1.34	1.37
24	c	514	CLA	C1C-NC	-2.04	1.34	1.37
24	b	603	CLA	C4B-CHC	2.04	1.46	1.41
24	b	618	CLA	C1B-CHB	2.04	1.46	1.41
25	D	402	PHO	CMC-C2C	-2.04	1.46	1.51
25	d	402	PHO	CMC-C2C	-2.04	1.46	1.51
24	b	611	CLA	C1C-NC	-2.04	1.34	1.37
24	C	503	CLA	C4B-CHC	2.04	1.46	1.41
24	B	614	CLA	C1C-NC	-2.03	1.34	1.37
24	b	616	CLA	C1C-NC	-2.03	1.34	1.37
24	D	404	CLA	C4B-CHC	2.03	1.46	1.41
24	d	404	CLA	C4B-CHC	2.03	1.46	1.41
31	c	520	LMG	O3-C3	-2.03	1.38	1.43
24	B	605	CLA	C1B-CHB	2.03	1.46	1.41
24	D	403	CLA	C4B-CHC	2.03	1.46	1.41
24	d	403	CLA	C4B-CHC	2.03	1.46	1.41
27	A	412	SQD	O4-C4	-2.03	1.38	1.43
24	B	601	CLA	C4B-CHC	2.02	1.46	1.41
24	d	401	CLA	C1B-CHB	2.02	1.46	1.41
24	B	612	CLA	C4B-CHC	2.02	1.46	1.41
24	b	613	CLA	C4B-NB	-2.02	1.33	1.35
36	z	101	LMT	O1'-C1'	-2.02	1.36	1.40
24	c	510	CLA	C1B-CHB	2.01	1.46	1.41
36	i	102	LMT	O3B-C3B	-2.01	1.38	1.43
24	C	507	CLA	C1B-CHB	2.01	1.46	1.41
24	c	507	CLA	C1B-CHB	2.01	1.46	1.41
24	b	614	CLA	C4B-CHC	2.01	1.46	1.41
34	E	103	HEM	FE-NB	2.01	2.06	1.96
34	e	103	HEM	FE-NB	2.01	2.06	1.96
24	B	607	CLA	C4B-CHC	2.01	1.46	1.41
24	b	609	CLA	C4B-CHC	2.01	1.46	1.41
24	B	601	CLA	C1A-CHA	2.01	1.51	1.43
24	b	603	CLA	C1A-CHA	2.01	1.51	1.43
25	A	407	PHO	CMD-C2D	-2.00	1.46	1.51
25	a	407	PHO	CMD-C2D	-2.00	1.46	1.51
25	D	402	PHO	C1C-NC	-2.00	1.32	1.38
24	C	514	CLA	C1B-CHB	2.00	1.46	1.41
24	c	514	CLA	C1B-CHB	2.00	1.46	1.41
25	d	402	PHO	C1C-NC	-2.00	1.32	1.38
33	C	518	DGD	O2E-C2E	-2.00	1.38	1.43
33	c	518	DGD	O2E-C2E	-2.00	1.38	1.43

All (2468) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	C1D-ND-C4D	-10.13	99.14	106.33
24	D	404	CLA	C1D-ND-C4D	-10.06	99.19	106.33
24	C	512	CLA	C1D-ND-C4D	-9.87	99.32	106.33
24	c	512	CLA	C1D-ND-C4D	-9.87	99.32	106.33
24	B	613	CLA	C1D-ND-C4D	-9.86	99.33	106.33
24	b	615	CLA	C1D-ND-C4D	-9.84	99.34	106.33
24	b	609	CLA	C2D-C1D-ND	9.79	117.31	110.10
24	B	607	CLA	C2D-C1D-ND	9.78	117.31	110.10
24	B	607	CLA	C1D-ND-C4D	-9.71	99.44	106.33
24	C	505	CLA	C1D-ND-C4D	-9.68	99.46	106.33
24	c	505	CLA	C1D-ND-C4D	-9.68	99.46	106.33
24	b	609	CLA	C1D-ND-C4D	-9.67	99.47	106.33
27	L	101	SQD	O6-C1-C2	9.57	123.25	108.30
27	l	101	SQD	O6-C1-C2	9.56	123.23	108.30
24	C	514	CLA	C1D-ND-C4D	-9.52	99.58	106.33
24	b	615	CLA	C2D-C1D-ND	9.50	117.11	110.10
24	c	514	CLA	C1D-ND-C4D	-9.49	99.59	106.33
24	B	613	CLA	C2D-C1D-ND	9.49	117.09	110.10
24	C	512	CLA	C2D-C1D-ND	9.36	117.00	110.10
24	c	512	CLA	C2D-C1D-ND	9.36	117.00	110.10
24	B	615	CLA	C1D-ND-C4D	-9.23	99.78	106.33
24	b	617	CLA	C1D-ND-C4D	-9.23	99.78	106.33
24	B	601	CLA	C1D-ND-C4D	-9.23	99.78	106.33
24	b	603	CLA	C1D-ND-C4D	-9.23	99.78	106.33
24	B	602	CLA	C1D-ND-C4D	-9.13	99.85	106.33
24	b	604	CLA	C1D-ND-C4D	-9.12	99.85	106.33
24	B	615	CLA	C2D-C1D-ND	9.02	116.75	110.10
24	b	617	CLA	C2D-C1D-ND	9.02	116.75	110.10
24	B	605	CLA	C1D-ND-C4D	-8.99	99.95	106.33
24	b	607	CLA	C1D-ND-C4D	-8.99	99.95	106.33
24	C	509	CLA	C1D-ND-C4D	-8.96	99.97	106.33
24	c	509	CLA	C1D-ND-C4D	-8.96	99.97	106.33
24	D	401	CLA	C1D-ND-C4D	-8.85	100.05	106.33
24	d	401	CLA	C1D-ND-C4D	-8.85	100.05	106.33
24	C	503	CLA	C1D-ND-C4D	-8.82	100.07	106.33
24	c	503	CLA	C1D-ND-C4D	-8.82	100.07	106.33
24	a	406	CLA	C1D-ND-C4D	-8.78	100.10	106.33
24	B	603	CLA	C1D-ND-C4D	-8.76	100.11	106.33
24	b	605	CLA	C1D-ND-C4D	-8.76	100.11	106.33
24	A	406	CLA	C1D-ND-C4D	-8.76	100.11	106.33
24	C	509	CLA	C2D-C1D-ND	8.76	116.56	110.10
24	c	509	CLA	C2D-C1D-ND	8.76	116.56	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	408	CLA	C1D-ND-C4D	-8.73	100.14	106.33
24	A	408	CLA	C1D-ND-C4D	-8.72	100.14	106.33
24	B	606	CLA	C2D-C1D-ND	8.72	116.53	110.10
24	b	608	CLA	C2D-C1D-ND	8.72	116.53	110.10
24	b	612	CLA	C2D-C1D-ND	8.70	116.52	110.10
24	d	404	CLA	C2D-C1D-ND	8.68	116.50	110.10
24	C	505	CLA	C2D-C1D-ND	8.64	116.47	110.10
24	b	612	CLA	C1D-ND-C4D	-8.63	100.21	106.33
24	D	404	CLA	C2D-C1D-ND	8.61	116.45	110.10
24	c	505	CLA	C2D-C1D-ND	8.61	116.45	110.10
24	a	408	CLA	C2D-C1D-ND	8.57	116.42	110.10
24	A	408	CLA	C2D-C1D-ND	8.57	116.42	110.10
24	c	502	CLA	C1D-ND-C4D	-8.55	100.26	106.33
24	B	606	CLA	C1D-ND-C4D	-8.48	100.31	106.33
24	b	608	CLA	C1D-ND-C4D	-8.48	100.31	106.33
24	c	513	CLA	C1D-ND-C4D	-8.46	100.32	106.33
24	C	502	CLA	C1D-ND-C4D	-8.46	100.33	106.33
24	C	513	CLA	C1D-ND-C4D	-8.45	100.33	106.33
24	C	503	CLA	C2D-C1D-ND	8.42	116.31	110.10
24	c	503	CLA	C2D-C1D-ND	8.42	116.31	110.10
24	B	616	CLA	C1D-ND-C4D	-8.39	100.38	106.33
24	b	618	CLA	C1D-ND-C4D	-8.39	100.38	106.33
24	B	605	CLA	C2D-C1D-ND	8.38	116.28	110.10
24	b	607	CLA	C2D-C1D-ND	8.38	116.28	110.10
24	C	504	CLA	C1D-ND-C4D	-8.37	100.39	106.33
24	c	504	CLA	C1D-ND-C4D	-8.37	100.39	106.33
24	C	513	CLA	C2D-C1D-ND	8.35	116.25	110.10
24	c	513	CLA	C2D-C1D-ND	8.34	116.25	110.10
27	a	410	SQD	O6-C1-C2	8.34	121.33	108.30
27	A	410	SQD	O6-C1-C2	8.31	121.28	108.30
24	C	511	CLA	CMD-C2D-C1D	8.31	139.35	124.71
24	c	511	CLA	CMD-C2D-C1D	8.31	139.35	124.71
24	B	614	CLA	C1D-ND-C4D	-8.30	100.44	106.33
24	b	616	CLA	C1D-ND-C4D	-8.30	100.44	106.33
24	B	610	CLA	C2D-C1D-ND	8.30	116.22	110.10
24	b	604	CLA	C2D-C1D-ND	8.26	116.19	110.10
24	B	602	CLA	C2D-C1D-ND	8.26	116.19	110.10
24	C	510	CLA	C1D-ND-C4D	-8.25	100.47	106.33
24	c	510	CLA	C1D-ND-C4D	-8.25	100.47	106.33
24	b	611	CLA	C1D-ND-C4D	-8.25	100.47	106.33
24	B	609	CLA	C1D-ND-C4D	-8.24	100.48	106.33
24	B	610	CLA	C1D-ND-C4D	-8.18	100.52	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	502	CLA	C2D-C1D-ND	8.12	116.09	110.10
24	C	508	CLA	C2D-C1D-ND	8.11	116.08	110.10
24	c	508	CLA	C2D-C1D-ND	8.09	116.06	110.10
24	C	502	CLA	C2D-C1D-ND	8.08	116.06	110.10
24	c	508	CLA	C1D-ND-C4D	-7.99	100.66	106.33
24	C	508	CLA	C1D-ND-C4D	-7.99	100.66	106.33
24	c	514	CLA	C2D-C1D-ND	7.99	115.99	110.10
24	C	514	CLA	C2D-C1D-ND	7.98	115.99	110.10
24	D	401	CLA	C2D-C1D-ND	7.94	115.96	110.10
24	d	401	CLA	C2D-C1D-ND	7.94	115.96	110.10
24	B	601	CLA	C2D-C1D-ND	7.94	115.96	110.10
24	b	603	CLA	C2D-C1D-ND	7.94	115.96	110.10
24	b	614	CLA	C1D-ND-C4D	-7.82	100.78	106.33
24	C	507	CLA	C1D-ND-C4D	-7.80	100.80	106.33
24	C	504	CLA	C2D-C1D-ND	7.78	115.84	110.10
24	c	504	CLA	C2D-C1D-ND	7.78	115.84	110.10
24	c	507	CLA	C1D-ND-C4D	-7.78	100.81	106.33
24	B	616	CLA	C2D-C1D-ND	7.78	115.83	110.10
24	b	618	CLA	C2D-C1D-ND	7.78	115.83	110.10
24	B	612	CLA	C1D-ND-C4D	-7.73	100.84	106.33
24	C	511	CLA	C1D-ND-C4D	-7.72	100.85	106.33
24	c	511	CLA	C1D-ND-C4D	-7.72	100.85	106.33
24	B	611	CLA	C2D-C1D-ND	7.65	115.74	110.10
24	C	506	CLA	C1D-ND-C4D	-7.63	100.91	106.33
24	c	506	CLA	C1D-ND-C4D	-7.63	100.91	106.33
24	b	613	CLA	C2D-C1D-ND	7.62	115.72	110.10
24	B	611	CLA	C1D-ND-C4D	-7.58	100.95	106.33
24	b	613	CLA	C1D-ND-C4D	-7.57	100.96	106.33
24	b	614	CLA	C2D-C1D-ND	7.52	115.65	110.10
24	B	612	CLA	C2D-C1D-ND	7.52	115.64	110.10
24	B	609	CLA	C2D-C1D-ND	7.51	115.64	110.10
24	B	614	CLA	C2D-C1D-ND	7.51	115.64	110.10
24	b	616	CLA	C2D-C1D-ND	7.51	115.64	110.10
24	b	611	CLA	C2D-C1D-ND	7.49	115.63	110.10
24	A	406	CLA	C2D-C1D-ND	7.48	115.61	110.10
24	a	406	CLA	C2D-C1D-ND	7.48	115.61	110.10
24	C	504	CLA	CMD-C2D-C1D	7.40	137.76	124.71
24	c	504	CLA	CMD-C2D-C1D	7.40	137.76	124.71
24	D	403	CLA	C1D-ND-C4D	-7.38	101.09	106.33
24	d	403	CLA	C1D-ND-C4D	-7.38	101.09	106.33
24	A	405	CLA	CMD-C2D-C1D	7.36	137.68	124.71
24	a	405	CLA	CMD-C2D-C1D	7.36	137.68	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	CMD-C2D-C1D	7.12	137.25	124.71
24	c	510	CLA	CMD-C2D-C1D	7.12	137.25	124.71
24	C	507	CLA	C2D-C1D-ND	7.09	115.33	110.10
24	c	507	CLA	C2D-C1D-ND	7.05	115.30	110.10
24	B	606	CLA	CHD-C1D-ND	-7.04	117.98	124.45
24	b	608	CLA	CHD-C1D-ND	-7.04	117.98	124.45
24	C	506	CLA	CHD-C4C-C3C	-7.02	114.53	124.84
24	c	506	CLA	CHD-C4C-C3C	-7.02	114.53	124.84
24	b	606	CLA	CMD-C2D-C1D	7.02	137.08	124.71
24	d	404	CLA	CMD-C2D-C1D	7.00	137.05	124.71
24	d	403	CLA	CMD-C2D-C1D	7.00	137.05	124.71
24	B	604	CLA	CMD-C2D-C1D	7.00	137.05	124.71
24	D	404	CLA	CMD-C2D-C1D	6.98	137.02	124.71
24	D	403	CLA	CMD-C2D-C1D	6.97	136.99	124.71
24	d	404	CLA	CHD-C1D-ND	-6.96	118.06	124.45
24	D	404	CLA	CHD-C1D-ND	-6.92	118.10	124.45
24	B	606	CLA	CMD-C2D-C1D	6.91	136.89	124.71
24	b	608	CLA	CMD-C2D-C1D	6.91	136.89	124.71
24	b	604	CLA	CMD-C2D-C1D	6.91	136.88	124.71
24	B	602	CLA	CMD-C2D-C1D	6.90	136.88	124.71
24	C	502	CLA	CMD-C2D-C1D	6.89	136.85	124.71
24	c	502	CLA	CMD-C2D-C1D	6.88	136.84	124.71
24	B	603	CLA	C2D-C1D-ND	6.86	115.16	110.10
24	b	605	CLA	C2D-C1D-ND	6.86	115.16	110.10
24	B	605	CLA	CMD-C2D-C1D	6.85	136.78	124.71
24	b	607	CLA	CMD-C2D-C1D	6.85	136.78	124.71
24	C	510	CLA	C2D-C1D-ND	6.82	115.13	110.10
24	b	606	CLA	C2C-C1C-NC	6.76	116.31	109.97
24	c	510	CLA	C2D-C1D-ND	6.73	115.06	110.10
24	B	604	CLA	C2C-C1C-NC	6.73	116.28	109.97
24	A	406	CLA	CMD-C2D-C1D	6.72	136.56	124.71
24	b	604	CLA	CHD-C1D-ND	-6.72	118.28	124.45
24	a	406	CLA	CMD-C2D-C1D	6.71	136.54	124.71
24	c	507	CLA	CMD-C2D-C1D	6.71	136.54	124.71
24	B	612	CLA	CHD-C4C-C3C	-6.71	114.97	124.84
24	C	507	CLA	CMD-C2D-C1D	6.70	136.52	124.71
24	b	614	CLA	CHD-C4C-C3C	-6.70	115.00	124.84
27	D	407	SQD	O6-C1-C2	6.70	118.76	108.30
27	d	407	SQD	O6-C1-C2	6.69	118.75	108.30
24	B	602	CLA	CHD-C1D-ND	-6.69	118.31	124.45
24	C	505	CLA	CHD-C1D-ND	-6.68	118.31	124.45
24	c	505	CLA	CHD-C1D-ND	-6.68	118.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	C1D-ND-C4D	-6.61	101.64	106.33
24	b	606	CLA	C1D-ND-C4D	-6.60	101.64	106.33
24	B	610	CLA	CHD-C4C-C3C	-6.59	115.15	124.84
24	b	612	CLA	CHD-C4C-C3C	-6.57	115.18	124.84
24	B	605	CLA	CHD-C4C-C3C	-6.57	115.18	124.84
24	b	607	CLA	CHD-C4C-C3C	-6.57	115.18	124.84
24	d	403	CLA	C2D-C1D-ND	6.56	114.94	110.10
24	C	505	CLA	CMD-C2D-C1D	6.56	136.28	124.71
24	C	506	CLA	O2D-CGD-CBD	6.56	122.93	111.27
24	c	506	CLA	O2D-CGD-CBD	6.56	122.93	111.27
24	B	608	CLA	C1D-ND-C4D	-6.56	101.68	106.33
24	c	505	CLA	CMD-C2D-C1D	6.55	136.26	124.71
24	D	403	CLA	C2D-C1D-ND	6.51	114.90	110.10
24	b	603	CLA	O2D-CGD-CBD	6.50	122.81	111.27
24	b	610	CLA	C1D-ND-C4D	-6.49	101.73	106.33
24	B	601	CLA	O2D-CGD-CBD	6.48	122.79	111.27
24	b	604	CLA	O2D-CGD-CBD	6.42	122.67	111.27
24	C	512	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	c	512	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	C	508	CLA	CMD-C2D-C1D	6.40	135.99	124.71
24	B	602	CLA	O2D-CGD-CBD	6.39	122.62	111.27
24	c	508	CLA	CMD-C2D-C1D	6.37	135.94	124.71
24	c	508	CLA	C2C-C1C-NC	6.34	115.91	109.97
24	C	508	CLA	C2C-C1C-NC	6.31	115.89	109.97
24	C	507	CLA	C2C-C1C-NC	6.31	115.88	109.97
24	c	507	CLA	C2C-C1C-NC	6.31	115.88	109.97
24	b	615	CLA	CMD-C2D-C1D	6.30	135.81	124.71
24	A	405	CLA	C1D-ND-C4D	-6.29	101.86	106.33
24	a	405	CLA	C1D-ND-C4D	-6.29	101.86	106.33
24	B	616	CLA	CHD-C4C-C3C	-6.29	115.60	124.84
24	b	618	CLA	CHD-C4C-C3C	-6.29	115.60	124.84
24	B	613	CLA	CMD-C2D-C1D	6.28	135.79	124.71
24	D	403	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
24	d	403	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
24	c	508	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
24	C	508	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
24	B	616	CLA	CMD-C2D-C1D	6.22	135.68	124.71
24	b	618	CLA	CMD-C2D-C1D	6.22	135.68	124.71
24	C	514	CLA	C4A-NA-C1A	-6.20	103.92	106.71
24	C	507	CLA	CHD-C1D-ND	-6.18	118.77	124.45
24	c	507	CLA	CHD-C1D-ND	-6.18	118.77	124.45
24	D	401	CLA	CHD-C1D-ND	-6.18	118.78	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	CHD-C1D-ND	-6.18	118.78	124.45
24	C	511	CLA	C2C-C1C-NC	6.17	115.75	109.97
24	c	511	CLA	C2C-C1C-NC	6.17	115.75	109.97
24	d	401	CLA	C2C-C1C-NC	6.16	115.74	109.97
24	c	514	CLA	C4A-NA-C1A	-6.15	103.94	106.71
24	B	603	CLA	CMD-C2D-C1D	6.14	135.54	124.71
24	b	605	CLA	CMD-C2D-C1D	6.14	135.54	124.71
24	D	401	CLA	C2C-C1C-NC	6.14	115.72	109.97
24	b	606	CLA	C2D-C1D-ND	6.13	114.62	110.10
24	B	615	CLA	CMD-C2D-C1D	6.10	135.47	124.71
24	b	617	CLA	CMD-C2D-C1D	6.09	135.44	124.71
24	C	512	CLA	CMD-C2D-C1D	6.08	135.44	124.71
24	c	512	CLA	CMD-C2D-C1D	6.08	135.44	124.71
24	B	604	CLA	C2D-C1D-ND	6.07	114.58	110.10
24	B	609	CLA	CMD-C2D-C1D	6.05	135.38	124.71
24	b	610	CLA	C2C-C1C-NC	6.04	115.63	109.97
24	B	608	CLA	C2C-C1C-NC	6.03	115.62	109.97
24	b	611	CLA	CMD-C2D-C1D	6.02	135.32	124.71
24	C	503	CLA	C2C-C1C-NC	6.01	115.61	109.97
24	c	503	CLA	C2C-C1C-NC	6.01	115.61	109.97
24	B	615	CLA	CHD-C1D-ND	-6.00	118.94	124.45
24	b	617	CLA	CHD-C1D-ND	-6.00	118.94	124.45
24	C	506	CLA	C3C-C4C-NC	5.99	117.29	110.57
24	c	506	CLA	C3C-C4C-NC	5.99	117.29	110.57
24	B	609	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
24	c	514	CLA	CMD-C2D-C1D	5.97	135.24	124.71
24	b	611	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
24	B	609	CLA	C2C-C1C-NC	5.96	115.56	109.97
24	C	514	CLA	CMD-C2D-C1D	5.96	135.22	124.71
24	D	403	CLA	C2C-C1C-NC	5.96	115.56	109.97
24	d	403	CLA	C2C-C1C-NC	5.96	115.55	109.97
24	B	601	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	b	611	CLA	C2C-C1C-NC	5.94	115.54	109.97
24	b	603	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
24	C	508	CLA	O2D-CGD-CBD	5.93	121.80	111.27
24	c	508	CLA	O2D-CGD-CBD	5.93	121.80	111.27
24	C	514	CLA	CHD-C1D-ND	-5.91	119.03	124.45
24	B	614	CLA	O2D-CGD-CBD	5.89	121.73	111.27
24	b	616	CLA	O2D-CGD-CBD	5.89	121.73	111.27
24	C	509	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	c	509	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	c	514	CLA	CHD-C1D-ND	-5.85	119.08	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	CMD-C2D-C1D	5.84	135.00	124.71
24	B	607	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
24	c	506	CLA	CMD-C2D-C1D	5.83	134.98	124.71
24	B	603	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	B	615	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	b	617	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	b	609	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
24	b	605	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	C	504	CLA	CHD-C1D-ND	-5.81	119.12	124.45
24	c	504	CLA	CHD-C1D-ND	-5.81	119.12	124.45
24	c	502	CLA	C2C-C1C-NC	5.80	115.41	109.97
24	c	502	CLA	CHD-C1D-ND	-5.80	119.12	124.45
24	C	502	CLA	C2C-C1C-NC	5.80	115.41	109.97
24	C	509	CLA	O2D-CGD-CBD	5.80	121.57	111.27
24	c	509	CLA	O2D-CGD-CBD	5.80	121.57	111.27
24	b	612	CLA	C2C-C1C-NC	5.80	115.40	109.97
24	C	513	CLA	O2D-CGD-CBD	5.79	121.56	111.27
24	c	513	CLA	O2D-CGD-CBD	5.79	121.56	111.27
24	B	601	CLA	CMD-C2D-C1D	5.79	134.92	124.71
24	b	603	CLA	CMD-C2D-C1D	5.79	134.92	124.71
24	b	616	CLA	C2C-C1C-NC	5.78	115.39	109.97
24	B	614	CLA	C2C-C1C-NC	5.78	115.39	109.97
24	C	510	CLA	CHD-C1D-ND	-5.78	119.14	124.45
24	A	408	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
24	a	408	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
24	B	610	CLA	C2C-C1C-NC	5.77	115.38	109.97
24	C	502	CLA	CHD-C1D-ND	-5.77	119.15	124.45
24	C	502	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
24	c	502	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
24	B	606	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	b	608	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	c	510	CLA	CHD-C1D-ND	-5.73	119.19	124.45
24	A	406	CLA	C2C-C1C-NC	5.71	115.32	109.97
24	a	406	CLA	C2C-C1C-NC	5.71	115.32	109.97
24	C	510	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
24	b	611	CLA	CHD-C1D-ND	-5.70	119.22	124.45
24	A	405	CLA	C2C-C1C-NC	5.70	115.31	109.97
24	a	405	CLA	C2C-C1C-NC	5.70	115.31	109.97
24	c	510	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
30	a	414	BCT	O2-C-O1	5.68	134.29	119.55
24	c	508	CLA	CHD-C1D-ND	-5.68	119.23	124.45
24	A	408	CLA	CMD-C2D-C1D	5.68	134.72	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	414	BCT	O2-C-O1	5.68	134.27	119.55
24	A	408	CLA	C2C-C1C-NC	5.67	115.28	109.97
24	a	408	CLA	C2C-C1C-NC	5.67	115.28	109.97
24	a	408	CLA	CMD-C2D-C1D	5.67	134.70	124.71
24	B	613	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
24	C	508	CLA	CHD-C1D-ND	-5.66	119.25	124.45
24	B	606	CLA	C3C-C4C-NC	5.66	116.92	110.57
24	b	608	CLA	C3C-C4C-NC	5.66	116.92	110.57
24	B	602	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
24	b	615	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
24	B	612	CLA	C3C-C4C-NC	5.65	116.91	110.57
24	B	609	CLA	CHD-C1D-ND	-5.65	119.26	124.45
24	B	611	CLA	C2C-C1C-NC	5.64	115.26	109.97
24	b	613	CLA	C2C-C1C-NC	5.64	115.26	109.97
24	B	613	CLA	CHD-C1D-ND	-5.63	119.28	124.45
24	B	607	CLA	O2D-CGD-CBD	5.63	121.27	111.27
24	B	601	CLA	C2C-C1C-NC	5.63	115.25	109.97
24	b	604	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
24	b	615	CLA	CHD-C1D-ND	-5.62	119.29	124.45
24	B	603	CLA	O2D-CGD-CBD	5.62	121.26	111.27
24	b	605	CLA	O2D-CGD-CBD	5.62	121.26	111.27
24	B	606	CLA	O2D-CGD-CBD	5.61	121.25	111.27
24	b	608	CLA	O2D-CGD-CBD	5.61	121.25	111.27
24	C	513	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
24	c	513	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
24	b	614	CLA	C3C-C4C-NC	5.60	116.85	110.57
24	b	609	CLA	O2D-CGD-CBD	5.60	121.21	111.27
24	b	618	CLA	O2D-CGD-CBD	5.59	121.21	111.27
24	D	401	CLA	C1C-C2C-C3C	-5.59	101.08	106.96
24	d	401	CLA	C1C-C2C-C3C	-5.59	101.08	106.96
24	C	505	CLA	C2C-C1C-NC	5.59	115.21	109.97
24	c	505	CLA	C2C-C1C-NC	5.59	115.21	109.97
24	B	616	CLA	O2D-CGD-CBD	5.59	121.21	111.27
24	b	616	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
24	B	614	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
24	c	514	CLA	O2D-CGD-CBD	5.58	121.18	111.27
24	C	506	CLA	C2D-C1D-ND	5.58	114.22	110.10
24	B	606	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
24	b	608	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
24	c	506	CLA	C2D-C1D-ND	5.54	114.19	110.10
24	b	603	CLA	C2C-C1C-NC	5.54	115.17	109.97
24	C	514	CLA	O2D-CGD-CBD	5.54	121.11	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C2C-C1C-NC	5.53	115.15	109.97
24	c	510	CLA	C2C-C1C-NC	5.53	115.15	109.97
24	B	603	CLA	CHD-C1D-ND	-5.53	119.38	124.45
24	b	605	CLA	CHD-C1D-ND	-5.53	119.38	124.45
24	D	401	CLA	CMD-C2D-C1D	5.52	134.43	124.71
24	b	612	CLA	C4A-NA-C1A	-5.51	104.23	106.71
24	B	605	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	b	607	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	b	615	CLA	C3D-C2D-C1D	-5.50	98.32	105.83
24	d	401	CLA	CMD-C2D-C1D	5.50	134.41	124.71
24	B	607	CLA	CMD-C2D-C1D	5.50	134.40	124.71
24	c	510	CLA	O2D-CGD-CBD	5.49	121.02	111.27
24	a	406	CLA	CHD-C1D-ND	-5.48	119.41	124.45
24	B	613	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
24	C	510	CLA	O2D-CGD-CBD	5.47	120.99	111.27
24	b	609	CLA	CMD-C2D-C1D	5.47	134.36	124.71
24	B	607	CLA	C2C-C1C-NC	5.46	115.09	109.97
24	C	512	CLA	CHD-C1D-ND	-5.45	119.44	124.45
24	c	512	CLA	CHD-C1D-ND	-5.45	119.44	124.45
24	B	615	CLA	C2C-C1C-NC	5.45	115.08	109.97
24	C	505	CLA	O2D-CGD-CBD	5.45	120.95	111.27
24	c	505	CLA	O2D-CGD-CBD	5.44	120.94	111.27
24	C	503	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
24	b	609	CLA	C2C-C1C-NC	5.44	115.07	109.97
24	b	617	CLA	C2C-C1C-NC	5.44	115.07	109.97
24	c	503	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
24	A	406	CLA	CHD-C1D-ND	-5.41	119.48	124.45
24	D	403	CLA	C3C-C4C-NC	5.38	116.60	110.57
24	C	511	CLA	CHD-C1D-ND	-5.38	119.51	124.45
24	c	511	CLA	CHD-C1D-ND	-5.38	119.51	124.45
24	d	403	CLA	C3C-C4C-NC	5.37	116.59	110.57
24	C	513	CLA	C2C-C1C-NC	5.37	115.00	109.97
24	B	604	CLA	O2D-CGD-CBD	5.37	120.81	111.27
24	a	406	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
24	c	506	CLA	C2C-C1C-NC	5.36	114.99	109.97
24	b	606	CLA	O2D-CGD-CBD	5.35	120.78	111.27
24	C	509	CLA	CHD-C1D-ND	-5.34	119.54	124.45
24	c	509	CLA	CHD-C1D-ND	-5.34	119.54	124.45
24	C	504	CLA	C4A-NA-C1A	-5.33	104.31	106.71
27	A	410	SQD	O9-S-C6	5.33	113.27	106.94
24	c	513	CLA	C2C-C1C-NC	5.33	114.96	109.97
24	A	406	CLA	CHD-C4C-C3C	-5.33	117.01	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
24	c	514	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
24	c	504	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
27	a	410	SQD	O9-S-C6	5.32	113.26	106.94
24	C	506	CLA	C2C-C1C-NC	5.31	114.95	109.97
24	C	504	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
24	b	615	CLA	C2C-C1C-NC	5.31	114.94	109.97
35	h	101	RRX	C16-C17-C18	-5.31	119.74	127.31
24	A	405	CLA	C4A-NA-C1A	-5.30	104.32	106.71
24	a	405	CLA	C4A-NA-C1A	-5.30	104.32	106.71
24	C	505	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
24	B	613	CLA	C2C-C1C-NC	5.30	114.93	109.97
24	b	610	CLA	C4A-NA-C1A	-5.29	104.33	106.71
35	H	101	RRX	C16-C17-C18	-5.28	119.77	127.31
24	C	502	CLA	O2D-CGD-CBD	5.27	120.63	111.27
24	c	502	CLA	O2D-CGD-CBD	5.27	120.63	111.27
24	B	604	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
24	b	606	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
24	c	505	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
24	C	509	CLA	C3C-C4C-NC	5.22	116.42	110.57
24	c	509	CLA	C3C-C4C-NC	5.22	116.42	110.57
24	c	504	CLA	C4A-NA-C1A	-5.21	104.36	106.71
24	B	610	CLA	C3C-C4C-NC	5.21	116.41	110.57
24	c	503	CLA	O2D-CGD-CBD	5.21	120.52	111.27
24	B	606	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
24	b	608	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
24	C	503	CLA	O2D-CGD-CBD	5.20	120.50	111.27
24	b	614	CLA	O2D-CGD-CBD	5.19	120.50	111.27
24	B	612	CLA	O2D-CGD-CBD	5.19	120.49	111.27
24	D	404	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
24	C	509	CLA	C2C-C1C-NC	5.18	114.83	109.97
24	c	509	CLA	C2C-C1C-NC	5.18	114.83	109.97
24	D	401	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
24	d	401	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
24	d	404	CLA	CHD-C4C-C3C	-5.17	117.23	124.84
24	D	404	CLA	CHD-C4C-C3C	-5.17	117.23	124.84
24	A	405	CLA	CHD-C1D-ND	-5.17	119.70	124.45
24	a	405	CLA	CHD-C1D-ND	-5.17	119.70	124.45
24	d	404	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
24	C	512	CLA	C2C-C1C-NC	5.16	114.81	109.97
24	c	512	CLA	C2C-C1C-NC	5.16	114.81	109.97
24	b	609	CLA	C3D-C2D-C1D	-5.16	98.79	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
24	b	612	CLA	C3C-C4C-NC	5.15	116.35	110.57
24	B	608	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
24	b	610	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
24	B	608	CLA	C4A-NA-C1A	-5.11	104.41	106.71
24	a	408	CLA	CHD-C1D-ND	-5.11	119.76	124.45
24	A	408	CLA	CHD-C1D-ND	-5.10	119.77	124.45
24	B	615	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
24	b	617	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
24	B	608	CLA	C2D-C1D-ND	5.09	113.86	110.10
24	A	408	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
24	a	408	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
27	d	407	SQD	O9-S-C6	5.09	112.99	106.94
24	C	512	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
24	c	512	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
24	A	408	CLA	O2D-CGD-CBD	5.08	120.30	111.27
24	a	408	CLA	O2D-CGD-CBD	5.08	120.30	111.27
27	D	407	SQD	O9-S-C6	5.08	112.97	106.94
24	B	614	CLA	CMD-C2D-C1D	5.08	133.66	124.71
24	b	616	CLA	CMD-C2D-C1D	5.08	133.66	124.71
24	c	504	CLA	CAC-C3C-C4C	5.07	131.39	124.81
24	b	604	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
24	B	602	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
24	C	504	CLA	CAC-C3C-C4C	5.06	131.37	124.81
24	D	404	CLA	C2C-C1C-NC	5.05	114.70	109.97
24	d	404	CLA	C2C-C1C-NC	5.05	114.70	109.97
24	C	504	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
24	c	504	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
24	B	607	CLA	CHD-C1D-ND	-5.03	119.83	124.45
24	c	508	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
24	b	609	CLA	CHD-C1D-ND	-5.01	119.85	124.45
24	C	508	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
24	B	616	CLA	CHD-C1D-ND	-5.00	119.86	124.45
24	b	618	CLA	CHD-C1D-ND	-5.00	119.86	124.45
24	b	610	CLA	C2D-C1D-ND	5.00	113.79	110.10
24	C	502	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
24	c	502	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
24	C	512	CLA	C3C-C4C-NC	4.97	116.15	110.57
24	c	512	CLA	C3C-C4C-NC	4.97	116.15	110.57
24	c	507	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
24	A	405	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
24	a	405	CLA	CHD-C4C-C3C	-4.97	117.54	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
24	b	613	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
24	C	507	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
24	B	604	CLA	C1C-C2C-C3C	-4.94	101.76	106.96
24	b	606	CLA	C1C-C2C-C3C	-4.94	101.76	106.96
24	A	405	CLA	C2D-C1D-ND	4.94	113.74	110.10
24	a	405	CLA	C2D-C1D-ND	4.94	113.74	110.10
24	B	605	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
24	b	607	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
24	b	613	CLA	O2D-CGD-CBD	4.92	120.01	111.27
24	B	611	CLA	O2D-CGD-CBD	4.91	119.99	111.27
24	c	504	CLA	C3C-C4C-NC	4.91	116.08	110.57
24	C	504	CLA	C2C-C1C-NC	4.90	114.56	109.97
24	c	504	CLA	C2C-C1C-NC	4.90	114.56	109.97
24	C	504	CLA	C3C-C4C-NC	4.89	116.06	110.57
24	C	511	CLA	CHD-C4C-C3C	-4.89	117.65	124.84
24	c	511	CLA	CHD-C4C-C3C	-4.89	117.65	124.84
24	b	612	CLA	O2D-CGD-CBD	4.89	119.96	111.27
24	A	406	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
28	a	411	PL9	C7-C3-C4	4.88	120.84	116.88
24	a	406	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
28	A	411	PL9	C7-C3-C4	4.86	120.83	116.88
24	B	605	CLA	O2D-CGD-CBD	4.86	119.91	111.27
24	b	607	CLA	O2D-CGD-CBD	4.86	119.91	111.27
24	C	511	CLA	C2D-C1D-ND	4.84	113.67	110.10
24	c	511	CLA	C2D-C1D-ND	4.84	113.67	110.10
24	B	609	CLA	C1C-C2C-C3C	-4.84	101.87	106.96
24	A	406	CLA	O2D-CGD-CBD	4.84	119.87	111.27
24	a	406	CLA	O2D-CGD-CBD	4.84	119.87	111.27
24	B	610	CLA	O2D-CGD-CBD	4.83	119.85	111.27
24	b	611	CLA	O2D-CGD-CBD	4.83	119.85	111.27
24	C	509	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
24	c	509	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
24	b	612	CLA	CMD-C2D-C1D	4.82	133.22	124.71
24	B	609	CLA	O2D-CGD-CBD	4.82	119.84	111.27
24	b	611	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
24	B	610	CLA	CMD-C2D-C1D	4.80	133.18	124.71
24	C	505	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
24	B	603	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	b	605	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	C	508	CLA	C1C-C2C-C3C	-4.79	101.92	106.96
24	B	612	CLA	C2C-C1C-NC	4.78	114.45	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	CMB-C2B-C3B	4.78	133.62	124.68
24	b	610	CLA	CMB-C2B-C3B	4.78	133.62	124.68
24	d	401	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	b	613	CLA	CAC-C3C-C4C	4.78	131.01	124.81
24	B	611	CLA	CMD-C2D-C1D	4.77	133.12	124.71
24	b	613	CLA	CMD-C2D-C1D	4.77	133.12	124.71
24	c	508	CLA	C1C-C2C-C3C	-4.77	101.94	106.96
24	C	511	CLA	O2D-CGD-CBD	4.77	119.74	111.27
24	c	511	CLA	O2D-CGD-CBD	4.77	119.74	111.27
24	b	612	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
24	c	514	CLA	CMB-C2B-C3B	4.76	133.59	124.68
24	B	611	CLA	CAC-C3C-C4C	4.76	130.99	124.81
24	c	505	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
24	C	514	CLA	CMB-C2B-C3B	4.75	133.57	124.68
24	D	401	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
24	b	614	CLA	C2C-C1C-NC	4.73	114.41	109.97
24	B	601	CLA	CHD-C1D-ND	-4.73	120.11	124.45
24	D	403	CLA	C4A-NA-C1A	-4.73	104.58	106.71
24	b	603	CLA	CHD-C1D-ND	-4.72	120.11	124.45
24	B	602	CLA	C2C-C1C-NC	4.72	114.40	109.97
24	b	604	CLA	C2C-C1C-NC	4.72	114.40	109.97
24	B	610	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	b	613	CLA	CHD-C1D-ND	-4.71	120.13	124.45
24	C	509	CLA	CMD-C2D-C1D	4.70	133.00	124.71
24	c	509	CLA	CMD-C2D-C1D	4.70	133.00	124.71
24	b	611	CLA	C4A-NA-C1A	-4.70	104.59	106.71
34	e	103	HEM	CBA-CAA-C2A	-4.70	104.60	112.62
24	b	610	CLA	CMD-C2D-C1D	4.69	132.98	124.71
24	C	513	CLA	C3C-C4C-NC	4.69	115.83	110.57
24	c	513	CLA	C3C-C4C-NC	4.69	115.83	110.57
24	B	611	CLA	CHD-C1D-ND	-4.68	120.15	124.45
24	B	609	CLA	C4A-NA-C1A	-4.68	104.60	106.71
34	E	103	HEM	CBA-CAA-C2A	-4.68	104.64	112.62
24	D	404	CLA	CMB-C2B-C3B	4.67	133.42	124.68
24	d	404	CLA	CMB-C2B-C3B	4.67	133.42	124.68
27	A	412	SQD	O7-S-C6	4.66	112.48	106.94
27	a	412	SQD	O7-S-C6	4.66	112.48	106.94
24	B	611	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
24	C	507	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
24	C	503	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	608	CLA	CMD-C2D-C1D	4.64	132.88	124.71
24	b	613	CLA	C3D-C2D-C1D	-4.64	99.50	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	c	503	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	b	607	CLA	C2C-C1C-NC	4.63	114.31	109.97
24	D	401	CLA	O2D-CGD-CBD	4.62	119.48	111.27
24	d	401	CLA	O2D-CGD-CBD	4.62	119.48	111.27
24	d	404	CLA	O2D-CGD-CBD	4.61	119.45	111.27
24	d	404	CLA	C3D-C4D-ND	4.60	117.68	110.24
24	D	404	CLA	O2D-CGD-CBD	4.60	119.44	111.27
24	B	616	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
24	b	618	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
24	B	616	CLA	C3C-C4C-NC	4.59	115.72	110.57
24	b	618	CLA	C3C-C4C-NC	4.59	115.72	110.57
24	D	404	CLA	C3D-C4D-ND	4.59	117.66	110.24
24	d	403	CLA	C4A-NA-C1A	-4.58	104.65	106.71
24	B	605	CLA	C2C-C1C-NC	4.57	114.25	109.97
24	A	408	CLA	C3C-C4C-NC	4.56	115.69	110.57
24	a	408	CLA	C3C-C4C-NC	4.56	115.69	110.57
24	C	514	CLA	C2C-C1C-NC	4.56	114.24	109.97
24	c	514	CLA	C2C-C1C-NC	4.56	114.24	109.97
24	B	605	CLA	C3C-C4C-NC	4.55	115.68	110.57
24	b	607	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	c	514	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
24	b	604	CLA	C4A-NA-C1A	-4.52	104.67	106.71
24	C	514	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
24	C	514	CLA	C3D-C4D-ND	4.51	117.53	110.24
24	c	514	CLA	C3D-C4D-ND	4.51	117.53	110.24
24	C	511	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
24	c	511	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
24	A	405	CLA	CAC-C3C-C4C	4.49	130.63	124.81
24	a	405	CLA	CAC-C3C-C4C	4.49	130.63	124.81
27	l	101	SQD	O8-S-C6	4.47	112.86	105.74
24	b	606	CLA	CHD-C1D-ND	-4.46	120.35	124.45
24	B	602	CLA	C4A-NA-C1A	-4.46	104.70	106.71
24	B	615	CLA	C3C-C4C-NC	4.46	115.57	110.57
24	b	617	CLA	C3C-C4C-NC	4.46	115.57	110.57
27	L	101	SQD	O8-S-C6	4.45	112.84	105.74
24	c	503	CLA	CMD-C2D-C1D	4.45	132.56	124.71
24	B	616	CLA	C4C-C3C-C2C	-4.45	100.41	106.90
24	C	503	CLA	CMD-C2D-C1D	4.45	132.56	124.71
24	C	503	CLA	CHD-C1D-ND	-4.45	120.36	124.45
24	c	503	CLA	CHD-C1D-ND	-4.45	120.36	124.45
24	b	618	CLA	C4C-C3C-C2C	-4.45	100.41	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	601	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	b	603	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	b	612	CLA	CHD-C1D-ND	-4.45	120.37	124.45
27	A	410	SQD	O9-S-O7	-4.44	98.57	113.95
24	B	604	CLA	CHD-C1D-ND	-4.44	120.37	124.45
27	a	412	SQD	O9-S-O7	-4.44	98.60	113.95
27	a	410	SQD	O9-S-O7	-4.43	98.61	113.95
24	b	616	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
24	B	614	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
27	A	412	SQD	O9-S-O7	-4.42	98.65	113.95
24	A	405	CLA	CAA-C2A-C3A	-4.41	100.70	112.78
24	a	405	CLA	CAA-C2A-C3A	-4.40	100.73	112.78
24	B	609	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	b	611	CLA	C3D-C2D-C1D	-4.39	99.85	105.83
24	B	612	CLA	CMC-C2C-C1C	4.38	131.70	125.04
24	A	406	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
24	a	406	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
24	C	505	CLA	C3D-C4D-ND	4.37	117.31	110.24
24	c	505	CLA	C3D-C4D-ND	4.37	117.31	110.24
24	B	614	CLA	CHD-C1D-ND	-4.37	120.44	124.45
24	b	616	CLA	CHD-C1D-ND	-4.37	120.44	124.45
24	C	511	CLA	C3D-C4D-ND	4.37	117.31	110.24
24	c	511	CLA	C3D-C4D-ND	4.37	117.31	110.24
24	b	603	CLA	C3C-C4C-NC	4.36	115.47	110.57
24	D	403	CLA	CHD-C1D-ND	-4.36	120.44	124.45
24	d	403	CLA	CHD-C1D-ND	-4.36	120.44	124.45
24	B	601	CLA	C3C-C4C-NC	4.36	115.47	110.57
24	C	513	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	c	513	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	b	614	CLA	CMC-C2C-C1C	4.36	131.68	125.04
24	A	405	CLA	C3B-C4B-NB	4.36	114.85	109.21
24	a	405	CLA	C3B-C4B-NB	4.36	114.85	109.21
28	D	406	PL9	C7-C3-C4	4.36	120.42	116.88
28	d	406	PL9	C7-C3-C4	4.36	120.42	116.88
27	A	412	SQD	O6-C1-C2	4.35	115.10	108.30
27	a	412	SQD	O6-C1-C2	4.35	115.10	108.30
24	B	608	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
24	b	618	CLA	C2C-C1C-NC	4.33	114.03	109.97
24	d	401	CLA	C3D-C4D-ND	4.32	117.23	110.24
24	B	608	CLA	C3C-C4C-NC	4.32	115.42	110.57
24	C	509	CLA	C3D-C4D-ND	4.32	117.22	110.24
24	c	509	CLA	C3D-C4D-ND	4.32	117.22	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	C3B-C4B-NB	4.32	114.79	109.21
24	c	508	CLA	C3B-C4B-NB	4.32	114.79	109.21
24	B	616	CLA	C2C-C1C-NC	4.31	114.01	109.97
24	D	401	CLA	C3D-C4D-ND	4.30	117.20	110.24
24	A	406	CLA	C3D-C4D-ND	4.30	117.20	110.24
24	a	406	CLA	C3D-C4D-ND	4.30	117.20	110.24
24	b	610	CLA	C3C-C4C-NC	4.29	115.38	110.57
24	b	610	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
24	C	508	CLA	C3C-C4C-NC	4.29	115.38	110.57
35	H	101	RRX	C20-C21-C22	-4.27	121.21	127.31
35	h	101	RRX	C20-C21-C22	-4.27	121.21	127.31
24	C	507	CLA	C3B-C4B-NB	4.27	114.73	109.21
24	C	509	CLA	C3B-C4B-NB	4.26	114.72	109.21
24	c	509	CLA	C3B-C4B-NB	4.26	114.72	109.21
24	c	507	CLA	C3B-C4B-NB	4.26	114.72	109.21
24	c	508	CLA	C3C-C4C-NC	4.26	115.35	110.57
24	c	505	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
24	C	505	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
24	b	611	CLA	C3B-C4B-NB	4.25	114.70	109.21
24	b	605	CLA	O2A-CGA-CBA	4.24	125.22	111.91
24	C	509	CLA	CAC-C3C-C4C	4.24	130.31	124.81
24	C	507	CLA	O2D-CGD-CBD	4.24	118.80	111.27
24	c	507	CLA	O2D-CGD-CBD	4.24	118.80	111.27
24	B	603	CLA	O2A-CGA-CBA	4.24	125.20	111.91
24	c	509	CLA	CAC-C3C-C4C	4.24	130.31	124.81
24	C	506	CLA	C1D-CHD-C4C	-4.23	116.92	126.06
24	c	506	CLA	C1D-CHD-C4C	-4.23	116.92	126.06
35	H	101	RRX	C33-C5-C6	-4.23	119.78	124.53
24	C	512	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	c	512	CLA	C3D-C4D-ND	4.23	117.08	110.24
24	C	510	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
24	C	513	CLA	CHD-C1D-ND	-4.22	120.57	124.45
24	c	513	CLA	CHD-C1D-ND	-4.22	120.58	124.45
24	B	601	CLA	C3D-C4D-ND	4.22	117.07	110.24
24	b	603	CLA	C3D-C4D-ND	4.22	117.07	110.24
32	B	625	LHG	O4-P-O5	4.22	133.10	112.24
32	b	627	LHG	O4-P-O5	4.22	133.10	112.24
24	B	611	CLA	C3C-C4C-NC	4.22	115.30	110.57
24	b	613	CLA	C3C-C4C-NC	4.22	115.30	110.57
24	C	513	CLA	CMD-C2D-C1D	4.22	132.14	124.71
24	c	513	CLA	CMD-C2D-C1D	4.22	132.14	124.71
24	B	609	CLA	C3B-C4B-NB	4.20	114.65	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	401	CLA	C3B-C4B-NB	4.20	114.65	109.21
24	d	401	CLA	C3B-C4B-NB	4.20	114.65	109.21
24	C	509	CLA	C4C-C3C-C2C	-4.20	100.77	106.90
24	c	509	CLA	C4C-C3C-C2C	-4.20	100.77	106.90
24	c	510	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
24	B	603	CLA	C3D-C4D-ND	4.19	117.02	110.24
24	b	605	CLA	C3D-C4D-ND	4.19	117.02	110.24
35	h	101	RRX	C33-C5-C6	-4.19	119.82	124.53
27	A	412	SQD	O47-C7-C8	4.19	120.52	111.50
24	b	606	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
24	B	614	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
24	b	616	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
32	d	408	LHG	O4-P-O5	4.17	132.87	112.24
32	D	408	LHG	O4-P-O5	4.17	132.86	112.24
27	a	412	SQD	O47-C7-C8	4.17	120.48	111.50
24	d	403	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
24	C	502	CLA	C3C-C4C-NC	4.16	115.23	110.57
24	c	502	CLA	C3C-C4C-NC	4.16	115.23	110.57
24	B	610	CLA	C4A-NA-C1A	-4.16	104.84	106.71
24	B	604	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
24	c	505	CLA	CMB-C2B-C3B	4.14	132.42	124.68
24	C	510	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
24	c	510	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
24	B	614	CLA	C3D-C4D-ND	4.13	116.91	110.24
24	b	616	CLA	C3D-C4D-ND	4.13	116.91	110.24
24	D	403	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
24	b	611	CLA	C3D-C4D-ND	4.12	116.91	110.24
24	C	505	CLA	CMB-C2B-C3B	4.12	132.39	124.68
24	B	613	CLA	CAC-C3C-C4C	4.12	130.16	124.81
24	B	603	CLA	C3C-C4C-NC	4.12	115.19	110.57
24	B	609	CLA	C3D-C4D-ND	4.12	116.90	110.24
27	l	101	SQD	O47-C7-C8	4.11	120.37	111.50
24	b	615	CLA	CAC-C3C-C4C	4.11	130.14	124.81
24	c	502	CLA	C4A-NA-C1A	-4.11	104.86	106.71
24	b	609	CLA	C3D-C4D-ND	4.10	116.88	110.24
24	B	614	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	b	616	CLA	C3C-C4C-NC	4.10	115.17	110.57
27	L	101	SQD	O47-C7-C8	4.10	120.33	111.50
24	B	607	CLA	C3D-C4D-ND	4.09	116.86	110.24
24	B	602	CLA	C3D-C4D-ND	4.09	116.86	110.24
24	b	604	CLA	C3D-C4D-ND	4.09	116.86	110.24
24	b	612	CLA	CMB-C2B-C3B	4.09	132.33	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CMB-C2B-C3B	4.09	132.33	124.68
24	b	608	CLA	CMB-C2B-C3B	4.09	132.33	124.68
24	B	607	CLA	C3C-C4C-NC	4.09	115.16	110.57
27	D	407	SQD	O47-C7-C8	4.08	120.29	111.50
27	d	407	SQD	O47-C7-C8	4.08	120.29	111.50
24	A	405	CLA	C3C-C4C-NC	4.08	115.14	110.57
24	a	405	CLA	C3C-C4C-NC	4.08	115.14	110.57
24	b	609	CLA	C3C-C4C-NC	4.07	115.14	110.57
24	B	613	CLA	C3B-C4B-NB	4.07	114.47	109.21
24	b	615	CLA	C3B-C4B-NB	4.07	114.47	109.21
24	B	610	CLA	CHD-C1D-ND	-4.07	120.72	124.45
26	C	521	BCR	C24-C23-C22	-4.06	120.10	126.23
26	c	521	BCR	C24-C23-C22	-4.06	120.10	126.23
24	b	607	CLA	CMC-C2C-C1C	4.06	131.22	125.04
24	B	602	CLA	CAA-C2A-C3A	-4.05	101.69	112.78
24	b	611	CLA	CMC-C2C-C1C	4.05	131.21	125.04
32	D	409	LHG	O4-P-O5	4.05	132.25	112.24
32	d	409	LHG	O4-P-O5	4.05	132.25	112.24
24	b	604	CLA	CAA-C2A-C3A	-4.05	101.69	112.78
24	c	510	CLA	CMB-C2B-C3B	4.05	132.25	124.68
24	B	605	CLA	CMC-C2C-C1C	4.05	131.20	125.04
24	B	607	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	b	609	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	B	610	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
24	b	612	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
24	b	605	CLA	C3C-C4C-NC	4.04	115.10	110.57
24	C	508	CLA	C1D-CHD-C4C	-4.03	117.35	126.06
24	c	508	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
24	B	615	CLA	C3D-C4D-ND	4.03	116.76	110.24
24	b	617	CLA	C3D-C4D-ND	4.03	116.76	110.24
24	B	609	CLA	CMC-C2C-C1C	4.03	131.18	125.04
24	b	618	CLA	CMB-C2B-C3B	4.03	132.22	124.68
24	B	604	CLA	C3C-C4C-NC	4.03	115.09	110.57
24	C	507	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	c	507	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	b	606	CLA	C3C-C4C-NC	4.02	115.08	110.57
24	B	606	CLA	C4C-C3C-C2C	-4.01	101.05	106.90
24	b	608	CLA	C4C-C3C-C2C	-4.01	101.05	106.90
24	C	506	CLA	C4C-C3C-C2C	-4.01	101.05	106.90
24	c	506	CLA	C4C-C3C-C2C	-4.01	101.05	106.90
24	b	612	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
24	c	506	CLA	C4A-NA-C1A	-4.01	104.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	CMB-C2B-C3B	4.01	132.17	124.68
24	C	514	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	c	514	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	C	510	CLA	CMB-C2B-C3B	4.00	132.16	124.68
24	B	616	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
24	b	618	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
24	C	506	CLA	C4A-NA-C1A	-3.99	104.91	106.71
24	c	503	CLA	C3D-C4D-ND	3.99	116.69	110.24
24	b	618	CLA	C3B-C4B-NB	3.99	114.37	109.21
24	C	503	CLA	C3C-C4C-NC	3.99	115.04	110.57
24	C	503	CLA	C3D-C4D-ND	3.99	116.69	110.24
27	D	407	SQD	O9-S-O7	-3.99	100.16	113.95
27	d	407	SQD	O9-S-O7	-3.99	100.16	113.95
24	B	614	CLA	CMC-C2C-C1C	3.98	131.10	125.04
24	b	616	CLA	CMC-C2C-C1C	3.98	131.10	125.04
24	c	503	CLA	C1-C2-C3	-3.98	119.16	126.04
24	C	502	CLA	C4A-NA-C1A	-3.98	104.92	106.71
32	E	101	LHG	O4-P-O5	3.98	131.91	112.24
32	e	101	LHG	O4-P-O5	3.98	131.91	112.24
24	C	510	CLA	C4A-NA-C1A	-3.97	104.92	106.71
24	c	510	CLA	C4A-NA-C1A	-3.97	104.92	106.71
24	C	503	CLA	C1-C2-C3	-3.97	119.17	126.04
24	c	503	CLA	C3C-C4C-NC	3.96	115.02	110.57
33	C	517	DGD	O3G-C3G-C2G	-3.96	101.34	110.90
24	B	616	CLA	C3B-C4B-NB	3.96	114.33	109.21
24	C	506	CLA	C3D-C4D-ND	3.96	116.64	110.24
24	A	408	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
24	a	408	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
24	B	605	CLA	C3D-C4D-ND	3.95	116.63	110.24
24	b	607	CLA	C3D-C4D-ND	3.95	116.63	110.24
24	c	506	CLA	C3D-C4D-ND	3.95	116.62	110.24
33	c	517	DGD	O3G-C3G-C2G	-3.95	101.38	110.90
24	c	504	CLA	C4C-C3C-C2C	-3.94	101.15	106.90
24	B	601	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
24	A	408	CLA	C3D-C4D-ND	3.94	116.61	110.24
24	a	408	CLA	C3D-C4D-ND	3.94	116.61	110.24
24	B	613	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	B	604	CLA	C3B-C4B-NB	3.94	114.31	109.21
24	b	606	CLA	C3B-C4B-NB	3.94	114.31	109.21
32	d	410	LHG	O4-P-O5	3.94	131.69	112.24
32	D	410	LHG	O4-P-O5	3.93	131.68	112.24
24	b	603	CLA	C1D-CHD-C4C	-3.93	117.58	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	403	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
24	d	403	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
24	A	405	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
24	a	405	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
24	B	602	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
24	B	612	CLA	C1D-CHD-C4C	-3.93	117.59	126.06
24	B	613	CLA	C3D-C4D-ND	3.93	116.59	110.24
24	b	615	CLA	C3D-C4D-ND	3.93	116.59	110.24
24	C	504	CLA	C4C-C3C-C2C	-3.92	101.18	106.90
27	D	407	SQD	O7-S-C6	3.92	111.60	106.94
35	H	101	RRX	C11-C10-C9	-3.92	121.72	127.31
35	h	101	RRX	C11-C10-C9	-3.92	121.72	127.31
24	B	615	CLA	O2D-CGD-CBD	3.92	118.23	111.27
24	b	617	CLA	O2D-CGD-CBD	3.92	118.23	111.27
24	C	502	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
24	b	614	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
24	b	615	CLA	C3C-C4C-NC	3.91	114.96	110.57
27	L	101	SQD	C4-C3-C2	3.91	117.65	110.82
27	l	101	SQD	C4-C3-C2	3.91	117.65	110.82
24	C	505	CLA	C3C-C4C-NC	3.90	114.95	110.57
24	C	510	CLA	C3C-C4C-NC	3.90	114.95	110.57
25	a	407	PHO	CMB-C2B-C3B	3.90	131.98	124.68
27	a	412	SQD	C4-C3-C2	3.90	117.63	110.82
25	A	407	PHO	CMB-C2B-C3B	3.90	131.97	124.68
24	c	502	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
24	B	608	CLA	C3D-C4D-ND	3.89	116.53	110.24
24	b	604	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
27	A	412	SQD	C4-C3-C2	3.89	117.61	110.82
24	c	514	CLA	CAC-C3C-C4C	3.89	129.86	124.81
27	d	407	SQD	O7-S-C6	3.89	111.56	106.94
24	B	605	CLA	C4-C3-C5	3.89	121.81	115.27
24	b	607	CLA	C4-C3-C5	3.89	121.81	115.27
24	c	510	CLA	C3D-C4D-ND	3.88	116.51	110.24
24	B	616	CLA	C3D-C4D-ND	3.88	116.51	110.24
24	b	618	CLA	C3D-C4D-ND	3.88	116.51	110.24
24	C	514	CLA	CAC-C3C-C4C	3.88	129.84	124.81
24	b	610	CLA	C3D-C4D-ND	3.87	116.50	110.24
24	B	612	CLA	CAC-C3C-C4C	3.86	129.82	124.81
24	C	510	CLA	C3D-C4D-ND	3.86	116.48	110.24
24	C	511	CLA	C3B-C4B-NB	3.85	114.19	109.21
24	c	510	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	A	406	CLA	C4A-NA-C1A	-3.85	104.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406	CLA	C4A-NA-C1A	-3.85	104.97	106.71
34	E	103	HEM	CBD-CAD-C3D	-3.85	101.93	112.63
34	e	103	HEM	CBD-CAD-C3D	-3.85	101.94	112.63
24	c	511	CLA	C3B-C4B-NB	3.84	114.18	109.21
24	c	505	CLA	C3C-C4C-NC	3.84	114.88	110.57
24	B	610	CLA	CMB-C2B-C3B	3.84	131.86	124.68
24	b	605	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
24	B	606	CLA	C4A-NA-C1A	-3.83	104.98	106.71
24	b	608	CLA	C4A-NA-C1A	-3.83	104.98	106.71
24	C	504	CLA	CMB-C2B-C3B	3.83	131.84	124.68
24	b	614	CLA	CAC-C3C-C4C	3.82	129.77	124.81
33	C	518	DGD	O6D-C1D-O3G	-3.81	100.94	109.97
24	B	603	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
24	c	510	CLA	C3B-C4B-NB	3.81	114.14	109.21
33	c	518	DGD	O6D-C1D-O3G	-3.81	100.95	109.97
24	D	401	CLA	CMB-C2B-C3B	3.81	131.80	124.68
24	d	401	CLA	CMB-C2B-C3B	3.81	131.80	124.68
27	A	410	SQD	O8-S-C6	3.80	111.80	105.74
27	a	410	SQD	O8-S-C6	3.80	111.80	105.74
24	B	601	CLA	C3B-C4B-NB	3.80	114.13	109.21
24	b	603	CLA	C3B-C4B-NB	3.80	114.13	109.21
24	b	610	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
24	c	504	CLA	CMB-C2B-C3B	3.80	131.78	124.68
24	c	513	CLA	C3D-C4D-ND	3.80	116.38	110.24
24	C	510	CLA	C3B-C4B-NB	3.79	114.12	109.21
24	b	614	CLA	C4C-C3C-C2C	-3.79	101.37	106.90
24	C	513	CLA	C3D-C4D-ND	3.79	116.37	110.24
24	B	604	CLA	C1-C2-C3	-3.79	119.49	126.04
25	D	402	PHO	CMB-C2B-C3B	3.79	131.77	124.68
25	d	402	PHO	CMB-C2B-C3B	3.79	131.77	124.68
24	c	505	CLA	C3B-C4B-NB	3.78	114.10	109.21
24	A	406	CLA	C3C-C4C-NC	3.78	114.81	110.57
24	B	612	CLA	C4C-C3C-C2C	-3.78	101.38	106.90
24	B	610	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
24	a	406	CLA	C3C-C4C-NC	3.78	114.81	110.57
24	C	512	CLA	O2D-CGD-CBD	3.78	117.98	111.27
24	c	512	CLA	O2D-CGD-CBD	3.78	117.98	111.27
24	B	603	CLA	CAA-C2A-C3A	-3.78	102.44	112.78
24	b	605	CLA	CAA-C2A-C3A	-3.78	102.44	112.78
24	B	611	CLA	C3D-C4D-ND	3.78	116.35	110.24
24	b	613	CLA	C3D-C4D-ND	3.78	116.35	110.24
24	D	403	CLA	CAA-C2A-C3A	-3.77	102.44	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
24	c	503	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
24	C	507	CLA	C3D-C4D-ND	3.77	116.34	110.24
24	b	606	CLA	C1-C2-C3	-3.77	119.52	126.04
24	B	603	CLA	C3D-C2D-C1D	-3.77	100.69	105.83
24	b	605	CLA	C3D-C2D-C1D	-3.77	100.69	105.83
24	B	606	CLA	C3D-C4D-ND	3.77	116.33	110.24
24	b	608	CLA	C3D-C4D-ND	3.77	116.33	110.24
24	c	507	CLA	C3D-C4D-ND	3.76	116.33	110.24
24	B	604	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
24	b	606	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
24	d	403	CLA	CAA-C2A-C3A	-3.76	102.48	112.78
24	A	405	CLA	CMB-C2B-C3B	3.75	131.70	124.68
24	a	405	CLA	CMB-C2B-C3B	3.75	131.70	124.68
24	C	507	CLA	C3C-C4C-NC	3.75	114.78	110.57
24	c	507	CLA	C3C-C4C-NC	3.75	114.78	110.57
24	B	611	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	C	511	CLA	CMD-C2D-C3D	-3.75	119.00	127.61
24	c	511	CLA	CMD-C2D-C3D	-3.75	119.00	127.61
24	B	608	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
24	C	505	CLA	C3B-C4B-NB	3.74	114.04	109.21
24	c	502	CLA	C3D-C4D-ND	3.73	116.28	110.24
35	H	101	RRX	C38-C26-C25	-3.73	120.34	124.53
24	A	405	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
24	a	405	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
36	i	102	LMT	O1B-C4'-C3'	3.73	117.19	107.28
24	b	613	CLA	C3B-C4B-NB	3.73	114.03	109.21
24	C	502	CLA	C3D-C4D-ND	3.71	116.24	110.24
24	c	510	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
36	I	102	LMT	O1B-C4'-C3'	3.71	117.15	107.28
24	C	510	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
24	B	612	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
24	B	608	CLA	CHD-C1D-ND	-3.70	121.06	124.45
24	b	614	CLA	C3D-C2D-C1D	-3.69	100.79	105.83
24	C	503	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	C	511	CLA	C3C-C4C-NC	3.68	114.70	110.57
24	c	511	CLA	C3C-C4C-NC	3.68	114.70	110.57
24	c	503	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	C	504	CLA	C3D-C4D-ND	3.68	116.19	110.24
24	c	504	CLA	C3D-C4D-ND	3.68	116.19	110.24
24	B	607	CLA	CAA-CBA-CGA	3.68	124.00	113.25
24	b	609	CLA	CAA-CBA-CGA	3.68	124.00	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	C4A-NA-C1A	-3.67	105.05	106.71
24	c	511	CLA	C4A-NA-C1A	-3.67	105.05	106.71
24	d	404	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
24	D	404	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
24	D	404	CLA	C3B-C4B-NB	3.67	113.95	109.21
24	d	404	CLA	C3B-C4B-NB	3.67	113.95	109.21
24	B	612	CLA	C3D-C4D-ND	3.66	116.17	110.24
24	b	614	CLA	C3D-C4D-ND	3.66	116.16	110.24
24	C	507	CLA	CHC-C1C-C2C	-3.66	116.61	126.72
24	c	507	CLA	CHC-C1C-C2C	-3.66	116.61	126.72
24	b	612	CLA	C3D-C4D-ND	3.66	116.15	110.24
24	B	611	CLA	C4A-NA-C1A	-3.65	105.06	106.71
24	b	613	CLA	C4A-NA-C1A	-3.65	105.06	106.71
35	h	101	RRX	C38-C26-C25	-3.65	120.43	124.53
24	b	617	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	c	514	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
24	B	615	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
28	D	406	PL9	C36-C34-C33	-3.64	113.75	121.12
28	d	406	PL9	C36-C34-C33	-3.64	113.75	121.12
24	C	507	CLA	CMB-C2B-C3B	3.64	131.49	124.68
24	C	514	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
24	c	507	CLA	CMB-C2B-C3B	3.63	131.47	124.68
24	C	513	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
24	B	612	CLA	CMB-C2B-C3B	3.62	131.45	124.68
24	C	509	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
24	c	509	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
24	b	616	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
24	b	614	CLA	CMB-C2B-C3B	3.62	131.45	124.68
24	B	614	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
24	B	611	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
24	b	613	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
24	D	403	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
24	d	403	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
24	B	612	CLA	C4A-NA-C1A	-3.59	105.09	106.71
24	c	513	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
24	B	615	CLA	C4A-NA-C1A	-3.58	105.09	106.71
24	b	617	CLA	C4A-NA-C1A	-3.58	105.09	106.71
24	B	616	CLA	CAC-C3C-C4C	3.58	129.45	124.81
24	b	618	CLA	CAC-C3C-C4C	3.58	129.45	124.81
24	B	610	CLA	C3D-C4D-ND	3.57	116.02	110.24
24	B	601	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
24	b	603	CLA	C4C-C3C-C2C	-3.57	101.70	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
24	b	608	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
24	b	605	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
24	D	401	CLA	CBC-CAC-C3C	-3.56	102.61	112.43
24	B	610	CLA	C4C-C3C-C2C	-3.55	101.72	106.90
24	B	603	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
24	B	608	CLA	O2D-CGD-CBD	3.55	117.57	111.27
24	A	406	CLA	C1D-CHD-C4C	-3.55	118.41	126.06
24	d	401	CLA	CBC-CAC-C3C	-3.55	102.66	112.43
24	B	607	CLA	C3B-C4B-NB	3.54	113.79	109.21
24	a	406	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
24	b	609	CLA	C3B-C4B-NB	3.54	113.78	109.21
24	b	610	CLA	O2D-CGD-CBD	3.53	117.55	111.27
24	b	610	CLA	CHD-C1D-ND	-3.53	121.21	124.45
24	C	512	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
24	c	512	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
24	D	401	CLA	CAA-C2A-C3A	-3.51	103.16	112.78
24	d	401	CLA	CAA-C2A-C3A	-3.51	103.16	112.78
27	A	410	SQD	C4-C3-C2	3.51	116.95	110.82
24	A	405	CLA	C3D-C4D-ND	3.51	115.91	110.24
24	a	405	CLA	C3D-C4D-ND	3.51	115.91	110.24
35	H	101	RRX	C15-C14-C13	-3.50	122.31	127.31
35	h	101	RRX	C15-C14-C13	-3.50	122.31	127.31
24	b	609	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
24	C	510	CLA	C1-O2A-CGA	3.50	125.63	116.44
26	B	627	BCR	C2-C1-C6	3.50	115.86	110.48
26	T	101	BCR	C2-C1-C6	3.50	115.86	110.48
24	b	614	CLA	O2A-CGA-CBA	3.50	122.88	111.91
27	a	410	SQD	C4-C3-C2	3.50	116.93	110.82
24	B	607	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
24	D	403	CLA	C3D-C4D-ND	3.49	115.89	110.24
24	d	403	CLA	C3D-C4D-ND	3.49	115.89	110.24
38	V	201	HEC	CMC-C2C-C1C	-3.49	123.09	128.46
24	B	612	CLA	O2A-CGA-CBA	3.49	122.86	111.91
24	c	510	CLA	C1-O2A-CGA	3.49	125.60	116.44
35	h	101	RRX	C24-C23-C22	-3.48	120.97	126.23
24	B	605	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
24	b	614	CLA	C4A-NA-C1A	-3.47	105.14	106.71
24	b	607	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
38	v	201	HEC	CMC-C2C-C1C	-3.46	123.14	128.46
24	B	607	CLA	C4-C3-C5	3.46	121.09	115.27
24	b	609	CLA	C4-C3-C5	3.46	121.09	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	410	SQD	O47-C7-C8	3.46	118.95	111.50
24	B	602	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
24	b	604	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
24	b	616	CLA	CAC-C3C-C4C	3.45	129.29	124.81
24	B	614	CLA	CAC-C3C-C4C	3.45	129.29	124.81
24	b	613	CLA	CMB-C2B-C3B	3.45	131.14	124.68
24	B	611	CLA	CMB-C2B-C3B	3.45	131.14	124.68
27	a	410	SQD	O47-C7-C8	3.45	118.94	111.50
36	i	102	LMT	C3'-C4'-C5'	-3.45	103.01	110.93
24	D	401	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
24	d	401	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
35	H	101	RRX	C24-C23-C22	-3.45	121.02	126.23
24	C	513	CLA	C4A-NA-C1A	-3.44	105.16	106.71
24	c	513	CLA	C4A-NA-C1A	-3.44	105.16	106.71
24	B	602	CLA	C3C-C4C-NC	3.44	114.43	110.57
24	b	604	CLA	C3C-C4C-NC	3.44	114.43	110.57
36	I	102	LMT	C3'-C4'-C5'	-3.44	103.05	110.93
24	B	609	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
27	A	410	SQD	O7-S-C6	3.43	111.02	106.94
24	B	603	CLA	C4A-NA-C1A	-3.43	105.17	106.71
24	b	605	CLA	C4A-NA-C1A	-3.43	105.17	106.71
24	B	603	CLA	O2A-CGA-O1A	-3.43	114.94	123.59
24	b	605	CLA	O2A-CGA-O1A	-3.43	114.94	123.59
24	C	512	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
24	c	512	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
24	b	605	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
27	a	410	SQD	O7-S-C6	3.41	110.99	106.94
24	B	605	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
24	b	607	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
24	b	611	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
24	C	502	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
24	c	502	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
24	B	603	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
24	b	612	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
24	C	513	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
24	c	513	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
24	B	616	CLA	C4A-NA-C1A	-3.39	105.18	106.71
24	B	613	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
24	B	609	CLA	CHD-C4C-NC	3.39	129.54	124.20
24	B	604	CLA	CHC-C1C-C2C	-3.38	117.36	126.72
24	b	606	CLA	CHC-C1C-C2C	-3.38	117.36	126.72
24	C	513	CLA	C3B-C4B-NB	3.38	113.58	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C3C-C4C-NC	3.38	114.36	110.57
24	b	611	CLA	C3C-C4C-NC	3.38	114.36	110.57
24	b	615	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
24	b	611	CLA	CHD-C4C-NC	3.37	129.52	124.20
24	D	403	CLA	C3B-C4B-NB	3.37	113.57	109.21
24	d	403	CLA	C3B-C4B-NB	3.37	113.57	109.21
24	c	506	CLA	C1-C2-C3	-3.37	120.22	126.04
24	D	403	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
24	d	403	CLA	C4C-C3C-C2C	-3.36	101.99	106.90
24	b	616	CLA	C1-C2-C3	-3.36	120.22	126.04
24	A	405	CLA	CHC-C1C-C2C	-3.36	117.42	126.72
24	C	508	CLA	C3D-C4D-ND	3.36	115.67	110.24
24	c	508	CLA	C3D-C4D-ND	3.36	115.67	110.24
24	c	513	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
24	C	502	CLA	CAC-C3C-C4C	3.35	129.16	124.81
24	a	405	CLA	CHC-C1C-C2C	-3.35	117.45	126.72
24	B	603	CLA	C3B-C4B-NB	3.35	113.54	109.21
24	b	605	CLA	C3B-C4B-NB	3.35	113.54	109.21
24	c	513	CLA	C3B-C4B-NB	3.35	113.54	109.21
24	C	513	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
24	B	614	CLA	C1-C2-C3	-3.35	120.25	126.04
24	C	503	CLA	CAC-C3C-C4C	3.35	129.16	124.81
24	b	607	CLA	C4A-NA-C1A	-3.34	105.20	106.71
24	B	611	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
24	C	512	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
24	c	512	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
24	C	506	CLA	C1-C2-C3	-3.34	120.27	126.04
24	B	602	CLA	CMB-C2B-C3B	3.33	130.92	124.68
35	h	101	RRX	C7-C8-C9	-3.33	121.20	126.23
35	H	101	RRX	C7-C8-C9	-3.33	121.20	126.23
24	b	604	CLA	CMB-C2B-C3B	3.33	130.91	124.68
24	A	405	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
24	a	405	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
24	c	502	CLA	CAC-C3C-C4C	3.33	129.13	124.81
24	b	615	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
28	d	406	PL9	C7-C8-C9	-3.33	121.25	126.79
27	l	101	SQD	O7-S-C6	3.33	110.89	106.94
24	B	602	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
24	b	613	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
24	C	505	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
24	B	601	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
24	B	606	CLA	C3B-C4B-NB	3.32	113.50	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	B	610	CLA	CAA-C2A-C3A	-3.32	103.70	112.78
24	b	605	CLA	C4-C3-C5	3.31	120.84	115.27
24	B	601	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
24	B	614	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
24	b	616	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
24	c	505	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
24	c	503	CLA	CAC-C3C-C4C	3.31	129.10	124.81
27	L	101	SQD	O7-S-C6	3.31	110.87	106.94
24	A	408	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
24	a	408	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
24	B	615	CLA	C1D-CHD-C4C	-3.31	118.93	126.06
24	b	617	CLA	C1D-CHD-C4C	-3.31	118.93	126.06
24	B	613	CLA	O2D-CGD-CBD	3.31	117.14	111.27
24	b	615	CLA	O2D-CGD-CBD	3.31	117.14	111.27
24	C	507	CLA	CBC-CAC-C3C	-3.31	103.32	112.43
24	c	507	CLA	CBC-CAC-C3C	-3.31	103.32	112.43
31	c	522	LMG	O1-C1-C2	-3.30	103.14	108.30
31	C	522	LMG	O1-C1-C2	-3.30	103.15	108.30
24	b	618	CLA	C4A-NA-C1A	-3.30	105.22	106.71
28	D	406	PL9	C7-C8-C9	-3.30	121.30	126.79
24	b	603	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
24	A	408	CLA	C4-C3-C5	3.30	120.82	115.27
24	b	604	CLA	C1D-CHD-C4C	-3.30	118.95	126.06
24	d	404	CLA	C3C-C4C-NC	3.29	114.27	110.57
24	D	404	CLA	C3C-C4C-NC	3.29	114.26	110.57
24	C	504	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
24	c	504	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
24	B	603	CLA	C4-C3-C5	3.29	120.81	115.27
24	B	602	CLA	C3B-C4B-NB	3.29	113.47	109.21
24	b	604	CLA	C3B-C4B-NB	3.29	113.47	109.21
24	a	408	CLA	C4-C3-C5	3.29	120.80	115.27
24	b	603	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
38	v	201	HEC	CBD-CAD-C3D	-3.28	107.02	112.62
24	d	404	CLA	CAC-C3C-C4C	3.28	129.06	124.81
24	C	507	CLA	CAC-C3C-C4C	3.28	129.06	124.81
24	c	507	CLA	CAC-C3C-C4C	3.28	129.06	124.81
38	V	201	HEC	CBD-CAD-C3D	-3.28	107.03	112.62
24	C	514	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
24	c	514	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
24	c	514	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
24	b	614	CLA	CHD-C1D-ND	-3.27	121.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
24	c	503	CLA	C3B-C4B-NB	3.26	113.43	109.21
24	B	614	CLA	C3B-C4B-NB	3.26	113.42	109.21
24	B	605	CLA	C4A-NA-C1A	-3.25	105.24	106.71
24	b	613	CLA	CHC-C1C-C2C	-3.25	117.72	126.72
24	C	514	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
24	b	616	CLA	C3B-C4B-NB	3.25	113.41	109.21
24	C	507	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
24	B	613	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
24	B	611	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
24	D	404	CLA	CAC-C3C-C4C	3.25	129.02	124.81
24	C	513	CLA	CMC-C2C-C1C	3.24	129.98	125.04
24	c	507	CLA	CAA-C2A-C3A	-3.24	103.89	112.78
24	C	507	CLA	CAA-C2A-C3A	-3.24	103.91	112.78
24	A	405	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
24	a	405	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
24	C	512	CLA	C3B-C4B-NB	3.23	113.39	109.21
24	c	512	CLA	C3B-C4B-NB	3.23	113.39	109.21
24	C	503	CLA	C3B-C4B-NB	3.23	113.39	109.21
24	b	614	CLA	C3B-C4B-NB	3.23	113.38	109.21
24	c	513	CLA	CMC-C2C-C1C	3.22	129.95	125.04
24	B	615	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
27	l	101	SQD	O9-S-O7	-3.22	102.80	113.95
24	C	504	CLA	C3B-C4B-NB	3.22	113.38	109.21
24	c	504	CLA	C3B-C4B-NB	3.22	113.38	109.21
24	B	612	CLA	C3B-C4B-NB	3.22	113.37	109.21
24	b	617	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
24	C	502	CLA	CMB-C2B-C3B	3.21	130.69	124.68
24	c	502	CLA	CMB-C2B-C3B	3.21	130.69	124.68
24	C	513	CLA	CAC-C3C-C4C	3.21	128.98	124.81
24	c	513	CLA	CAC-C3C-C4C	3.21	128.98	124.81
24	C	513	CLA	CMB-C2B-C3B	3.21	130.69	124.68
24	b	612	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
27	L	101	SQD	O9-S-O7	-3.21	102.85	113.95
24	c	513	CLA	CMB-C2B-C3B	3.21	130.68	124.68
24	C	506	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	c	506	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	A	408	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
24	a	408	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
24	D	401	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
24	A	406	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
24	a	406	CLA	CAA-C2A-C3A	-3.19	104.03	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	CAA-CBA-CGA	3.19	122.58	113.25
24	d	401	CLA	C4A-NA-C1A	-3.19	105.27	106.71
24	d	401	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
24	c	505	CLA	CAA-CBA-CGA	3.19	122.56	113.25
26	B	619	BCR	C2-C1-C6	3.19	115.39	110.48
24	b	611	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
26	b	621	BCR	C2-C1-C6	3.18	115.38	110.48
24	C	511	CLA	CMB-C2B-C3B	3.18	130.62	124.68
24	c	511	CLA	CMB-C2B-C3B	3.18	130.62	124.68
28	a	411	PL9	C7-C3-C2	-3.17	119.12	123.30
24	c	506	CLA	C1C-C2C-C3C	-3.17	103.62	106.96
24	b	608	CLA	C4-C3-C5	3.17	120.60	115.27
38	V	201	HEC	CMB-C2B-C1B	-3.17	123.59	128.46
24	B	606	CLA	C4-C3-C5	3.17	120.60	115.27
24	B	608	CLA	C3D-C2D-C1D	-3.17	101.51	105.83
24	b	611	CLA	CED-O2D-CGD	3.16	123.09	115.94
24	C	511	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
24	c	511	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
24	C	506	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
24	b	618	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
24	B	609	CLA	CBC-CAC-C3C	-3.16	103.73	112.43
24	B	609	CLA	CED-O2D-CGD	3.16	123.08	115.94
38	v	201	HEC	CMB-C2B-C1B	-3.16	123.61	128.46
24	B	606	CLA	CAA-C2A-C3A	-3.15	104.14	112.78
24	b	608	CLA	CAA-C2A-C3A	-3.15	104.14	112.78
24	B	616	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
24	B	613	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
24	b	611	CLA	CBC-CAC-C3C	-3.15	103.75	112.43
24	b	615	CLA	C4A-NA-C1A	-3.15	105.29	106.71
28	A	411	PL9	C7-C3-C2	-3.14	119.17	123.30
24	c	504	CLA	CMC-C2C-C1C	3.14	129.82	125.04
24	b	607	CLA	CHD-C4C-NC	3.14	129.14	124.20
33	C	517	DGD	C6D-O5D-C1E	3.13	119.86	113.74
33	c	517	DGD	C6D-O5D-C1E	3.13	119.86	113.74
24	B	605	CLA	CHD-C4C-NC	3.13	129.13	124.20
24	C	504	CLA	CMC-C2C-C1C	3.12	129.80	125.04
24	C	508	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
24	b	615	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
24	D	404	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
24	d	404	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
24	b	610	CLA	C3D-C2D-C1D	-3.12	101.58	105.83
24	B	609	CLA	CHC-C1C-C2C	-3.12	118.10	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	CHC-C1C-C2C	-3.12	118.10	126.72
24	b	614	CLA	CMD-C2D-C1D	3.11	130.20	124.71
24	C	507	CLA	C4A-NA-C1A	-3.11	105.31	106.71
24	c	507	CLA	C4A-NA-C1A	-3.11	105.31	106.71
24	C	502	CLA	C3B-C4B-NB	3.11	113.23	109.21
28	D	406	PL9	C40-C39-C41	3.11	120.50	115.27
28	d	406	PL9	C40-C39-C41	3.11	120.50	115.27
26	B	627	BCR	C3-C4-C5	-3.10	108.54	114.08
26	T	101	BCR	C3-C4-C5	-3.10	108.54	114.08
24	B	613	CLA	C1-C2-C3	-3.10	120.68	126.04
24	a	408	CLA	C3B-C4B-NB	3.10	113.22	109.21
24	C	502	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	c	502	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	c	502	CLA	C3B-C4B-NB	3.10	113.22	109.21
24	B	612	CLA	CHD-C1D-ND	-3.10	121.61	124.45
24	A	408	CLA	C3B-C4B-NB	3.10	113.22	109.21
33	C	518	DGD	O5D-C6D-C5D	-3.10	103.32	109.05
24	C	503	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
24	B	604	CLA	C3D-C4D-ND	3.09	115.24	110.24
24	D	401	CLA	C4A-NA-C1A	-3.09	105.32	106.71
24	B	608	CLA	C1-C2-C3	-3.09	120.71	126.04
24	B	608	CLA	C3B-C4B-NB	3.08	113.20	109.21
26	a	409	BCR	C24-C23-C22	-3.08	121.58	126.23
24	c	503	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
24	b	606	CLA	C3D-C4D-ND	3.08	115.22	110.24
24	b	615	CLA	C1-C2-C3	-3.08	120.71	126.04
24	b	612	CLA	O2A-CGA-CBA	3.08	121.58	111.91
24	B	613	CLA	C4A-NA-C1A	-3.08	105.32	106.71
24	c	509	CLA	CMB-C2B-C3B	3.07	130.43	124.68
24	B	603	CLA	CMB-C2B-C3B	3.07	130.43	124.68
24	b	605	CLA	CMB-C2B-C3B	3.07	130.43	124.68
26	A	409	BCR	C24-C23-C22	-3.07	121.59	126.23
24	B	602	CLA	CHD-C4C-NC	3.07	129.04	124.20
24	b	612	CLA	C3B-C4B-NB	3.07	113.18	109.21
24	B	608	CLA	O2A-CGA-CBA	3.07	121.54	111.91
24	C	511	CLA	C3D-C2D-C1D	-3.07	101.65	105.83
24	c	511	CLA	C3D-C2D-C1D	-3.07	101.65	105.83
25	a	407	PHO	CMA-C3A-C4A	-3.07	107.66	114.38
24	b	610	CLA	C1-C2-C3	-3.06	120.74	126.04
33	c	518	DGD	O5D-C6D-C5D	-3.06	103.38	109.05
24	C	506	CLA	C3B-C4B-NB	3.06	113.17	109.21
24	c	506	CLA	C3B-C4B-NB	3.06	113.17	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	407	PHO	CMA-C3A-C4A	-3.06	107.67	114.38
24	C	503	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
24	c	503	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
24	C	514	CLA	C3B-C4B-NB	3.06	113.16	109.21
24	C	509	CLA	CMB-C2B-C3B	3.06	130.40	124.68
24	b	610	CLA	O2A-CGA-CBA	3.05	121.49	111.91
26	B	618	BCR	C27-C26-C25	3.05	127.16	122.73
24	B	604	CLA	O2A-CGA-CBA	3.05	121.48	111.91
24	C	508	CLA	CMB-C2B-C3B	3.05	130.38	124.68
24	c	508	CLA	CMB-C2B-C3B	3.05	130.38	124.68
24	b	604	CLA	CHD-C4C-NC	3.05	129.01	124.20
24	c	508	CLA	CHD-C4C-NC	3.05	129.01	124.20
26	b	620	BCR	C27-C26-C25	3.05	127.15	122.73
24	b	610	CLA	C3B-C4B-NB	3.04	113.14	109.21
24	C	514	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
24	c	514	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
24	D	403	CLA	O2D-CGD-CBD	3.04	116.67	111.27
24	B	612	CLA	CMD-C2D-C1D	3.04	130.07	124.71
24	C	505	CLA	C4-C3-C5	3.04	120.38	115.27
24	C	505	CLA	CHB-C4A-NA	3.04	128.71	124.51
24	c	505	CLA	CHB-C4A-NA	3.04	128.71	124.51
24	d	403	CLA	O2D-CGD-CBD	3.03	116.66	111.27
24	B	603	CLA	CMC-C2C-C1C	3.03	129.65	125.04
24	b	605	CLA	CMC-C2C-C1C	3.03	129.65	125.04
27	D	407	SQD	C4-C3-C2	3.03	116.11	110.82
27	d	407	SQD	C4-C3-C2	3.03	116.11	110.82
24	c	505	CLA	C4-C3-C5	3.03	120.36	115.27
24	C	508	CLA	CHD-C4C-NC	3.02	128.97	124.20
24	b	606	CLA	O2A-CGA-CBA	3.02	121.40	111.91
32	D	408	LHG	O8-C23-C24	3.02	121.39	111.91
32	d	408	LHG	O8-C23-C24	3.02	121.39	111.91
24	A	406	CLA	C3B-C4B-NB	3.02	113.11	109.21
24	a	406	CLA	C3B-C4B-NB	3.02	113.11	109.21
33	C	518	DGD	O3G-C3G-C2G	-3.02	103.62	110.90
24	B	604	CLA	CMC-C2C-C1C	3.02	129.63	125.04
24	b	606	CLA	CMC-C2C-C1C	3.02	129.63	125.04
24	C	502	CLA	CBC-CAC-C3C	-3.01	104.12	112.43
24	c	502	CLA	CBC-CAC-C3C	-3.01	104.13	112.43
24	c	514	CLA	C3B-C4B-NB	3.01	113.10	109.21
33	c	518	DGD	O3G-C3G-C2G	-3.01	103.64	110.90
24	C	512	CLA	CMB-C2B-C3B	3.01	130.31	124.68
24	c	512	CLA	CMB-C2B-C3B	3.01	130.31	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
24	c	502	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
24	B	610	CLA	O2A-CGA-CBA	3.01	121.35	111.91
38	v	201	HEC	CMC-C2C-C3C	3.01	129.35	125.82
24	B	601	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
24	C	510	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
24	c	510	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
24	C	513	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
38	V	201	HEC	CMC-C2C-C3C	2.99	129.34	125.82
24	b	603	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
24	D	401	CLA	CHD-C4C-NC	2.99	128.91	124.20
24	d	401	CLA	CHD-C4C-NC	2.99	128.91	124.20
24	C	509	CLA	C1D-CHD-C4C	-2.98	119.62	126.06
24	c	509	CLA	C1D-CHD-C4C	-2.98	119.62	126.06
24	B	603	CLA	CAC-C3C-C4C	2.98	128.68	124.81
24	B	605	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	b	607	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	B	605	CLA	CAC-C3C-C4C	2.98	128.68	124.81
24	b	607	CLA	CAC-C3C-C4C	2.98	128.68	124.81
24	b	610	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
24	D	403	CLA	CMC-C2C-C1C	2.98	129.57	125.04
24	B	608	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
26	c	516	BCR	C2-C1-C6	2.97	115.06	110.48
24	d	403	CLA	CMC-C2C-C1C	2.97	129.57	125.04
24	C	502	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
24	C	514	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
27	l	101	SQD	O5-C5-C4	2.97	115.09	109.69
24	c	513	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
24	c	514	CLA	CAA-C2A-C3A	-2.96	104.66	112.78
26	c	515	BCR	C15-C14-C13	-2.96	123.08	127.31
27	L	101	SQD	O5-C5-C4	2.96	115.06	109.69
24	b	603	CLA	C1-C2-C3	-2.96	120.93	126.04
27	D	407	SQD	C45-O47-C7	2.95	125.06	117.79
27	d	407	SQD	C45-O47-C7	2.95	125.06	117.79
24	C	514	CLA	O2A-CGA-CBA	2.95	121.18	111.91
24	c	514	CLA	O2A-CGA-CBA	2.95	121.18	111.91
24	c	502	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
35	h	101	RRX	C23-C24-C25	-2.95	118.91	127.20
27	a	412	SQD	O8-S-C6	2.95	110.44	105.74
26	C	516	BCR	C2-C1-C6	2.95	115.02	110.48
24	C	505	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
24	C	506	CLA	CMB-C2B-C3B	2.94	130.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	CMB-C2B-C3B	2.94	130.19	124.68
24	B	608	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
24	C	511	CLA	CAC-C3C-C4C	2.94	128.63	124.81
24	c	511	CLA	CAC-C3C-C4C	2.94	128.63	124.81
24	c	512	CLA	C4-C3-C5	2.94	120.21	115.27
24	d	401	CLA	C3C-C4C-NC	2.94	113.86	110.57
24	D	401	CLA	C3C-C4C-NC	2.94	113.86	110.57
24	C	511	CLA	C1D-CHD-C4C	-2.94	119.72	126.06
24	c	511	CLA	C1D-CHD-C4C	-2.94	119.72	126.06
24	b	605	CLA	CAC-C3C-C4C	2.93	128.62	124.81
24	D	401	CLA	O2A-CGA-CBA	2.93	121.11	111.91
24	d	401	CLA	O2A-CGA-CBA	2.93	121.11	111.91
24	b	605	CLA	CBA-CAA-C2A	2.93	122.52	113.86
24	C	510	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	c	510	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	b	615	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
35	H	101	RRX	C23-C24-C25	-2.93	118.97	127.20
24	C	503	CLA	C4A-NA-C1A	-2.93	105.39	106.71
24	B	601	CLA	C1-C2-C3	-2.93	120.98	126.04
24	B	611	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
24	b	613	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
24	B	605	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	B	607	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	b	607	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	C	514	CLA	CMC-C2C-C1C	2.92	129.49	125.04
27	L	101	SQD	O47-C7-O49	-2.92	116.64	123.70
24	b	614	CLA	C4-C3-C5	2.92	120.19	115.27
24	B	603	CLA	CBA-CAA-C2A	2.92	122.49	113.86
24	C	512	CLA	C4-C3-C5	2.92	120.19	115.27
24	b	610	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
27	A	412	SQD	O8-S-C6	2.92	110.39	105.74
24	B	613	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
24	c	514	CLA	CMC-C2C-C1C	2.92	129.48	125.04
31	c	520	LMG	O6-C1-O1	-2.92	103.07	109.97
24	b	609	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
26	c	515	BCR	C7-C8-C9	-2.92	121.83	126.23
27	l	101	SQD	O47-C7-O49	-2.91	116.67	123.70
24	c	505	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	B	612	CLA	C4-C3-C5	2.90	120.16	115.27
24	C	508	CLA	O1D-CGD-CBD	-2.90	118.54	124.48
26	C	515	BCR	C15-C14-C13	-2.90	123.17	127.31
24	c	508	CLA	O1D-CGD-CBD	-2.90	118.55	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	515	BCR	C7-C8-C9	-2.90	121.85	126.23
24	b	616	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	B	602	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	b	604	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
25	D	402	PHO	CMC-C2C-C3C	2.89	130.40	124.94
24	A	408	CLA	CHB-C4A-NA	2.89	128.51	124.51
24	a	408	CLA	CHB-C4A-NA	2.89	128.51	124.51
33	C	517	DGD	O6D-C1D-O3G	-2.89	103.12	109.97
24	C	503	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
24	c	503	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
24	C	507	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
24	c	507	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
33	c	519	DGD	CDB-CCB-CBB	-2.88	99.79	114.42
24	B	615	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
24	B	615	CLA	C3B-C4B-NB	2.88	112.94	109.21
24	b	617	CLA	C3B-C4B-NB	2.88	112.94	109.21
25	d	402	PHO	CMC-C2C-C3C	2.88	130.37	124.94
33	c	517	DGD	O6D-C1D-O3G	-2.88	103.16	109.97
33	C	519	DGD	CDB-CCB-CBB	-2.88	99.81	114.42
24	B	614	CLA	CMB-C2B-C3B	2.88	130.06	124.68
24	A	408	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
24	a	408	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
24	b	617	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
31	C	520	LMG	O6-C1-O1	-2.88	103.17	109.97
24	B	604	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	b	606	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	A	406	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
24	a	406	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
24	c	508	CLA	CBC-CAC-C3C	-2.87	104.52	112.43
24	C	508	CLA	CBC-CAC-C3C	-2.87	104.53	112.43
24	B	603	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
24	c	510	CLA	C1-C2-C3	-2.87	121.08	126.04
24	A	408	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
24	a	408	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
34	e	103	HEM	C4C-CHD-C1D	2.86	126.34	122.56
24	C	505	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
24	c	505	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
24	C	510	CLA	CMC-C2C-C1C	2.86	129.40	125.04
24	c	510	CLA	CMC-C2C-C1C	2.86	129.40	125.04
24	C	509	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
24	c	509	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
27	d	407	SQD	C1-C2-C3	-2.86	104.05	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C1-C2-C3	-2.85	121.11	126.04
24	b	604	CLA	C1-C2-C3	-2.85	121.11	126.04
27	D	407	SQD	C1-C2-C3	-2.85	104.07	110.00
24	B	616	CLA	CHD-C4C-NC	2.84	128.68	124.20
24	b	618	CLA	CHD-C4C-NC	2.84	128.68	124.20
34	E	103	HEM	C4C-CHD-C1D	2.84	126.30	122.56
32	b	627	LHG	O8-C23-C24	2.84	120.81	111.91
24	B	609	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	B	606	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	b	608	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	C	510	CLA	C1-C2-C3	-2.83	121.15	126.04
32	B	625	LHG	O8-C23-C24	2.83	120.78	111.91
24	D	403	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
24	d	403	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
24	b	605	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
27	A	412	SQD	O5-C5-C4	2.82	114.81	109.69
24	A	405	CLA	C7-C6-C5	-2.82	105.71	113.36
26	B	618	BCR	C38-C26-C27	-2.81	108.22	113.62
24	c	510	CLA	CHD-C4C-NC	2.81	128.63	124.20
24	B	606	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
24	b	608	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
24	a	405	CLA	C7-C6-C5	-2.81	105.74	113.36
24	c	503	CLA	C4A-NA-C1A	-2.80	105.44	106.71
24	B	607	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
24	b	609	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
24	b	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
27	a	412	SQD	O5-C5-C4	2.80	114.78	109.69
28	a	411	PL9	C12-C13-C14	-2.80	120.91	127.66
26	b	620	BCR	C30-C25-C26	-2.80	118.67	122.61
24	B	604	CLA	C6-C7-C8	-2.80	106.87	115.92
26	T	101	BCR	C15-C16-C17	-2.80	117.74	123.47
24	C	510	CLA	C4C-C3C-C2C	-2.79	102.82	106.90
26	b	620	BCR	C38-C26-C27	-2.79	108.25	113.62
28	A	411	PL9	C12-C13-C14	-2.79	120.93	127.66
24	C	510	CLA	CHD-C4C-NC	2.79	128.60	124.20
26	B	618	BCR	C30-C25-C26	-2.79	118.68	122.61
24	b	605	CLA	CHD-C4C-NC	2.79	128.60	124.20
31	C	522	LMG	O6-C5-C4	2.79	114.76	109.69
24	C	510	CLA	O2A-CGA-CBA	2.79	120.66	111.91
24	c	510	CLA	O2A-CGA-CBA	2.79	120.66	111.91
26	B	627	BCR	C15-C16-C17	-2.79	117.77	123.47
24	b	606	CLA	C6-C7-C8	-2.79	106.91	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	414	BCT	O3-C-O1	-2.78	112.32	119.55
31	C	501	LMG	O6-C1-O1	-2.78	103.39	109.97
24	D	404	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
24	d	404	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
33	C	519	DGD	O6D-C1D-O3G	-2.78	103.39	109.97
33	c	519	DGD	O6D-C1D-O3G	-2.78	103.39	109.97
24	B	608	CLA	C11-C12-C13	-2.78	106.94	115.92
24	c	510	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
24	D	404	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	d	404	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	C	513	CLA	O2A-CGA-CBA	2.77	120.61	111.91
24	c	513	CLA	O2A-CGA-CBA	2.77	120.61	111.91
31	c	522	LMG	O6-C5-C4	2.77	114.73	109.69
30	A	414	BCT	O3-C-O1	-2.77	112.35	119.55
28	a	411	PL9	C27-C28-C29	-2.77	120.99	127.66
24	b	610	CLA	C11-C12-C13	-2.77	106.97	115.92
24	B	607	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	b	609	CLA	CHD-C4C-NC	2.77	128.57	124.20
31	c	501	LMG	O6-C1-O1	-2.77	103.42	109.97
27	L	101	SQD	C1-C2-C3	-2.77	104.24	110.00
31	d	411	LMG	C6-C5-C4	-2.77	106.53	113.00
24	B	602	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
24	b	604	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
24	B	612	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
27	l	101	SQD	C1-C2-C3	-2.75	104.27	110.00
31	D	411	LMG	C6-C5-C4	-2.75	106.57	113.00
24	A	406	CLA	CBC-CAC-C3C	-2.75	104.86	112.43
24	a	406	CLA	CBC-CAC-C3C	-2.75	104.86	112.43
28	A	411	PL9	C27-C28-C29	-2.75	121.05	127.66
24	B	603	CLA	CHD-C4C-NC	2.74	128.53	124.20
27	a	412	SQD	O9-S-C6	2.74	110.20	106.94
26	C	516	BCR	C27-C26-C25	2.74	126.71	122.73
24	C	506	CLA	CAC-C3C-C4C	2.74	128.37	124.81
24	c	506	CLA	CAC-C3C-C4C	2.74	128.37	124.81
26	c	516	BCR	C27-C26-C25	2.74	126.71	122.73
24	D	404	CLA	O2A-CGA-CBA	2.74	120.50	111.91
24	B	608	CLA	CMC-C2C-C1C	2.73	129.20	125.04
24	D	404	CLA	CAA-C2A-C3A	-2.73	105.29	112.78
24	b	615	CLA	CHD-C4C-NC	2.73	128.51	124.20
24	d	404	CLA	O2A-CGA-CBA	2.73	120.48	111.91
24	b	612	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
24	b	616	CLA	CAA-C2A-C3A	-2.73	105.31	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	B	604	CLA	CAC-C3C-C4C	2.73	128.35	124.81
24	b	606	CLA	CAC-C3C-C4C	2.73	128.35	124.81
31	c	522	LMG	C1-C2-C3	-2.72	104.32	110.00
24	D	404	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	d	404	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	B	613	CLA	CHD-C4C-NC	2.72	128.49	124.20
24	D	404	CLA	CHD-C4C-NC	2.72	128.49	124.20
24	d	404	CLA	CHD-C4C-NC	2.72	128.49	124.20
24	d	404	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
24	b	616	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
24	B	614	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
24	B	607	CLA	CAC-C3C-C4C	2.72	128.34	124.81
27	A	412	SQD	O9-S-C6	2.72	110.17	106.94
24	B	614	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
24	C	511	CLA	O2A-CGA-CBA	2.72	120.44	111.91
28	A	411	PL9	C22-C23-C24	-2.71	121.12	127.66
24	C	502	CLA	CAA-C2A-C3A	-2.71	105.34	112.78
24	c	502	CLA	CAA-C2A-C3A	-2.71	105.34	112.78
35	H	101	RRX	C8-C7-C6	-2.71	119.58	127.20
31	C	501	LMG	C1-C2-C3	-2.71	104.34	110.00
33	C	517	DGD	CDB-CCB-CBB	-2.71	100.65	114.42
28	a	411	PL9	C22-C23-C24	-2.71	121.13	127.66
24	C	512	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
24	c	512	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
35	h	101	RRX	C8-C7-C6	-2.71	119.59	127.20
24	B	610	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
33	c	517	DGD	CDB-CCB-CBB	-2.71	100.68	114.42
24	B	610	CLA	C3B-C4B-NB	2.71	112.71	109.21
24	b	609	CLA	CAC-C3C-C4C	2.71	128.32	124.81
24	b	603	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	b	614	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
24	b	612	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	b	610	CLA	CMC-C2C-C1C	2.70	129.15	125.04
24	C	513	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
26	B	618	BCR	C24-C23-C22	-2.70	122.16	126.23
26	b	620	BCR	C24-C23-C22	-2.70	122.16	126.23
31	c	501	LMG	C1-C2-C3	-2.70	104.37	110.00
31	C	522	LMG	C1-C2-C3	-2.70	104.38	110.00
24	B	601	CLA	O2A-CGA-CBA	2.70	120.37	111.91
24	B	601	CLA	CHD-C4C-NC	2.69	128.44	124.20
24	D	404	CLA	CHB-C4A-NA	2.69	128.23	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	c	513	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
24	B	610	CLA	CHD-C4C-NC	2.68	128.43	124.20
24	c	504	CLA	O2D-CGD-CBD	2.68	116.03	111.27
33	h	102	DGD	CDB-CCB-CBB	-2.68	100.82	114.42
24	b	615	CLA	O2A-CGA-CBA	2.68	120.31	111.91
24	B	603	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
24	b	605	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
33	H	102	DGD	CDB-CCB-CBB	-2.67	100.84	114.42
24	C	512	CLA	CHD-C4C-NC	2.67	128.41	124.20
24	c	512	CLA	CHD-C4C-NC	2.67	128.41	124.20
24	C	506	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	c	506	CLA	CHD-C1D-ND	-2.67	122.00	124.45
24	b	603	CLA	CHD-C4C-NC	2.67	128.41	124.20
24	B	616	CLA	CBC-CAC-C3C	-2.67	105.07	112.43
24	b	618	CLA	CBC-CAC-C3C	-2.67	105.07	112.43
24	B	613	CLA	O2A-CGA-CBA	2.67	120.28	111.91
24	d	403	CLA	O2A-CGA-CBA	2.67	120.28	111.91
24	b	615	CLA	CMB-C2B-C3B	2.67	129.67	124.68
24	B	603	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
24	b	605	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
24	C	502	CLA	C1-C2-C3	-2.67	121.43	126.04
24	c	502	CLA	C1-C2-C3	-2.67	121.43	126.04
24	D	403	CLA	O2A-CGA-CBA	2.66	120.27	111.91
24	B	608	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
36	z	101	LMT	O5B-C5B-C4B	2.66	114.53	109.69
24	b	610	CLA	CMB-C2B-C1B	-2.66	124.38	128.46
28	D	406	PL9	O1-C4-C3	-2.66	117.79	120.72
28	d	406	PL9	O1-C4-C3	-2.66	117.79	120.72
24	C	502	CLA	CHD-C4C-NC	2.66	128.39	124.20
24	c	502	CLA	CHD-C4C-NC	2.66	128.39	124.20
25	d	402	PHO	O2D-CGD-O1D	-2.66	118.64	123.84
36	Z	101	LMT	O5B-C5B-C4B	2.65	114.51	109.69
24	B	613	CLA	CMB-C2B-C3B	2.65	129.64	124.68
25	D	402	PHO	O2D-CGD-O1D	-2.65	118.65	123.84
33	C	518	DGD	CDB-CCB-CBB	-2.65	100.96	114.42
24	C	504	CLA	O2D-CGD-CBD	2.65	115.98	111.27
24	B	614	CLA	C4-C3-C5	2.65	119.73	115.27
33	c	518	DGD	CDB-CCB-CBB	-2.65	100.98	114.42
24	D	404	CLA	CGD-CBD-CAD	-2.65	102.16	110.73
26	Y	101	BCR	C29-C30-C25	2.64	114.55	110.48
26	y	101	BCR	C29-C30-C25	2.64	114.55	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	H	101	RRX	C16-C15-C14	-2.64	118.07	123.47
36	Z	101	LMT	O5B-C5B-C6B	2.64	113.00	106.44
24	C	506	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
36	J	102	LMT	C3'-C4'-C5'	-2.63	105.54	110.24
36	j	102	LMT	C3'-C4'-C5'	-2.63	105.54	110.24
24	d	404	CLA	CGD-CBD-CAD	-2.63	102.20	110.73
25	D	402	PHO	O1D-CGD-CBD	2.63	129.12	124.74
24	a	406	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
26	c	515	BCR	C15-C16-C17	-2.63	118.08	123.47
35	h	101	RRX	C16-C15-C14	-2.63	118.09	123.47
26	C	516	BCR	C11-C10-C9	-2.63	123.56	127.31
26	c	516	BCR	C11-C10-C9	-2.63	123.56	127.31
36	z	101	LMT	O5B-C5B-C6B	2.63	112.97	106.44
26	C	515	BCR	C15-C16-C17	-2.63	118.09	123.47
24	A	405	CLA	CMD-C2D-C3D	-2.63	121.57	127.61
24	a	405	CLA	CMD-C2D-C3D	-2.63	121.57	127.61
25	d	402	PHO	O1D-CGD-CBD	2.63	129.11	124.74
24	b	614	CLA	CAA-C2A-C3A	-2.62	105.59	112.78
24	c	506	CLA	C3D-C2D-C1D	-2.62	102.25	105.83
24	B	612	CLA	CAA-C2A-C3A	-2.62	105.59	112.78
34	E	103	HEM	C4B-CHC-C1C	2.62	126.02	122.56
24	B	611	CLA	C1-C2-C3	-2.62	121.51	126.04
24	b	613	CLA	C1-C2-C3	-2.62	121.51	126.04
24	A	406	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
24	b	616	CLA	C4-C3-C5	2.62	119.68	115.27
24	b	611	CLA	CAC-C3C-C4C	2.62	128.20	124.81
24	b	614	CLA	CMA-C3A-C4A	-2.61	104.75	111.77
24	C	508	CLA	CMC-C2C-C1C	2.61	129.01	125.04
24	c	508	CLA	CMC-C2C-C1C	2.61	129.01	125.04
24	C	514	CLA	CMA-C3A-C4A	-2.61	104.76	111.77
24	c	514	CLA	CMA-C3A-C4A	-2.61	104.76	111.77
24	B	602	CLA	C1-O2A-CGA	2.61	123.28	116.44
24	b	604	CLA	C1-O2A-CGA	2.61	123.28	116.44
24	C	513	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	c	513	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	B	612	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
32	D	408	LHG	C20-C19-C18	-2.60	101.20	114.42
24	B	601	CLA	CAC-C3C-C4C	2.60	128.19	124.81
24	b	603	CLA	CAC-C3C-C4C	2.60	128.19	124.81
25	A	407	PHO	CBA-CAA-C2A	-2.60	106.20	113.81
24	C	511	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
24	c	511	CLA	CAA-C2A-C3A	-2.60	105.65	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	521	BCR	C2-C1-C6	2.60	114.48	110.48
32	d	408	LHG	C20-C19-C18	-2.60	101.23	114.42
32	D	408	LHG	C11-C10-C9	-2.60	101.24	114.42
28	D	406	PL9	C7-C3-C2	-2.59	119.89	123.30
28	d	406	PL9	C7-C3-C2	-2.59	119.89	123.30
33	c	518	DGD	C3D-C4D-C5D	-2.59	105.61	110.24
26	c	521	BCR	C2-C1-C6	2.59	114.47	110.48
32	d	408	LHG	C11-C10-C9	-2.59	101.26	114.42
24	D	401	CLA	CAA-CBA-CGA	2.59	120.83	113.25
24	d	401	CLA	CAA-CBA-CGA	2.59	120.83	113.25
28	D	406	PL9	C8-C7-C3	2.59	119.31	111.98
33	C	518	DGD	C3D-C4D-C5D	-2.59	105.62	110.24
34	e	103	HEM	C4B-CHC-C1C	2.59	125.98	122.56
24	b	618	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
24	d	401	CLA	CAC-C3C-C2C	2.59	131.96	127.53
24	B	616	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
28	d	406	PL9	C8-C7-C3	2.59	119.29	111.98
31	b	622	LMG	O7-C10-O9	-2.59	117.45	123.70
24	D	401	CLA	CAC-C3C-C2C	2.59	131.95	127.53
31	D	411	LMG	C1-C2-C3	-2.59	104.61	110.00
24	D	403	CLA	CAC-C3C-C4C	2.58	128.16	124.81
25	D	402	PHO	C1-C2-C3	-2.58	121.58	126.04
25	d	402	PHO	C1-C2-C3	-2.58	121.58	126.04
25	a	407	PHO	CBA-CAA-C2A	-2.58	106.27	113.81
24	C	512	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
24	c	512	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
31	d	411	LMG	C1-C2-C3	-2.58	104.63	110.00
31	C	520	LMG	C38-C37-C36	-2.57	101.36	114.42
24	C	504	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
31	d	411	LMG	O2-C2-C1	-2.57	103.79	110.05
26	A	409	BCR	C27-C26-C25	2.57	126.47	122.73
26	a	409	BCR	C27-C26-C25	2.57	126.47	122.73
26	Y	101	BCR	C1-C6-C5	-2.57	118.99	122.61
31	C	522	LMG	O2-C2-C1	-2.57	103.80	110.05
31	c	520	LMG	C38-C37-C36	-2.57	101.38	114.42
24	a	408	CLA	CED-O2D-CGD	2.57	121.75	115.94
31	D	411	LMG	O2-C2-C1	-2.57	103.81	110.05
31	C	522	LMG	C40-C39-C38	-2.57	101.39	114.42
24	D	404	CLA	C1-C2-C3	-2.57	121.60	126.04
24	d	404	CLA	C1-C2-C3	-2.57	121.60	126.04
31	c	522	LMG	C40-C39-C38	-2.57	101.39	114.42
24	B	609	CLA	CAC-C3C-C4C	2.57	128.14	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C4-C3-C5	2.57	119.59	115.27
24	b	618	CLA	C4-C3-C5	2.57	119.59	115.27
31	B	620	LMG	O7-C10-O9	-2.57	117.50	123.70
26	y	101	BCR	C1-C6-C5	-2.57	119.00	122.61
24	c	504	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
31	c	522	LMG	O2-C2-C1	-2.56	103.83	110.05
24	C	511	CLA	CBC-CAC-C3C	-2.56	105.38	112.43
24	c	511	CLA	CBC-CAC-C3C	-2.56	105.38	112.43
24	A	408	CLA	CED-O2D-CGD	2.56	121.72	115.94
24	C	506	CLA	CMC-C2C-C1C	2.55	128.93	125.04
27	d	407	SQD	O8-S-C6	2.55	109.81	105.74
24	b	612	CLA	C1-C2-C3	-2.55	121.63	126.04
27	D	407	SQD	O8-S-C6	2.55	109.80	105.74
24	b	614	CLA	CHB-C4A-NA	2.55	128.04	124.51
33	H	102	DGD	C3E-C4E-C5E	-2.55	105.69	110.24
33	h	102	DGD	C3E-C4E-C5E	-2.55	105.69	110.24
24	d	403	CLA	CAC-C3C-C4C	2.55	128.12	124.81
24	B	605	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
24	b	607	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
24	c	506	CLA	CMC-C2C-C1C	2.55	128.91	125.04
24	a	406	CLA	CHD-C4C-NC	2.55	128.21	124.20
24	c	507	CLA	CED-O2D-CGD	2.54	121.69	115.94
24	c	512	CLA	C4A-NA-C1A	-2.54	105.56	106.71
31	C	501	LMG	O3-C3-C2	-2.54	104.47	110.35
24	b	613	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
24	c	505	CLA	CED-O2D-CGD	2.54	121.68	115.94
24	B	610	CLA	C1-C2-C3	-2.54	121.65	126.04
24	C	505	CLA	C1-O2A-CGA	2.54	123.10	116.44
24	C	505	CLA	CED-O2D-CGD	2.54	121.67	115.94
24	B	604	CLA	CAA-C2A-C3A	-2.54	105.84	112.78
24	b	606	CLA	CAA-C2A-C3A	-2.54	105.84	112.78
24	C	511	CLA	C4C-C3C-C2C	-2.53	103.20	106.90
24	c	511	CLA	C4C-C3C-C2C	-2.53	103.20	106.90
24	c	505	CLA	C1-O2A-CGA	2.53	123.09	116.44
26	C	515	BCR	C27-C26-C25	2.53	126.41	122.73
26	c	515	BCR	C27-C26-C25	2.53	126.41	122.73
24	c	504	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
24	B	612	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	A	409	BCR	C15-C14-C13	-2.53	123.70	127.31
26	a	409	BCR	C15-C14-C13	-2.53	123.70	127.31
31	c	501	LMG	O3-C3-C2	-2.53	104.51	110.35
24	C	507	CLA	CED-O2D-CGD	2.53	121.65	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	CBC-CAC-C3C	-2.53	105.47	112.43
24	C	506	CLA	CHD-C4C-NC	2.52	128.18	124.20
24	c	506	CLA	CHD-C4C-NC	2.52	128.18	124.20
24	c	504	CLA	O2A-CGA-CBA	2.52	119.82	111.91
24	C	504	CLA	O2A-CGA-CBA	2.52	119.82	111.91
33	H	102	DGD	C6D-C5D-C4D	2.52	117.35	112.09
33	h	102	DGD	C6D-C5D-C4D	2.52	117.35	112.09
24	C	504	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
24	B	611	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
24	c	508	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
24	b	614	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
24	A	406	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	C	509	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
24	c	509	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
24	B	614	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
24	B	611	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
24	b	614	CLA	CHD-C4C-NC	2.51	128.15	124.20
24	b	616	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
24	b	617	CLA	CHD-C4C-NC	2.50	128.15	124.20
24	C	508	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
24	B	615	CLA	CHD-C4C-NC	2.50	128.15	124.20
31	C	520	LMG	C40-C39-C38	-2.50	101.73	114.42
24	A	406	CLA	CED-O2D-CGD	2.50	121.59	115.94
24	a	406	CLA	CED-O2D-CGD	2.50	121.59	115.94
35	H	101	RRX	C10-C11-C12	-2.50	115.42	123.22
35	h	101	RRX	C10-C11-C12	-2.50	115.42	123.22
27	A	412	SQD	O48-C23-O10	-2.50	117.29	123.59
24	b	610	CLA	CAC-C3C-C4C	2.50	128.05	124.81
24	c	504	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
24	b	616	CLA	CHD-C4C-NC	2.50	128.14	124.20
24	B	616	CLA	CHC-C1C-NC	2.50	127.99	124.20
24	b	618	CLA	CHC-C1C-NC	2.50	127.99	124.20
24	C	504	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
27	a	412	SQD	O48-C23-O10	-2.49	117.30	123.59
24	B	601	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
24	b	603	CLA	CBC-CAC-C3C	-2.49	105.56	112.43
24	C	505	CLA	C4A-NA-C1A	-2.49	105.59	106.71
24	c	505	CLA	C4A-NA-C1A	-2.49	105.59	106.71
24	B	614	CLA	CHD-C4C-NC	2.49	128.13	124.20
24	B	610	CLA	CMC-C2C-C1C	2.49	128.83	125.04
24	B	608	CLA	CAC-C3C-C4C	2.49	128.04	124.81
26	B	619	BCR	C27-C26-C25	2.49	126.34	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	621	BCR	C27-C26-C25	2.49	126.34	122.73
24	b	618	CLA	O2A-CGA-CBA	2.48	119.71	111.91
31	c	520	LMG	C40-C39-C38	-2.48	101.81	114.42
24	B	613	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
24	b	615	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
24	C	503	CLA	CHD-C4C-NC	2.48	128.11	124.20
24	c	503	CLA	CHD-C4C-NC	2.48	128.11	124.20
24	B	612	CLA	CHD-C4C-NC	2.48	128.11	124.20
24	c	504	CLA	C4-C3-C5	2.48	119.44	115.27
24	d	403	CLA	CMA-C3A-C2A	-2.48	103.83	113.83
24	B	612	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
24	D	403	CLA	CMA-C3A-C2A	-2.48	103.84	113.83
24	A	405	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
24	a	405	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
24	B	612	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
24	A	405	CLA	CMC-C2C-C1C	2.47	128.81	125.04
24	a	405	CLA	CMC-C2C-C1C	2.47	128.81	125.04
27	L	101	SQD	O48-C23-O10	-2.47	117.35	123.59
24	B	602	CLA	CAC-C3C-C4C	2.47	128.02	124.81
24	b	604	CLA	CAC-C3C-C4C	2.47	128.02	124.81
24	B	616	CLA	O2A-CGA-CBA	2.47	119.66	111.91
27	D	407	SQD	O48-C23-C24	2.47	119.66	111.91
24	B	611	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
24	b	613	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
26	b	619	BCR	C29-C30-C25	2.47	114.28	110.48
26	B	617	BCR	C29-C30-C25	2.47	114.28	110.48
24	C	504	CLA	C4-C3-C5	2.46	119.42	115.27
24	b	614	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
28	A	411	PL9	O2-C1-C6	2.46	124.86	120.59
28	a	411	PL9	O2-C1-C6	2.46	124.86	120.59
24	B	607	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
24	b	609	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
25	D	402	PHO	CMA-C3A-C4A	-2.46	108.99	114.38
25	d	402	PHO	CMA-C3A-C4A	-2.46	108.99	114.38
24	c	508	CLA	C1-C2-C3	-2.46	121.79	126.04
27	d	407	SQD	O48-C23-C24	2.46	119.62	111.91
24	c	505	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
24	C	502	CLA	CMC-C2C-C1C	2.46	128.78	125.04
24	B	607	CLA	O1D-CGD-CBD	-2.45	119.46	124.48
24	b	613	CLA	O2A-CGA-CBA	2.45	119.61	111.91
32	d	409	LHG	C20-C19-C18	-2.45	101.98	114.42
24	c	511	CLA	C4-C3-C5	2.45	119.39	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C4-C3-C5	2.45	119.39	115.27
24	b	604	CLA	C4-C3-C5	2.45	119.39	115.27
24	b	616	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
24	B	611	CLA	O2A-CGA-CBA	2.45	119.59	111.91
24	c	505	CLA	CMC-C2C-C1C	2.45	128.77	125.04
24	C	509	CLA	O2A-CGA-CBA	2.45	119.59	111.91
24	c	509	CLA	O2A-CGA-CBA	2.45	119.59	111.91
24	B	614	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
24	B	610	CLA	CAC-C3C-C4C	2.44	127.98	124.81
32	D	409	LHG	C20-C19-C18	-2.44	102.02	114.42
24	c	502	CLA	CMC-C2C-C1C	2.44	128.76	125.04
24	b	609	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
24	B	608	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
32	b	627	LHG	C11-C10-C9	-2.44	102.04	114.42
24	C	506	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
24	c	506	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
27	l	101	SQD	O48-C23-O10	-2.44	117.44	123.59
31	c	520	LMG	O8-C28-C29	2.44	119.56	111.91
32	d	410	LHG	O8-C23-C24	2.44	119.56	111.91
24	C	506	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
24	b	611	CLA	C1-C2-C3	-2.44	121.83	126.04
24	C	505	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
24	c	506	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
24	C	511	CLA	C4-C3-C5	2.44	119.37	115.27
24	B	604	CLA	C1-O2A-CGA	2.44	122.84	116.44
32	B	625	LHG	C11-C10-C9	-2.44	102.06	114.42
34	e	103	HEM	C4D-ND-C1D	2.43	107.59	105.07
34	E	103	HEM	C4D-ND-C1D	2.43	107.59	105.07
24	B	609	CLA	C1-C2-C3	-2.43	121.83	126.04
24	C	512	CLA	C4A-NA-C1A	-2.43	105.61	106.71
27	A	410	SQD	C1-C2-C3	-2.43	104.93	110.00
24	C	505	CLA	CMC-C2C-C1C	2.43	128.74	125.04
24	b	606	CLA	C1-O2A-CGA	2.43	122.82	116.44
31	C	520	LMG	O8-C28-C29	2.43	119.53	111.91
32	D	410	LHG	O8-C23-C24	2.43	119.53	111.91
24	a	408	CLA	OBD-CAD-C3D	-2.43	122.68	128.52
26	B	617	BCR	C38-C26-C27	-2.43	108.96	113.62
24	C	508	CLA	C1-C2-C3	-2.42	121.85	126.04
31	d	411	LMG	O6-C1-O1	-2.42	104.23	109.97
31	C	522	LMG	C38-C37-C36	-2.42	102.13	114.42
24	B	616	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
24	b	618	CLA	CAA-C2A-C3A	-2.42	106.15	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	O2A-CGA-CBA	2.42	119.50	111.91
24	b	609	CLA	O2A-CGA-CBA	2.42	119.50	111.91
31	C	501	LMG	C40-C39-C38	-2.42	102.14	114.42
31	c	501	LMG	C40-C39-C38	-2.42	102.14	114.42
24	C	505	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
24	c	505	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
24	b	612	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	B	610	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
36	M	101	LMT	C3'-C4'-C5'	-2.42	105.39	110.93
36	m	102	LMT	C3'-C4'-C5'	-2.42	105.39	110.93
26	b	619	BCR	C38-C26-C27	-2.41	108.98	113.62
31	c	522	LMG	C38-C37-C36	-2.41	102.17	114.42
26	A	409	BCR	C15-C16-C17	-2.41	118.53	123.47
24	b	612	CLA	CMC-C2C-C1C	2.41	128.71	125.04
24	B	607	CLA	CMC-C2C-C1C	2.41	128.71	125.04
24	b	609	CLA	CMC-C2C-C1C	2.41	128.71	125.04
24	b	610	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
26	a	409	BCR	C15-C16-C17	-2.41	118.54	123.47
24	A	408	CLA	OBD-CAD-C3D	-2.41	122.72	128.52
27	a	410	SQD	C1-C2-C3	-2.41	104.98	110.00
24	B	609	CLA	C1-O2A-CGA	2.41	122.76	116.44
24	c	505	CLA	CHD-C4C-NC	2.41	127.99	124.20
24	b	611	CLA	C1-O2A-CGA	2.41	122.75	116.44
33	c	518	DGD	CBB-CAB-C9B	-2.40	102.22	114.42
26	D	405	BCR	C1-C6-C5	-2.40	119.23	122.61
26	d	405	BCR	C1-C6-C5	-2.40	119.23	122.61
24	C	505	CLA	CHD-C4C-NC	2.40	127.99	124.20
24	b	603	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
24	b	604	CLA	CMA-C3A-C4A	-2.40	105.33	111.77
24	B	615	CLA	CED-O2D-CGD	2.40	121.36	115.94
24	C	514	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
24	c	514	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
33	C	517	DGD	CBB-CAB-C9B	-2.40	102.26	114.42
24	B	609	CLA	CHA-C1A-NA	-2.40	120.91	126.40
24	b	616	CLA	O2A-CGA-CBA	2.40	119.42	111.91
24	b	617	CLA	CED-O2D-CGD	2.39	121.35	115.94
24	B	606	CLA	C1D-CHD-C4C	-2.39	120.90	126.06
24	b	608	CLA	C1D-CHD-C4C	-2.39	120.90	126.06
24	B	614	CLA	O2A-CGA-CBA	2.39	119.41	111.91
31	d	411	LMG	C40-C39-C38	-2.39	102.29	114.42
33	c	517	DGD	CBB-CAB-C9B	-2.39	102.29	114.42
24	B	606	CLA	O2A-CGA-CBA	2.39	119.41	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	O2A-CGA-CBA	2.39	119.41	111.91
24	B	601	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
24	B	602	CLA	CMA-C3A-C4A	-2.39	105.35	111.77
24	b	609	CLA	CHB-C4A-NA	2.39	127.82	124.51
31	D	411	LMG	O6-C1-O1	-2.39	104.32	109.97
33	C	517	DGD	O5D-C6D-C5D	-2.39	104.63	109.05
33	c	517	DGD	O5D-C6D-C5D	-2.39	104.63	109.05
24	B	613	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
31	c	520	LMG	O3-C3-C2	-2.39	104.83	110.35
31	D	411	LMG	C40-C39-C38	-2.39	102.31	114.42
24	D	404	CLA	CMC-C2C-C1C	2.39	128.67	125.04
24	d	404	CLA	CMC-C2C-C1C	2.39	128.67	125.04
33	C	518	DGD	CBB-CAB-C9B	-2.39	102.31	114.42
24	A	408	CLA	CHD-C4C-NC	2.38	127.96	124.20
24	a	408	CLA	CHD-C4C-NC	2.38	127.96	124.20
24	A	405	CLA	CHA-C1A-NA	-2.38	120.94	126.40
24	a	405	CLA	CHA-C1A-NA	-2.38	120.94	126.40
24	B	607	CLA	CHB-C4A-NA	2.38	127.81	124.51
24	c	514	CLA	C4-C3-C5	2.38	119.28	115.27
24	B	605	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
24	b	606	CLA	CED-O2D-CGD	2.38	121.32	115.94
33	C	519	DGD	O3G-C3G-C2G	-2.38	105.16	110.90
33	c	519	DGD	O3G-C3G-C2G	-2.38	105.16	110.90
24	c	510	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	B	604	CLA	CMB-C2B-C3B	2.38	129.13	124.68
24	b	606	CLA	CMB-C2B-C3B	2.38	129.13	124.68
24	D	401	CLA	CMC-C2C-C3C	2.38	132.57	126.12
26	D	405	BCR	C2-C1-C6	2.37	114.13	110.48
26	d	405	BCR	C2-C1-C6	2.37	114.13	110.48
32	E	101	LHG	C11-C10-C9	-2.37	102.39	114.42
24	b	615	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
34	E	103	HEM	C3C-C4C-NC	-2.37	106.47	110.94
34	e	103	HEM	C3C-C4C-NC	-2.37	106.47	110.94
24	d	401	CLA	CMC-C2C-C3C	2.37	132.55	126.12
24	B	604	CLA	CED-O2D-CGD	2.37	121.29	115.94
24	B	604	CLA	C4C-C3C-C2C	-2.37	103.45	106.90
24	b	606	CLA	C4C-C3C-C2C	-2.37	103.45	106.90
24	b	611	CLA	CHA-C1A-NA	-2.37	120.98	126.40
24	B	608	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	b	607	CLA	CHC-C1C-C2C	-2.36	120.18	126.72
32	E	101	LHG	O8-C23-C24	2.36	119.33	111.91
32	e	101	LHG	O8-C23-C24	2.36	119.33	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	520	LMG	O3-C3-C2	-2.36	104.89	110.35
26	y	101	BCR	C38-C26-C27	-2.36	109.08	113.62
24	C	511	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
24	c	511	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
24	C	514	CLA	C4-C3-C5	2.36	119.24	115.27
32	e	101	LHG	C11-C10-C9	-2.36	102.45	114.42
26	B	627	BCR	C38-C26-C27	-2.36	109.08	113.62
26	T	101	BCR	C38-C26-C27	-2.36	109.08	113.62
24	B	607	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
26	a	409	BCR	C2-C1-C6	2.36	114.11	110.48
27	D	407	SQD	O48-C23-O10	-2.36	117.64	123.59
25	d	402	PHO	CBA-CAA-C2A	-2.36	106.92	113.81
24	c	514	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
26	B	617	BCR	C2-C1-C6	2.36	114.11	110.48
26	b	619	BCR	C2-C1-C6	2.36	114.11	110.48
26	D	405	BCR	C27-C26-C25	2.35	126.15	122.73
26	d	405	BCR	C27-C26-C25	2.35	126.15	122.73
24	C	514	CLA	CHD-C4C-NC	2.35	127.91	124.20
24	c	514	CLA	CHD-C4C-NC	2.35	127.91	124.20
24	C	510	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	C	516	BCR	C38-C26-C27	-2.35	109.10	113.62
26	c	516	BCR	C38-C26-C27	-2.35	109.10	113.62
24	A	408	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
24	a	408	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
24	C	509	CLA	C1-C2-C3	-2.35	121.98	126.04
24	c	509	CLA	C1-C2-C3	-2.35	121.98	126.04
26	A	409	BCR	C2-C1-C6	2.35	114.09	110.48
26	Y	101	BCR	C30-C25-C26	-2.34	119.31	122.61
36	Z	101	LMT	C3'-C4'-C5'	-2.34	105.55	110.93
24	C	514	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
28	A	411	PL9	C40-C39-C41	2.34	119.21	115.27
24	D	401	CLA	C1-C2-C3	-2.34	121.99	126.04
24	d	401	CLA	C1-C2-C3	-2.34	121.99	126.04
24	b	615	CLA	CMC-C2C-C1C	2.34	128.60	125.04
25	D	402	PHO	CBA-CAA-C2A	-2.34	106.97	113.81
24	b	609	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
26	y	101	BCR	C30-C25-C26	-2.34	119.32	122.61
24	B	612	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
24	b	617	CLA	CMC-C2C-C1C	2.34	128.59	125.04
36	z	101	LMT	C3'-C4'-C5'	-2.33	105.58	110.93
24	c	512	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
26	Y	101	BCR	C38-C26-C27	-2.33	109.14	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	401	CLA	CMA-C3A-C2A	-2.33	104.42	113.83
24	d	401	CLA	CMA-C3A-C2A	-2.33	104.42	113.83
24	C	512	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
27	d	407	SQD	O48-C23-O10	-2.33	117.71	123.59
24	b	614	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
24	b	603	CLA	C4-C3-C5	2.33	119.19	115.27
31	B	620	LMG	C40-C39-C38	-2.33	102.61	114.42
31	b	622	LMG	C40-C39-C38	-2.33	102.61	114.42
24	B	613	CLA	CMC-C2C-C1C	2.33	128.58	125.04
24	b	603	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	B	615	CLA	CMC-C2C-C1C	2.32	128.57	125.04
31	B	620	LMG	C38-C37-C36	-2.32	102.65	114.42
24	B	601	CLA	C4-C3-C5	2.32	119.17	115.27
24	B	615	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
24	b	617	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
28	a	411	PL9	C40-C39-C41	2.31	119.17	115.27
24	c	505	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
24	B	601	CLA	CMB-C2B-C3B	2.31	129.01	124.68
24	b	603	CLA	CMB-C2B-C3B	2.31	129.01	124.68
27	D	407	SQD	O47-C7-O49	-2.31	118.11	123.70
24	B	614	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
24	b	616	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
31	b	622	LMG	C38-C37-C36	-2.31	102.69	114.42
24	C	512	CLA	CAC-C3C-C4C	2.31	127.81	124.81
24	C	507	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
24	a	406	CLA	CAC-C3C-C4C	2.31	127.80	124.81
32	e	101	LHG	C27-C26-C25	-2.31	102.72	114.42
24	B	602	CLA	CHB-C4A-NA	2.31	127.70	124.51
24	c	507	CLA	CMB-C2B-C1B	-2.30	124.92	128.46
32	E	101	LHG	C20-C19-C18	-2.30	102.73	114.42
32	E	101	LHG	C27-C26-C25	-2.30	102.73	114.42
32	e	101	LHG	C20-C19-C18	-2.30	102.74	114.42
33	H	102	DGD	C3D-C4D-C5D	-2.30	106.14	110.24
27	a	410	SQD	O47-C7-O49	-2.30	118.14	123.70
24	B	615	CLA	CAC-C3C-C4C	2.30	127.80	124.81
24	b	617	CLA	CAC-C3C-C4C	2.30	127.80	124.81
24	b	616	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	A	406	CLA	O2A-CGA-CBA	2.30	119.13	111.91
28	a	411	PL9	C37-C38-C39	-2.30	122.12	127.66
24	B	601	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	B	613	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
27	A	410	SQD	O47-C7-O49	-2.30	118.15	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
24	a	406	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
28	A	411	PL9	C37-C38-C39	-2.30	122.13	127.66
24	b	603	CLA	O1D-CGD-CBD	-2.30	119.79	124.48
24	C	505	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
24	b	615	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
32	B	625	LHG	C27-C26-C25	-2.29	102.78	114.42
24	c	511	CLA	CED-O2D-CGD	2.29	121.12	115.94
24	A	406	CLA	CAC-C3C-C4C	2.29	127.79	124.81
27	d	407	SQD	O47-C7-O49	-2.29	118.16	123.70
24	b	606	CLA	CHD-C4C-NC	2.29	127.82	124.20
24	b	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	b	615	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
24	b	611	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
24	B	613	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
24	C	511	CLA	CED-O2D-CGD	2.29	121.12	115.94
24	B	604	CLA	CHD-C4C-NC	2.29	127.81	124.20
27	L	101	SQD	O48-C23-C24	2.29	119.09	111.91
33	h	102	DGD	C3D-C4D-C5D	-2.29	106.16	110.24
27	A	412	SQD	C46-C45-C44	-2.29	106.38	111.79
24	C	503	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
24	a	406	CLA	O2A-CGA-CBA	2.28	119.08	111.91
26	B	627	BCR	C27-C26-C25	2.28	126.05	122.73
26	T	101	BCR	C27-C26-C25	2.28	126.05	122.73
24	d	403	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
32	b	627	LHG	C27-C26-C25	-2.28	102.83	114.42
24	c	512	CLA	CAC-C3C-C4C	2.28	127.77	124.81
24	C	509	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
24	c	509	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
24	b	616	CLA	C4A-NA-C1A	-2.28	105.68	106.71
24	c	503	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
24	b	604	CLA	CHB-C4A-NA	2.28	127.66	124.51
24	B	615	CLA	C1-O2A-CGA	2.28	122.42	116.44
24	B	614	CLA	CHB-C4A-NA	2.28	127.66	124.51
33	C	519	DGD	C3G-C2G-C1G	-2.28	106.41	111.79
33	c	519	DGD	C3G-C2G-C1G	-2.28	106.41	111.79
26	D	405	BCR	C24-C23-C22	-2.27	122.80	126.23
26	d	405	BCR	C24-C23-C22	-2.27	122.80	126.23
28	A	411	PL9	O2-C1-C2	-2.27	116.58	121.78
28	a	411	PL9	O2-C1-C2	-2.27	116.58	121.78
24	A	408	CLA	CAC-C3C-C4C	2.27	127.76	124.81
24	a	408	CLA	CAC-C3C-C4C	2.27	127.76	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	411	LMG	C38-C37-C36	-2.27	102.90	114.42
27	l	101	SQD	O48-C23-C24	2.27	119.03	111.91
28	d	406	PL9	C22-C23-C24	-2.27	122.20	127.66
24	c	508	CLA	C4-C3-C5	2.27	119.09	115.27
24	d	403	CLA	CHD-C4C-NC	2.27	127.78	124.20
24	D	403	CLA	CHD-C4C-NC	2.27	127.78	124.20
24	B	607	CLA	C2A-C1A-CHA	-2.27	119.90	123.86
33	C	519	DGD	CBB-CAB-C9B	-2.27	102.92	114.42
27	A	410	SQD	O48-C23-C24	2.27	119.02	111.91
27	a	410	SQD	O48-C23-C24	2.27	119.02	111.91
24	B	601	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
27	a	412	SQD	C46-C45-C44	-2.26	106.43	111.79
24	B	606	CLA	CED-O2D-CGD	2.26	121.06	115.94
24	b	608	CLA	CED-O2D-CGD	2.26	121.06	115.94
24	B	604	CLA	C4A-NA-C1A	-2.26	105.69	106.71
31	d	411	LMG	C38-C37-C36	-2.26	102.93	114.42
24	b	608	CLA	CHB-C4A-NA	2.26	127.64	124.51
33	c	519	DGD	CBB-CAB-C9B	-2.26	102.93	114.42
24	C	508	CLA	C4-C3-C5	2.26	119.08	115.27
24	D	403	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
24	C	504	CLA	CHA-C1A-NA	-2.26	121.22	126.40
24	c	504	CLA	CHA-C1A-NA	-2.26	121.22	126.40
24	b	617	CLA	C1-O2A-CGA	2.26	122.37	116.44
24	c	514	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
24	B	605	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
24	b	607	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
24	B	610	CLA	C4-C3-C5	2.25	119.06	115.27
25	d	402	PHO	OBD-CAD-CBD	-2.25	122.52	125.82
24	D	401	CLA	CED-O2D-CGD	2.25	121.03	115.94
24	d	401	CLA	CED-O2D-CGD	2.25	121.03	115.94
32	d	408	LHG	C18-C17-C16	-2.25	103.01	114.42
24	d	401	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
24	b	609	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
28	D	406	PL9	C22-C23-C24	-2.25	122.25	127.66
24	C	514	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
32	D	408	LHG	C18-C17-C16	-2.25	103.03	114.42
26	c	516	BCR	C30-C25-C26	-2.24	119.45	122.61
25	A	407	PHO	C1B-NB-C4B	2.24	111.70	107.09
24	C	511	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
24	c	511	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
25	a	407	PHO	C1B-NB-C4B	2.24	111.69	107.09
24	b	608	CLA	CAC-C3C-C4C	2.24	127.72	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
33	h	102	DGD	O6D-C1D-O3G	-2.24	104.67	109.97
33	C	517	DGD	C1E-O6E-C5E	2.24	118.08	113.69
24	B	606	CLA	CHB-C4A-NA	2.24	127.60	124.51
33	H	102	DGD	O6D-C1D-O3G	-2.24	104.68	109.97
35	H	101	RRX	C33-C5-C4	2.23	117.91	113.62
24	b	618	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	c	512	CLA	CHA-C1A-NA	-2.23	121.28	126.40
28	A	411	PL9	C21-C19-C18	-2.23	116.60	121.12
36	I	102	LMT	O5B-C5B-C4B	2.23	113.75	109.69
24	c	508	CLA	CHB-C4A-NA	2.23	127.60	124.51
26	C	515	BCR	C33-C5-C6	-2.23	122.02	124.53
26	c	515	BCR	C33-C5-C6	-2.23	122.02	124.53
35	h	101	RRX	C33-C5-C4	2.23	117.90	113.62
24	A	408	CLA	C4A-NA-C1A	-2.23	105.70	106.71
24	B	602	CLA	CED-O2D-CGD	2.23	120.98	115.94
31	C	501	LMG	C38-C37-C36	-2.23	103.10	114.42
31	c	501	LMG	C38-C37-C36	-2.23	103.10	114.42
26	B	627	BCR	C1-C6-C5	-2.23	119.47	122.61
26	T	101	BCR	C1-C6-C5	-2.23	119.47	122.61
24	b	612	CLA	C4-C3-C5	2.23	119.02	115.27
24	B	606	CLA	CAC-C3C-C4C	2.23	127.70	124.81
28	D	406	PL9	C36-C37-C38	-2.23	104.57	111.88
28	d	406	PL9	C36-C37-C38	-2.23	104.57	111.88
24	B	610	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
26	C	516	BCR	C30-C25-C26	-2.23	119.48	122.61
24	D	401	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
24	A	406	CLA	C1-C2-C3	-2.22	122.20	126.04
24	C	508	CLA	CHB-C4A-NA	2.22	127.58	124.51
28	a	411	PL9	C21-C19-C18	-2.22	116.63	121.12
24	B	615	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	b	617	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	b	611	CLA	C4-C3-C5	2.22	119.00	115.27
24	C	512	CLA	CHA-C1A-NA	-2.22	121.32	126.40
24	c	507	CLA	CHD-C4C-NC	2.21	127.69	124.20
28	D	406	PL9	C31-C32-C33	-2.21	104.61	111.88
28	d	406	PL9	C31-C32-C33	-2.21	104.61	111.88
24	B	609	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
24	C	514	CLA	C1-C2-C3	-2.21	122.22	126.04
24	c	514	CLA	C1-C2-C3	-2.21	122.22	126.04
24	B	605	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
24	b	609	CLA	C1B-CHB-C4A	-2.21	125.74	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	c	514	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	B	612	CLA	CHA-C1A-NA	-2.21	121.34	126.40
24	a	406	CLA	C1-C2-C3	-2.21	122.22	126.04
24	D	404	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
24	C	505	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
26	C	521	BCR	C29-C30-C25	2.21	113.88	110.48
26	c	521	BCR	C29-C30-C25	2.21	113.88	110.48
24	a	408	CLA	C4A-NA-C1A	-2.21	105.71	106.71
24	C	510	CLA	CAC-C3C-C4C	2.21	127.67	124.81
25	D	402	PHO	OBD-CAD-CBD	-2.21	122.59	125.82
24	B	616	CLA	CHB-C4A-NA	2.21	127.56	124.51
36	i	102	LMT	O5B-C5B-C4B	2.20	113.70	109.69
33	c	517	DGD	C1E-O6E-C5E	2.20	118.02	113.69
24	C	505	CLA	CAC-C3C-C4C	2.20	127.67	124.81
24	b	611	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
25	A	407	PHO	C1-C2-C3	-2.20	122.23	126.04
25	a	407	PHO	C1-C2-C3	-2.20	122.23	126.04
24	d	404	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
24	b	606	CLA	C4A-NA-C1A	-2.20	105.72	106.71
24	B	607	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
24	b	604	CLA	CED-O2D-CGD	2.20	120.92	115.94
24	d	403	CLA	OBD-CAD-C3D	-2.20	123.22	128.52
24	C	508	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
31	c	520	LMG	O8-C28-O10	-2.19	118.05	123.59
24	C	507	CLA	CHD-C4C-NC	2.19	127.66	124.20
24	A	405	CLA	CAA-C2A-C1A	-2.19	104.79	111.97
24	b	614	CLA	CHA-C1A-NA	-2.19	121.37	126.40
28	a	411	PL9	C20-C19-C21	2.19	118.96	115.27
24	C	514	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
24	b	607	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	a	405	CLA	CAA-C2A-C1A	-2.19	104.79	111.97
24	d	403	CLA	CED-O2D-CGD	2.19	120.89	115.94
24	B	609	CLA	C4-C3-C5	2.19	118.95	115.27
28	A	411	PL9	C20-C19-C21	2.19	118.95	115.27
24	c	514	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
31	C	520	LMG	O8-C28-O10	-2.19	118.07	123.59
24	B	614	CLA	C4A-NA-C1A	-2.19	105.72	106.71
24	B	616	CLA	O1D-CGD-CBD	-2.18	120.01	124.48
24	b	618	CLA	O1D-CGD-CBD	-2.18	120.01	124.48
26	Y	101	BCR	C33-C5-C6	-2.18	122.08	124.53
26	y	101	BCR	C33-C5-C6	-2.18	122.08	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
24	b	613	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
24	d	404	CLA	CBC-CAC-C3C	-2.18	106.41	112.43
24	b	618	CLA	C1-C2-C3	-2.18	122.27	126.04
32	d	408	LHG	C27-C26-C25	-2.18	103.34	114.42
24	C	507	CLA	CHC-C1C-NC	2.18	127.51	124.20
24	c	507	CLA	CHC-C1C-NC	2.18	127.51	124.20
24	B	611	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
24	d	401	CLA	CHB-C4A-NA	2.18	127.53	124.51
24	C	511	CLA	CHD-C4C-NC	2.18	127.64	124.20
24	c	511	CLA	CHD-C4C-NC	2.18	127.64	124.20
24	C	510	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
24	A	408	CLA	CMB-C2B-C3B	2.18	128.75	124.68
24	a	408	CLA	CMB-C2B-C3B	2.18	128.75	124.68
26	A	409	BCR	C20-C21-C22	-2.18	124.20	127.31
24	B	616	CLA	C1-C2-C3	-2.18	122.28	126.04
24	B	606	CLA	CAC-C3C-C2C	2.18	131.25	127.53
24	C	507	CLA	C4-C3-C5	2.18	118.93	115.27
24	c	507	CLA	C4-C3-C5	2.18	118.93	115.27
32	D	408	LHG	C27-C26-C25	-2.18	103.38	114.42
24	C	508	CLA	CHA-C1A-NA	-2.17	121.42	126.40
24	c	508	CLA	CHA-C1A-NA	-2.17	121.42	126.40
32	d	409	LHG	C11-C10-C9	-2.17	103.39	114.42
24	c	508	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	B	609	CLA	CMA-C3A-C4A	-2.17	105.93	111.77
24	C	508	CLA	O2A-CGA-CBA	2.17	118.73	111.91
24	D	403	CLA	CED-O2D-CGD	2.17	120.85	115.94
24	c	508	CLA	O2A-CGA-CBA	2.17	118.72	111.91
24	D	404	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
24	b	610	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
24	D	403	CLA	OBD-CAD-C3D	-2.17	123.30	128.52
24	b	607	CLA	C3B-C4B-NB	2.17	112.02	109.21
25	A	407	PHO	CMC-C2C-C3C	2.17	129.03	124.94
24	B	608	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
32	D	409	LHG	O8-C23-C24	2.17	118.71	111.91
24	B	604	CLA	C11-C10-C8	-2.17	108.91	115.92
24	b	606	CLA	C11-C10-C8	-2.17	108.91	115.92
24	c	510	CLA	CAC-C3C-C4C	2.17	127.62	124.81
24	A	408	CLA	C1-O2A-CGA	2.17	122.13	116.44
24	C	506	CLA	C4-C3-C5	2.17	118.92	115.27
24	c	506	CLA	C4-C3-C5	2.17	118.92	115.27
26	B	627	BCR	C28-C27-C26	-2.17	110.21	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
24	b	609	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
32	D	410	LHG	C11-C10-C9	-2.17	103.43	114.42
32	d	410	LHG	C11-C10-C9	-2.17	103.43	114.42
33	C	518	DGD	C9B-C8B-C7B	-2.17	103.43	114.42
24	b	608	CLA	CAC-C3C-C2C	2.16	131.23	127.53
24	c	510	CLA	CBC-CAC-C3C	-2.16	106.47	112.43
24	c	510	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
24	b	617	CLA	C4-C3-C5	2.16	118.91	115.27
32	D	409	LHG	C11-C10-C9	-2.16	103.45	114.42
27	a	412	SQD	O48-C23-C24	2.16	118.68	111.91
25	a	407	PHO	CMC-C2C-C3C	2.16	129.01	124.94
32	d	409	LHG	O8-C23-C24	2.16	118.68	111.91
31	B	620	LMG	O2-C2-C1	-2.16	104.81	110.05
24	B	612	CLA	C1-C2-C3	-2.16	122.31	126.04
24	b	614	CLA	C1-C2-C3	-2.16	122.31	126.04
33	c	518	DGD	C9B-C8B-C7B	-2.16	103.48	114.42
27	D	407	SQD	O5-C1-C2	-2.16	105.79	110.35
24	c	505	CLA	CAC-C3C-C4C	2.15	127.61	124.81
27	A	412	SQD	O48-C23-C24	2.15	118.67	111.91
24	d	403	CLA	CAA-CBA-CGA	-2.15	106.96	113.25
24	C	512	CLA	CHB-C4A-NA	2.15	127.49	124.51
31	B	620	LMG	O8-C28-O10	-2.15	118.17	123.59
24	B	615	CLA	C4-C3-C5	2.15	118.89	115.27
26	T	101	BCR	C28-C27-C26	-2.15	110.24	114.08
26	B	627	BCR	C15-C14-C13	-2.15	124.24	127.31
31	b	622	LMG	O8-C28-O10	-2.15	118.17	123.59
24	C	510	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
31	b	622	LMG	O2-C2-C1	-2.15	104.83	110.05
24	c	512	CLA	CHB-C4A-NA	2.14	127.48	124.51
26	a	409	BCR	C20-C21-C22	-2.14	124.25	127.31
24	C	508	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
24	c	508	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
24	D	403	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
24	a	408	CLA	C1-O2A-CGA	2.14	122.06	116.44
26	T	101	BCR	C15-C14-C13	-2.14	124.26	127.31
24	D	403	CLA	CHA-C1A-NA	-2.14	121.50	126.40
27	d	407	SQD	O5-C1-C2	-2.14	105.82	110.35
24	B	602	CLA	O2A-CGA-CBA	2.14	118.62	111.91
24	b	604	CLA	O2A-CGA-CBA	2.14	118.62	111.91
33	C	519	DGD	C6D-O5D-C1E	2.14	117.91	113.74
33	c	519	DGD	C6D-O5D-C1E	2.14	117.91	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	CHA-C1A-NA	-2.13	121.51	126.40
24	D	401	CLA	CHB-C4A-NA	2.13	127.46	124.51
24	C	513	CLA	CHD-C4C-NC	2.13	127.57	124.20
24	c	513	CLA	CHD-C4C-NC	2.13	127.57	124.20
24	a	406	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
24	b	611	CLA	CMA-C3A-C2A	-2.13	105.23	113.83
24	A	406	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	B	612	CLA	CMA-C3A-C2A	-2.13	105.24	113.83
26	B	618	BCR	C35-C13-C14	-2.13	119.94	122.92
26	b	620	BCR	C35-C13-C14	-2.13	119.94	122.92
26	C	521	BCR	C27-C26-C25	2.13	125.82	122.73
26	c	521	BCR	C27-C26-C25	2.13	125.82	122.73
26	c	521	BCR	C15-C16-C17	-2.13	119.11	123.47
24	A	405	CLA	O2A-CGA-CBA	2.13	118.59	111.91
24	B	605	CLA	C3B-C4B-NB	2.13	111.96	109.21
26	C	521	BCR	C38-C26-C27	-2.13	109.53	113.62
26	c	521	BCR	C38-C26-C27	-2.13	109.53	113.62
24	C	510	CLA	CAA-C2A-C1A	2.12	118.94	111.97
24	c	510	CLA	CAA-C2A-C1A	2.12	118.94	111.97
28	A	411	PL9	C31-C32-C33	-2.12	104.90	111.88
26	C	515	BCR	C30-C25-C26	-2.12	119.62	122.61
26	c	515	BCR	C30-C25-C26	-2.12	119.62	122.61
28	a	411	PL9	C31-C32-C33	-2.12	104.90	111.88
24	b	614	CLA	CMA-C3A-C2A	-2.12	105.26	113.83
33	c	518	DGD	CAB-C9B-C8B	-2.12	103.64	114.42
32	B	625	LHG	C29-C28-C27	-2.12	103.65	114.42
33	C	518	DGD	CAB-C9B-C8B	-2.12	103.66	114.42
26	b	620	BCR	C15-C14-C13	-2.12	124.29	127.31
26	C	521	BCR	C15-C16-C17	-2.12	119.14	123.47
24	b	610	CLA	CBC-CAC-C3C	-2.11	106.60	112.43
24	a	405	CLA	O2A-CGA-CBA	2.11	118.54	111.91
24	b	618	CLA	CMA-C3A-C4A	-2.11	106.09	111.77
24	D	403	CLA	C1-C2-C3	-2.11	122.39	126.04
24	d	403	CLA	C1-C2-C3	-2.11	122.39	126.04
24	C	506	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
24	C	512	CLA	C6-C7-C8	-2.11	109.09	115.92
24	B	616	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
26	B	618	BCR	C40-C30-C25	2.11	113.72	110.30
26	b	620	BCR	C40-C30-C25	2.11	113.72	110.30
24	b	614	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
31	b	622	LMG	O6-C1-O1	-2.11	104.98	109.97
24	B	608	CLA	CBC-CAC-C3C	-2.11	106.62	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	405	BCR	C4-C5-C6	2.11	125.79	122.73
26	d	405	BCR	C4-C5-C6	2.11	125.79	122.73
24	c	506	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
26	C	515	BCR	C38-C26-C27	-2.11	109.57	113.62
26	c	515	BCR	C38-C26-C27	-2.11	109.57	113.62
31	B	620	LMG	O6-C1-O1	-2.11	104.98	109.97
24	A	406	CLA	CMB-C2B-C3B	2.11	128.62	124.68
24	a	406	CLA	CMB-C2B-C3B	2.11	128.62	124.68
24	D	403	CLA	C4-C3-C5	2.11	118.81	115.27
24	d	403	CLA	C4-C3-C5	2.11	118.81	115.27
28	A	411	PL9	C32-C33-C34	-2.11	122.59	127.66
28	a	411	PL9	C32-C33-C34	-2.11	122.59	127.66
24	B	604	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
32	b	627	LHG	C29-C28-C27	-2.10	103.74	114.42
24	B	615	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
24	b	617	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
24	B	612	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
24	b	610	CLA	CED-O2D-CGD	2.10	120.69	115.94
24	c	503	CLA	C4-C3-C5	2.10	118.81	115.27
24	C	512	CLA	O2A-CGA-CBA	2.10	118.50	111.91
24	B	608	CLA	CED-O2D-CGD	2.10	120.68	115.94
35	h	101	RRX	C30-C29-C28	-2.10	108.91	113.64
28	D	406	PL9	O2-C1-C2	-2.10	116.97	121.78
28	d	406	PL9	O2-C1-C2	-2.10	116.97	121.78
24	c	512	CLA	C6-C7-C8	-2.10	109.14	115.92
24	c	507	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
24	d	403	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
26	B	618	BCR	C15-C14-C13	-2.10	124.32	127.31
24	b	606	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
24	A	406	CLA	CAA-CBA-CGA	2.09	119.37	113.25
26	Y	101	BCR	C28-C27-C26	-2.09	110.34	114.08
24	c	514	CLA	C11-C10-C8	-2.09	109.16	115.92
24	D	403	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
24	C	514	CLA	C11-C10-C8	-2.09	109.16	115.92
31	C	522	LMG	O7-C10-O9	-2.09	118.65	123.70
24	B	605	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
24	b	607	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
26	Y	101	BCR	C4-C5-C6	2.09	125.76	122.73
26	y	101	BCR	C4-C5-C6	2.09	125.76	122.73
24	C	513	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
31	c	522	LMG	O7-C10-O9	-2.08	118.66	123.70
33	C	518	DGD	CEB-CDB-CCB	-2.08	103.84	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C28-C27-C26	-2.08	110.36	114.08
35	H	101	RRX	C30-C29-C28	-2.08	108.94	113.64
24	C	507	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
24	C	503	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
24	c	503	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
24	C	510	CLA	CED-O2D-CGD	2.08	120.64	115.94
24	c	510	CLA	CED-O2D-CGD	2.08	120.64	115.94
24	c	513	CLA	CBC-CAC-C3C	-2.08	106.69	112.43
33	c	518	DGD	CEB-CDB-CCB	-2.08	103.86	114.42
24	a	406	CLA	CAA-CBA-CGA	2.08	119.33	113.25
24	c	512	CLA	O2A-CGA-CBA	2.08	118.43	111.91
24	B	615	CLA	CMB-C2B-C3B	2.08	128.57	124.68
24	b	617	CLA	CMB-C2B-C3B	2.08	128.57	124.68
24	C	514	CLA	CMA-C3A-C2A	-2.08	105.45	113.83
24	c	514	CLA	CMA-C3A-C2A	-2.08	105.45	113.83
26	D	405	BCR	C38-C26-C27	-2.07	109.63	113.62
24	a	408	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
24	C	503	CLA	C4-C3-C5	2.07	118.76	115.27
26	C	515	BCR	C35-C13-C14	-2.07	120.02	122.92
24	C	512	CLA	CMC-C2C-C1C	2.07	128.19	125.04
24	c	512	CLA	CMC-C2C-C1C	2.07	128.19	125.04
32	D	409	LHG	C27-C26-C25	-2.07	103.92	114.42
24	b	616	CLA	CMA-C3A-C2A	-2.07	105.48	113.83
24	B	606	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	b	608	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
32	d	409	LHG	C27-C26-C25	-2.07	103.94	114.42
31	B	620	LMG	O3-C3-C2	-2.07	105.57	110.35
31	b	622	LMG	O3-C3-C2	-2.07	105.57	110.35
24	d	404	CLA	C6-C7-C8	-2.07	109.24	115.92
24	D	404	CLA	C6-C7-C8	-2.06	109.25	115.92
32	D	410	LHG	C27-C26-C25	-2.06	103.95	114.42
32	d	410	LHG	C27-C26-C25	-2.06	103.95	114.42
32	e	101	LHG	C18-C17-C16	-2.06	103.95	114.42
26	d	405	BCR	C38-C26-C27	-2.06	109.65	113.62
24	B	614	CLA	CMA-C3A-C2A	-2.06	105.51	113.83
24	A	408	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
32	E	101	LHG	C18-C17-C16	-2.06	103.97	114.42
28	D	406	PL9	C27-C28-C29	-2.06	122.70	127.66
28	d	406	PL9	C27-C28-C29	-2.06	122.70	127.66
24	B	608	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
33	C	519	DGD	O2D-C2D-C1D	-2.06	105.05	110.05
33	c	519	DGD	O2D-C2D-C1D	-2.06	105.05	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
24	C	510	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
24	c	510	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
24	a	406	CLA	CMC-C2C-C1C	2.05	128.17	125.04
26	d	405	BCR	C30-C25-C26	-2.05	119.72	122.61
24	b	610	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	a	409	BCR	C38-C26-C27	-2.04	109.69	113.62
31	c	501	LMG	O7-C10-O9	-2.04	118.77	123.70
36	j	102	LMT	C1'-C2'-C3'	2.04	114.25	110.00
27	a	412	SQD	C3-C4-C5	2.04	113.88	110.24
24	C	507	CLA	CHB-C4A-NA	2.04	127.33	124.51
24	c	507	CLA	CHB-C4A-NA	2.04	127.33	124.51
24	A	406	CLA	CMC-C2C-C1C	2.04	128.14	125.04
24	b	608	CLA	CMA-C3A-C2A	-2.03	105.62	113.83
24	B	610	CLA	CHB-C4A-NA	2.03	127.33	124.51
24	c	510	CLA	O2A-C1-C2	2.03	113.98	108.64
26	c	515	BCR	C35-C13-C14	-2.03	120.07	122.92
26	B	617	BCR	C27-C26-C25	2.03	125.68	122.73
27	L	101	SQD	C26-C25-C24	-2.03	105.89	113.19
24	C	510	CLA	O2A-C1-C2	2.03	113.97	108.64
24	B	605	CLA	C11-C10-C8	-2.03	109.35	115.92
24	B	608	CLA	C4-C3-C5	2.03	118.69	115.27
24	b	610	CLA	C4-C3-C5	2.03	118.69	115.27
26	A	409	BCR	C38-C26-C27	-2.03	109.71	113.62
24	C	509	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	c	509	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	d	401	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
24	B	603	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
26	D	405	BCR	C30-C25-C26	-2.03	119.76	122.61
24	B	608	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	B	606	CLA	CMA-C3A-C2A	-2.03	105.65	113.83
24	B	609	CLA	CMA-C3A-C2A	-2.03	105.65	113.83
24	B	604	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
27	l	101	SQD	C26-C25-C24	-2.03	105.90	113.19
32	d	409	LHG	C29-C28-C27	-2.03	104.14	114.42
24	c	511	CLA	CMC-C2C-C1C	2.03	128.12	125.04
24	b	605	CLA	CBC-CAC-C3C	-2.03	106.85	112.43
32	D	410	LHG	C20-C19-C18	-2.03	104.14	114.42
32	d	410	LHG	C20-C19-C18	-2.03	104.14	114.42
24	b	607	CLA	C11-C10-C8	-2.02	109.38	115.92
36	J	102	LMT	C1'-C2'-C3'	2.02	114.21	110.00
31	C	501	LMG	O7-C10-O9	-2.02	118.81	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	C	509	CLA	C4A-NA-C1A	-2.02	105.80	106.71
24	c	509	CLA	C4A-NA-C1A	-2.02	105.80	106.71
24	b	603	CLA	C6-C7-C8	-2.02	109.39	115.92
24	b	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
24	A	405	CLA	CHC-C1C-NC	2.02	127.27	124.20
24	c	509	CLA	C7-C6-C5	-2.02	107.88	113.36
35	h	101	RRX	C35-C13-C12	2.02	121.26	118.08
27	A	412	SQD	C3-C4-C5	2.02	113.84	110.24
26	b	619	BCR	C27-C26-C25	2.02	125.66	122.73
24	D	401	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
24	B	612	CLA	CED-O2D-CGD	2.01	120.49	115.94
24	B	601	CLA	C6-C7-C8	-2.01	109.41	115.92
24	B	610	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
32	D	409	LHG	C29-C28-C27	-2.01	104.22	114.42
25	A	407	PHO	OBD-CAD-CBD	-2.01	122.87	125.82
25	a	407	PHO	OBD-CAD-CBD	-2.01	122.87	125.82
24	b	604	CLA	CMA-C3A-C2A	-2.01	105.72	113.83
24	C	506	CLA	CHA-C1A-NA	-2.01	121.80	126.40
24	c	506	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	c	520	LMG	C1-C2-C3	-2.01	105.81	110.00
24	B	602	CLA	CMA-C3A-C2A	-2.01	105.73	113.83
24	B	604	CLA	CHA-C1A-NA	-2.01	121.80	126.40
24	b	614	CLA	CED-O2D-CGD	2.01	120.47	115.94
24	C	511	CLA	CMC-C2C-C1C	2.00	128.09	125.04
24	a	405	CLA	CHC-C1C-NC	2.00	127.24	124.20
24	c	510	CLA	C4-C3-C5	2.00	118.64	115.27
28	D	406	PL9	C20-C19-C21	2.00	118.64	115.27
28	d	406	PL9	C20-C19-C21	2.00	118.64	115.27
24	C	509	CLA	C7-C6-C5	-2.00	107.92	113.36
35	H	101	RRX	C35-C13-C12	2.00	121.23	118.08
31	c	520	LMG	O2-C2-C1	-2.00	105.19	110.05

All (61) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	408	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	609	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	C	502	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	D	401	CLA	ND
24	D	403	CLA	ND
24	D	404	CLA	ND
24	a	405	CLA	ND
24	a	408	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	609	CLA	ND
24	b	611	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	618	CLA	ND
24	c	502	CLA	ND

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Mol	Chain	Res	Type	Atom
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	d	401	CLA	ND
24	d	403	CLA	ND
24	d	404	CLA	ND

All (1464) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	603	CLA	C2-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6
24	B	605	CLA	C2-C3-C5-C6
24	B	605	CLA	C4-C3-C5-C6
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CHA-CBD-CGD-O1D
24	B	614	CLA	CHA-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CBD-CGD-O2D-CED
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	C2-C1-O2A-CGA
24	b	605	CLA	C2-C3-C5-C6
24	b	605	CLA	C4-C3-C5-C6
24	b	607	CLA	C2-C3-C5-C6
24	b	607	CLA	C4-C3-C5-C6
24	b	608	CLA	CHA-CBD-CGD-O1D
24	b	608	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CHA-CBD-CGD-O1D
24	b	616	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	503	CLA	CHA-CBD-CGD-O1D
24	c	503	CLA	CHA-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CBD-CGD-O2D-CED
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	C2-C1-O2A-CGA
26	A	409	BCR	C7-C8-C9-C34
26	B	618	BCR	C7-C8-C9-C34
26	B	619	BCR	C7-C8-C9-C10
26	B	619	BCR	C7-C8-C9-C34
26	B	619	BCR	C21-C22-C23-C24
26	B	619	BCR	C37-C22-C23-C24
26	B	627	BCR	C1-C6-C7-C8
26	B	627	BCR	C5-C6-C7-C8
26	B	627	BCR	C21-C22-C23-C24
26	B	627	BCR	C37-C22-C23-C24
26	C	521	BCR	C11-C10-C9-C8
26	C	521	BCR	C11-C10-C9-C34
26	D	405	BCR	C7-C8-C9-C34
26	D	405	BCR	C21-C22-C23-C24
26	D	405	BCR	C37-C22-C23-C24
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	T	101	BCR	C21-C22-C23-C24
26	T	101	BCR	C37-C22-C23-C24
26	Y	101	BCR	C5-C6-C7-C8
26	Y	101	BCR	C7-C8-C9-C34
26	Y	101	BCR	C20-C21-C22-C37
26	Y	101	BCR	C37-C22-C23-C24
26	a	409	BCR	C7-C8-C9-C34
26	b	620	BCR	C7-C8-C9-C34
26	b	621	BCR	C7-C8-C9-C10
26	b	621	BCR	C7-C8-C9-C34
26	b	621	BCR	C21-C22-C23-C24
26	b	621	BCR	C37-C22-C23-C24
26	c	521	BCR	C11-C10-C9-C8
26	c	521	BCR	C11-C10-C9-C34
26	d	405	BCR	C7-C8-C9-C34
26	d	405	BCR	C21-C22-C23-C24
26	d	405	BCR	C37-C22-C23-C24
26	y	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	y	101	BCR	C7-C8-C9-C34
26	y	101	BCR	C20-C21-C22-C37
26	y	101	BCR	C37-C22-C23-C24
27	A	412	SQD	C5-C6-S-O7
27	D	407	SQD	O49-C7-O47-C45
27	D	407	SQD	C24-C23-O48-C46
27	a	412	SQD	C5-C6-S-O7
27	d	407	SQD	O49-C7-O47-C45
27	d	407	SQD	C24-C23-O48-C46
28	A	411	PL9	C12-C13-C14-C15
28	A	411	PL9	C12-C13-C14-C16
28	A	411	PL9	C20-C19-C21-C22
28	A	411	PL9	C22-C23-C24-C25
28	A	411	PL9	C22-C23-C24-C26
28	A	411	PL9	C27-C28-C29-C31
28	D	406	PL9	C32-C33-C34-C35
28	a	411	PL9	C12-C13-C14-C15
28	a	411	PL9	C12-C13-C14-C16
28	a	411	PL9	C20-C19-C21-C22
28	a	411	PL9	C22-C23-C24-C25
28	a	411	PL9	C22-C23-C24-C26
28	a	411	PL9	C27-C28-C29-C31
28	d	406	PL9	C32-C33-C34-C35
31	C	501	LMG	O9-C10-O7-C8
31	c	501	LMG	O9-C10-O7-C8
32	B	625	LHG	C4-O6-P-O5
32	D	410	LHG	C4-O6-P-O4
32	E	101	LHG	O1-C1-C2-C3
32	E	101	LHG	C3-O3-P-O4
32	E	101	LHG	C3-O3-P-O5
32	b	627	LHG	C4-O6-P-O5
32	d	410	LHG	C4-O6-P-O4
32	e	101	LHG	O1-C1-C2-C3
32	e	101	LHG	C3-O3-P-O4
32	e	101	LHG	C3-O3-P-O5
35	H	101	RRX	C9-C10-C11-C12
35	h	101	RRX	C9-C10-C11-C12
36	Z	101	LMT	C2-C1-O1'-C1'
36	z	101	LMT	C2-C1-O1'-C1'
27	L	101	SQD	O10-C23-O48-C46
27	l	101	SQD	O10-C23-O48-C46
24	C	504	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	c	504	CLA	O1D-CGD-O2D-CED
24	D	404	CLA	CBD-CGD-O2D-CED
24	d	404	CLA	CBD-CGD-O2D-CED
36	I	102	LMT	C3'-C4'-O1B-C1B
36	i	102	LMT	C3'-C4'-O1B-C1B
27	D	407	SQD	O10-C23-O48-C46
27	d	407	SQD	O10-C23-O48-C46
24	A	408	CLA	C3-C5-C6-C7
24	B	601	CLA	C3-C5-C6-C7
24	B	604	CLA	C3-C5-C6-C7
24	B	614	CLA	C3-C5-C6-C7
24	C	514	CLA	C3-C5-C6-C7
24	a	408	CLA	C3-C5-C6-C7
24	b	603	CLA	C3-C5-C6-C7
24	b	606	CLA	C3-C5-C6-C7
24	b	616	CLA	C3-C5-C6-C7
24	c	514	CLA	C3-C5-C6-C7
27	D	407	SQD	C8-C7-O47-C45
27	d	407	SQD	C8-C7-O47-C45
36	I	102	LMT	C4'-C5'-C6'-O6'
36	i	102	LMT	C4'-C5'-C6'-O6'
24	B	606	CLA	C2A-CAA-CBA-CGA
24	b	608	CLA	C2A-CAA-CBA-CGA
27	L	101	SQD	C24-C23-O48-C46
27	l	101	SQD	C24-C23-O48-C46
31	C	522	LMG	C29-C28-O8-C9
31	c	522	LMG	C29-C28-O8-C9
28	A	411	PL9	C27-C28-C29-C30
28	a	411	PL9	C27-C28-C29-C30
32	D	409	LHG	O2-C2-C3-O3
32	d	409	LHG	O2-C2-C3-O3
24	C	510	CLA	CBA-CGA-O2A-C1
24	c	510	CLA	CBA-CGA-O2A-C1
24	B	606	CLA	CBD-CGD-O2D-CED
24	b	608	CLA	CBD-CGD-O2D-CED
36	I	102	LMT	O5'-C5'-C6'-O6'
36	i	102	LMT	O5'-C5'-C6'-O6'
24	C	510	CLA	O1A-CGA-O2A-C1
24	c	510	CLA	O1A-CGA-O2A-C1
28	D	406	PL9	C47-C48-C49-C50
28	d	406	PL9	C47-C48-C49-C50
24	A	408	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	614	CLA	C4-C3-C5-C6
24	a	408	CLA	C4-C3-C5-C6
24	b	616	CLA	C4-C3-C5-C6
24	A	408	CLA	C2-C3-C5-C6
24	B	614	CLA	C2-C3-C5-C6
24	a	408	CLA	C2-C3-C5-C6
24	b	616	CLA	C2-C3-C5-C6
28	D	406	PL9	C33-C34-C36-C37
28	d	406	PL9	C33-C34-C36-C37
36	I	102	LMT	O5B-C5B-C6B-O6B
36	J	102	LMT	O5'-C5'-C6'-O6'
36	i	102	LMT	O5B-C5B-C6B-O6B
36	j	102	LMT	O5'-C5'-C6'-O6'
31	C	522	LMG	O10-C28-O8-C9
31	c	522	LMG	O10-C28-O8-C9
28	A	411	PL9	C24-C26-C27-C28
28	D	406	PL9	C44-C46-C47-C48
28	a	411	PL9	C24-C26-C27-C28
28	d	406	PL9	C44-C46-C47-C48
36	J	102	LMT	C4'-C5'-C6'-O6'
36	j	102	LMT	C4'-C5'-C6'-O6'
24	C	507	CLA	CBD-CGD-O2D-CED
24	c	507	CLA	CBD-CGD-O2D-CED
32	D	408	LHG	C23-C24-C25-C26
32	d	408	LHG	C23-C24-C25-C26
36	I	102	LMT	C4B-C5B-C6B-O6B
36	i	102	LMT	C4B-C5B-C6B-O6B
36	M	101	LMT	O5'-C5'-C6'-O6'
36	m	102	LMT	O5'-C5'-C6'-O6'
31	C	522	LMG	C10-C11-C12-C13
31	c	522	LMG	C10-C11-C12-C13
27	A	412	SQD	O6-C44-C45-O47
27	a	412	SQD	O6-C44-C45-O47
31	B	620	LMG	O6-C5-C6-O5
31	b	622	LMG	O6-C5-C6-O5
26	B	627	BCR	C7-C8-C9-C34
26	T	101	BCR	C7-C8-C9-C34
26	B	627	BCR	C7-C8-C9-C10
26	T	101	BCR	C7-C8-C9-C10
31	c	522	LMG	O6-C5-C6-O5
32	E	101	LHG	C7-C8-C9-C10
32	e	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	C	522	LMG	O6-C5-C6-O5
24	B	607	CLA	C3-C5-C6-C7
24	b	609	CLA	C3-C5-C6-C7
24	B	616	CLA	C15-C16-C17-C18
24	b	618	CLA	C15-C16-C17-C18
27	A	410	SQD	C7-C8-C9-C10
27	D	407	SQD	C23-C24-C25-C26
27	a	410	SQD	C7-C8-C9-C10
27	d	407	SQD	C23-C24-C25-C26
24	C	504	CLA	C15-C16-C17-C18
24	C	507	CLA	C10-C11-C12-C13
24	C	513	CLA	C13-C15-C16-C17
24	c	504	CLA	C15-C16-C17-C18
24	c	507	CLA	C10-C11-C12-C13
24	c	513	CLA	C13-C15-C16-C17
28	A	411	PL9	C37-C38-C39-C40
28	a	411	PL9	C37-C38-C39-C40
31	C	520	LMG	O6-C5-C6-O5
24	A	406	CLA	C13-C15-C16-C17
24	B	604	CLA	C13-C15-C16-C17
24	C	508	CLA	C5-C6-C7-C8
24	a	406	CLA	C13-C15-C16-C17
24	b	606	CLA	C13-C15-C16-C17
24	b	616	CLA	C10-C11-C12-C13
24	c	508	CLA	C5-C6-C7-C8
24	D	404	CLA	O1D-CGD-O2D-CED
24	d	404	CLA	O1D-CGD-O2D-CED
31	c	520	LMG	O6-C5-C6-O5
31	C	522	LMG	C11-C10-O7-C8
24	B	601	CLA	C5-C6-C7-C8
24	b	603	CLA	C5-C6-C7-C8
24	B	611	CLA	C12-C13-C15-C16
24	B	613	CLA	C11-C10-C8-C7
24	D	403	CLA	C12-C13-C15-C16
24	b	613	CLA	C12-C13-C15-C16
24	b	615	CLA	C11-C10-C8-C7
24	d	403	CLA	C12-C13-C15-C16
24	B	614	CLA	C10-C11-C12-C13
24	C	513	CLA	C8-C10-C11-C12
27	D	407	SQD	O5-C1-O6-C44
27	d	407	SQD	O5-C1-O6-C44
33	C	518	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
24	c	513	CLA	C8-C10-C11-C12
31	C	501	LMG	C28-C29-C30-C31
31	c	501	LMG	C28-C29-C30-C31
24	A	405	CLA	C15-C16-C17-C18
24	a	405	CLA	C15-C16-C17-C18
31	C	520	LMG	C4-C5-C6-O5
31	c	520	LMG	C4-C5-C6-O5
24	B	608	CLA	C13-C15-C16-C17
24	b	610	CLA	C13-C15-C16-C17
24	B	614	CLA	CBD-CGD-O2D-CED
24	b	616	CLA	CBD-CGD-O2D-CED
31	c	522	LMG	C11-C10-O7-C8
32	D	409	LHG	C4-O6-P-O3
32	E	101	LHG	C3-O3-P-O6
32	d	409	LHG	C4-O6-P-O3
32	e	101	LHG	C3-O3-P-O6
24	C	513	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	CBA-CGA-O2A-C1
27	D	407	SQD	C7-C8-C9-C10
27	d	407	SQD	C7-C8-C9-C10
31	C	522	LMG	O9-C10-O7-C8
31	c	522	LMG	O9-C10-O7-C8
24	B	603	CLA	C10-C11-C12-C13
24	b	605	CLA	C10-C11-C12-C13
24	C	502	CLA	C2A-CAA-CBA-CGA
24	C	508	CLA	C2A-CAA-CBA-CGA
24	c	502	CLA	C2A-CAA-CBA-CGA
24	c	508	CLA	C2A-CAA-CBA-CGA
24	A	408	CLA	C16-C17-C18-C19
24	a	408	CLA	C16-C17-C18-C19
24	B	616	CLA	C3-C5-C6-C7
24	b	618	CLA	C3-C5-C6-C7
31	C	501	LMG	C11-C10-O7-C8
31	c	501	LMG	C11-C10-O7-C8
24	B	616	CLA	C5-C6-C7-C8
24	b	618	CLA	C5-C6-C7-C8
26	A	409	BCR	C20-C21-C22-C37
26	B	617	BCR	C35-C13-C14-C15
26	B	617	BCR	C20-C21-C22-C37
26	B	618	BCR	C16-C17-C18-C36
26	B	619	BCR	C20-C21-C22-C37
26	C	515	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
26	C	515	BCR	C35-C13-C14-C15
26	C	516	BCR	C11-C10-C9-C34
26	C	516	BCR	C16-C17-C18-C36
26	C	516	BCR	C20-C21-C22-C37
26	C	521	BCR	C35-C13-C14-C15
26	a	409	BCR	C20-C21-C22-C37
26	b	619	BCR	C35-C13-C14-C15
26	b	619	BCR	C20-C21-C22-C37
26	b	620	BCR	C16-C17-C18-C36
26	b	621	BCR	C20-C21-C22-C37
26	c	515	BCR	C11-C10-C9-C34
26	c	515	BCR	C35-C13-C14-C15
26	c	516	BCR	C11-C10-C9-C34
26	c	516	BCR	C16-C17-C18-C36
26	c	516	BCR	C20-C21-C22-C37
26	c	521	BCR	C35-C13-C14-C15
27	A	412	SQD	C12-C13-C14-C15
27	a	412	SQD	C12-C13-C14-C15
31	D	411	LMG	C14-C15-C16-C17
31	d	411	LMG	C14-C15-C16-C17
32	D	409	LHG	C32-C33-C34-C35
32	d	409	LHG	C32-C33-C34-C35
33	C	518	DGD	C4A-C5A-C6A-C7A
33	c	518	DGD	C4A-C5A-C6A-C7A
24	C	507	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C19
27	L	101	SQD	C29-C30-C31-C32
27	l	101	SQD	C29-C30-C31-C32
32	D	410	LHG	C31-C32-C33-C34
32	d	410	LHG	C31-C32-C33-C34
33	C	517	DGD	CCA-CDA-CEA-CFA
33	c	517	DGD	CCA-CDA-CEA-CFA
33	C	518	DGD	C8A-C9A-CAA-CBA
33	C	518	DGD	CAA-CBA-CCA-CDA
33	c	518	DGD	C8A-C9A-CAA-CBA
33	c	518	DGD	CAA-CBA-CCA-CDA
27	A	410	SQD	C13-C14-C15-C16
27	a	410	SQD	C13-C14-C15-C16
32	E	101	LHG	C32-C33-C34-C35
32	e	101	LHG	C32-C33-C34-C35
36	J	102	LMT	C11-C10-C9-C8
36	j	102	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	C	522	LMG	C17-C18-C19-C20
31	c	522	LMG	C17-C18-C19-C20
33	c	517	DGD	C6A-C7A-C8A-C9A
26	B	627	BCR	C20-C21-C22-C23
26	C	516	BCR	C16-C17-C18-C19
26	T	101	BCR	C20-C21-C22-C23
26	c	516	BCR	C16-C17-C18-C19
33	C	518	DGD	C2E-C1E-O5D-C6D
33	c	518	DGD	C2E-C1E-O5D-C6D
36	Z	101	LMT	C2'-C1'-O1'-C1
36	z	101	LMT	C2'-C1'-O1'-C1
31	B	620	LMG	C32-C33-C34-C35
31	C	522	LMG	C34-C35-C36-C37
31	b	622	LMG	C32-C33-C34-C35
31	c	520	LMG	C31-C32-C33-C34
31	c	522	LMG	C34-C35-C36-C37
32	D	410	LHG	C15-C16-C17-C18
33	C	517	DGD	C6A-C7A-C8A-C9A
33	C	518	DGD	C3B-C4B-C5B-C6B
33	c	518	DGD	C3B-C4B-C5B-C6B
24	B	610	CLA	C16-C17-C18-C19
24	B	615	CLA	C16-C17-C18-C19
24	C	507	CLA	C16-C17-C18-C20
24	b	612	CLA	C16-C17-C18-C19
24	b	617	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C20
27	A	410	SQD	C34-C35-C36-C37
27	a	410	SQD	C34-C35-C36-C37
31	C	520	LMG	C31-C32-C33-C34
31	C	522	LMG	C39-C40-C41-C42
31	D	411	LMG	C30-C31-C32-C33
31	d	411	LMG	C30-C31-C32-C33
32	d	410	LHG	C15-C16-C17-C18
24	B	603	CLA	C11-C10-C8-C9
24	B	605	CLA	C11-C12-C13-C14
24	B	611	CLA	C14-C13-C15-C16
24	B	613	CLA	C11-C10-C8-C9
24	b	605	CLA	C11-C10-C8-C9
24	b	607	CLA	C11-C12-C13-C14
24	b	613	CLA	C14-C13-C15-C16
24	b	615	CLA	C11-C10-C8-C9
31	B	620	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	C	501	LMG	C12-C13-C14-C15
31	D	411	LMG	C18-C19-C20-C21
31	b	622	LMG	C30-C31-C32-C33
31	c	501	LMG	C12-C13-C14-C15
31	c	522	LMG	C39-C40-C41-C42
31	d	411	LMG	C18-C19-C20-C21
32	B	625	LHG	C33-C34-C35-C36
32	E	101	LHG	C24-C25-C26-C27
32	b	627	LHG	C33-C34-C35-C36
32	e	101	LHG	C24-C25-C26-C27
36	J	102	LMT	C5-C6-C7-C8
36	j	102	LMT	C5-C6-C7-C8
31	B	620	LMG	C29-C30-C31-C32
31	C	522	LMG	C18-C19-C20-C21
31	b	622	LMG	C29-C30-C31-C32
31	c	522	LMG	C18-C19-C20-C21
33	C	517	DGD	CAA-CBA-CCA-CDA
33	c	517	DGD	CAA-CBA-CCA-CDA
32	D	410	LHG	O1-C1-C2-C3
32	d	410	LHG	O1-C1-C2-C3
27	A	410	SQD	C17-C18-C19-C20
27	a	410	SQD	C17-C18-C19-C20
27	a	412	SQD	C31-C32-C33-C34
32	B	625	LHG	C32-C33-C34-C35
33	C	518	DGD	C9A-CAA-CBA-CCA
33	c	518	DGD	C9A-CAA-CBA-CCA
27	L	101	SQD	C23-C24-C25-C26
27	l	101	SQD	C23-C24-C25-C26
32	b	627	LHG	C7-C8-C9-C10
27	A	412	SQD	C31-C32-C33-C34
27	a	412	SQD	C26-C27-C28-C29
31	C	520	LMG	C16-C17-C18-C19
31	D	411	LMG	C35-C36-C37-C38
31	c	520	LMG	C16-C17-C18-C19
31	d	411	LMG	C35-C36-C37-C38
32	D	408	LHG	C17-C18-C19-C20
32	D	408	LHG	C27-C28-C29-C30
32	E	101	LHG	C16-C17-C18-C19
32	b	627	LHG	C32-C33-C34-C35
32	d	408	LHG	C17-C18-C19-C20
32	d	408	LHG	C27-C28-C29-C30
32	e	101	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	C	518	DGD	C6B-C7B-C8B-C9B
33	H	102	DGD	C7A-C8A-C9A-CAA
33	c	517	DGD	C4B-C5B-C6B-C7B
33	c	518	DGD	C6B-C7B-C8B-C9B
33	h	102	DGD	C7A-C8A-C9A-CAA
36	Z	101	LMT	C7-C8-C9-C10
31	C	520	LMG	O6-C1-O1-C7
31	c	520	LMG	O6-C1-O1-C7
33	c	518	DGD	O6E-C1E-O5D-C6D
36	Z	101	LMT	O5'-C1'-O1'-C1
36	z	101	LMT	O5'-C1'-O1'-C1
27	A	410	SQD	C14-C15-C16-C17
27	A	412	SQD	C26-C27-C28-C29
27	D	407	SQD	C30-C31-C32-C33
27	L	101	SQD	C30-C31-C32-C33
27	a	410	SQD	C14-C15-C16-C17
27	l	101	SQD	C30-C31-C32-C33
33	C	517	DGD	C4B-C5B-C6B-C7B
36	z	101	LMT	C7-C8-C9-C10
27	A	412	SQD	C24-C25-C26-C27
27	L	101	SQD	C25-C26-C27-C28
27	a	412	SQD	C24-C25-C26-C27
27	d	407	SQD	C30-C31-C32-C33
27	l	101	SQD	C25-C26-C27-C28
31	C	522	LMG	C16-C17-C18-C19
31	D	411	LMG	C13-C14-C15-C16
31	c	522	LMG	C16-C17-C18-C19
31	d	411	LMG	C13-C14-C15-C16
32	D	408	LHG	C33-C34-C35-C36
32	e	101	LHG	C18-C19-C20-C21
33	C	517	DGD	C2B-C3B-C4B-C5B
33	c	517	DGD	C2B-C3B-C4B-C5B
32	B	625	LHG	C7-C8-C9-C10
27	A	412	SQD	C29-C30-C31-C32
27	a	412	SQD	C29-C30-C31-C32
32	E	101	LHG	C18-C19-C20-C21
32	d	408	LHG	C33-C34-C35-C36
24	B	601	CLA	CBA-CGA-O2A-C1
24	b	603	CLA	CBA-CGA-O2A-C1
36	I	102	LMT	C2-C1-O1'-C1'
36	i	102	LMT	C2-C1-O1'-C1'
31	C	520	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	D	411	LMG	C32-C33-C34-C35
31	c	520	LMG	C12-C13-C14-C15
31	d	411	LMG	C32-C33-C34-C35
32	B	625	LHG	C13-C14-C15-C16
32	b	627	LHG	C13-C14-C15-C16
33	h	102	DGD	C5B-C6B-C7B-C8B
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	513	CLA	O1A-CGA-O2A-C1
24	A	408	CLA	C16-C17-C18-C20
24	a	408	CLA	C16-C17-C18-C20
32	D	408	LHG	C29-C30-C31-C32
32	D	409	LHG	C14-C15-C16-C17
32	E	101	LHG	C17-C18-C19-C20
32	d	408	LHG	C29-C30-C31-C32
32	d	409	LHG	C14-C15-C16-C17
32	e	101	LHG	C17-C18-C19-C20
33	H	102	DGD	C5B-C6B-C7B-C8B
33	C	519	DGD	CBA-CCA-CDA-CEA
33	c	519	DGD	CBA-CCA-CDA-CEA
31	C	520	LMG	C32-C33-C34-C35
31	c	520	LMG	C32-C33-C34-C35
28	D	406	PL9	C13-C14-C16-C17
28	d	406	PL9	C13-C14-C16-C17
33	C	519	DGD	C5A-C6A-C7A-C8A
33	H	102	DGD	CBA-CCA-CDA-CEA
33	c	519	DGD	C5A-C6A-C7A-C8A
32	E	101	LHG	O1-C1-C2-O2
32	e	101	LHG	O1-C1-C2-O2
27	L	101	SQD	C12-C13-C14-C15
27	l	101	SQD	C12-C13-C14-C15
33	c	518	DGD	C6A-C7A-C8A-C9A
33	h	102	DGD	CBA-CCA-CDA-CEA
24	B	610	CLA	C16-C17-C18-C20
24	b	612	CLA	C16-C17-C18-C20
33	C	518	DGD	C6A-C7A-C8A-C9A
33	H	102	DGD	CCA-CDA-CEA-CFA
27	d	407	SQD	C34-C35-C36-C37
33	h	102	DGD	CCA-CDA-CEA-CFA
27	A	410	SQD	C12-C13-C14-C15
27	D	407	SQD	C34-C35-C36-C37
27	a	410	SQD	C12-C13-C14-C15
31	B	620	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
31	B	620	LMG	C38-C39-C40-C41
31	b	622	LMG	C31-C32-C33-C34
31	b	622	LMG	C38-C39-C40-C41
27	L	101	SQD	C11-C10-C9-C8
27	l	101	SQD	C11-C10-C9-C8
33	H	102	DGD	C7B-C8B-C9B-CAB
33	h	102	DGD	C7B-C8B-C9B-CAB
24	B	613	CLA	C8-C10-C11-C12
24	b	615	CLA	C8-C10-C11-C12
27	A	410	SQD	C30-C31-C32-C33
27	a	410	SQD	C30-C31-C32-C33
33	C	519	DGD	C7B-C8B-C9B-CAB
33	c	519	DGD	C7B-C8B-C9B-CAB
26	B	617	BCR	C1-C6-C7-C8
26	B	617	BCR	C5-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	Y	101	BCR	C1-C6-C7-C8
26	b	619	BCR	C1-C6-C7-C8
26	b	619	BCR	C5-C6-C7-C8
26	c	515	BCR	C1-C6-C7-C8
26	c	515	BCR	C5-C6-C7-C8
26	y	101	BCR	C1-C6-C7-C8
31	C	501	LMG	C18-C19-C20-C21
31	c	501	LMG	C18-C19-C20-C21
32	B	625	LHG	C16-C17-C18-C19
32	b	627	LHG	C16-C17-C18-C19
24	A	408	CLA	C5-C6-C7-C8
24	a	408	CLA	C5-C6-C7-C8
31	C	501	LMG	C39-C40-C41-C42
31	c	501	LMG	C39-C40-C41-C42
24	B	609	CLA	C4-C3-C5-C6
24	b	611	CLA	C4-C3-C5-C6
24	B	603	CLA	C11-C10-C8-C7
24	B	605	CLA	C11-C12-C13-C15
24	B	609	CLA	C2-C3-C5-C6
24	C	507	CLA	C11-C12-C13-C15
24	D	404	CLA	C11-C10-C8-C7
24	b	605	CLA	C11-C10-C8-C7
24	b	607	CLA	C11-C12-C13-C15
24	b	611	CLA	C2-C3-C5-C6
24	c	507	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	d	404	CLA	C11-C10-C8-C7
24	B	601	CLA	O1A-CGA-O2A-C1
24	b	603	CLA	O1A-CGA-O2A-C1
24	B	610	CLA	C13-C15-C16-C17
26	C	521	BCR	C19-C20-C21-C22
26	c	521	BCR	C19-C20-C21-C22
24	D	404	CLA	CBA-CGA-O2A-C1
24	d	404	CLA	CBA-CGA-O2A-C1
24	b	612	CLA	C13-C15-C16-C17
27	L	101	SQD	C31-C32-C33-C34
27	l	101	SQD	C31-C32-C33-C34
31	c	522	LMG	C31-C32-C33-C34
32	B	625	LHG	C34-C35-C36-C37
32	b	627	LHG	C34-C35-C36-C37
31	B	620	LMG	C15-C16-C17-C18
31	C	522	LMG	C31-C32-C33-C34
31	b	622	LMG	C15-C16-C17-C18
31	D	411	LMG	C17-C18-C19-C20
31	d	411	LMG	C17-C18-C19-C20
28	A	411	PL9	C32-C33-C34-C35
28	a	411	PL9	C32-C33-C34-C35
31	C	501	LMG	C19-C20-C21-C22
31	c	501	LMG	C19-C20-C21-C22
24	C	514	CLA	CBD-CGD-O2D-CED
24	c	514	CLA	CBD-CGD-O2D-CED
24	C	514	CLA	C16-C17-C18-C19
33	C	518	DGD	O6D-C1D-O3G-C3G
33	C	519	DGD	O6D-C1D-O3G-C3G
33	c	518	DGD	O6D-C1D-O3G-C3G
33	c	519	DGD	O6D-C1D-O3G-C3G
27	A	410	SQD	C33-C34-C35-C36
27	a	410	SQD	C33-C34-C35-C36
32	D	410	LHG	C16-C17-C18-C19
32	d	410	LHG	C16-C17-C18-C19
31	C	501	LMG	C13-C14-C15-C16
31	c	501	LMG	C13-C14-C15-C16
33	C	518	DGD	CCA-CDA-CEA-CFA
33	c	518	DGD	CCA-CDA-CEA-CFA
31	C	520	LMG	C2-C1-O1-C7
31	c	520	LMG	C2-C1-O1-C7
27	A	412	SQD	C13-C14-C15-C16
27	a	412	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	c	514	CLA	C16-C17-C18-C19
31	C	522	LMG	C38-C39-C40-C41
32	E	101	LHG	C15-C16-C17-C18
32	e	101	LHG	C15-C16-C17-C18
33	C	518	DGD	CBB-CCB-CDB-CEB
24	C	508	CLA	C4-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
31	c	522	LMG	C38-C39-C40-C41
33	c	518	DGD	CBB-CCB-CDB-CEB
24	C	507	CLA	C11-C12-C13-C14
24	D	404	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C12-C13-C14
24	d	404	CLA	C11-C10-C8-C9
28	D	406	PL9	C47-C48-C49-C51
28	d	406	PL9	C47-C48-C49-C51
32	D	410	LHG	C10-C11-C12-C13
32	d	410	LHG	C10-C11-C12-C13
33	C	518	DGD	C8B-C9B-CAB-CBB
33	c	518	DGD	C8B-C9B-CAB-CBB
31	D	411	LMG	O6-C5-C6-O5
31	d	411	LMG	O6-C5-C6-O5
24	A	406	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C1A-C2A-CAA-CBA
24	C	507	CLA	C1A-C2A-CAA-CBA
24	C	512	CLA	C1A-C2A-CAA-CBA
24	C	514	CLA	C1A-C2A-CAA-CBA
24	D	401	CLA	C1A-C2A-CAA-CBA
24	a	406	CLA	C1A-C2A-CAA-CBA
24	c	502	CLA	C1A-C2A-CAA-CBA
24	c	507	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
24	c	514	CLA	C1A-C2A-CAA-CBA
24	d	401	CLA	C1A-C2A-CAA-CBA
27	A	412	SQD	C11-C12-C13-C14
27	a	412	SQD	C11-C12-C13-C14
27	d	407	SQD	C11-C10-C9-C8
32	D	408	LHG	C7-C8-C9-C10
32	d	408	LHG	C7-C8-C9-C10
31	B	620	LMG	C4-C5-C6-O5
31	b	622	LMG	C4-C5-C6-O5
36	M	101	LMT	C4'-C5'-C6'-O6'
36	m	102	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
27	D	407	SQD	C11-C10-C9-C8
32	D	410	LHG	C12-C13-C14-C15
32	d	410	LHG	C12-C13-C14-C15
24	C	505	CLA	C15-C16-C17-C18
24	c	505	CLA	C15-C16-C17-C18
27	L	101	SQD	C13-C14-C15-C16
27	l	101	SQD	C13-C14-C15-C16
32	D	408	LHG	C11-C12-C13-C14
32	d	408	LHG	C11-C12-C13-C14
24	B	615	CLA	C16-C17-C18-C20
24	b	617	CLA	C16-C17-C18-C20
27	A	410	SQD	C31-C32-C33-C34
36	z	101	LMT	O5B-C5B-C6B-O6B
27	a	410	SQD	C31-C32-C33-C34
33	C	518	DGD	C2B-C3B-C4B-C5B
33	c	518	DGD	C2B-C3B-C4B-C5B
24	B	606	CLA	O1D-CGD-O2D-CED
24	b	608	CLA	O1D-CGD-O2D-CED
31	C	501	LMG	C36-C37-C38-C39
31	c	501	LMG	C36-C37-C38-C39
32	D	410	LHG	C28-C29-C30-C31
36	Z	101	LMT	O1'-C1-C2-C3
36	z	101	LMT	O1'-C1-C2-C3
36	Z	101	LMT	O5B-C5B-C6B-O6B
32	d	410	LHG	C28-C29-C30-C31
24	C	510	CLA	C8-C10-C11-C12
24	c	510	CLA	C8-C10-C11-C12
24	B	604	CLA	O1A-CGA-O2A-C1
24	D	404	CLA	O1A-CGA-O2A-C1
24	a	408	CLA	O1A-CGA-O2A-C1
24	d	404	CLA	O1A-CGA-O2A-C1
32	D	410	LHG	C29-C30-C31-C32
32	d	410	LHG	C29-C30-C31-C32
24	C	512	CLA	C3-C5-C6-C7
24	c	512	CLA	C3-C5-C6-C7
31	C	520	LMG	O1-C7-C8-C9
31	C	522	LMG	O1-C7-C8-C9
31	C	522	LMG	C40-C41-C42-C43
31	c	520	LMG	O1-C7-C8-C9
31	c	522	LMG	O1-C7-C8-C9
27	A	410	SQD	C29-C30-C31-C32
27	a	410	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
24	b	606	CLA	O1A-CGA-O2A-C1
33	C	518	DGD	C5D-C6D-O5D-C1E
33	c	518	DGD	C5D-C6D-O5D-C1E
31	c	522	LMG	C40-C41-C42-C43
27	A	410	SQD	C32-C33-C34-C35
27	a	410	SQD	C32-C33-C34-C35
31	c	501	LMG	C17-C18-C19-C20
24	A	408	CLA	O1A-CGA-O2A-C1
31	C	501	LMG	C17-C18-C19-C20
31	C	501	LMG	C30-C31-C32-C33
31	c	501	LMG	C30-C31-C32-C33
31	d	411	LMG	C39-C40-C41-C42
31	D	411	LMG	C39-C40-C41-C42
24	a	408	CLA	CBA-CGA-O2A-C1
32	B	625	LHG	C30-C31-C32-C33
32	b	627	LHG	C30-C31-C32-C33
32	D	410	LHG	C32-C33-C34-C35
32	d	410	LHG	C32-C33-C34-C35
26	B	617	BCR	C11-C10-C9-C34
26	b	619	BCR	C11-C10-C9-C34
33	C	517	DGD	O6E-C5E-C6E-O5E
33	c	517	DGD	O6E-C5E-C6E-O5E
31	B	620	LMG	C37-C38-C39-C40
31	b	622	LMG	C37-C38-C39-C40
31	c	522	LMG	C4-C5-C6-O5
24	A	408	CLA	CBA-CGA-O2A-C1
24	B	604	CLA	CBA-CGA-O2A-C1
24	b	606	CLA	CBA-CGA-O2A-C1
36	I	102	LMT	C3-C4-C5-C6
36	i	102	LMT	C3-C4-C5-C6
36	I	102	LMT	C2-C3-C4-C5
36	i	102	LMT	C2-C3-C4-C5
24	B	616	CLA	C10-C11-C12-C13
24	b	618	CLA	C10-C11-C12-C13
24	B	613	CLA	C2-C1-O2A-CGA
24	B	614	CLA	C2-C1-O2A-CGA
24	b	615	CLA	C2-C1-O2A-CGA
24	b	616	CLA	C2-C1-O2A-CGA
24	C	507	CLA	O1D-CGD-O2D-CED
24	c	507	CLA	O1D-CGD-O2D-CED
27	L	101	SQD	C10-C11-C12-C13
32	B	625	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	b	627	LHG	C14-C15-C16-C17
31	C	522	LMG	C4-C5-C6-O5
27	l	101	SQD	C10-C11-C12-C13
31	D	411	LMG	C37-C38-C39-C40
27	A	410	SQD	C11-C12-C13-C14
27	D	407	SQD	C10-C11-C12-C13
27	d	407	SQD	C10-C11-C12-C13
31	d	411	LMG	C37-C38-C39-C40
27	a	410	SQD	C11-C12-C13-C14
31	C	520	LMG	C40-C41-C42-C43
31	c	520	LMG	C40-C41-C42-C43
26	B	619	BCR	C11-C10-C9-C8
26	b	621	BCR	C11-C10-C9-C8
24	d	401	CLA	C2C-C3C-CAC-CBC
27	A	412	SQD	C27-C28-C29-C30
24	D	401	CLA	C2C-C3C-CAC-CBC
27	a	412	SQD	C27-C28-C29-C30
24	A	406	CLA	C6-C7-C8-C10
24	A	408	CLA	C11-C10-C8-C7
24	B	614	CLA	C11-C12-C13-C15
24	C	505	CLA	C12-C13-C15-C16
24	D	404	CLA	C6-C7-C8-C10
24	a	406	CLA	C6-C7-C8-C10
24	a	408	CLA	C11-C10-C8-C7
24	b	616	CLA	C11-C12-C13-C15
24	c	505	CLA	C12-C13-C15-C16
24	d	404	CLA	C6-C7-C8-C10
24	A	406	CLA	C6-C7-C8-C9
24	A	408	CLA	C11-C10-C8-C9
24	B	614	CLA	C11-C12-C13-C14
24	C	505	CLA	C14-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C9
24	C	513	CLA	C11-C10-C8-C9
24	D	403	CLA	C14-C13-C15-C16
24	D	404	CLA	C6-C7-C8-C9
24	a	406	CLA	C6-C7-C8-C9
24	a	408	CLA	C11-C10-C8-C9
24	b	616	CLA	C11-C12-C13-C14
24	c	505	CLA	C14-C13-C15-C16
24	c	507	CLA	C11-C10-C8-C9
24	c	513	CLA	C11-C10-C8-C9
24	d	403	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	d	404	CLA	C6-C7-C8-C9
33	C	519	DGD	CAB-CBB-CCB-CDB
33	c	519	DGD	CAB-CBB-CCB-CDB
24	B	613	CLA	C13-C15-C16-C17
24	D	404	CLA	C8-C10-C11-C12
24	b	615	CLA	C13-C15-C16-C17
24	d	404	CLA	C8-C10-C11-C12
24	C	514	CLA	C16-C17-C18-C20
32	B	625	LHG	O6-C4-C5-C6
32	b	627	LHG	O6-C4-C5-C6
28	A	411	PL9	C39-C41-C42-C43
28	a	411	PL9	C39-C41-C42-C43
33	C	518	DGD	CBA-CCA-CDA-CEA
33	c	518	DGD	CBA-CCA-CDA-CEA
24	C	514	CLA	C4-C3-C5-C6
24	c	514	CLA	C4-C3-C5-C6
24	c	514	CLA	C16-C17-C18-C20
32	B	625	LHG	C12-C13-C14-C15
32	b	627	LHG	C12-C13-C14-C15
24	C	502	CLA	CBA-CGA-O2A-C1
24	c	502	CLA	CBA-CGA-O2A-C1
27	A	410	SQD	C35-C36-C37-C38
32	D	408	LHG	C25-C26-C27-C28
32	d	408	LHG	C25-C26-C27-C28
33	H	102	DGD	CCB-CDB-CEB-CFB
33	h	102	DGD	CCB-CDB-CEB-CFB
36	J	102	LMT	C6-C7-C8-C9
36	j	102	LMT	C6-C7-C8-C9
27	a	410	SQD	C35-C36-C37-C38
33	H	102	DGD	CDB-CEB-CFB-CGB
33	h	102	DGD	CDB-CEB-CFB-CGB
24	B	612	CLA	CBA-CGA-O2A-C1
24	b	614	CLA	CBA-CGA-O2A-C1
27	A	412	SQD	C24-C23-O48-C46
27	a	412	SQD	C24-C23-O48-C46
24	C	514	CLA	C5-C6-C7-C8
24	c	514	CLA	C5-C6-C7-C8
27	A	412	SQD	O6-C44-C45-C46
27	a	412	SQD	O6-C44-C45-C46
32	E	101	LHG	C29-C30-C31-C32
32	e	101	LHG	C29-C30-C31-C32
31	c	501	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
33	C	517	DGD	O6D-C5D-C6D-O5D
33	c	517	DGD	O6D-C5D-C6D-O5D
27	a	412	SQD	C25-C26-C27-C28
31	C	501	LMG	C20-C21-C22-C23
27	A	412	SQD	C25-C26-C27-C28
32	E	101	LHG	C34-C35-C36-C37
32	e	101	LHG	C34-C35-C36-C37
31	C	520	LMG	C11-C12-C13-C14
31	c	520	LMG	C11-C12-C13-C14
32	D	410	LHG	C11-C12-C13-C14
32	d	410	LHG	C11-C12-C13-C14
32	D	409	LHG	O6-C4-C5-O7
32	d	409	LHG	O6-C4-C5-O7
27	d	407	SQD	C32-C33-C34-C35
27	D	407	SQD	C32-C33-C34-C35
27	a	410	SQD	C16-C17-C18-C19
33	c	519	DGD	C2A-C3A-C4A-C5A
31	C	522	LMG	O7-C8-C9-O8
32	E	101	LHG	O7-C5-C6-O8
32	e	101	LHG	O7-C5-C6-O8
27	A	410	SQD	C16-C17-C18-C19
31	c	522	LMG	C11-C12-C13-C14
33	C	519	DGD	C2A-C3A-C4A-C5A
32	D	409	LHG	C1-C2-C3-O3
32	d	409	LHG	C1-C2-C3-O3
31	C	522	LMG	C11-C12-C13-C14
27	L	101	SQD	O49-C7-O47-C45
24	C	514	CLA	C2-C3-C5-C6
24	c	514	CLA	C2-C3-C5-C6
31	c	501	LMG	C32-C33-C34-C35
24	C	503	CLA	C14-C13-C15-C16
24	c	503	CLA	C14-C13-C15-C16
31	C	501	LMG	C32-C33-C34-C35
32	D	409	LHG	C11-C10-C9-C8
32	d	409	LHG	C11-C10-C9-C8
31	c	522	LMG	C15-C16-C17-C18
24	C	511	CLA	C8-C10-C11-C12
24	c	511	CLA	C8-C10-C11-C12
31	B	620	LMG	C18-C19-C20-C21
31	b	622	LMG	C18-C19-C20-C21
33	C	519	DGD	C9A-CAA-CBA-CCA
33	c	519	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	C16-C17-C18-C20
24	c	504	CLA	C16-C17-C18-C20
26	A	409	BCR	C1-C6-C7-C8
26	A	409	BCR	C5-C6-C7-C8
26	A	409	BCR	C23-C24-C25-C26
26	B	619	BCR	C5-C6-C7-C8
26	B	619	BCR	C23-C24-C25-C26
26	B	619	BCR	C23-C24-C25-C30
26	C	521	BCR	C1-C6-C7-C8
26	C	521	BCR	C5-C6-C7-C8
26	a	409	BCR	C1-C6-C7-C8
26	a	409	BCR	C5-C6-C7-C8
26	a	409	BCR	C23-C24-C25-C26
26	b	621	BCR	C5-C6-C7-C8
26	b	621	BCR	C23-C24-C25-C26
26	b	621	BCR	C23-C24-C25-C30
26	c	521	BCR	C1-C6-C7-C8
26	c	521	BCR	C5-C6-C7-C8
24	b	612	CLA	C8-C10-C11-C12
32	D	409	LHG	C30-C31-C32-C33
32	d	408	LHG	C30-C31-C32-C33
32	d	409	LHG	C30-C31-C32-C33
33	C	517	DGD	C8A-C9A-CAA-CBA
33	C	519	DGD	C6B-C7B-C8B-C9B
33	c	517	DGD	C8A-C9A-CAA-CBA
33	c	519	DGD	C6B-C7B-C8B-C9B
32	D	408	LHG	C30-C31-C32-C33
33	H	102	DGD	C5A-C6A-C7A-C8A
33	h	102	DGD	C5A-C6A-C7A-C8A
26	B	617	BCR	C21-C22-C23-C24
26	b	619	BCR	C21-C22-C23-C24
24	B	610	CLA	C8-C10-C11-C12
31	d	411	LMG	C21-C22-C23-C24
27	l	101	SQD	O49-C7-O47-C45
31	D	411	LMG	C21-C22-C23-C24
32	B	625	LHG	C10-C11-C12-C13
32	b	627	LHG	C10-C11-C12-C13
32	D	409	LHG	O6-C4-C5-C6
32	d	409	LHG	O6-C4-C5-C6
31	C	522	LMG	C15-C16-C17-C18
36	M	101	LMT	C6-C7-C8-C9
24	B	616	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C11-C10-C8-C7
24	C	513	CLA	C11-C10-C8-C7
24	b	618	CLA	C6-C7-C8-C10
24	c	507	CLA	C11-C10-C8-C7
24	c	513	CLA	C11-C10-C8-C7
33	C	517	DGD	C4D-C5D-C6D-O5D
33	c	517	DGD	C4D-C5D-C6D-O5D
33	C	518	DGD	C5A-C6A-C7A-C8A
36	m	102	LMT	C6-C7-C8-C9
32	E	101	LHG	C9-C10-C11-C12
32	e	101	LHG	C9-C10-C11-C12
33	c	518	DGD	C5A-C6A-C7A-C8A
24	B	612	CLA	C10-C11-C12-C13
24	b	614	CLA	C10-C11-C12-C13
24	B	612	CLA	O1A-CGA-O2A-C1
27	D	407	SQD	C9-C10-C11-C12
27	d	407	SQD	C9-C10-C11-C12
26	B	627	BCR	C35-C13-C14-C15
26	C	516	BCR	C35-C13-C14-C15
26	T	101	BCR	C35-C13-C14-C15
26	c	516	BCR	C35-C13-C14-C15
24	C	510	CLA	C10-C11-C12-C13
24	c	510	CLA	C10-C11-C12-C13
24	C	506	CLA	CBA-CGA-O2A-C1
24	c	506	CLA	CBA-CGA-O2A-C1
31	B	620	LMG	O8-C28-C29-C30
31	b	622	LMG	O8-C28-C29-C30
31	C	520	LMG	C36-C37-C38-C39
31	c	520	LMG	C36-C37-C38-C39
32	D	409	LHG	C33-C34-C35-C36
32	d	409	LHG	C33-C34-C35-C36
24	b	614	CLA	O1A-CGA-O2A-C1
24	B	603	CLA	CAD-CBD-CGD-O2D
24	B	610	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	511	CLA	CAD-CBD-CGD-O2D
24	b	605	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	b	616	CLA	CAD-CBD-CGD-O2D
24	c	511	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C13-C15-C16-C17
24	C	512	CLA	C5-C6-C7-C8
24	a	405	CLA	C13-C15-C16-C17
33	C	517	DGD	O1A-C1A-O1G-C1G
33	c	517	DGD	O1A-C1A-O1G-C1G
24	C	514	CLA	O1D-CGD-O2D-CED
24	c	514	CLA	O1D-CGD-O2D-CED
31	C	501	LMG	C7-C8-C9-O8
31	C	522	LMG	C7-C8-C9-O8
31	c	501	LMG	C7-C8-C9-O8
32	E	101	LHG	C4-C5-C6-O8
32	e	101	LHG	C4-C5-C6-O8
32	B	625	LHG	O6-C4-C5-O7
32	b	627	LHG	O6-C4-C5-O7
24	c	512	CLA	C5-C6-C7-C8
31	C	520	LMG	C35-C36-C37-C38
31	c	520	LMG	C35-C36-C37-C38
24	B	601	CLA	CHA-CBD-CGD-O1D
24	B	601	CLA	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O1D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	D	401	CLA	CHA-CBD-CGD-O2D
24	b	603	CLA	CHA-CBD-CGD-O1D
24	b	603	CLA	CHA-CBD-CGD-O2D
24	c	505	CLA	CHA-CBD-CGD-O1D
24	c	505	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O2D
24	C	506	CLA	O1A-CGA-O2A-C1
24	c	506	CLA	O1A-CGA-O2A-C1
33	C	519	DGD	C2D-C1D-O3G-C3G
33	c	519	DGD	C2D-C1D-O3G-C3G
27	A	410	SQD	O6-C44-C45-O47
27	a	410	SQD	O6-C44-C45-O47
31	C	501	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
31	C	522	LMG	O1-C7-C8-O7
31	c	501	LMG	O7-C8-C9-O8
31	c	522	LMG	O1-C7-C8-O7
31	c	522	LMG	O7-C8-C9-O8
27	L	101	SQD	C18-C19-C20-C21
31	C	501	LMG	C35-C36-C37-C38
31	C	522	LMG	C13-C14-C15-C16
31	c	501	LMG	C35-C36-C37-C38
31	c	520	LMG	C15-C16-C17-C18
31	c	522	LMG	C30-C31-C32-C33
27	l	101	SQD	C18-C19-C20-C21
31	C	520	LMG	C15-C16-C17-C18
24	C	502	CLA	O1A-CGA-O2A-C1
24	c	502	CLA	O1A-CGA-O2A-C1
32	e	101	LHG	C23-C24-C25-C26
24	c	508	CLA	C2-C3-C5-C6
24	B	603	CLA	C6-C7-C8-C9
24	b	605	CLA	C6-C7-C8-C9
24	B	614	CLA	O1D-CGD-O2D-CED
24	b	616	CLA	O1D-CGD-O2D-CED
31	C	522	LMG	C30-C31-C32-C33
32	D	408	LHG	C24-C25-C26-C27
32	d	408	LHG	C24-C25-C26-C27
36	M	101	LMT	C7-C8-C9-C10
36	m	102	LMT	C7-C8-C9-C10
32	E	101	LHG	C23-C24-C25-C26
32	D	408	LHG	C34-C35-C36-C37
32	d	408	LHG	C34-C35-C36-C37
27	A	412	SQD	C5-C6-S-O8
27	L	101	SQD	C5-C6-S-O8
27	a	412	SQD	C5-C6-S-O8
27	l	101	SQD	C5-C6-S-O8
24	B	605	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C2A-CAA-CBA-CGA
24	b	612	CLA	C2A-CAA-CBA-CGA
36	z	101	LMT	C2B-C1B-O1B-C4'
26	C	516	BCR	C7-C8-C9-C34
26	c	516	BCR	C7-C8-C9-C34
33	C	519	DGD	C3A-C4A-C5A-C6A
33	c	519	DGD	C3A-C4A-C5A-C6A
36	Z	101	LMT	C2B-C1B-O1B-C4'
31	c	522	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	612	CLA	C1A-C2A-CAA-CBA
24	b	614	CLA	C1A-C2A-CAA-CBA
32	D	410	LHG	C4-O6-P-O3
32	d	410	LHG	C4-O6-P-O3
36	Z	101	LMT	C1-C2-C3-C4
24	C	508	CLA	C2-C3-C5-C6
25	A	407	PHO	C2-C3-C5-C6
25	a	407	PHO	C2-C3-C5-C6
31	C	520	LMG	C20-C21-C22-C23
31	c	520	LMG	C20-C21-C22-C23
32	D	409	LHG	C12-C13-C14-C15
32	d	409	LHG	C12-C13-C14-C15
32	D	409	LHG	C4-O6-P-O5
32	d	409	LHG	C4-O6-P-O5
24	A	405	CLA	C16-C17-C18-C20
24	a	405	CLA	C16-C17-C18-C20
36	z	101	LMT	C1-C2-C3-C4
24	D	404	CLA	C13-C15-C16-C17
24	d	404	CLA	C13-C15-C16-C17
32	B	625	LHG	C11-C10-C9-C8
32	b	627	LHG	C11-C10-C9-C8
24	B	601	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	b	603	CLA	CAD-CBD-CGD-O1D
24	c	505	CLA	CAD-CBD-CGD-O1D
24	c	507	CLA	CAD-CBD-CGD-O1D
33	H	102	DGD	O2G-C1B-C2B-C3B
33	h	102	DGD	O2G-C1B-C2B-C3B
33	C	519	DGD	C9B-CAB-CBB-CCB
33	c	519	DGD	C9B-CAB-CBB-CCB
24	A	406	CLA	C11-C10-C8-C7
24	B	603	CLA	C6-C7-C8-C10
24	C	508	CLA	C6-C7-C8-C10
24	C	508	CLA	C12-C13-C15-C16
24	C	514	CLA	C12-C13-C15-C16
24	a	406	CLA	C11-C10-C8-C7
24	b	605	CLA	C6-C7-C8-C10
24	c	508	CLA	C6-C7-C8-C10
24	c	508	CLA	C12-C13-C15-C16
24	c	514	CLA	C12-C13-C15-C16
31	c	522	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
24	b	613	CLA	O1A-CGA-O2A-C1
31	C	520	LMG	O1-C7-C8-O7
31	c	520	LMG	O1-C7-C8-O7
24	B	611	CLA	O1A-CGA-O2A-C1
31	C	522	LMG	C8-C7-O1-C1
31	c	522	LMG	C8-C7-O1-C1
33	C	517	DGD	C5B-C6B-C7B-C8B
33	c	517	DGD	C5B-C6B-C7B-C8B
25	A	407	PHO	C4-C3-C5-C6
25	a	407	PHO	C4-C3-C5-C6
31	B	620	LMG	C13-C14-C15-C16
31	b	622	LMG	C13-C14-C15-C16
24	A	406	CLA	C11-C10-C8-C9
24	B	616	CLA	C6-C7-C8-C9
24	C	508	CLA	C14-C13-C15-C16
24	a	406	CLA	C11-C10-C8-C9
24	b	618	CLA	C6-C7-C8-C9
24	c	508	CLA	C14-C13-C15-C16
28	D	406	PL9	C39-C41-C42-C43
28	d	406	PL9	C39-C41-C42-C43
32	E	101	LHG	C33-C34-C35-C36
26	c	515	BCR	C15-C16-C17-C18
32	e	101	LHG	C33-C34-C35-C36
36	I	102	LMT	C6-C7-C8-C9
36	i	102	LMT	C6-C7-C8-C9
33	C	518	DGD	CDA-CEA-CFA-CGA
24	B	602	CLA	C8-C10-C11-C12
24	b	604	CLA	C8-C10-C11-C12
33	C	517	DGD	CBA-CCA-CDA-CEA
33	c	517	DGD	CBA-CCA-CDA-CEA
33	c	518	DGD	CDA-CEA-CFA-CGA
24	A	408	CLA	C8-C10-C11-C12
24	a	408	CLA	C8-C10-C11-C12
24	c	509	CLA	C13-C15-C16-C17
32	B	625	LHG	C9-C10-C11-C12
32	b	627	LHG	C9-C10-C11-C12
24	C	503	CLA	O1D-CGD-O2D-CED
24	c	503	CLA	O1D-CGD-O2D-CED
24	B	610	CLA	C2A-CAA-CBA-CGA
31	B	620	LMG	O9-C10-O7-C8
31	b	622	LMG	O9-C10-O7-C8
33	C	517	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
33	c	517	DGD	O1B-C1B-O2G-C2G
24	C	509	CLA	C13-C15-C16-C17
31	c	501	LMG	C31-C32-C33-C34
31	C	501	LMG	C31-C32-C33-C34
36	z	101	LMT	O5B-C1B-O1B-C4'
31	B	620	LMG	C34-C35-C36-C37
31	b	622	LMG	C34-C35-C36-C37
31	c	520	LMG	C22-C23-C24-C25
26	C	515	BCR	C15-C16-C17-C18
31	C	520	LMG	C22-C23-C24-C25
26	C	515	BCR	C23-C24-C25-C30
26	C	516	BCR	C23-C24-C25-C30
26	c	515	BCR	C23-C24-C25-C30
26	c	516	BCR	C23-C24-C25-C30
31	D	411	LMG	C20-C21-C22-C23
36	Z	101	LMT	O5B-C1B-O1B-C4'
31	d	411	LMG	C20-C21-C22-C23
24	B	611	CLA	CBA-CGA-O2A-C1
24	C	512	CLA	CBA-CGA-O2A-C1
24	b	613	CLA	CBA-CGA-O2A-C1
24	c	512	CLA	CBA-CGA-O2A-C1
32	E	101	LHG	C25-C26-C27-C28
32	e	101	LHG	C25-C26-C27-C28
24	A	405	CLA	C16-C17-C18-C19
24	a	405	CLA	C16-C17-C18-C19
26	D	405	BCR	C20-C21-C22-C23
26	d	405	BCR	C20-C21-C22-C23
33	C	518	DGD	C2D-C1D-O3G-C3G
33	c	518	DGD	C2D-C1D-O3G-C3G
32	B	625	LHG	C4-O6-P-O3
32	b	627	LHG	C4-O6-P-O3
33	c	518	DGD	C1A-C2A-C3A-C4A
33	C	518	DGD	C1A-C2A-C3A-C4A
31	C	501	LMG	O1-C7-C8-C9
31	c	501	LMG	O1-C7-C8-C9
24	C	503	CLA	CBD-CGD-O2D-CED
31	C	501	LMG	C11-C12-C13-C14
24	C	508	CLA	C6-C7-C8-C9
24	C	514	CLA	C14-C13-C15-C16
24	c	508	CLA	C6-C7-C8-C9
24	c	514	CLA	C14-C13-C15-C16
31	c	501	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	h	102	DGD	CDA-CEA-CFA-CGA
24	c	503	CLA	CBD-CGD-O2D-CED
31	B	620	LMG	O10-C28-O8-C9
31	b	622	LMG	O10-C28-O8-C9
32	D	410	LHG	C2-C3-O3-P
32	d	410	LHG	C2-C3-O3-P
33	H	102	DGD	CDA-CEA-CFA-CGA
33	H	102	DGD	C9B-CAB-CBB-CCB
33	h	102	DGD	C9B-CAB-CBB-CCB
24	b	612	CLA	CBD-CGD-O2D-CED
32	E	101	LHG	C11-C10-C9-C8
32	e	101	LHG	C11-C10-C9-C8
27	A	412	SQD	C34-C35-C36-C37
27	a	412	SQD	C34-C35-C36-C37
33	C	517	DGD	O6E-C1E-O5D-C6D
33	c	517	DGD	O6E-C1E-O5D-C6D
24	D	401	CLA	C4C-C3C-CAC-CBC
24	d	401	CLA	C4C-C3C-CAC-CBC
28	D	406	PL9	C15-C14-C16-C17
28	d	406	PL9	C15-C14-C16-C17
24	B	611	CLA	C2-C3-C5-C6
24	b	613	CLA	C2-C3-C5-C6
27	l	101	SQD	C14-C15-C16-C17
24	B	608	CLA	C2-C1-O2A-CGA
24	b	610	CLA	C2-C1-O2A-CGA
27	L	101	SQD	C14-C15-C16-C17
27	A	410	SQD	C11-C10-C9-C8
27	a	410	SQD	C11-C10-C9-C8
36	I	102	LMT	C5'-C4'-O1B-C1B
36	i	102	LMT	C5'-C4'-O1B-C1B
31	C	501	LMG	C33-C34-C35-C36
31	c	501	LMG	C33-C34-C35-C36
24	B	611	CLA	C4-C3-C5-C6
24	b	613	CLA	C4-C3-C5-C6
28	A	411	PL9	C4-C3-C7-C8
28	a	411	PL9	C4-C3-C7-C8
24	C	507	CLA	C6-C7-C8-C9
24	c	507	CLA	C6-C7-C8-C9
31	C	522	LMG	C32-C33-C34-C35
31	c	522	LMG	C32-C33-C34-C35
32	D	409	LHG	C25-C26-C27-C28
33	C	517	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
32	d	409	LHG	C25-C26-C27-C28
33	c	517	DGD	C7A-C8A-C9A-CAA
32	D	410	LHG	C17-C18-C19-C20
28	D	406	PL9	C12-C13-C14-C16
27	A	412	SQD	C32-C33-C34-C35
32	d	410	LHG	C17-C18-C19-C20
24	C	512	CLA	O1A-CGA-O2A-C1
26	B	619	BCR	C36-C18-C19-C20
26	C	521	BCR	C37-C22-C23-C24
26	b	621	BCR	C36-C18-C19-C20
26	c	521	BCR	C37-C22-C23-C24
27	a	412	SQD	C32-C33-C34-C35
36	z	101	LMT	C3-C4-C5-C6
24	c	506	CLA	C13-C15-C16-C17
31	d	411	LMG	C12-C13-C14-C15
24	B	604	CLA	C1A-C2A-CAA-CBA
24	b	606	CLA	C1A-C2A-CAA-CBA
31	D	411	LMG	C12-C13-C14-C15
36	Z	101	LMT	C3-C4-C5-C6
24	B	601	CLA	C6-C7-C8-C10
24	C	511	CLA	C2-C3-C5-C6
24	D	401	CLA	C11-C10-C8-C7
24	b	603	CLA	C6-C7-C8-C10
24	c	511	CLA	C2-C3-C5-C6
24	d	401	CLA	C11-C10-C8-C7
24	C	506	CLA	C13-C15-C16-C17
24	c	512	CLA	O1A-CGA-O2A-C1
24	C	504	CLA	C2A-CAA-CBA-CGA
24	c	504	CLA	C2A-CAA-CBA-CGA
24	B	602	CLA	C15-C16-C17-C18
24	b	604	CLA	C15-C16-C17-C18
32	D	408	LHG	C18-C19-C20-C21
32	d	408	LHG	C18-C19-C20-C21
31	D	411	LMG	C36-C37-C38-C39
24	B	607	CLA	CBD-CGD-O2D-CED
31	d	411	LMG	C36-C37-C38-C39
33	H	102	DGD	C4A-C5A-C6A-C7A
33	h	102	DGD	C4A-C5A-C6A-C7A
31	D	411	LMG	C10-C11-C12-C13
31	d	411	LMG	C10-C11-C12-C13
24	B	605	CLA	O1A-CGA-O2A-C1
24	b	607	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	618	BCR	C11-C10-C9-C8
26	b	620	BCR	C11-C10-C9-C8
26	C	516	BCR	C6-C7-C8-C9
26	c	516	BCR	C6-C7-C8-C9
24	B	615	CLA	C4-C3-C5-C6
24	C	513	CLA	C2-C1-O2A-CGA
24	c	513	CLA	C2-C1-O2A-CGA
28	d	406	PL9	C12-C13-C14-C16
24	b	609	CLA	CBD-CGD-O2D-CED
33	H	102	DGD	CBB-CCB-CDB-CEB
33	h	102	DGD	CBB-CCB-CDB-CEB
24	B	605	CLA	C10-C11-C12-C13
31	C	520	LMG	C11-C10-O7-C8
31	c	520	LMG	C11-C10-O7-C8
24	b	607	CLA	C10-C11-C12-C13
24	C	504	CLA	C16-C17-C18-C19
24	c	504	CLA	C16-C17-C18-C19
26	A	409	BCR	C23-C24-C25-C30
26	B	618	BCR	C1-C6-C7-C8
26	B	619	BCR	C1-C6-C7-C8
26	C	515	BCR	C23-C24-C25-C26
26	C	516	BCR	C1-C6-C7-C8
26	C	521	BCR	C23-C24-C25-C30
26	D	405	BCR	C23-C24-C25-C30
26	a	409	BCR	C23-C24-C25-C30
26	b	620	BCR	C1-C6-C7-C8
26	b	621	BCR	C1-C6-C7-C8
26	c	515	BCR	C23-C24-C25-C26
26	c	516	BCR	C1-C6-C7-C8
26	c	521	BCR	C23-C24-C25-C30
26	d	405	BCR	C23-C24-C25-C30
35	H	101	RRX	C23-C24-C25-C30
35	h	101	RRX	C23-C24-C25-C30
27	a	410	SQD	C18-C19-C20-C21
27	D	407	SQD	C45-C44-O6-C1
27	d	407	SQD	C45-C44-O6-C1
33	C	517	DGD	C5D-C6D-O5D-C1E
33	c	517	DGD	C5D-C6D-O5D-C1E
27	d	407	SQD	C26-C27-C28-C29
25	D	402	PHO	C8-C10-C11-C12
25	d	402	PHO	C8-C10-C11-C12
27	D	407	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
24	b	617	CLA	C4-C3-C5-C6
33	c	518	DGD	C3A-C4A-C5A-C6A
24	C	506	CLA	C2-C3-C5-C6
24	c	506	CLA	C2-C3-C5-C6
33	C	518	DGD	C3A-C4A-C5A-C6A
27	A	410	SQD	C18-C19-C20-C21
24	d	404	CLA	C10-C11-C12-C13
31	c	520	LMG	C38-C39-C40-C41
24	A	408	CLA	C15-C16-C17-C18
24	D	404	CLA	C10-C11-C12-C13
24	a	408	CLA	C15-C16-C17-C18
38	v	201	HEC	CAD-CBD-CGD-O2D
31	C	520	LMG	C29-C30-C31-C32
31	c	520	LMG	C29-C30-C31-C32
24	b	617	CLA	C11-C10-C8-C9
38	V	201	HEC	CAD-CBD-CGD-O2D
31	C	520	LMG	C38-C39-C40-C41
32	B	625	LHG	O2-C2-C3-O3
32	b	627	LHG	O2-C2-C3-O3
24	b	614	CLA	C8-C10-C11-C12
24	C	511	CLA	CAA-CBA-CGA-O2A
24	c	511	CLA	CAA-CBA-CGA-O2A
24	B	607	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
24	c	510	CLA	CAD-CBD-CGD-O2D
24	c	513	CLA	CAD-CBD-CGD-O2D
25	A	407	PHO	CAD-CBD-CGD-O2D
25	a	407	PHO	CAD-CBD-CGD-O2D
32	B	625	LHG	O9-C7-O7-C5
32	b	627	LHG	O9-C7-O7-C5
24	B	610	CLA	CBD-CGD-O2D-CED
24	B	612	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	C	511	CLA	C2-C1-O2A-CGA
24	c	511	CLA	C2-C1-O2A-CGA
33	c	518	DGD	C7B-C8B-C9B-CAB
24	C	513	CLA	CAA-CBA-CGA-O2A
24	c	513	CLA	CAA-CBA-CGA-O2A
27	D	407	SQD	O47-C7-C8-C9
27	d	407	SQD	O47-C7-C8-C9
31	C	520	LMG	O7-C10-C11-C12
32	E	101	LHG	O8-C23-C24-C25
32	e	101	LHG	O8-C23-C24-C25
33	C	518	DGD	C7B-C8B-C9B-CAB
33	C	519	DGD	C4B-C5B-C6B-C7B
31	C	520	LMG	C37-C38-C39-C40
31	c	520	LMG	O7-C10-C11-C12
33	c	519	DGD	C4B-C5B-C6B-C7B
26	A	409	BCR	C17-C18-C19-C20
26	C	515	BCR	C7-C8-C9-C10
26	a	409	BCR	C17-C18-C19-C20
26	c	515	BCR	C7-C8-C9-C10
27	L	101	SQD	C44-C45-C46-O48
27	l	101	SQD	C44-C45-C46-O48
33	C	519	DGD	C1G-C2G-C3G-O3G
33	c	519	DGD	C1G-C2G-C3G-O3G
31	c	520	LMG	C37-C38-C39-C40
38	V	201	HEC	CAD-CBD-CGD-O1D
24	C	513	CLA	O2A-C1-C2-C3
24	D	403	CLA	O2A-C1-C2-C3
24	c	513	CLA	O2A-C1-C2-C3
24	d	403	CLA	O2A-C1-C2-C3
24	B	605	CLA	CBA-CGA-O2A-C1
32	E	101	LHG	C24-C23-O8-C6
32	e	101	LHG	C24-C23-O8-C6
27	l	101	SQD	C17-C18-C19-C20
38	v	201	HEC	CAD-CBD-CGD-O1D
27	L	101	SQD	C17-C18-C19-C20
24	B	616	CLA	CHA-CBD-CGD-O1D
24	B	616	CLA	CHA-CBD-CGD-O2D
24	D	401	CLA	CHA-CBD-CGD-O1D
24	b	618	CLA	CHA-CBD-CGD-O1D
24	b	618	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O1D
27	A	410	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	a	410	SQD	O47-C7-C8-C9
24	b	607	CLA	CBA-CGA-O2A-C1
26	b	619	BCR	C20-C21-C22-C23
33	H	102	DGD	C6B-C7B-C8B-C9B
24	B	613	CLA	CAA-CBA-CGA-O2A
24	b	615	CLA	CAA-CBA-CGA-O2A
31	d	411	LMG	O7-C10-C11-C12
36	z	101	LMT	C4-C5-C6-C7
27	L	101	SQD	O47-C45-C46-O48
27	l	101	SQD	O47-C45-C46-O48
27	A	412	SQD	C23-C24-C25-C26
27	a	412	SQD	C23-C24-C25-C26
32	d	409	LHG	C34-C35-C36-C37
33	h	102	DGD	C6B-C7B-C8B-C9B
24	B	616	CLA	CAA-CBA-CGA-O2A
24	C	506	CLA	CAA-CBA-CGA-O2A
24	b	618	CLA	CAA-CBA-CGA-O2A
31	D	411	LMG	O7-C10-C11-C12
32	B	625	LHG	O7-C7-C8-C9
32	b	627	LHG	O7-C7-C8-C9
33	C	519	DGD	O1G-C1A-C2A-C3A
33	c	519	DGD	O1G-C1A-C2A-C3A
25	D	402	PHO	CHA-CBD-CGD-O1D
25	d	402	PHO	CHA-CBD-CGD-O1D
32	D	409	LHG	C34-C35-C36-C37
24	C	513	CLA	C3-C5-C6-C7
24	c	513	CLA	C3-C5-C6-C7
27	a	410	SQD	C8-C7-O47-C45
24	c	506	CLA	CAA-CBA-CGA-O2A
36	Z	101	LMT	C4-C5-C6-C7
24	B	601	CLA	C6-C7-C8-C9
24	B	615	CLA	C11-C10-C8-C9
24	D	401	CLA	C11-C10-C8-C9
24	b	603	CLA	C6-C7-C8-C9
24	d	401	CLA	C11-C10-C8-C9
26	A	409	BCR	C19-C20-C21-C22
26	a	409	BCR	C19-C20-C21-C22
32	D	409	LHG	C17-C18-C19-C20
27	A	410	SQD	C15-C16-C17-C18
32	d	409	LHG	C17-C18-C19-C20
27	L	101	SQD	O47-C7-C8-C9
27	l	101	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	A	410	SQD	C8-C7-O47-C45
28	D	406	PL9	C11-C12-C13-C14
28	d	406	PL9	C11-C12-C13-C14
24	c	511	CLA	CAA-CBA-CGA-O1A
27	a	410	SQD	C15-C16-C17-C18
24	C	511	CLA	CAA-CBA-CGA-O1A
33	C	517	DGD	O1B-C1B-C2B-C3B
33	c	517	DGD	O1B-C1B-C2B-C3B
24	C	511	CLA	O1D-CGD-O2D-CED
24	C	503	CLA	C1A-C2A-CAA-CBA
24	c	503	CLA	C1A-C2A-CAA-CBA
24	D	403	CLA	C2-C1-O2A-CGA
24	d	403	CLA	C2-C1-O2A-CGA
31	B	620	LMG	C39-C40-C41-C42
31	b	622	LMG	C39-C40-C41-C42
24	C	513	CLA	CAA-CBA-CGA-O1A
24	c	513	CLA	CAA-CBA-CGA-O1A
31	B	620	LMG	C35-C36-C37-C38
27	L	101	SQD	O6-C44-C45-C46
27	l	101	SQD	O6-C44-C45-C46
31	C	501	LMG	C4-C5-C6-O5
24	A	405	CLA	C2A-CAA-CBA-CGA
24	B	603	CLA	C2A-CAA-CBA-CGA
24	a	405	CLA	C2A-CAA-CBA-CGA
24	c	511	CLA	O1D-CGD-O2D-CED
31	b	622	LMG	C35-C36-C37-C38
24	B	616	CLA	CAA-CBA-CGA-O1A
24	b	618	CLA	CAA-CBA-CGA-O1A
33	C	519	DGD	O1A-C1A-C2A-C3A
33	c	519	DGD	O1A-C1A-C2A-C3A
31	c	501	LMG	C4-C5-C6-O5
26	C	516	BCR	C5-C6-C7-C8
26	C	516	BCR	C23-C24-C25-C26
26	C	521	BCR	C23-C24-C25-C26
26	c	516	BCR	C5-C6-C7-C8
26	c	516	BCR	C23-C24-C25-C26
26	c	521	BCR	C23-C24-C25-C26
24	c	513	CLA	C15-C16-C17-C18
34	e	103	HEM	CAA-CBA-CGA-O2A
32	D	409	LHG	C11-C12-C13-C14
24	b	605	CLA	C2A-CAA-CBA-CGA
27	D	407	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
32	d	409	LHG	C11-C12-C13-C14
34	E	103	HEM	CAA-CBA-CGA-O1A
34	E	103	HEM	CAA-CBA-CGA-O2A
34	e	103	HEM	CAA-CBA-CGA-O1A
24	C	511	CLA	C4-C3-C5-C6
24	c	511	CLA	C4-C3-C5-C6
24	B	605	CLA	CAD-CBD-CGD-O1D
24	B	609	CLA	CAD-CBD-CGD-O1D
24	C	514	CLA	CAD-CBD-CGD-O1D
24	b	607	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	c	514	CLA	CAD-CBD-CGD-O1D
27	A	410	SQD	C5-C6-S-O7
27	a	410	SQD	C5-C6-S-O7
27	d	407	SQD	C33-C34-C35-C36
24	b	605	CLA	C11-C12-C13-C14
32	D	410	LHG	C19-C20-C21-C22
32	d	410	LHG	C19-C20-C21-C22
24	C	506	CLA	CAA-CBA-CGA-O1A
24	c	506	CLA	CAA-CBA-CGA-O1A
32	E	101	LHG	O10-C23-C24-C25
32	e	101	LHG	O10-C23-C24-C25
25	D	402	PHO	C5-C6-C7-C8
25	d	402	PHO	C5-C6-C7-C8
24	B	615	CLA	C11-C10-C8-C7
24	b	617	CLA	C11-C10-C8-C7
31	C	501	LMG	C10-C11-C12-C13
31	c	501	LMG	C10-C11-C12-C13
24	B	610	CLA	C15-C16-C17-C18
24	C	506	CLA	O1D-CGD-O2D-CED
24	C	513	CLA	C15-C16-C17-C18
32	d	409	LHG	C26-C27-C28-C29
33	C	519	DGD	CCB-CDB-CEB-CFB
24	B	613	CLA	CAA-CBA-CGA-O1A
24	B	612	CLA	C13-C15-C16-C17
24	b	612	CLA	C15-C16-C17-C18
24	c	506	CLA	O1D-CGD-O2D-CED
33	c	519	DGD	CCB-CDB-CEB-CFB
32	D	409	LHG	C9-C10-C11-C12
32	d	409	LHG	C9-C10-C11-C12
24	b	615	CLA	CAA-CBA-CGA-O1A
27	D	407	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
27	l	101	SQD	O49-C7-C8-C9
32	D	409	LHG	C26-C27-C28-C29
24	B	615	CLA	C5-C6-C7-C8
24	D	401	CLA	C15-C16-C17-C18
24	b	614	CLA	C13-C15-C16-C17
24	d	401	CLA	C15-C16-C17-C18
27	d	407	SQD	O10-C23-C24-C25
33	C	518	DGD	O1B-C1B-C2B-C3B
33	c	518	DGD	O1B-C1B-C2B-C3B
24	C	506	CLA	C4-C3-C5-C6
24	c	506	CLA	C4-C3-C5-C6

There are no ring outliers.

110 monomers are involved in 185 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	604	CLA	1	0
24	C	508	CLA	4	0
24	b	609	CLA	1	0
32	E	101	LHG	1	0
27	a	412	SQD	1	0
24	a	406	CLA	2	0
34	e	103	HEM	3	0
33	H	102	DGD	1	0
24	c	512	CLA	3	0
36	j	102	LMT	1	0
24	C	506	CLA	4	0
31	D	411	LMG	1	0
24	c	504	CLA	3	0
27	A	410	SQD	1	0
24	D	403	CLA	2	0
24	b	611	CLA	2	0
33	c	518	DGD	3	0
24	b	606	CLA	2	0
26	B	617	BCR	1	0
26	b	620	BCR	1	0
24	d	401	CLA	1	0
27	A	412	SQD	1	0
24	A	408	CLA	3	0
26	B	627	BCR	3	0
28	D	406	PL9	2	0
25	d	402	PHO	2	0

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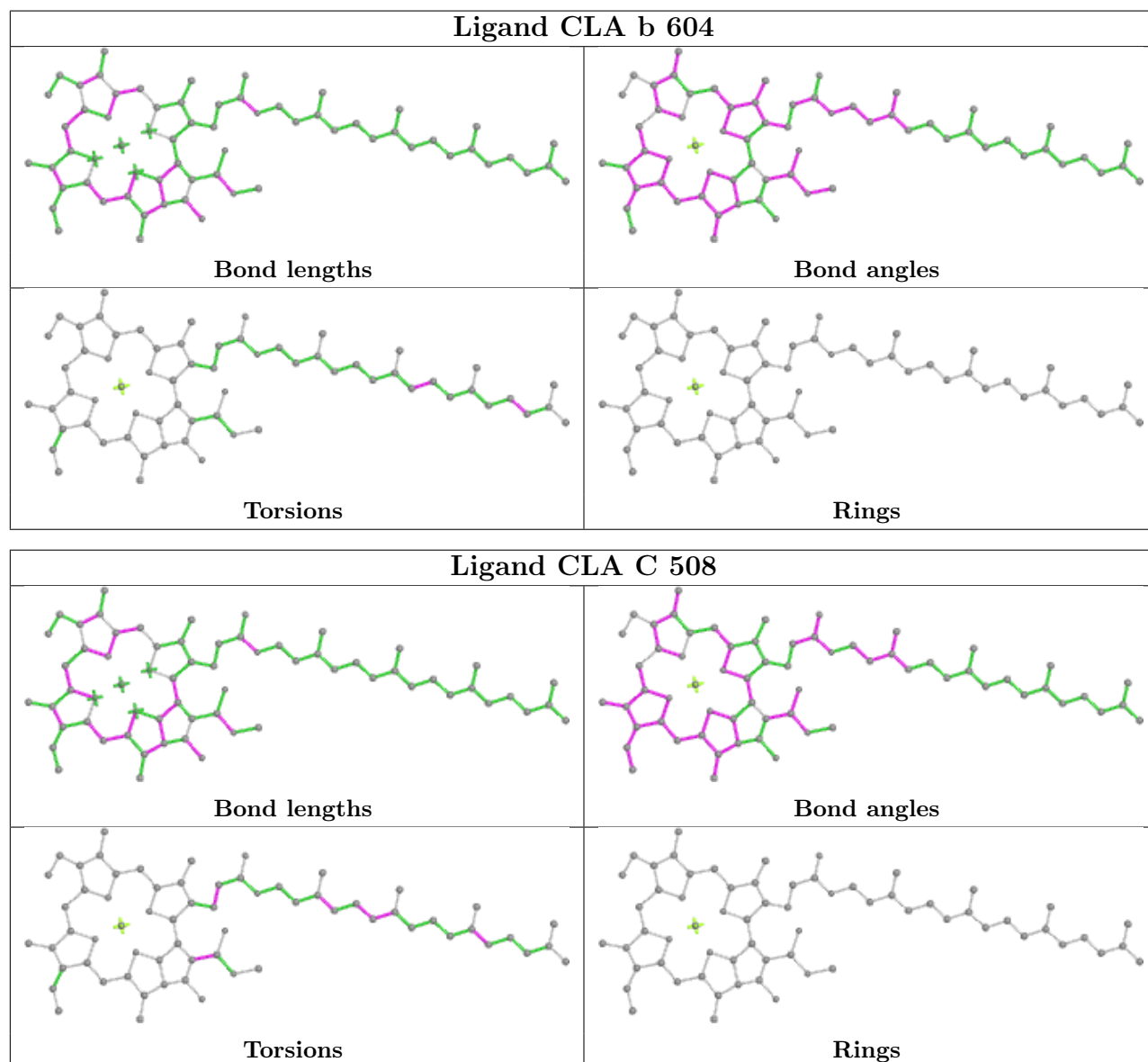
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	503	CLA	1	0
31	d	411	LMG	1	0
24	b	603	CLA	1	0
24	b	610	CLA	1	0
26	a	409	BCR	1	0
24	b	614	CLA	2	0
31	c	522	LMG	3	0
24	c	510	CLA	2	0
24	B	613	CLA	1	0
24	c	505	CLA	2	0
24	b	613	CLA	2	0
36	i	102	LMT	2	0
35	h	101	RRX	9	0
24	D	404	CLA	1	0
24	C	511	CLA	3	0
26	T	101	BCR	1	0
24	c	508	CLA	4	0
24	B	609	CLA	2	0
32	d	410	LHG	1	0
31	c	520	LMG	2	0
33	C	518	DGD	3	0
26	C	521	BCR	2	0
34	E	103	HEM	3	0
24	C	512	CLA	3	0
24	A	406	CLA	2	0
36	J	102	LMT	1	0
24	b	618	CLA	2	0
27	L	101	SQD	1	0
28	d	406	PL9	1	0
24	b	617	CLA	3	0
24	C	502	CLA	2	0
26	C	516	BCR	1	0
24	c	511	CLA	3	0
33	C	519	DGD	3	0
36	I	102	LMT	2	0
28	A	411	PL9	2	0
24	C	505	CLA	2	0
32	D	410	LHG	1	0
24	c	502	CLA	2	0
31	b	622	LMG	2	0
24	B	615	CLA	3	0
24	D	401	CLA	1	0

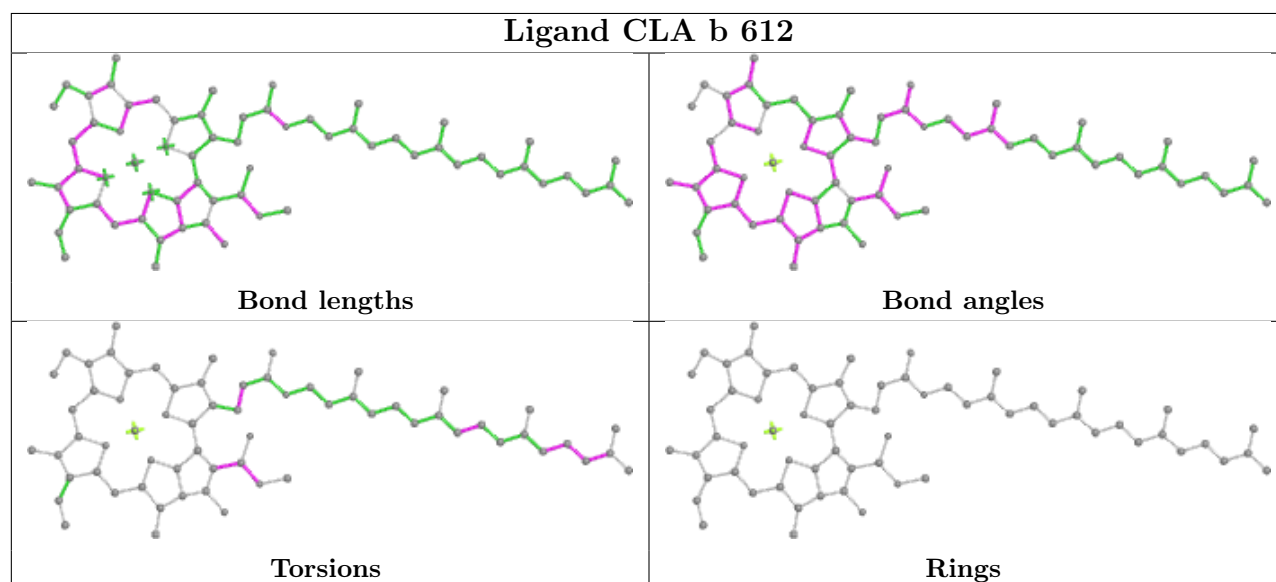
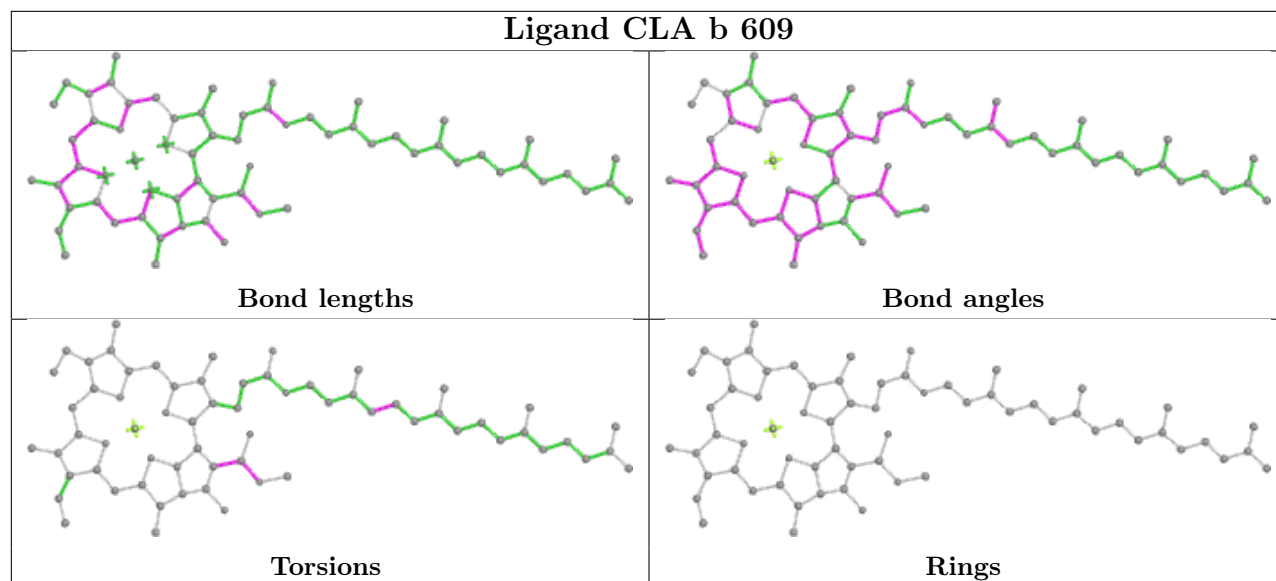
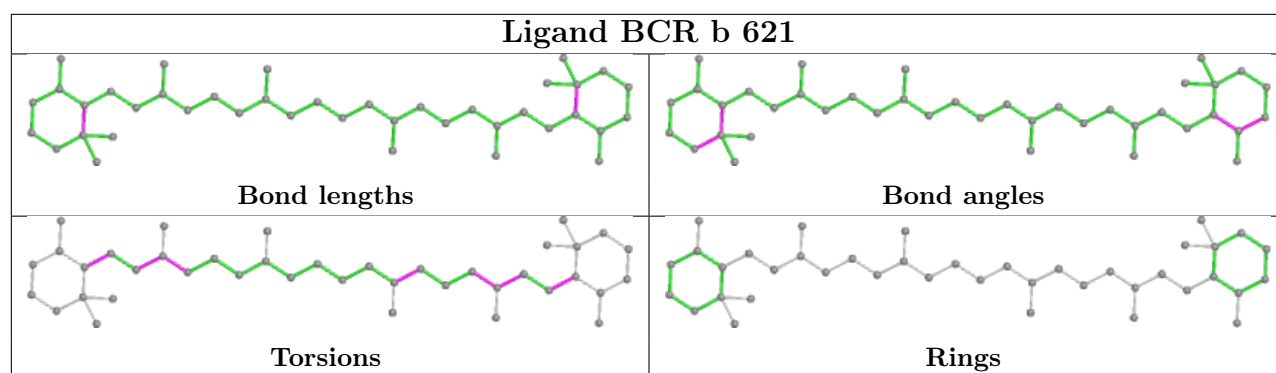
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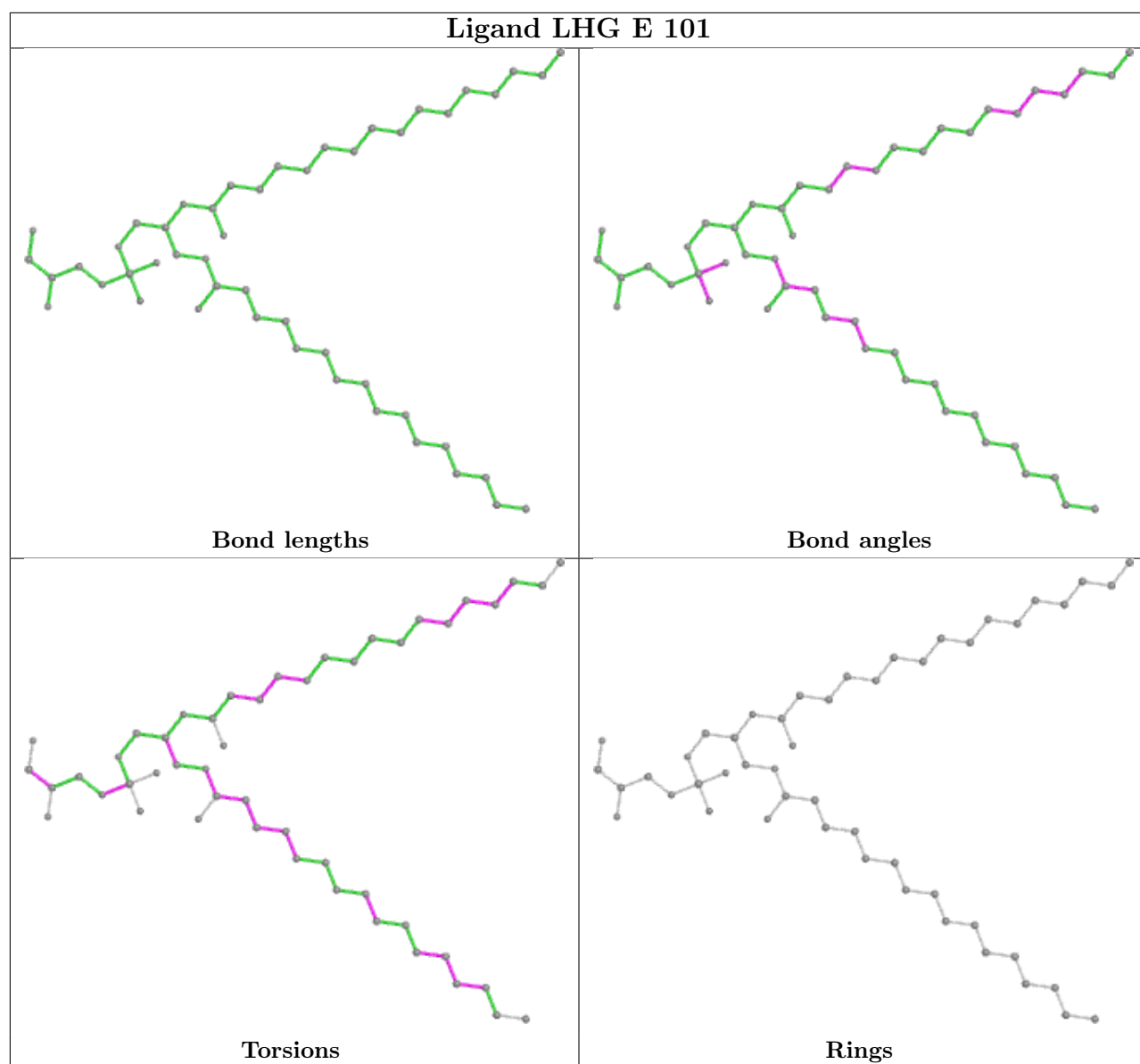
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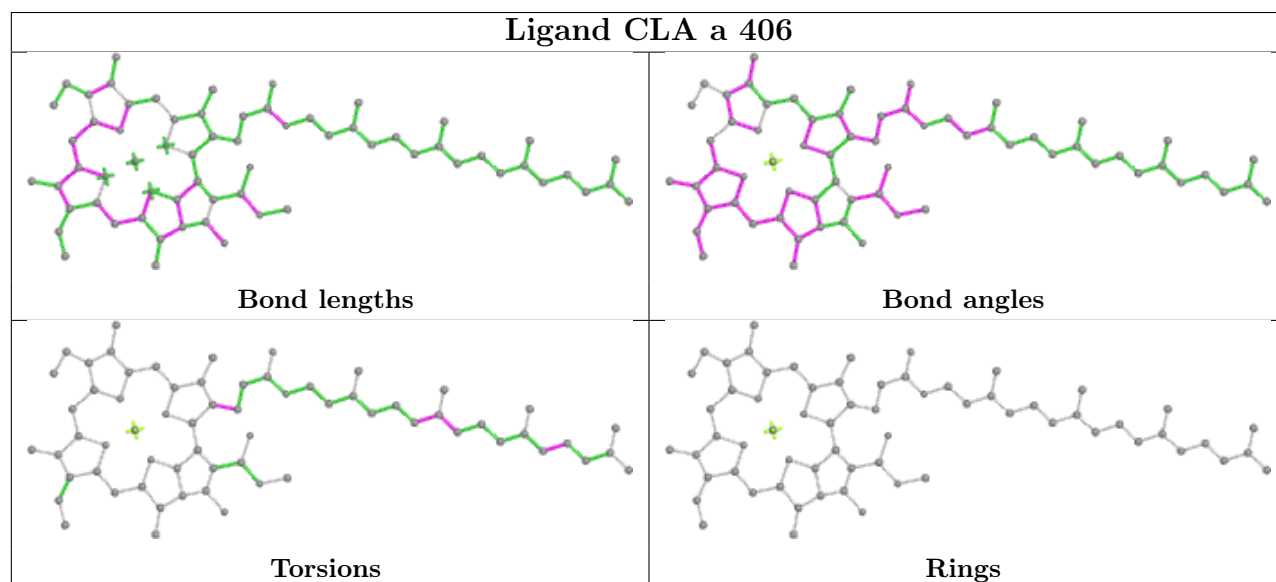
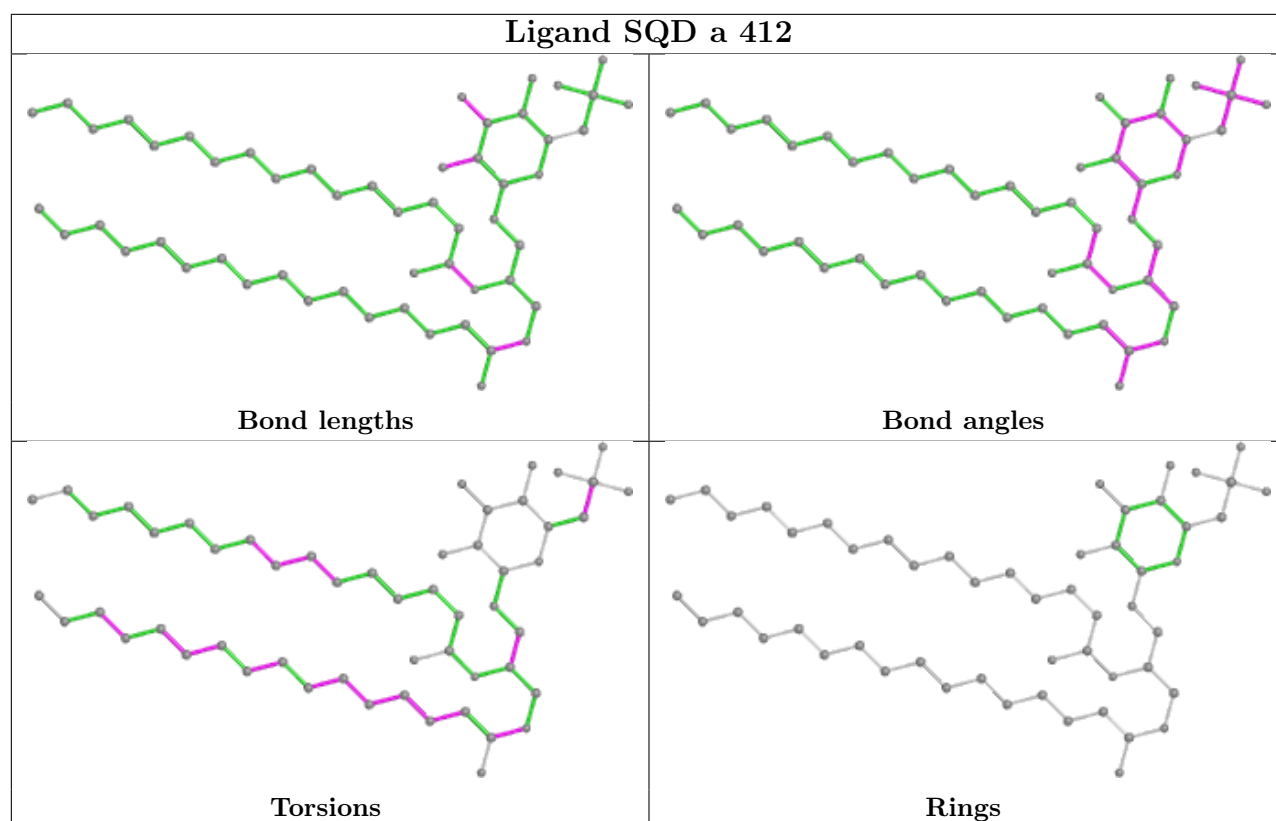
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	514	CLA	2	0
24	C	514	CLA	1	0
24	C	510	CLA	2	0
24	d	403	CLA	2	0
24	B	605	CLA	2	0
24	b	616	CLA	1	0
26	B	618	BCR	5	0
31	C	522	LMG	3	0
26	Y	101	BCR	1	0
24	C	509	CLA	3	0
24	d	404	CLA	1	0
27	l	101	SQD	1	0
26	c	516	BCR	2	0
24	B	608	CLA	1	0
32	B	625	LHG	2	0
24	C	504	CLA	3	0
33	c	519	DGD	3	0
24	c	503	CLA	1	0
24	a	408	CLA	3	0
24	B	612	CLA	3	0
31	C	520	LMG	2	0
26	C	515	BCR	3	0
24	B	611	CLA	1	0
35	H	101	RRX	7	0
24	B	607	CLA	1	0
26	A	409	BCR	1	0
26	c	515	BCR	2	0
32	d	409	LHG	2	0
24	c	506	CLA	4	0
28	a	411	PL9	2	0
31	B	620	LMG	2	0
33	h	102	DGD	2	0
24	c	509	CLA	3	0
32	b	627	LHG	2	0
32	e	101	LHG	1	0
25	D	402	PHO	1	0
32	D	409	LHG	2	0
24	B	604	CLA	1	0
24	B	616	CLA	1	0
24	b	607	CLA	2	0
27	a	410	SQD	2	0
24	B	614	CLA	1	0

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

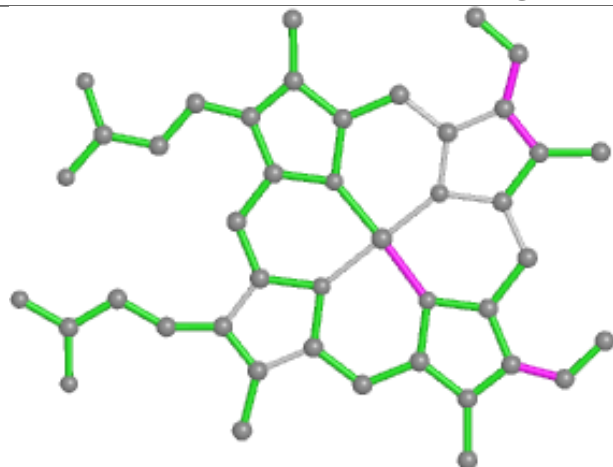




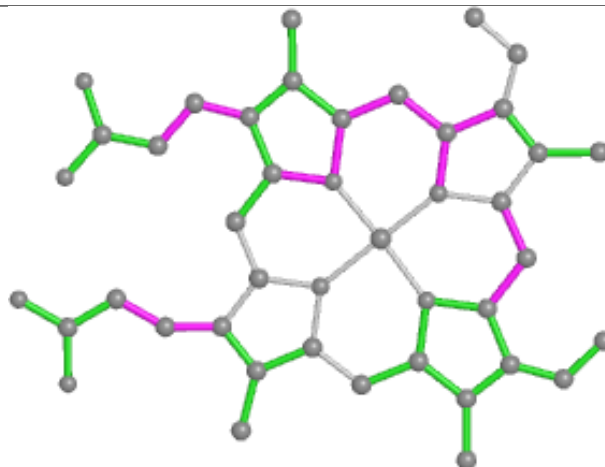




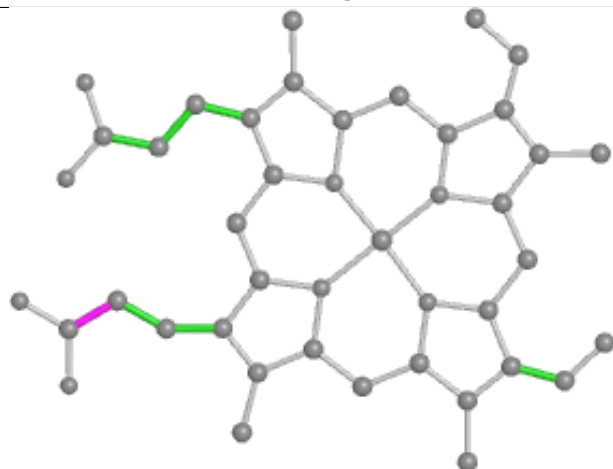
Ligand HEM e 103



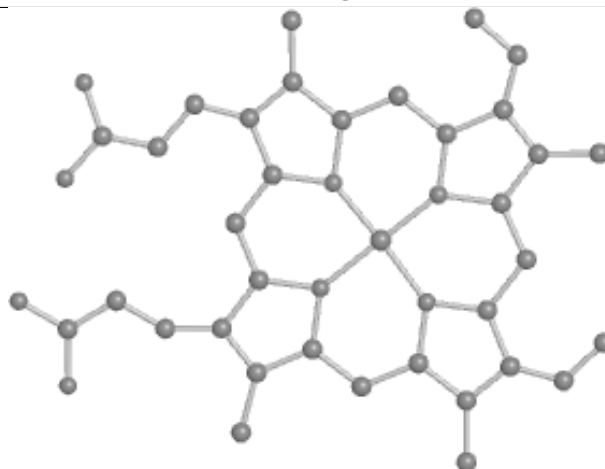
Bond lengths



Bond angles

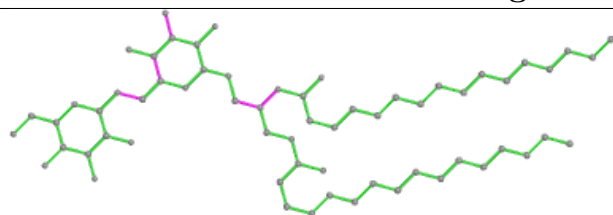


Torsions

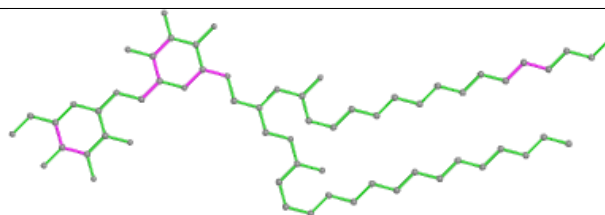


Rings

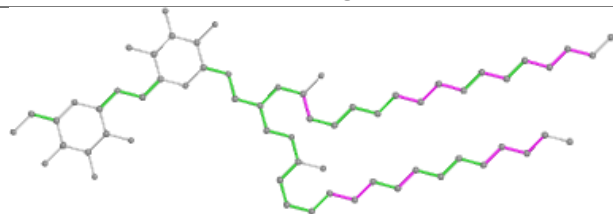
Ligand DGD H 102



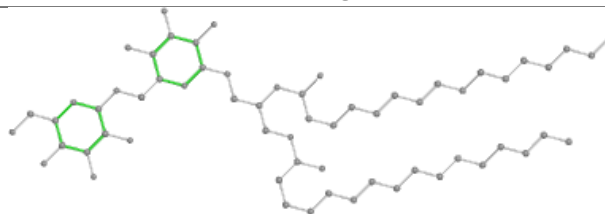
Bond lengths



Bond angles

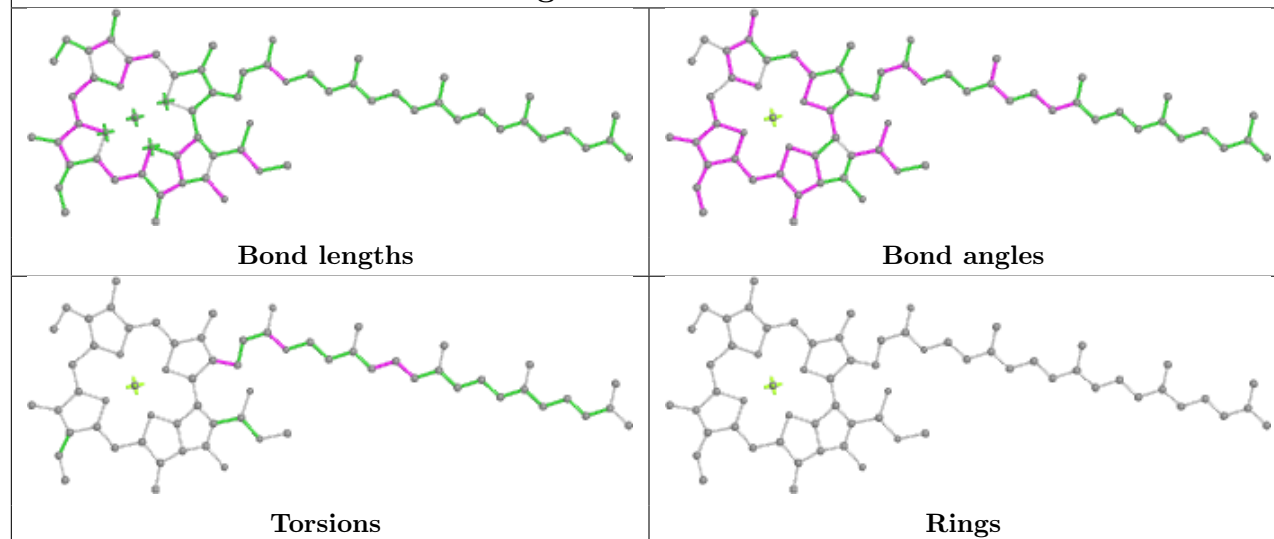


Torsions

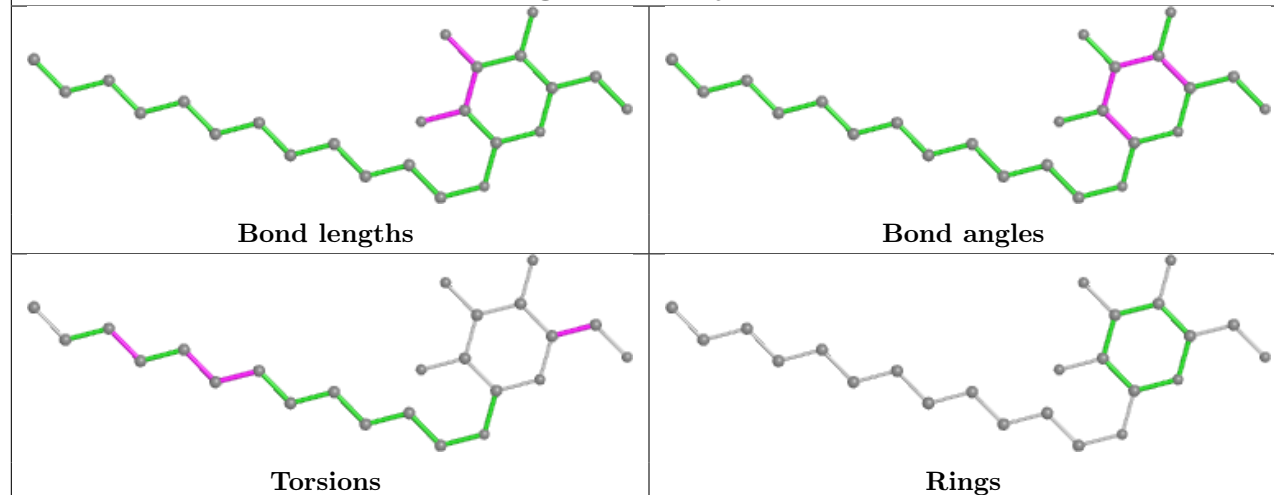


Rings

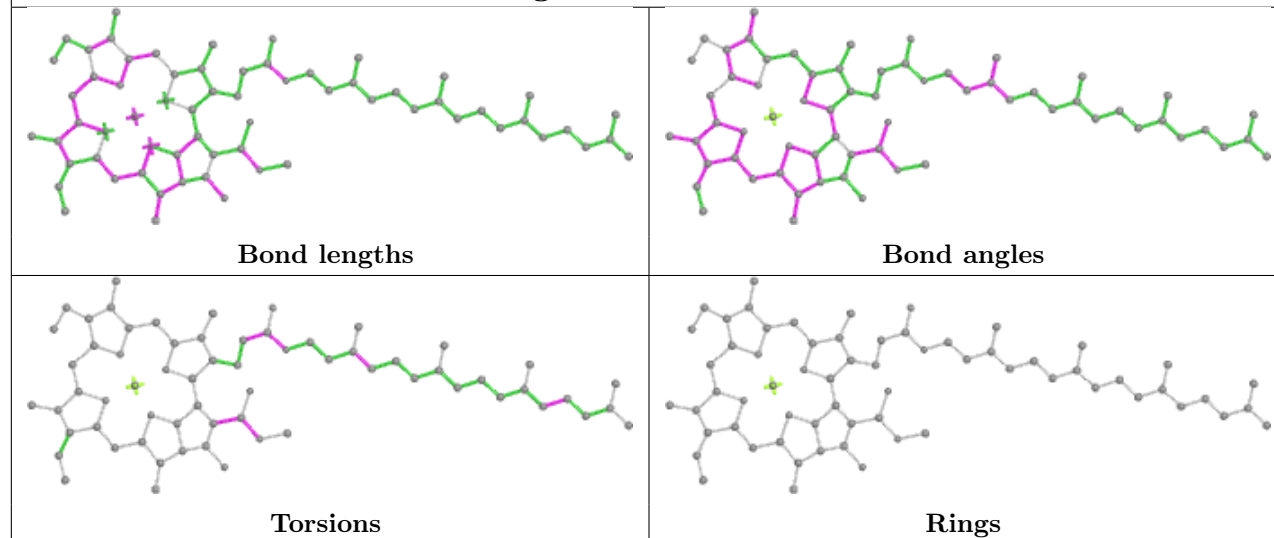
Ligand CLA c 512

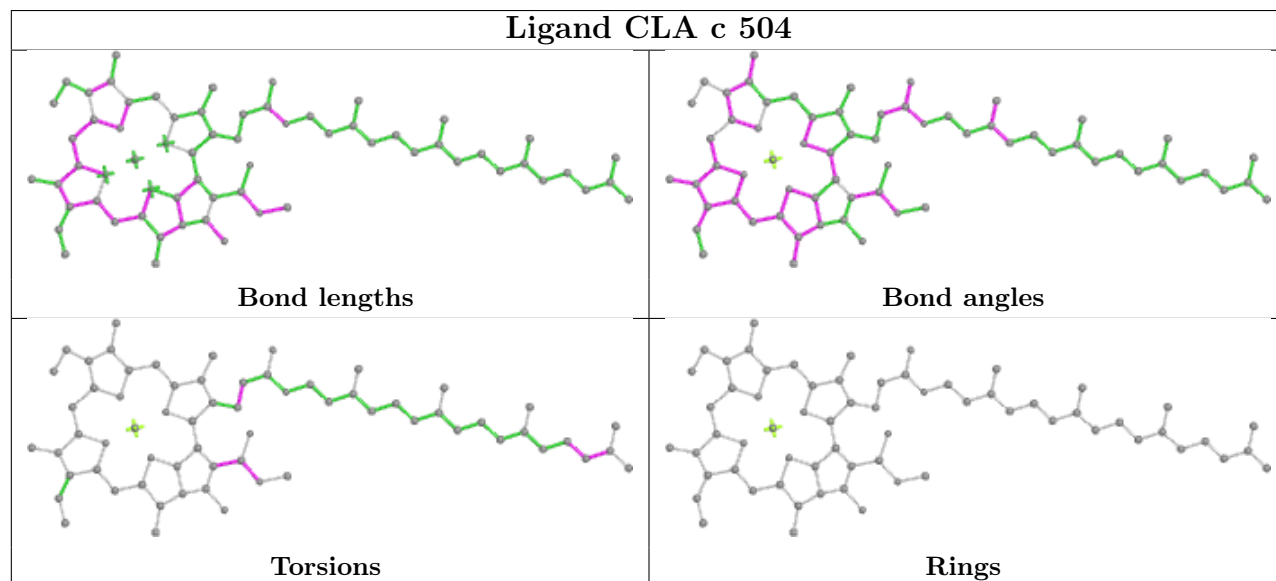
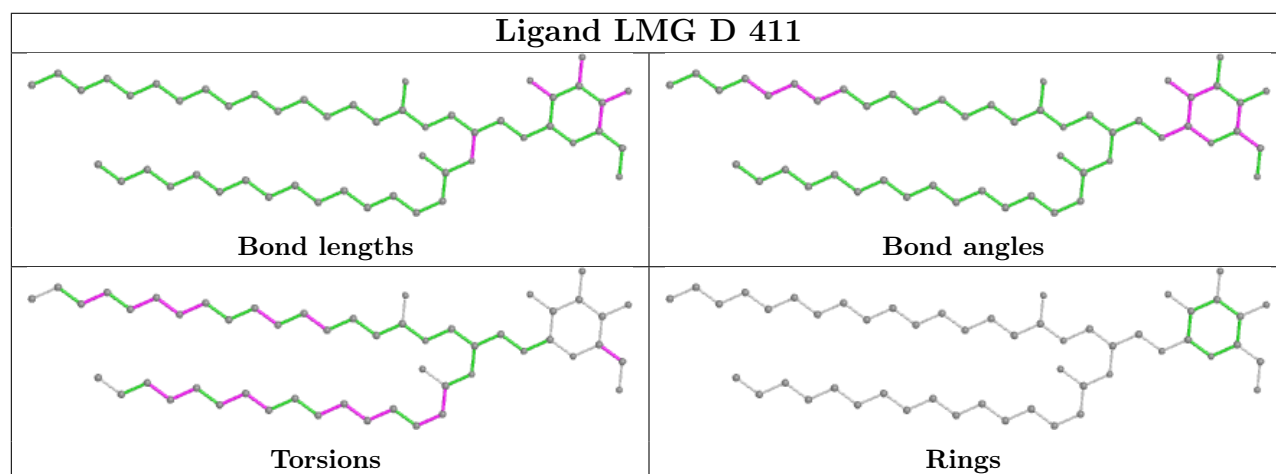
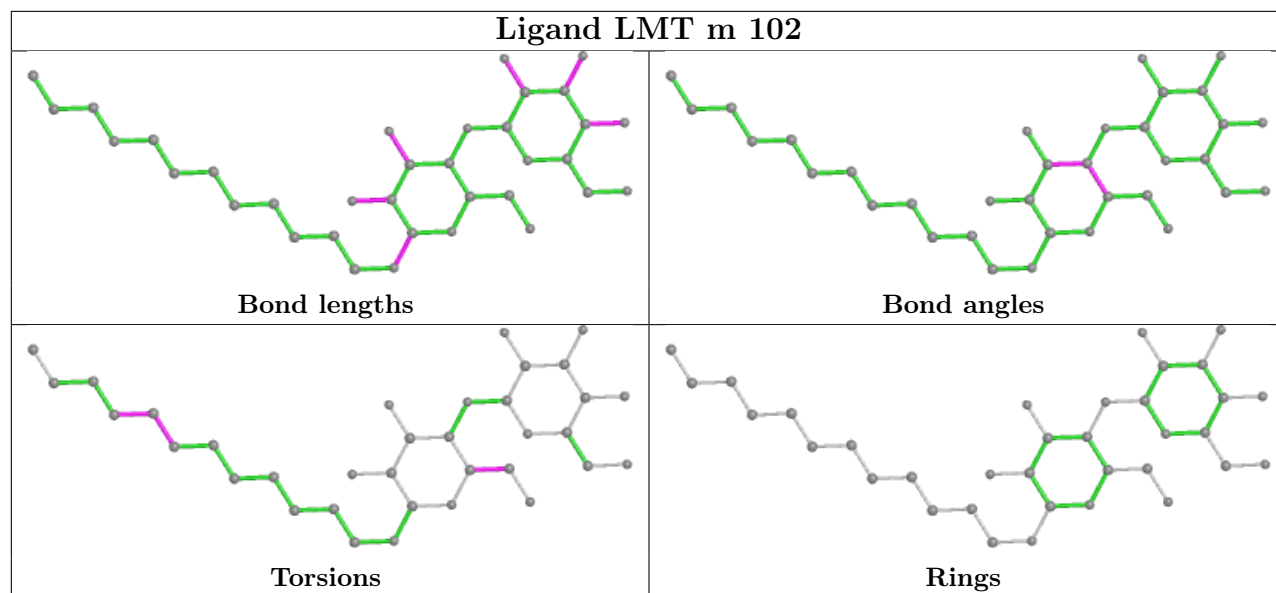


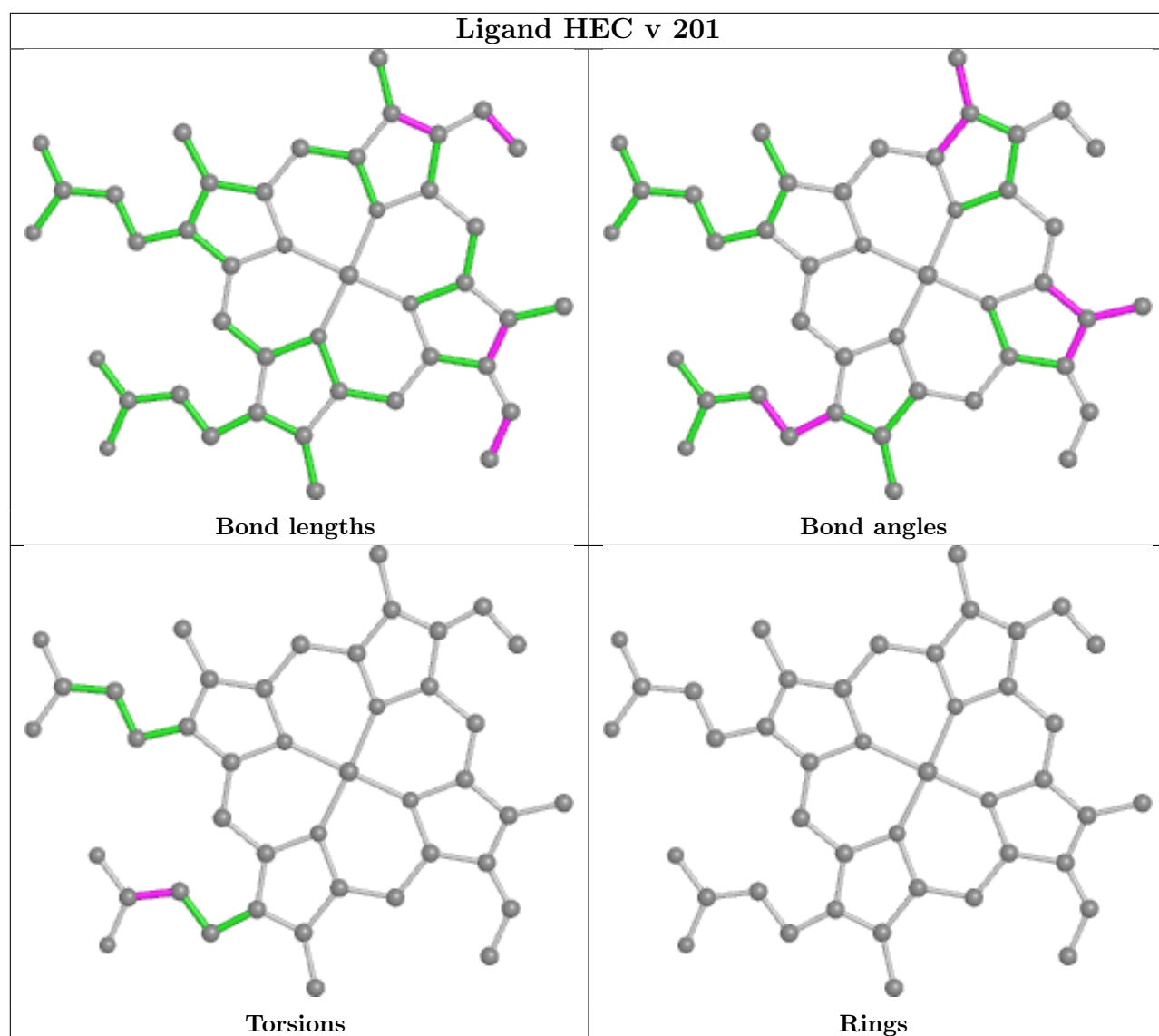
Ligand LMT j 102

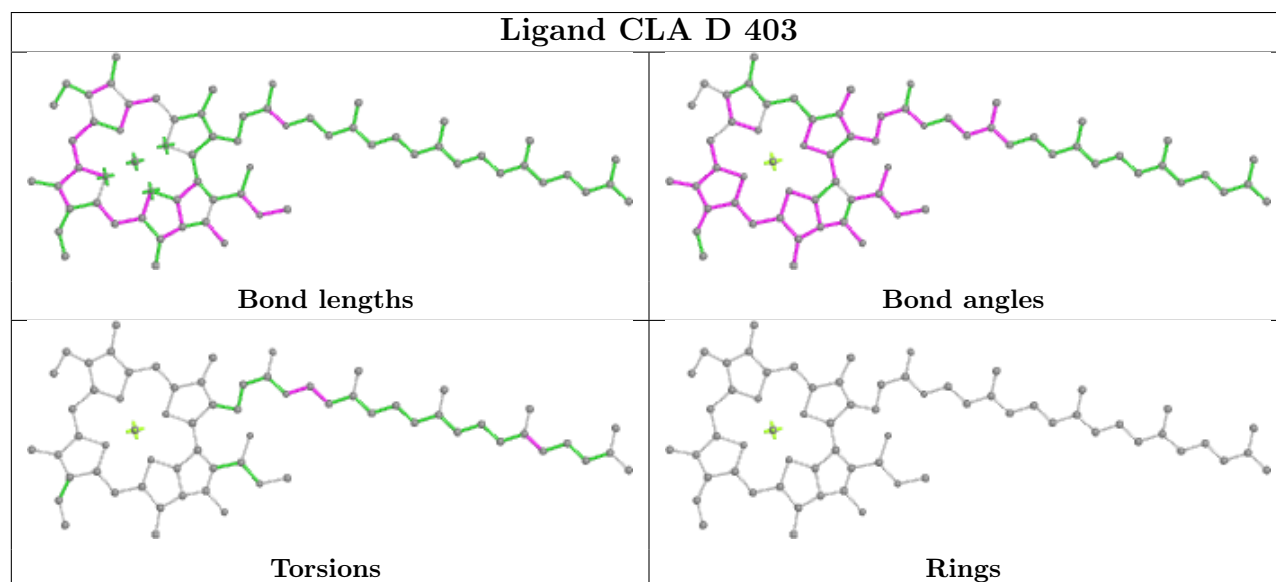
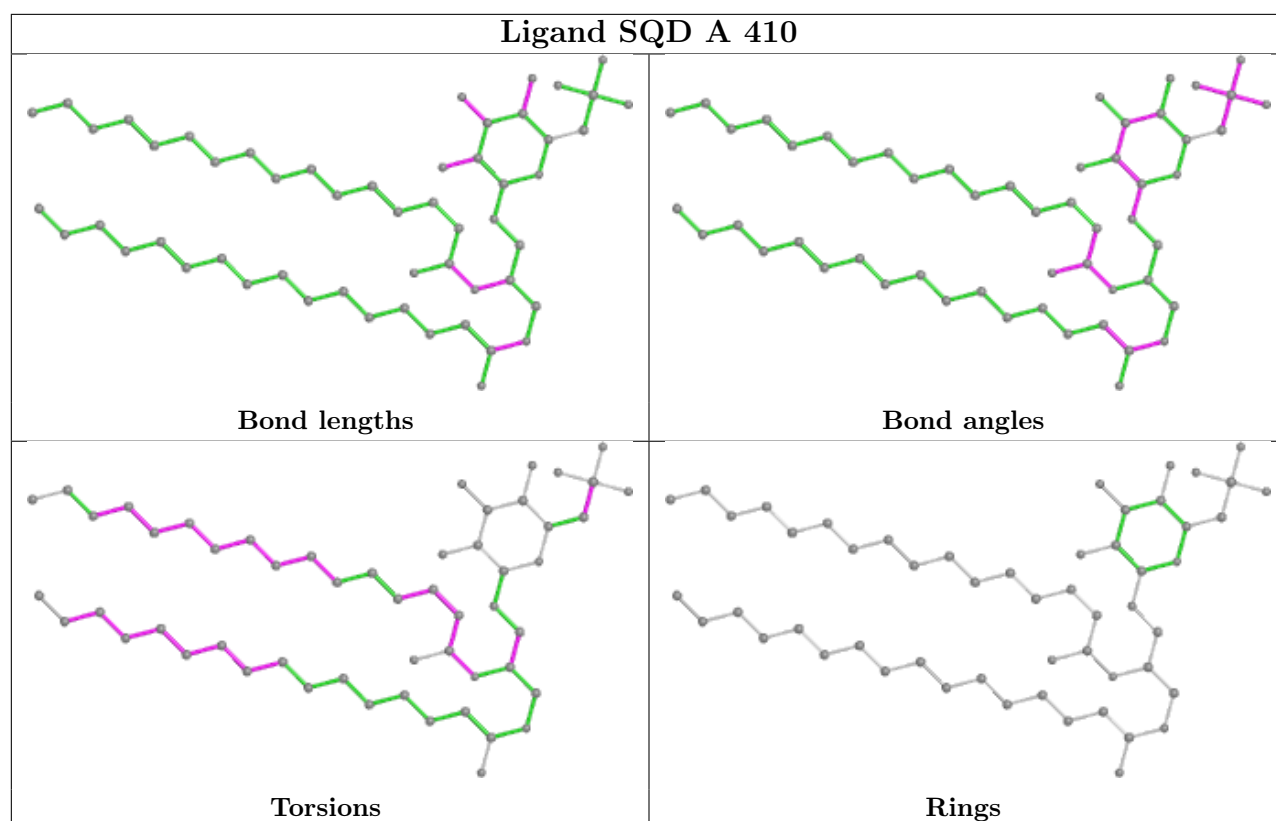


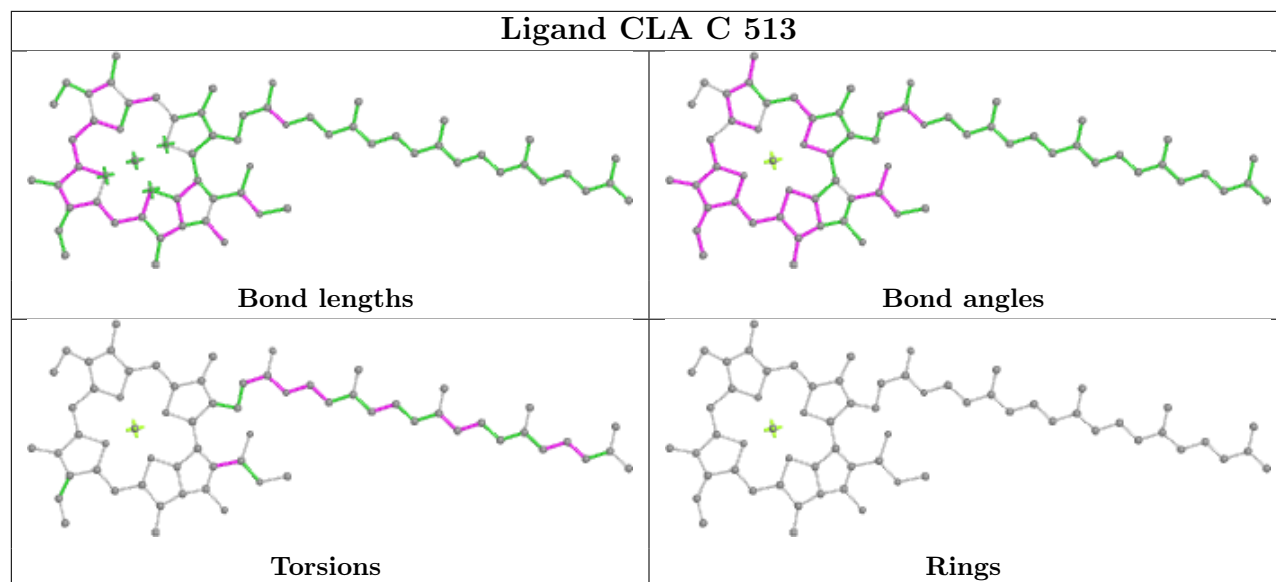
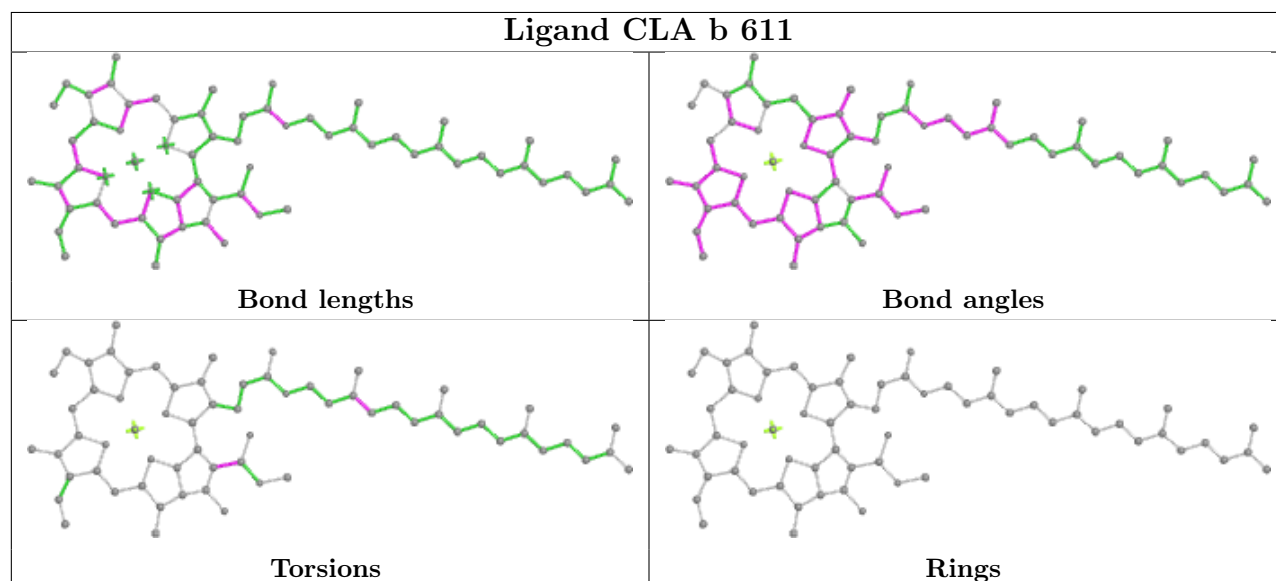
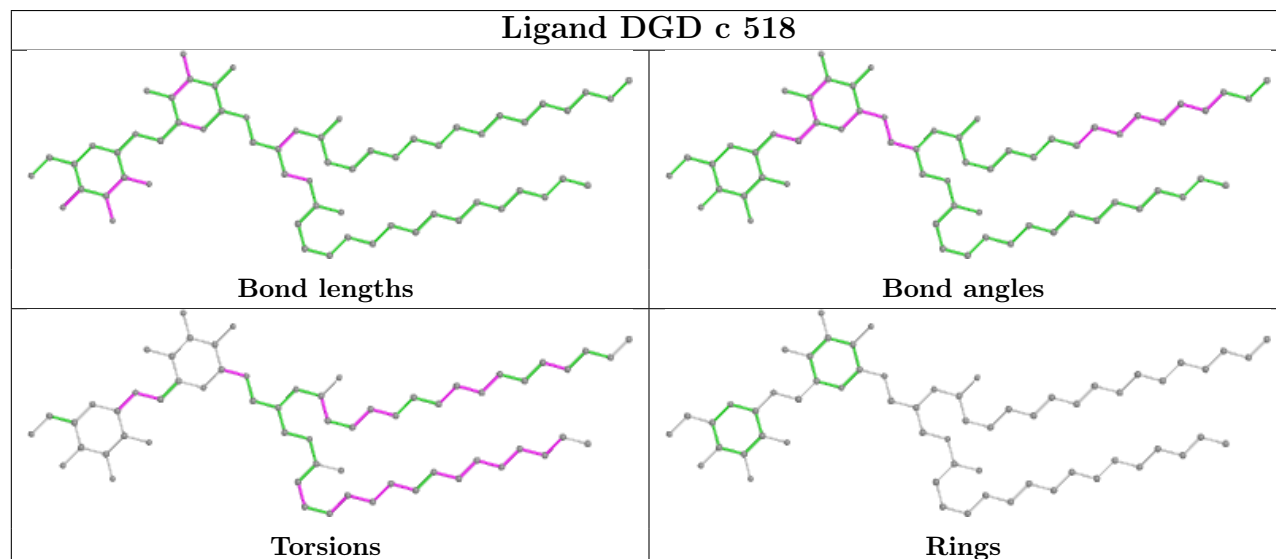
Ligand CLA C 506

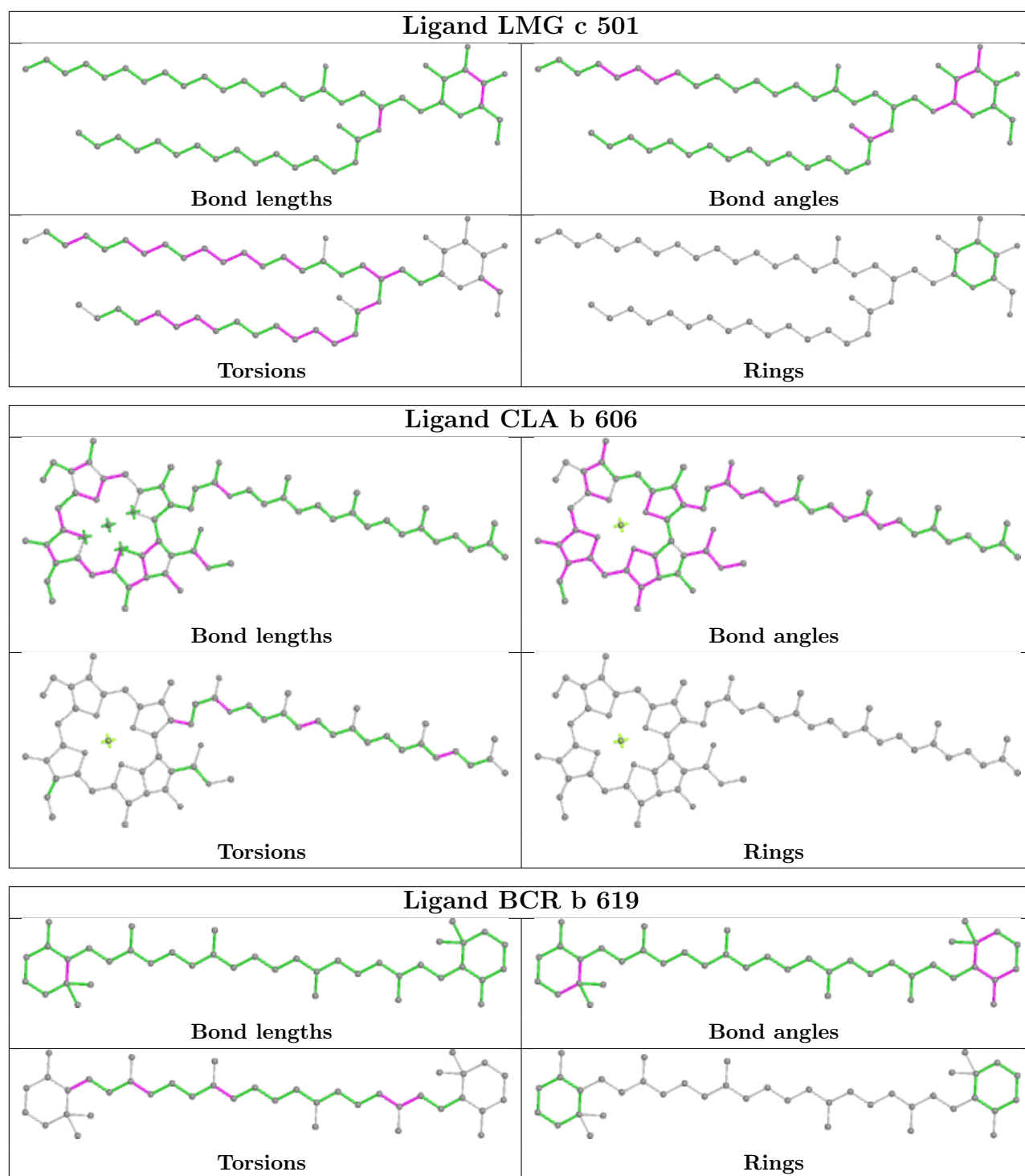


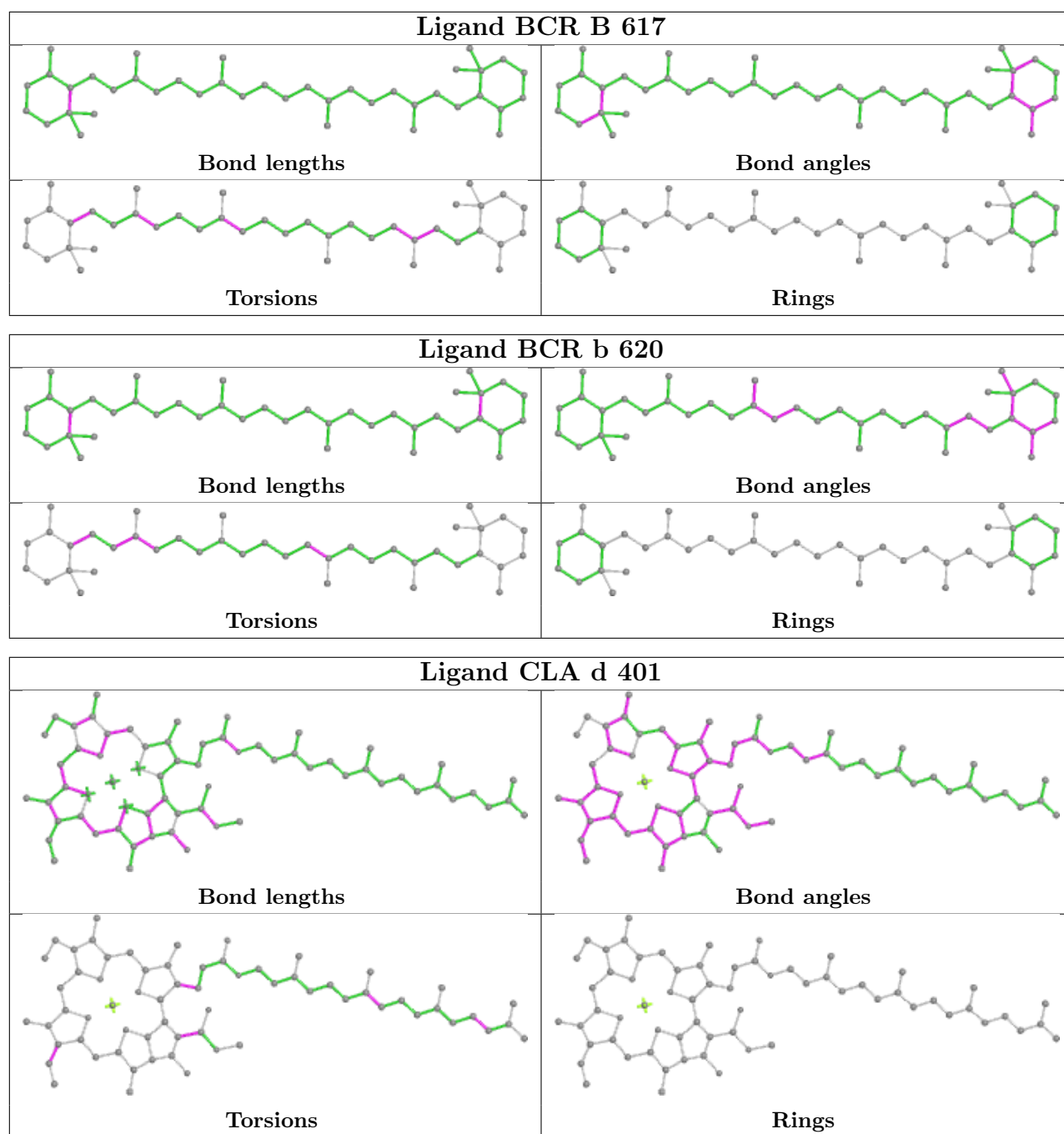


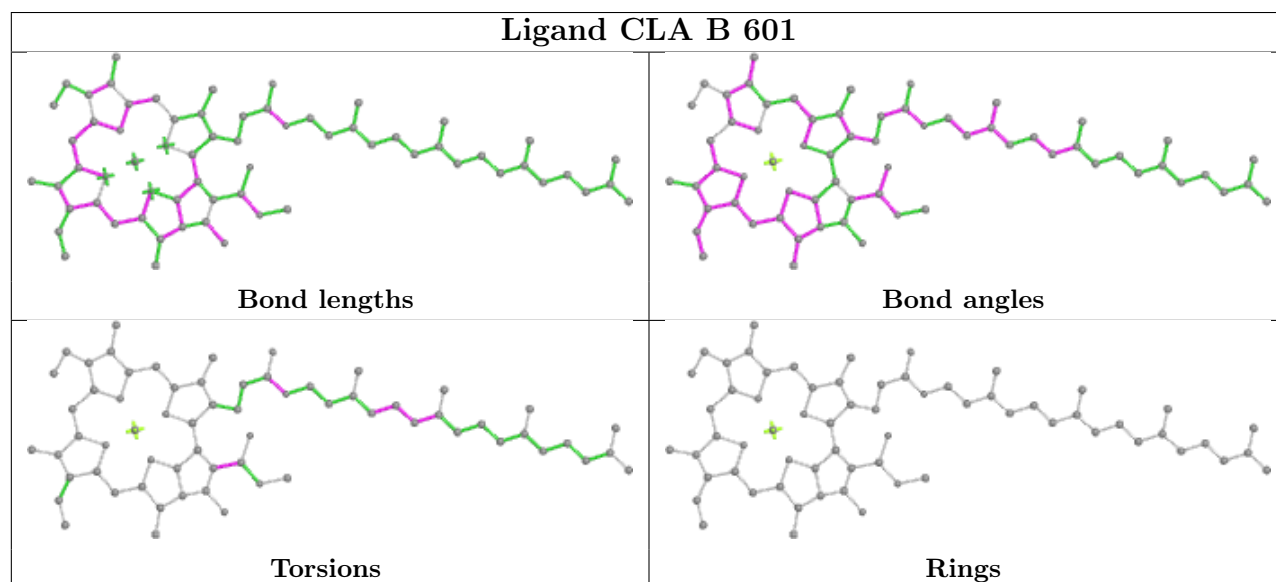
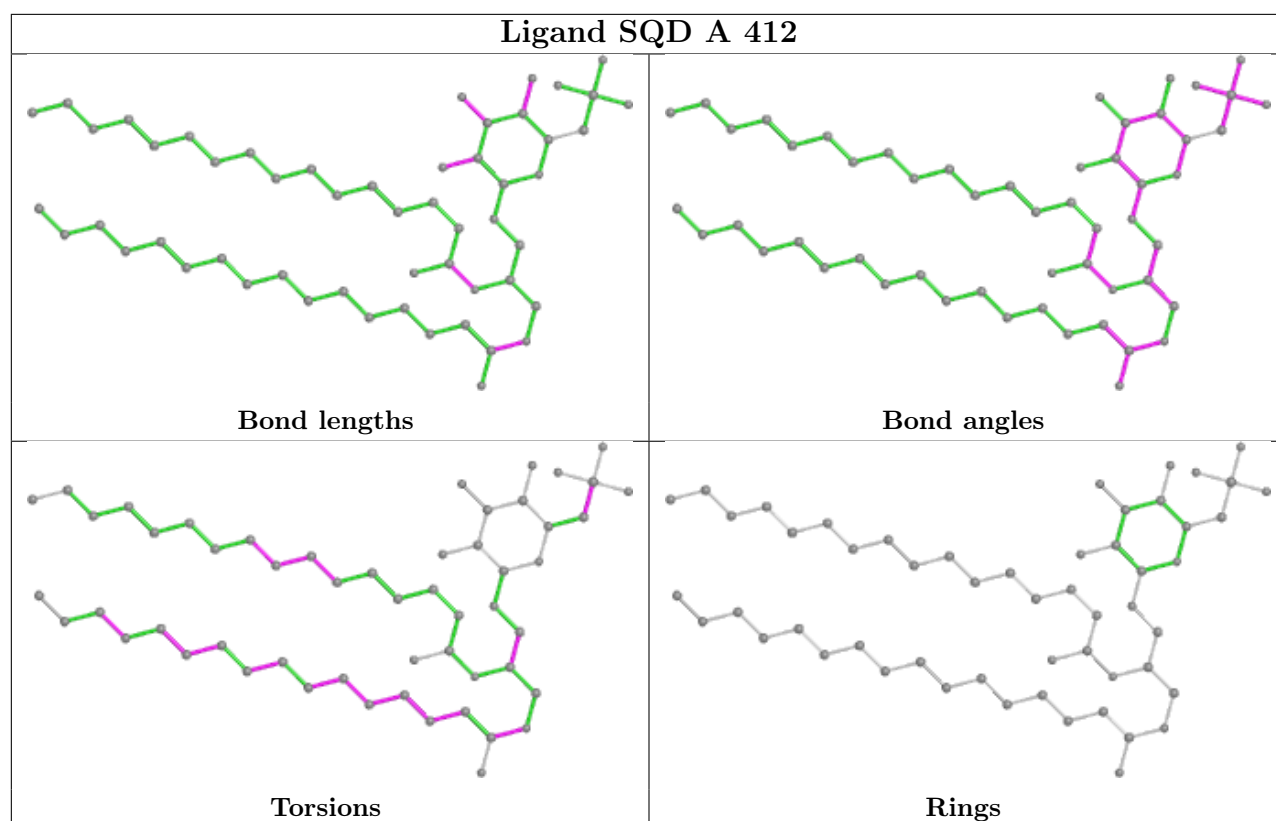


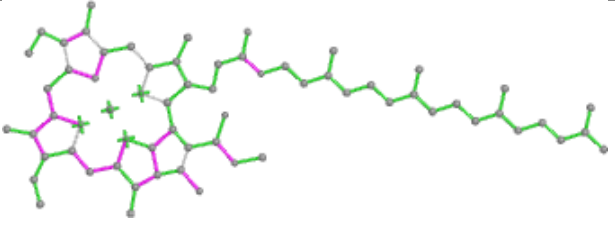
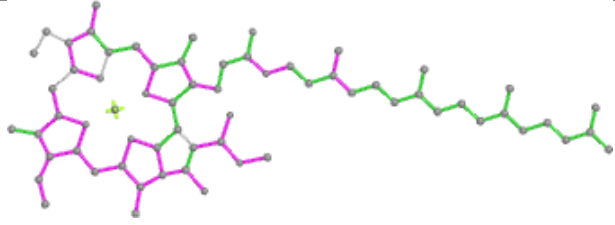
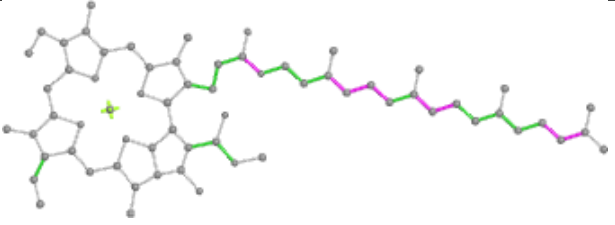
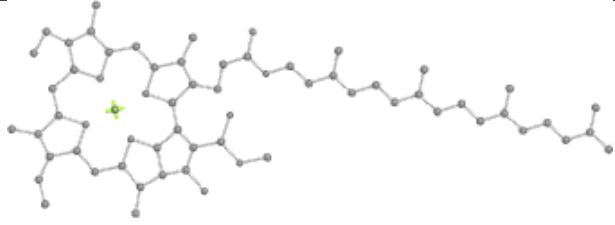
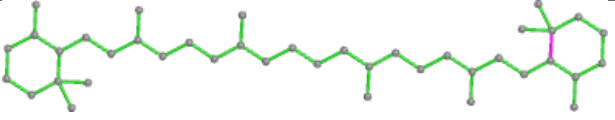
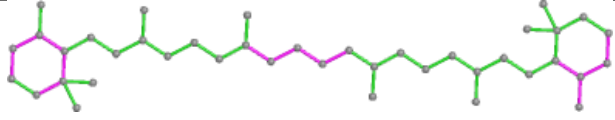
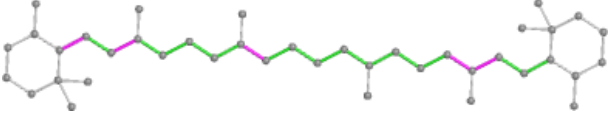
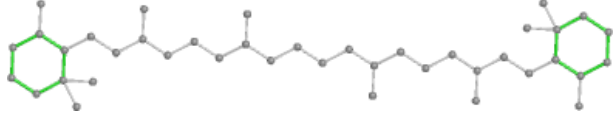
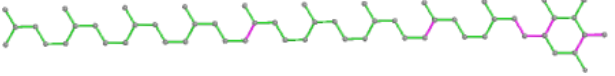
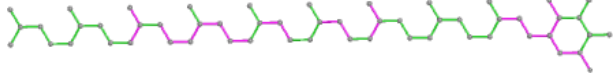
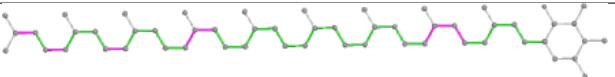
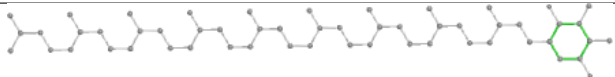


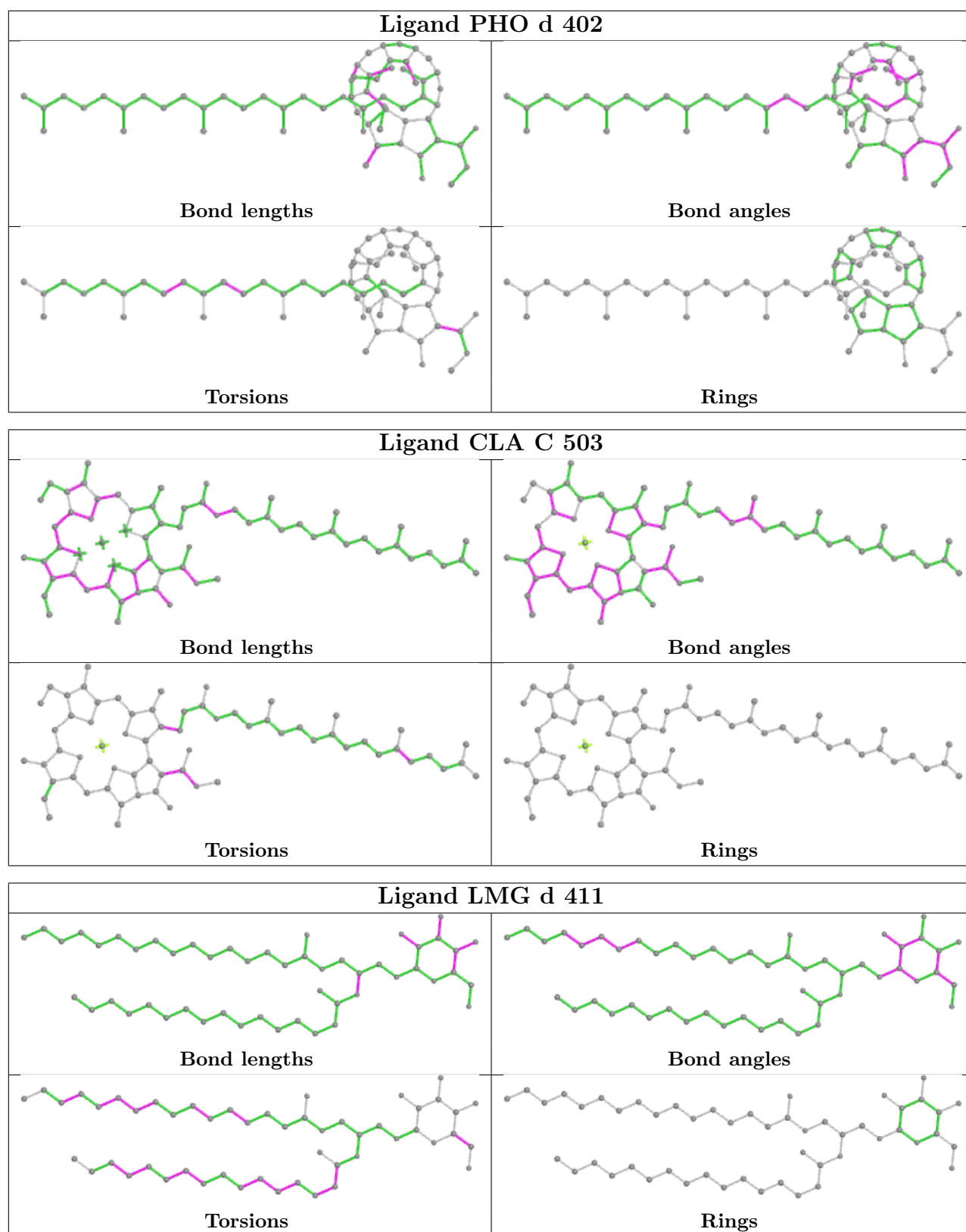
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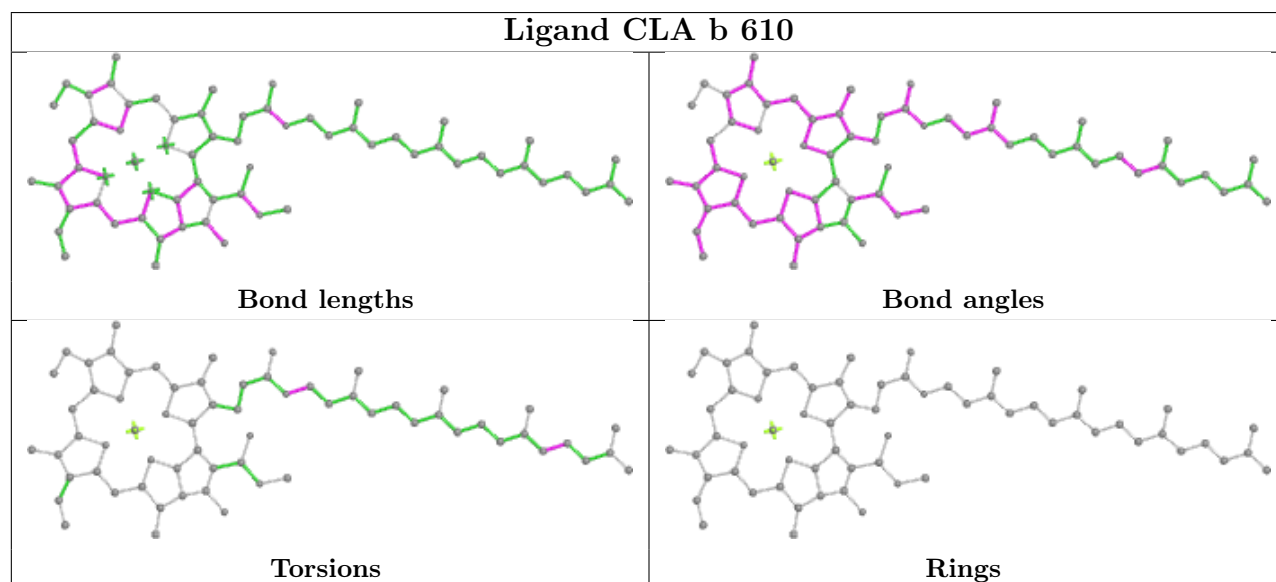
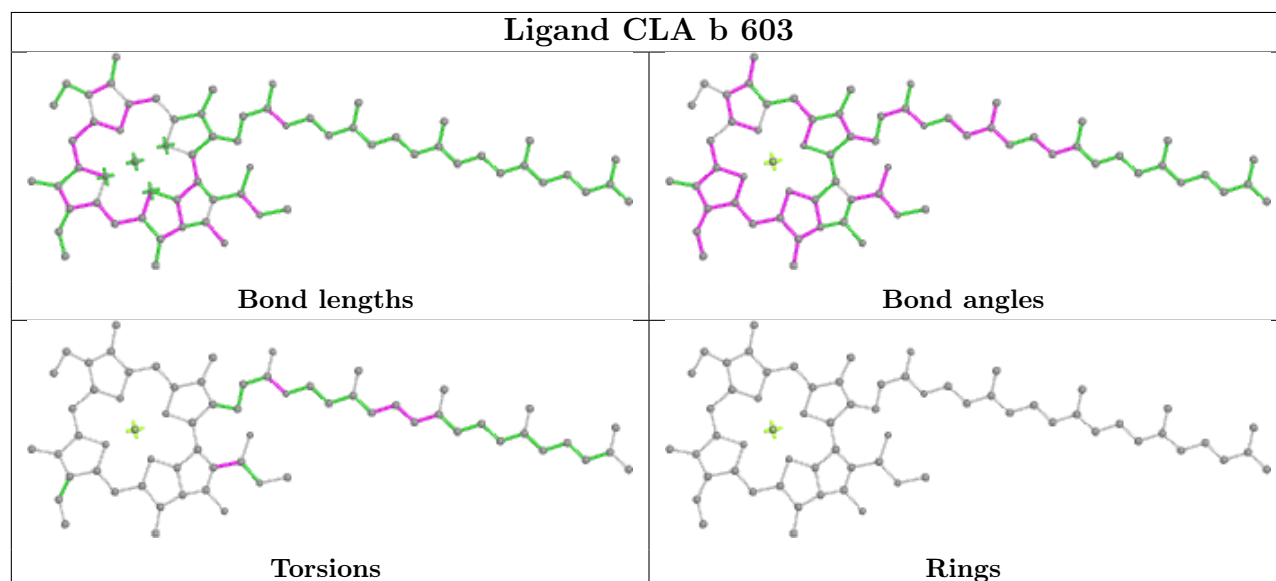
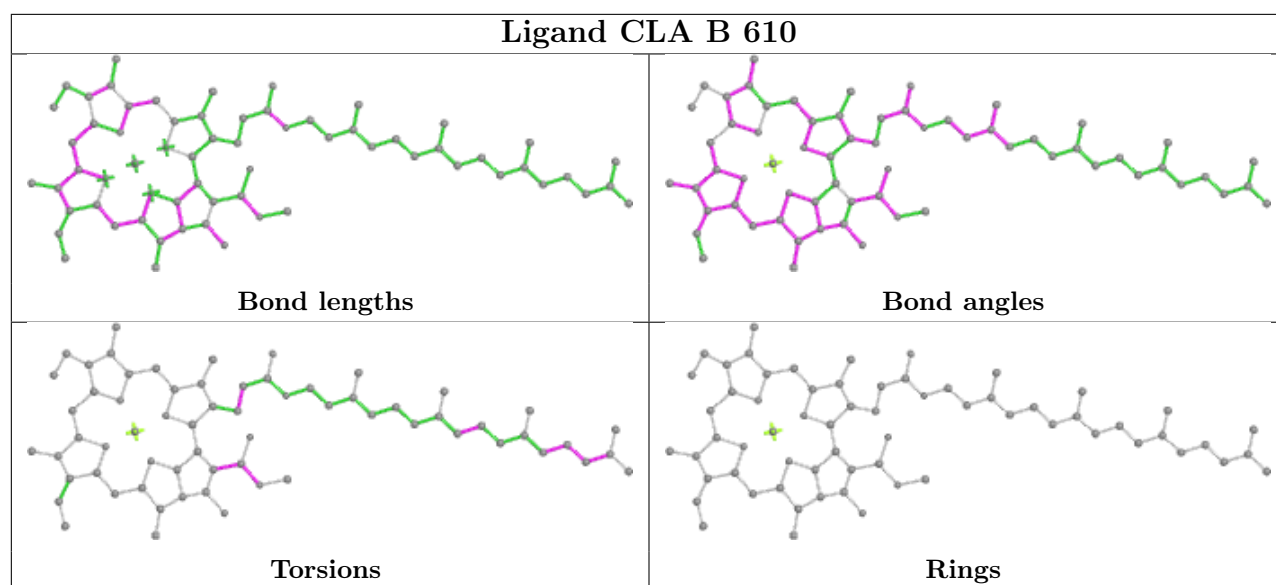


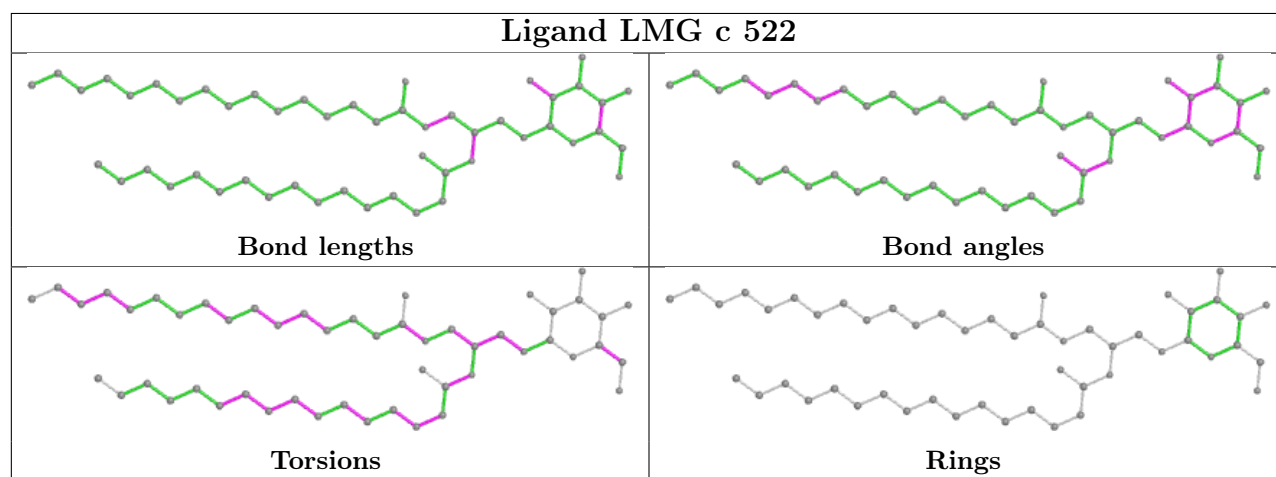
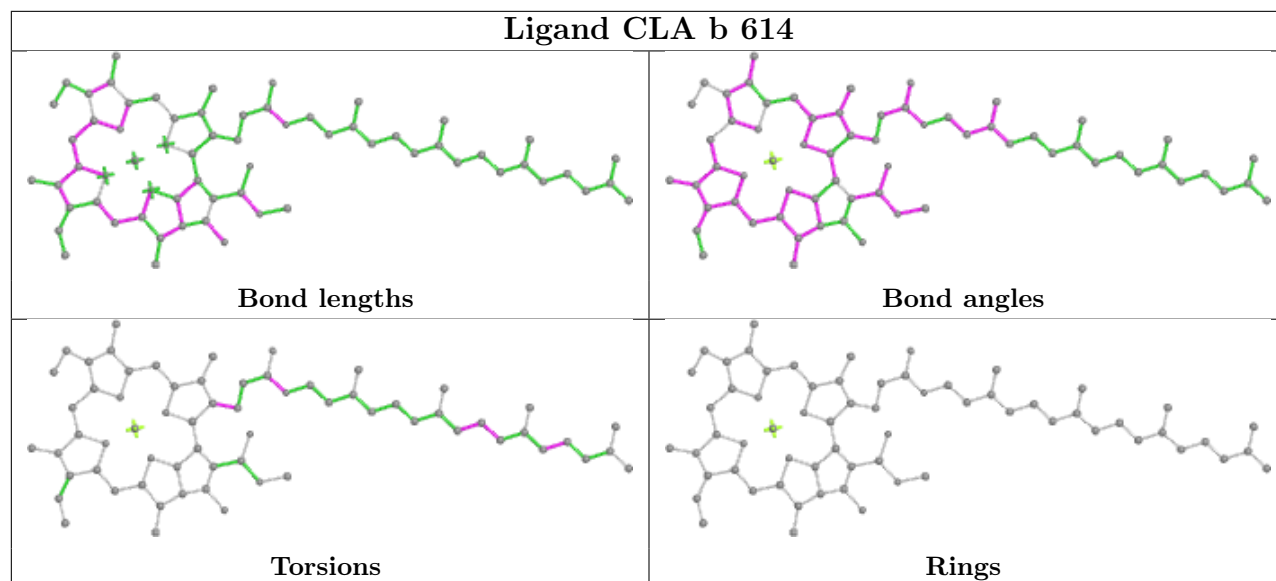
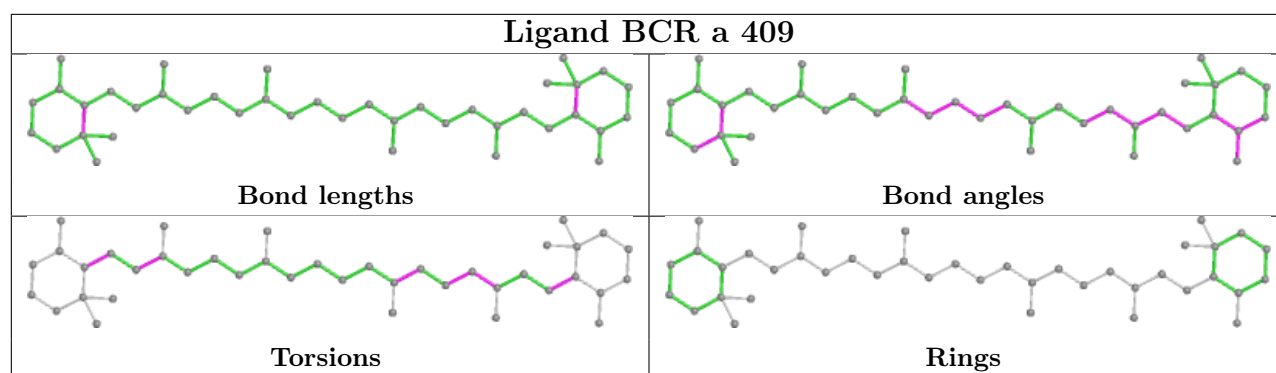




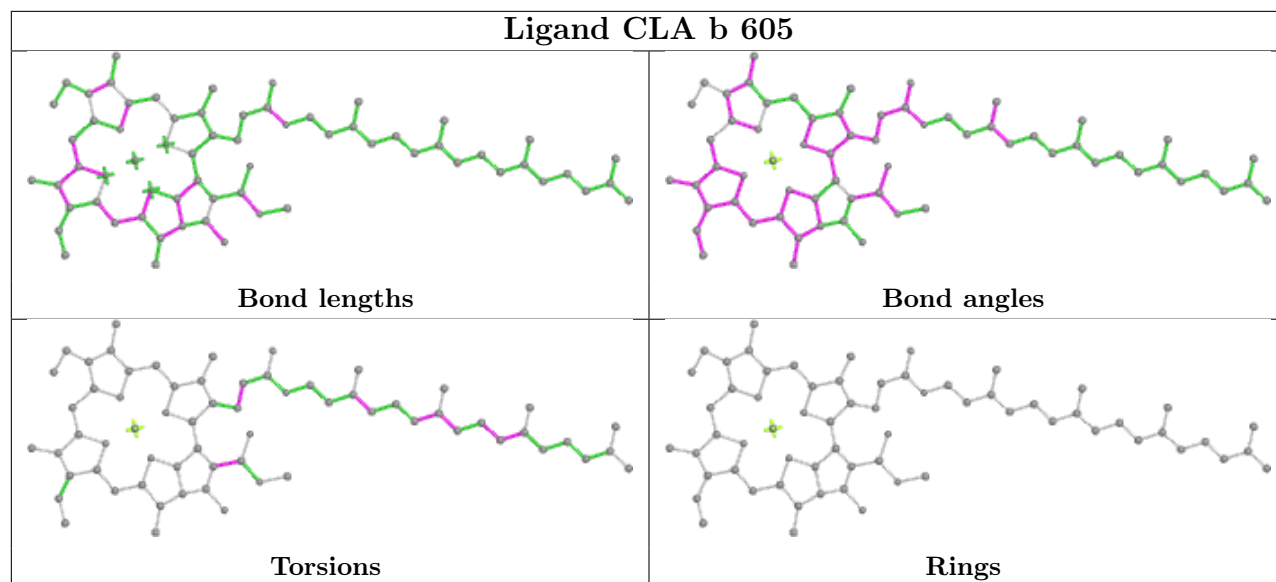
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 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 627	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PL9 D 406	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



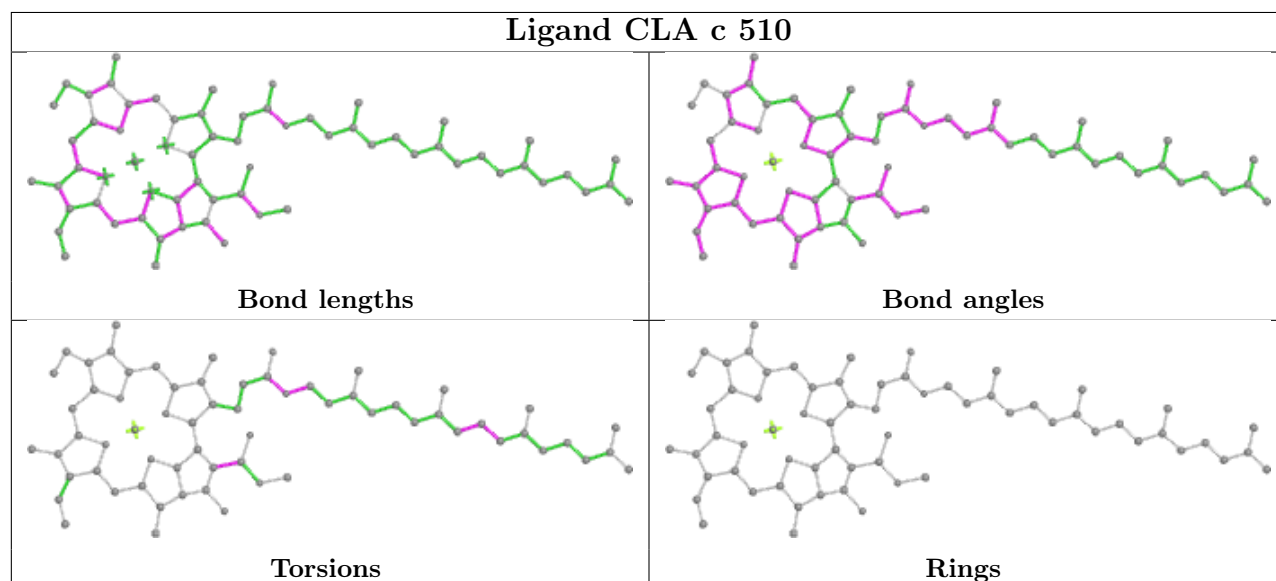




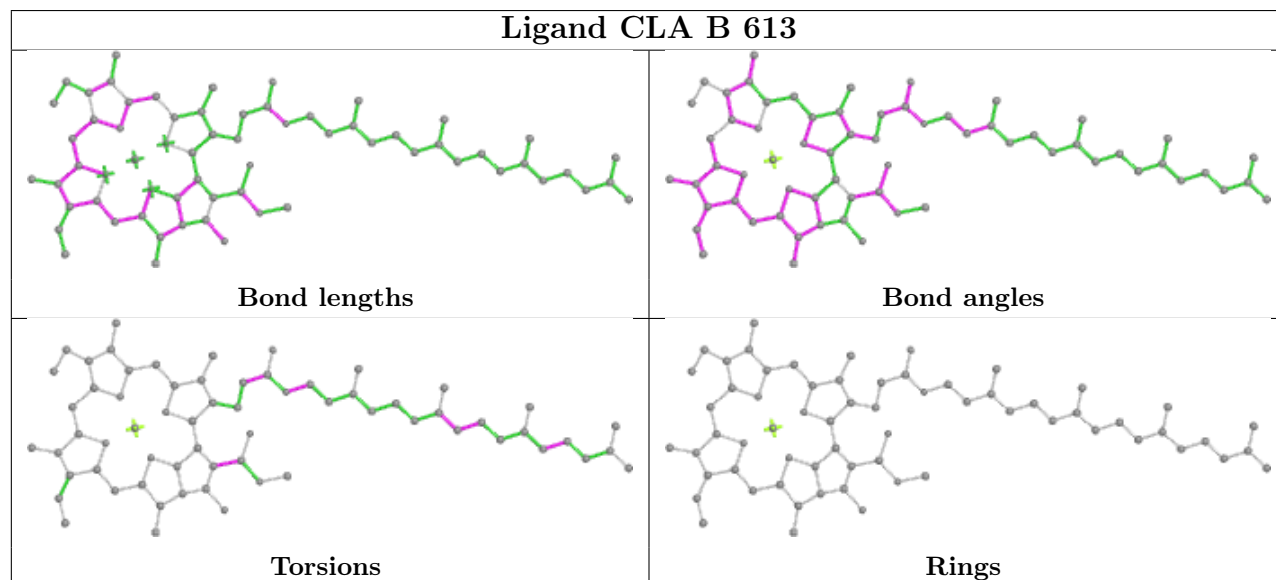
Ligand CLA b 605



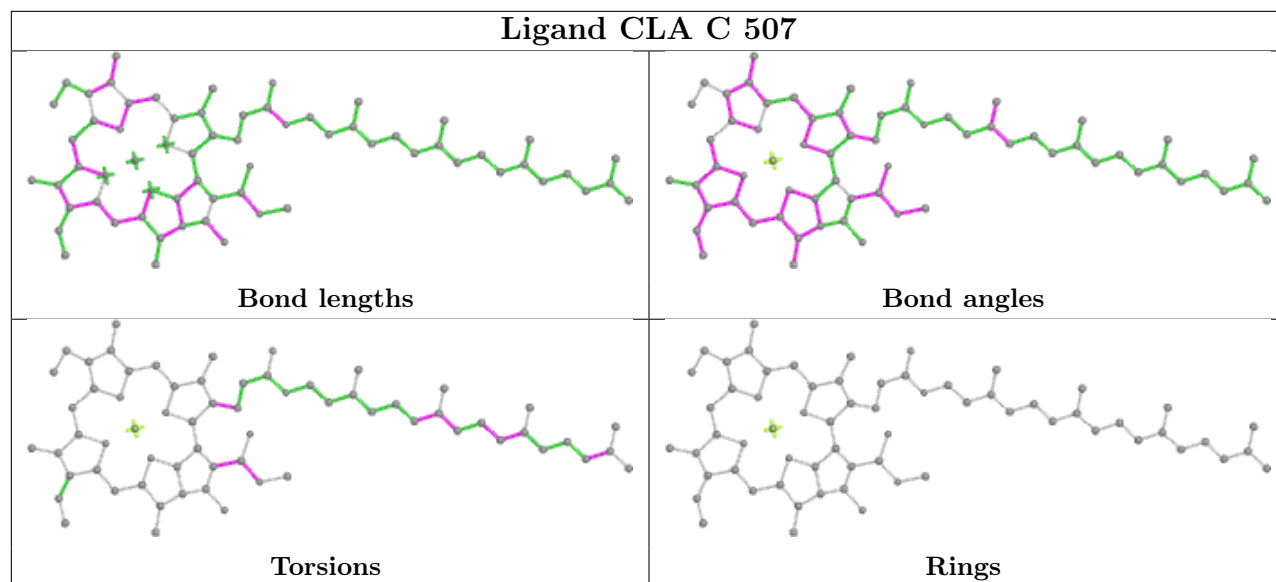
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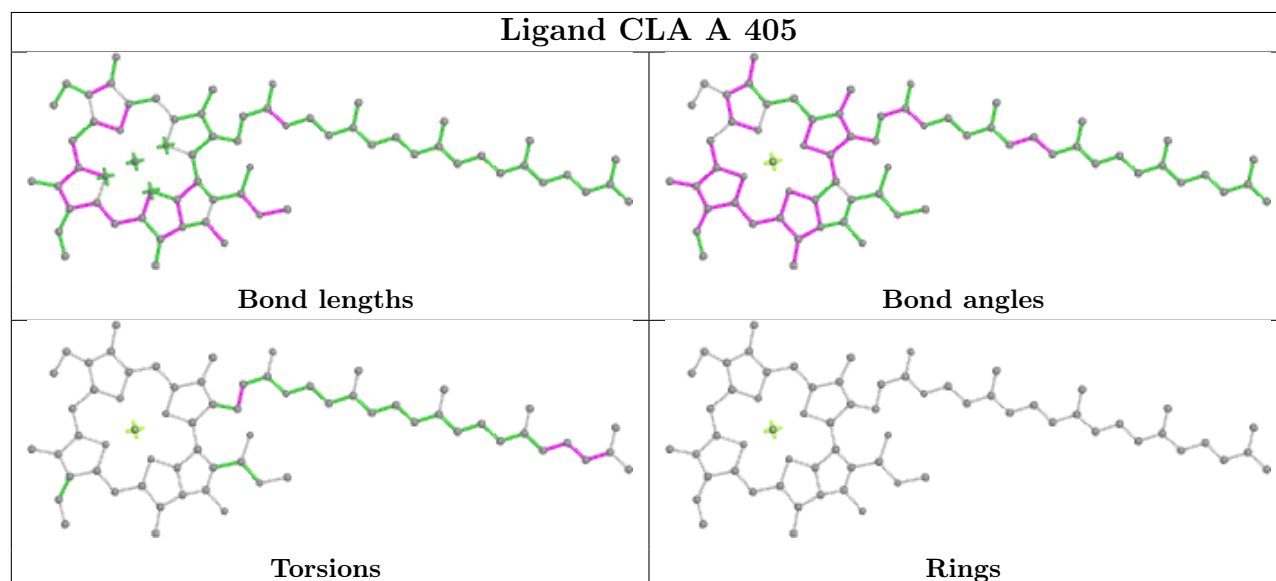
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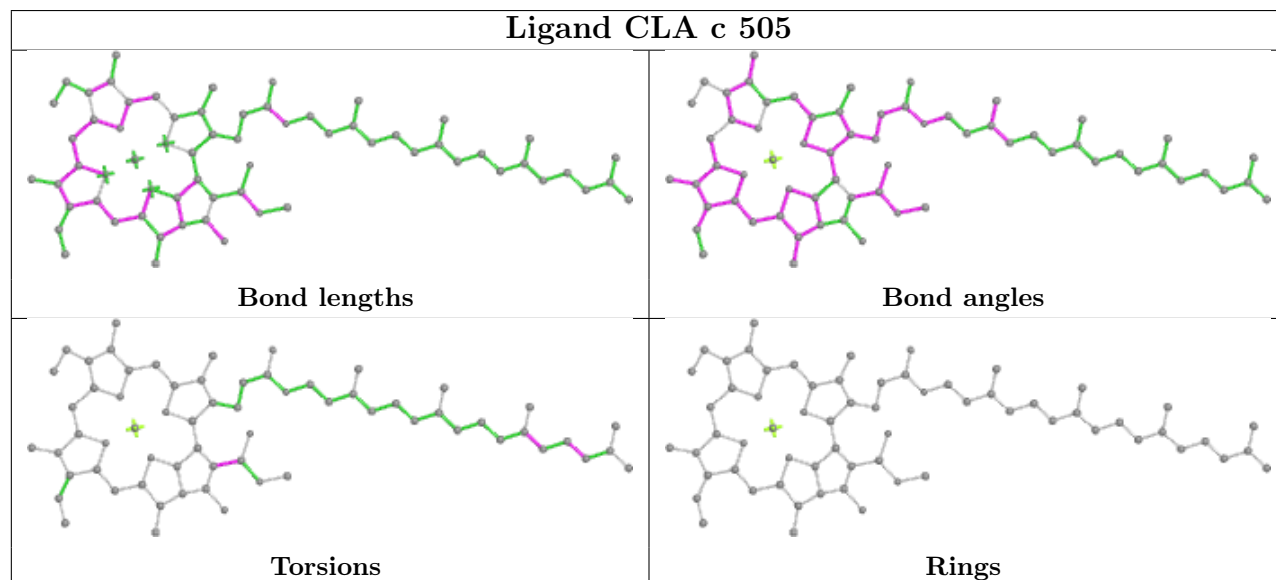
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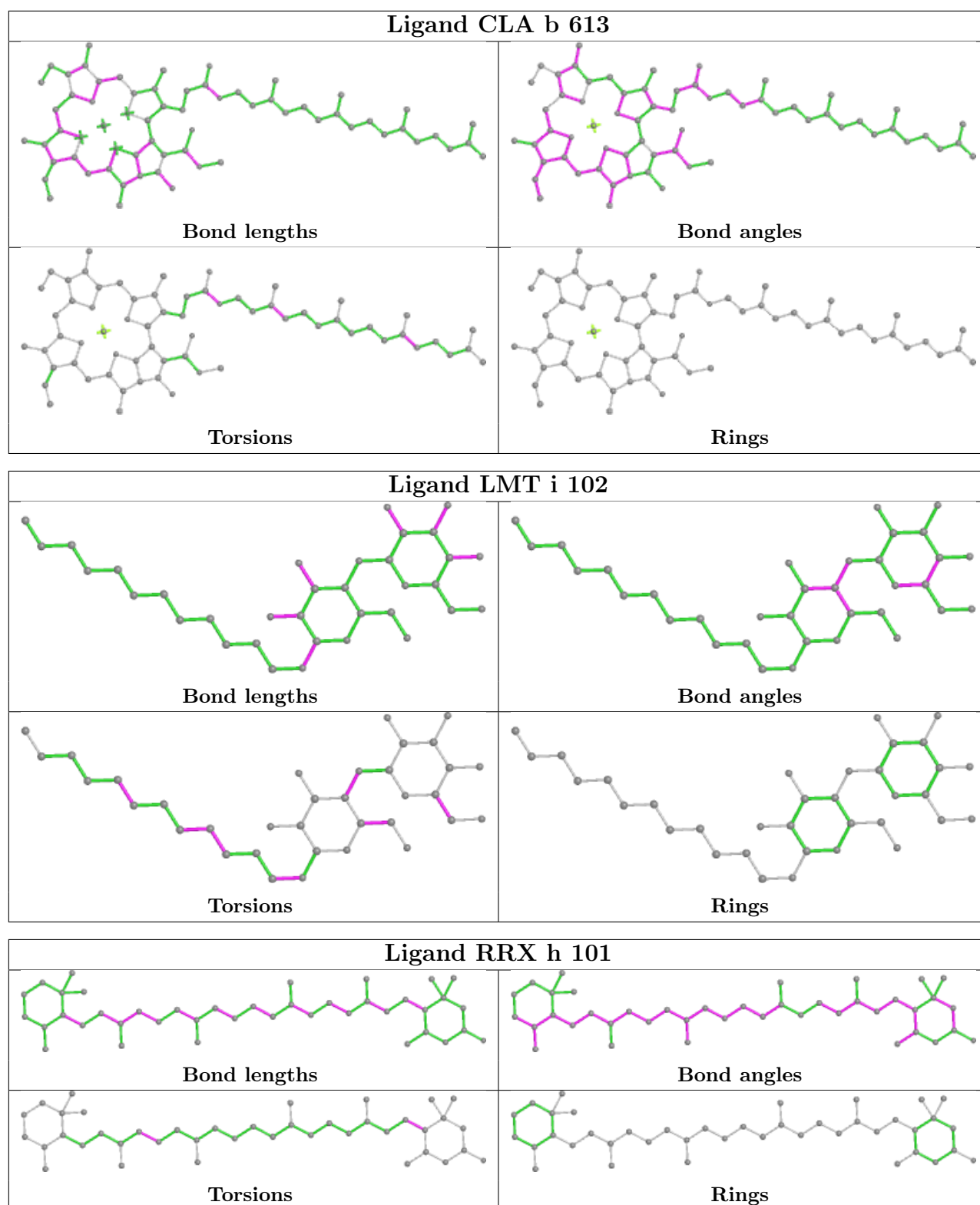


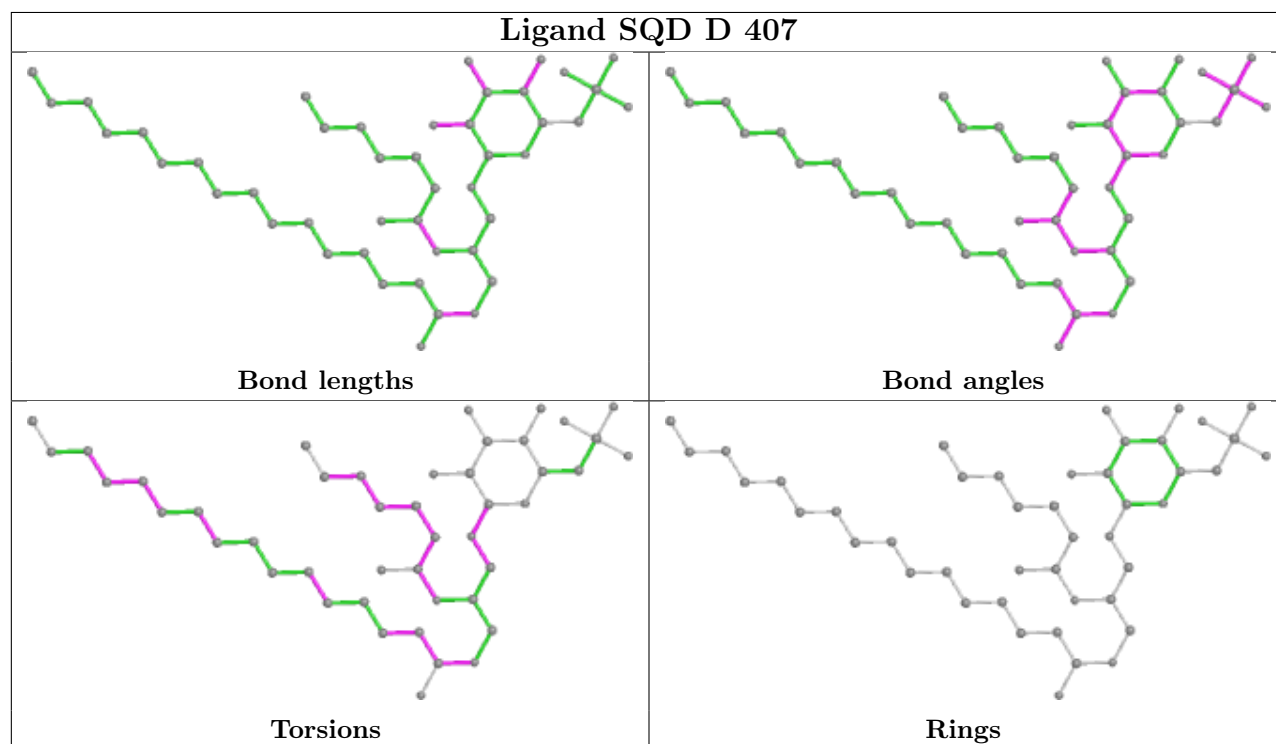
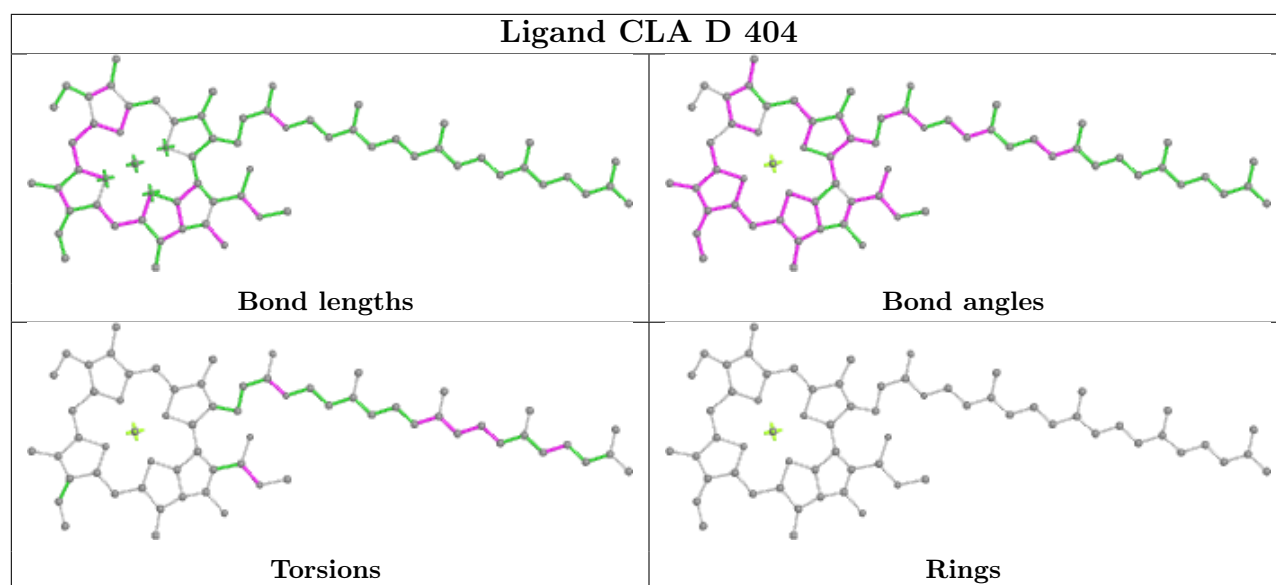
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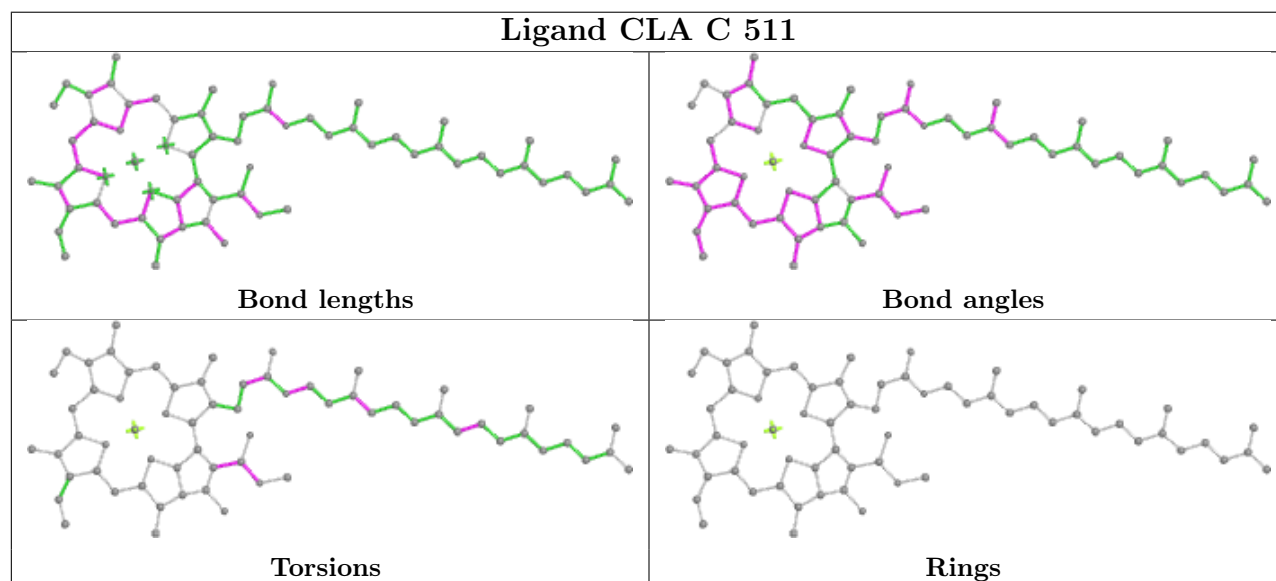
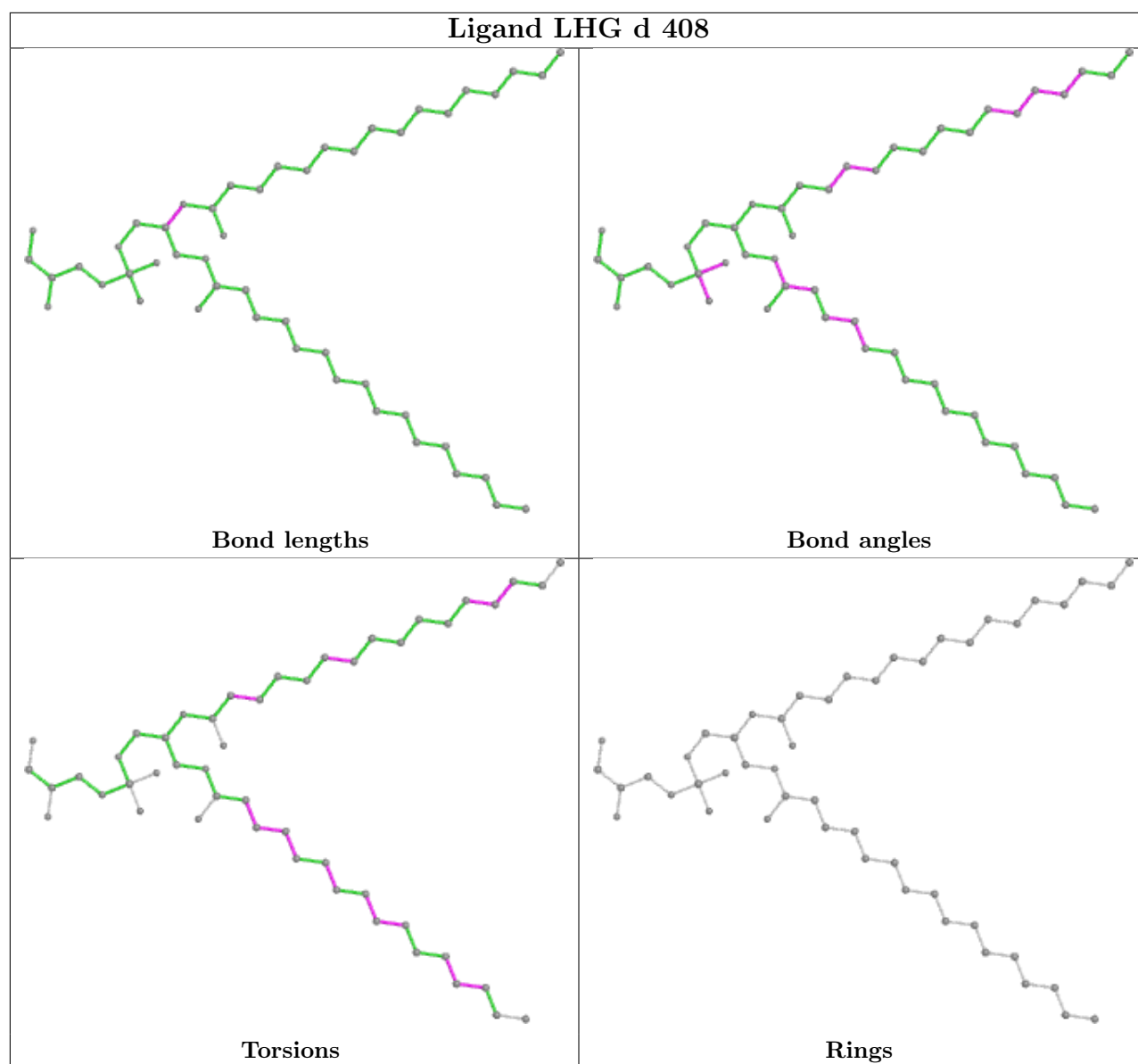


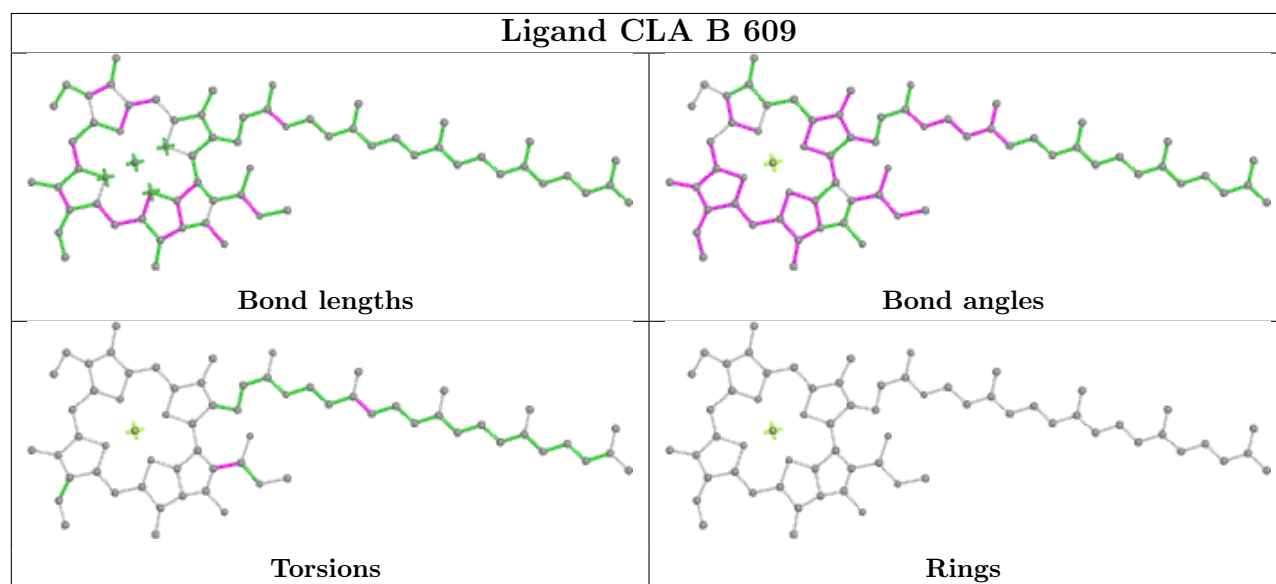
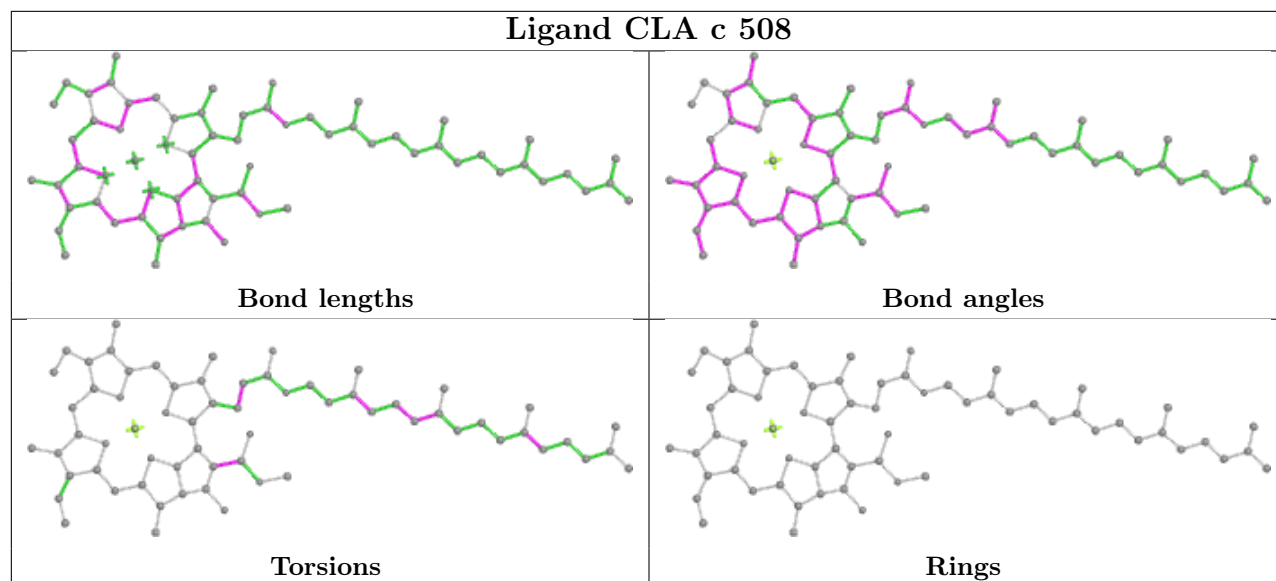
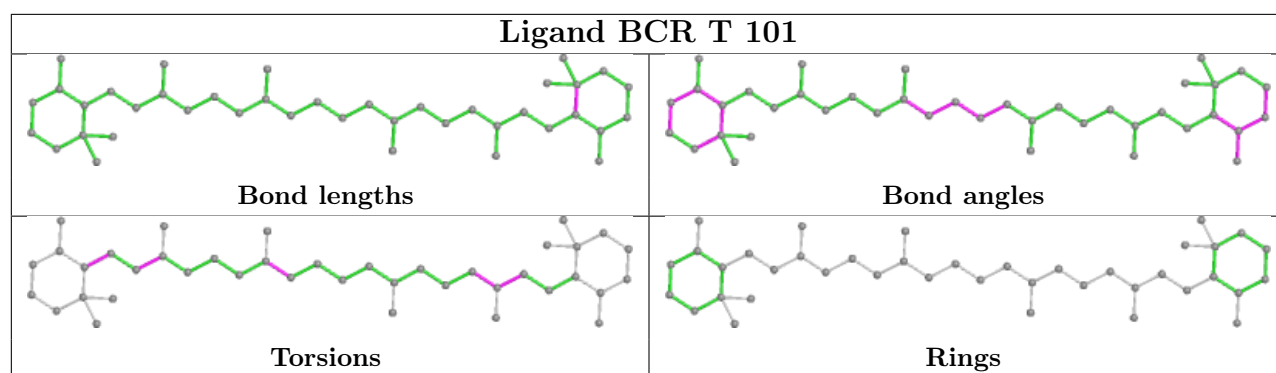
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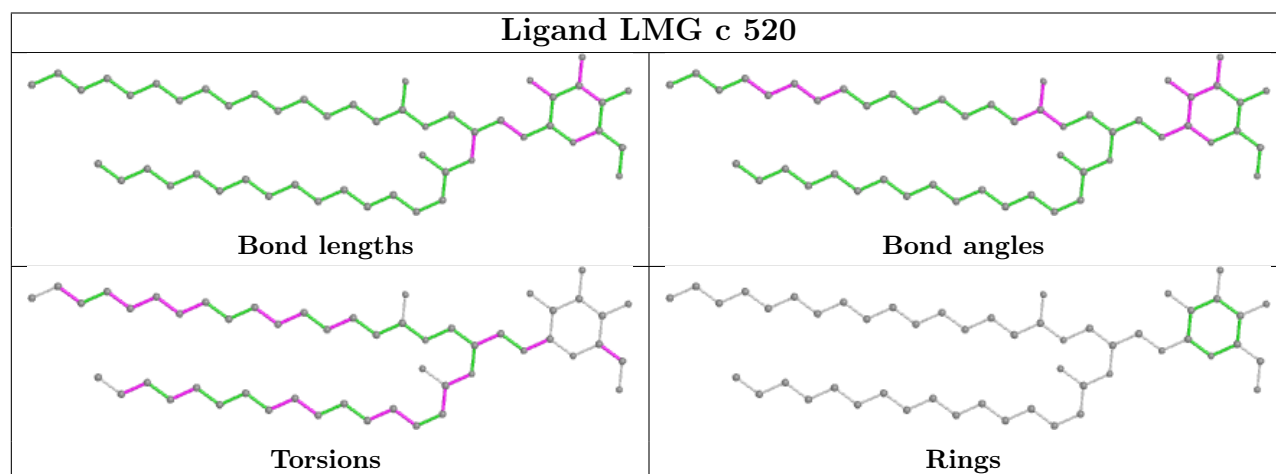
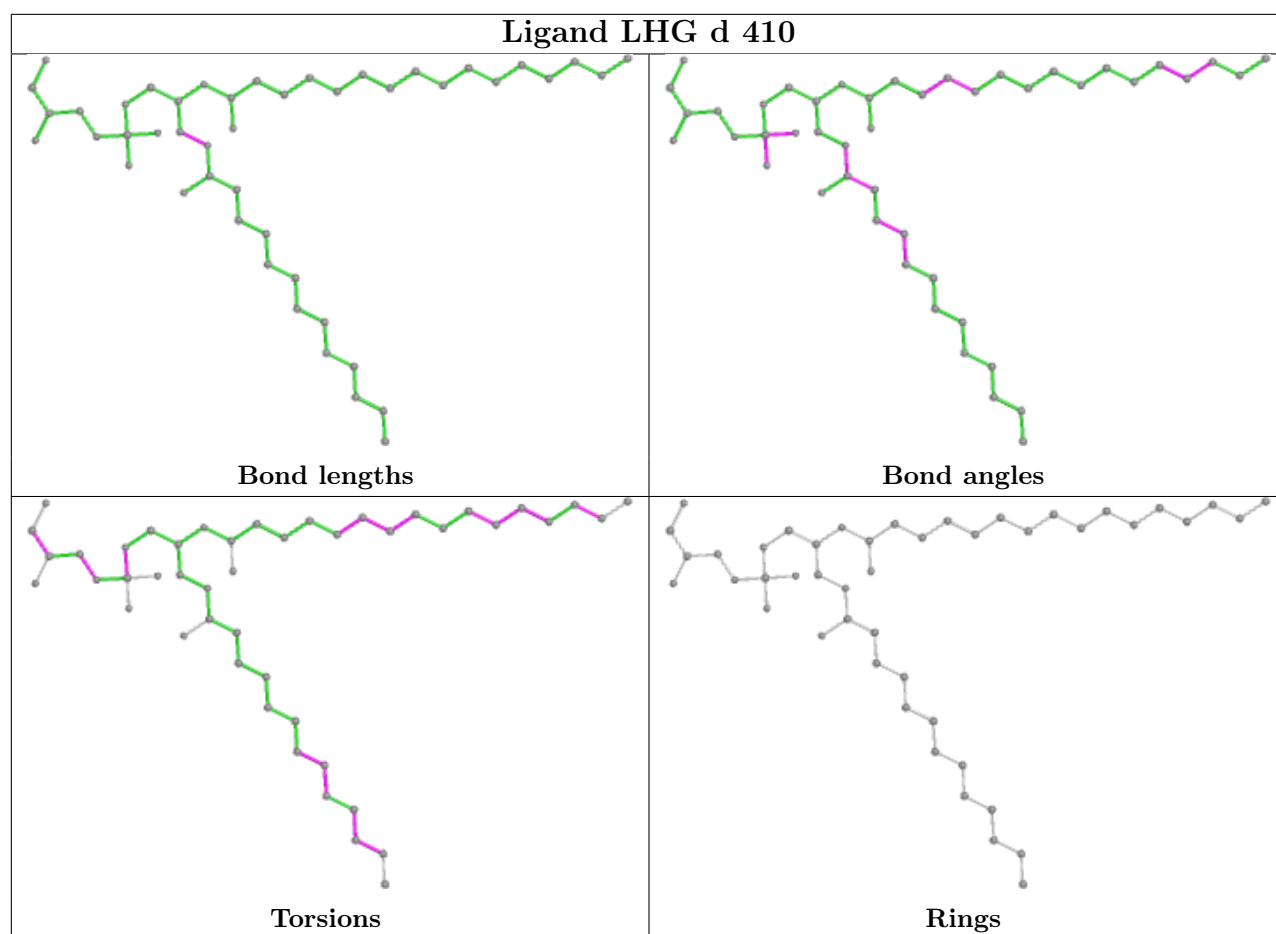


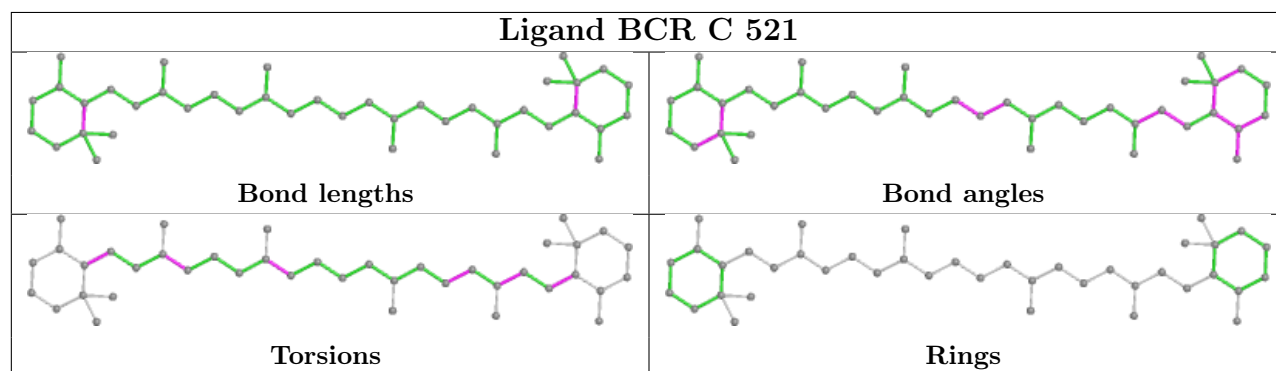
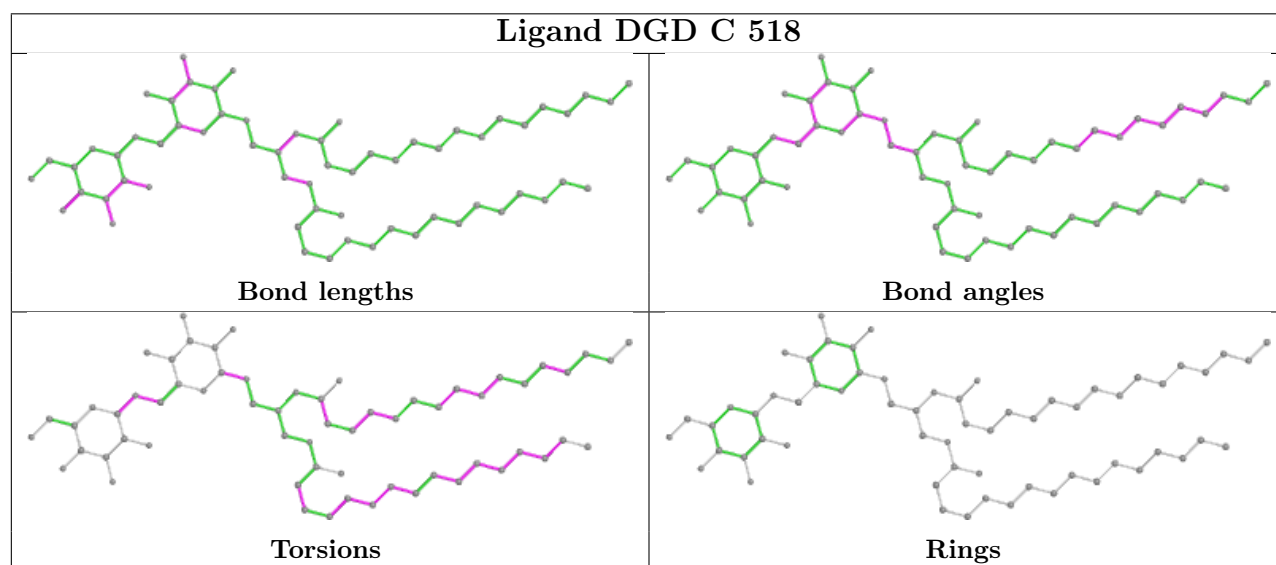
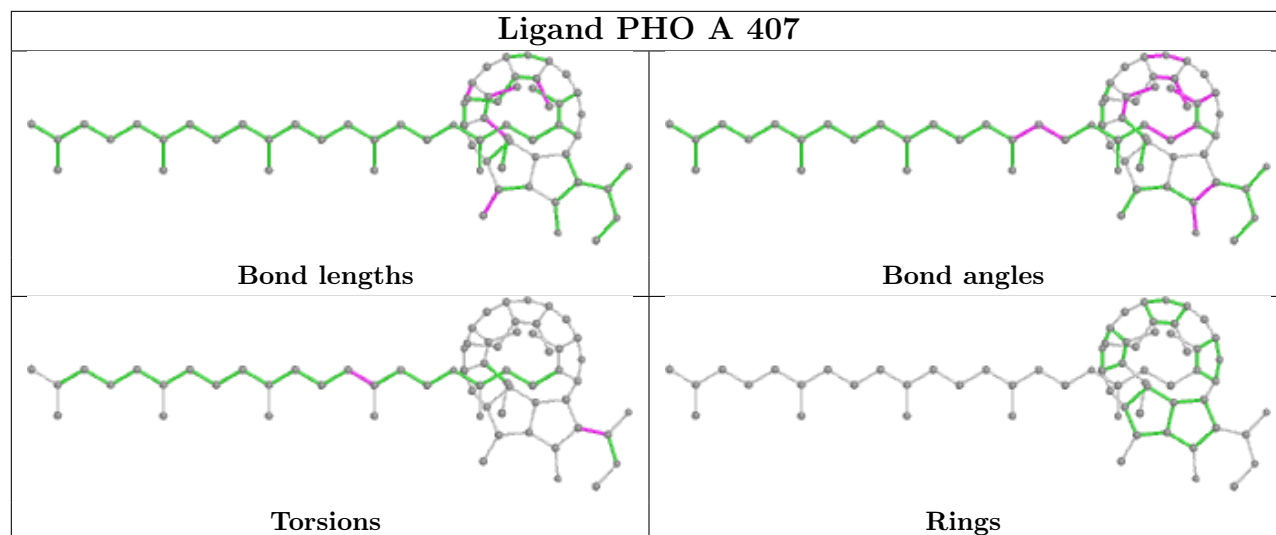


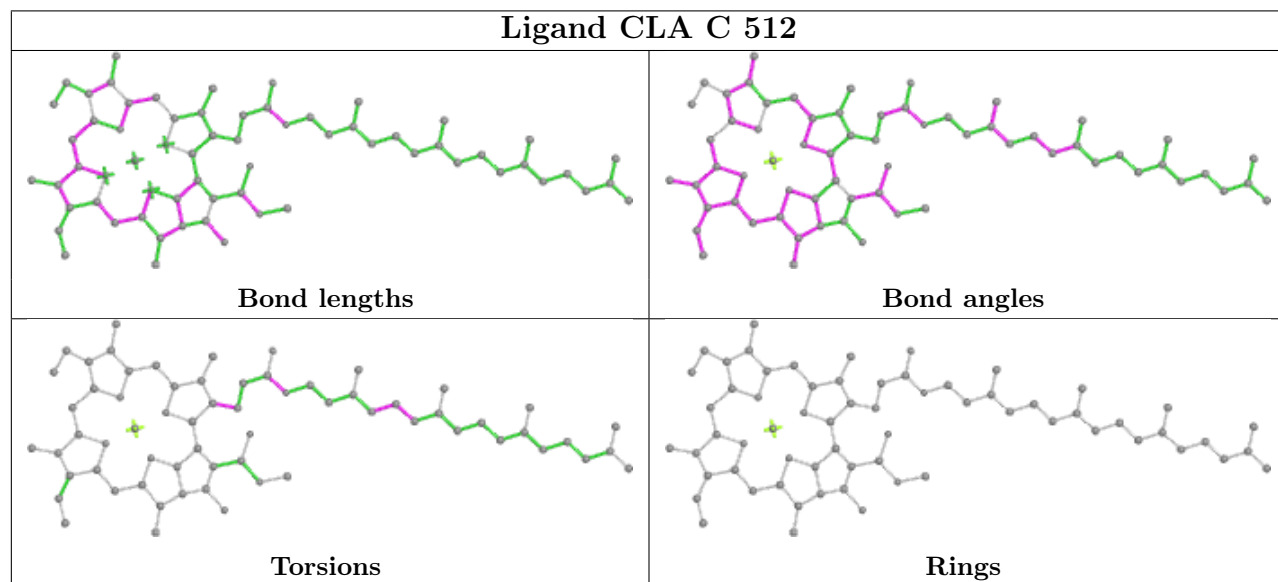
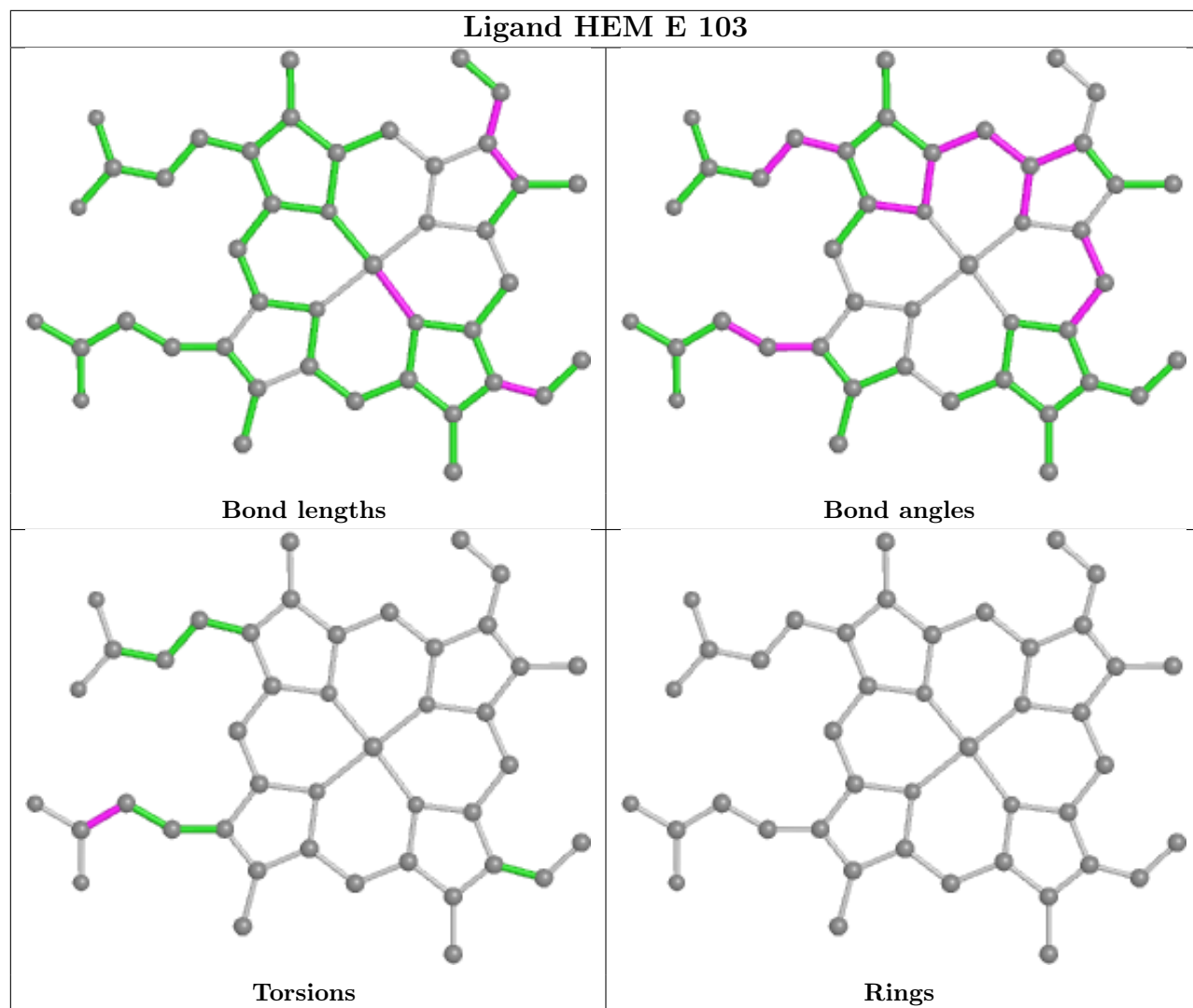




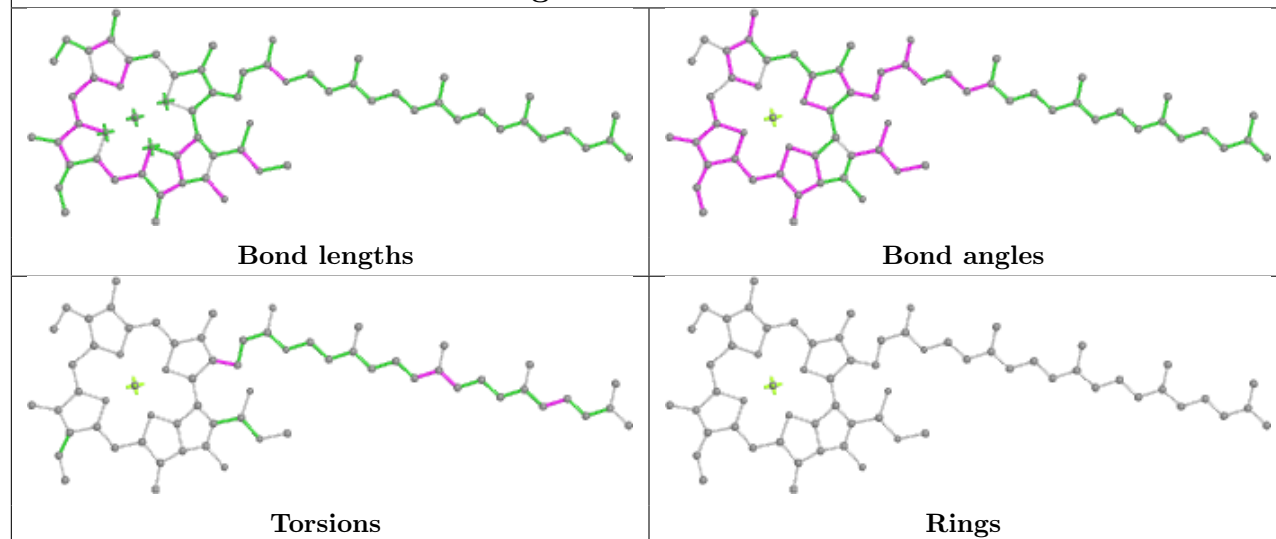




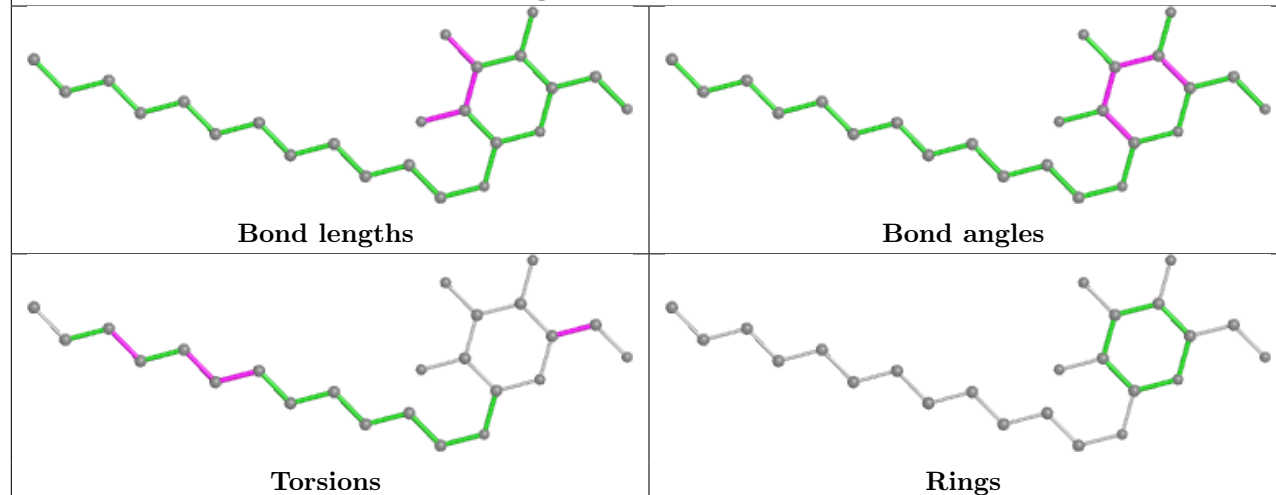




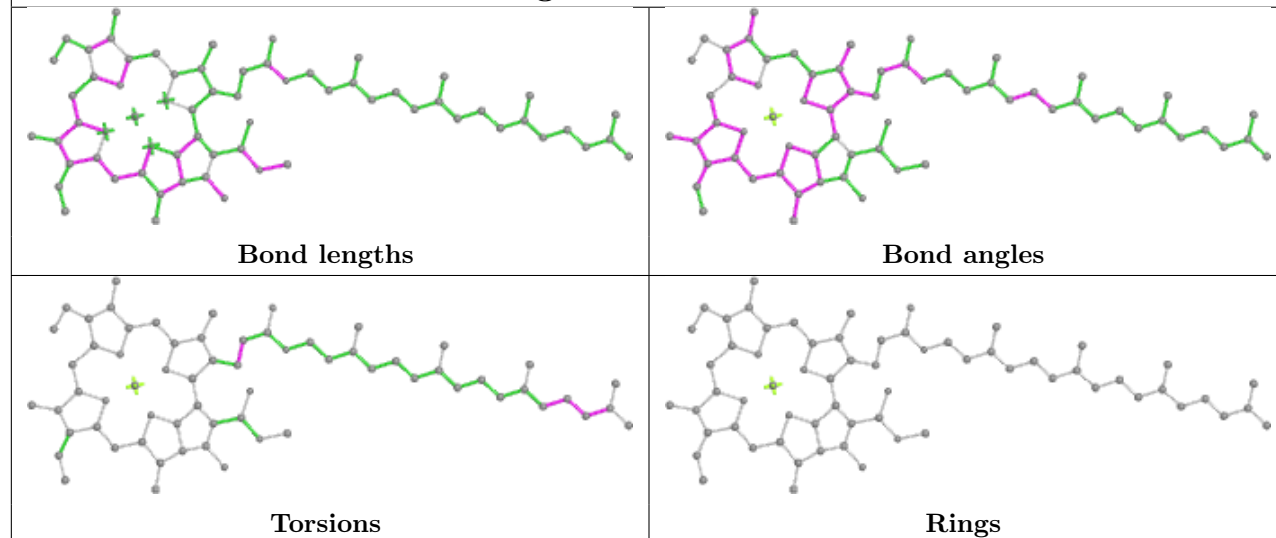
Ligand CLA A 406

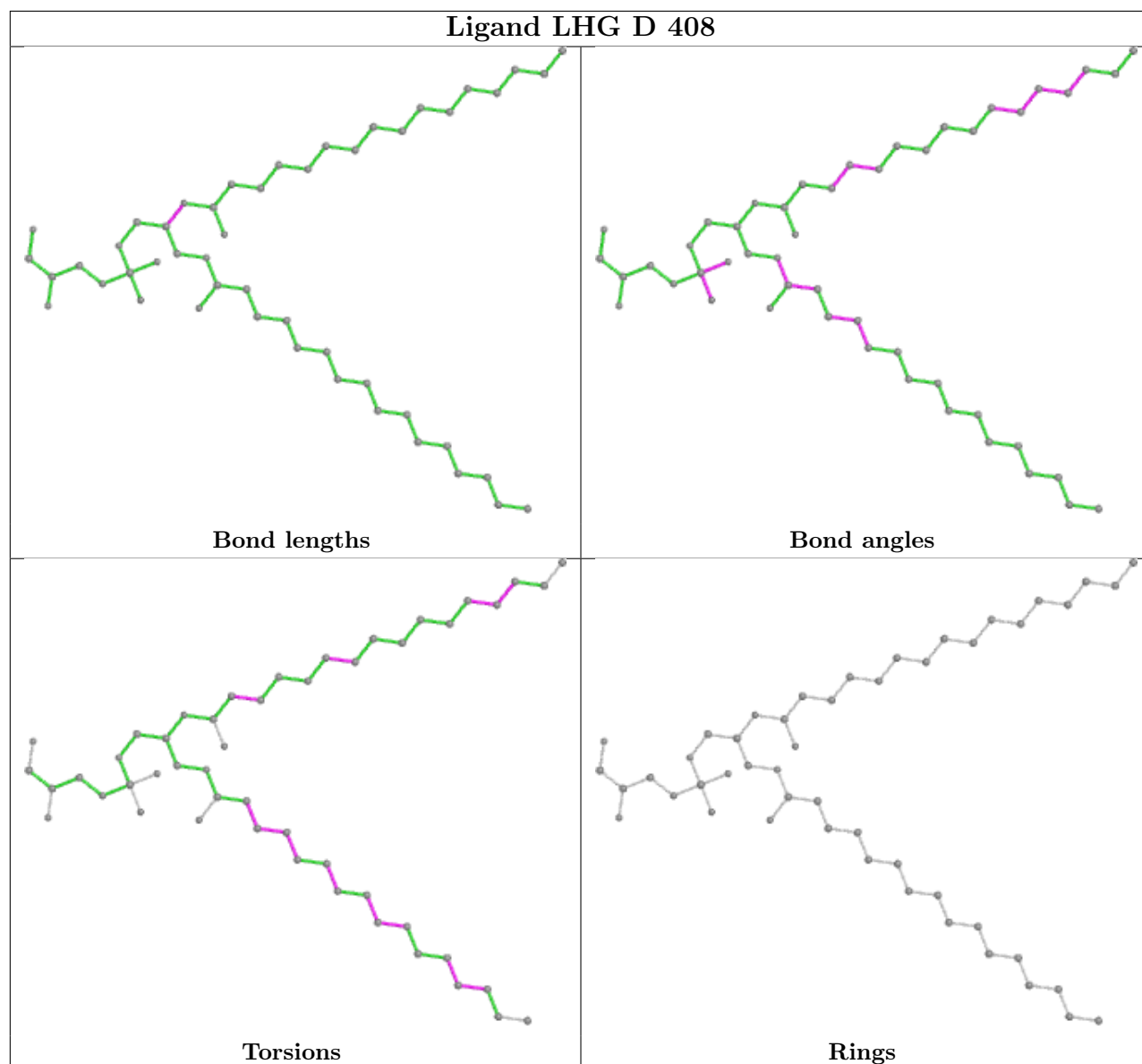
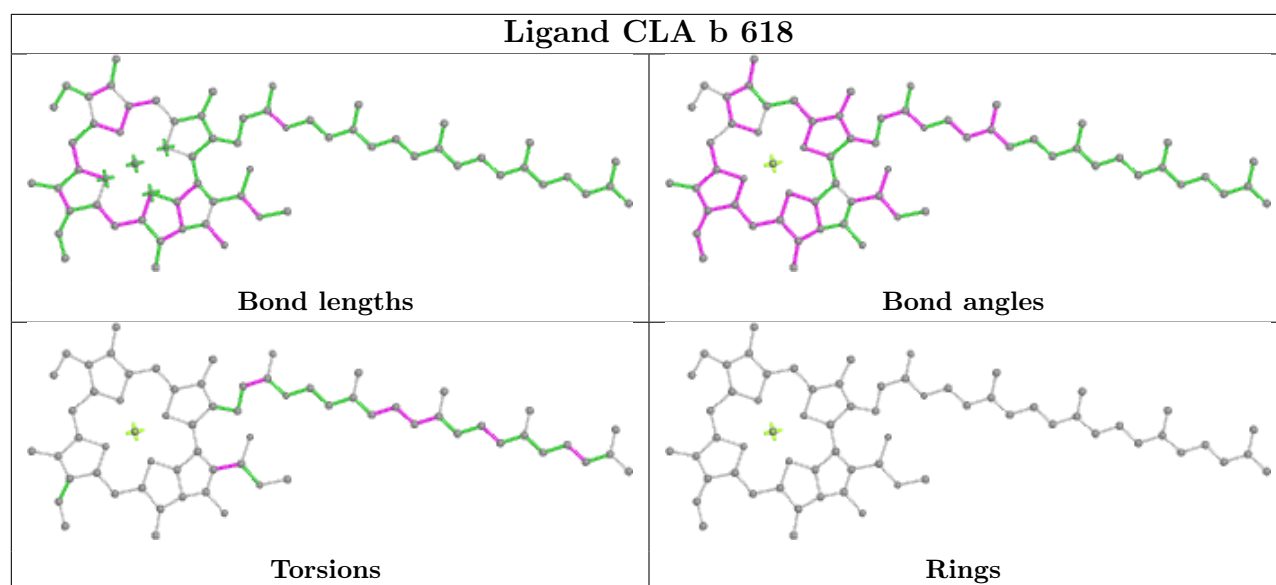


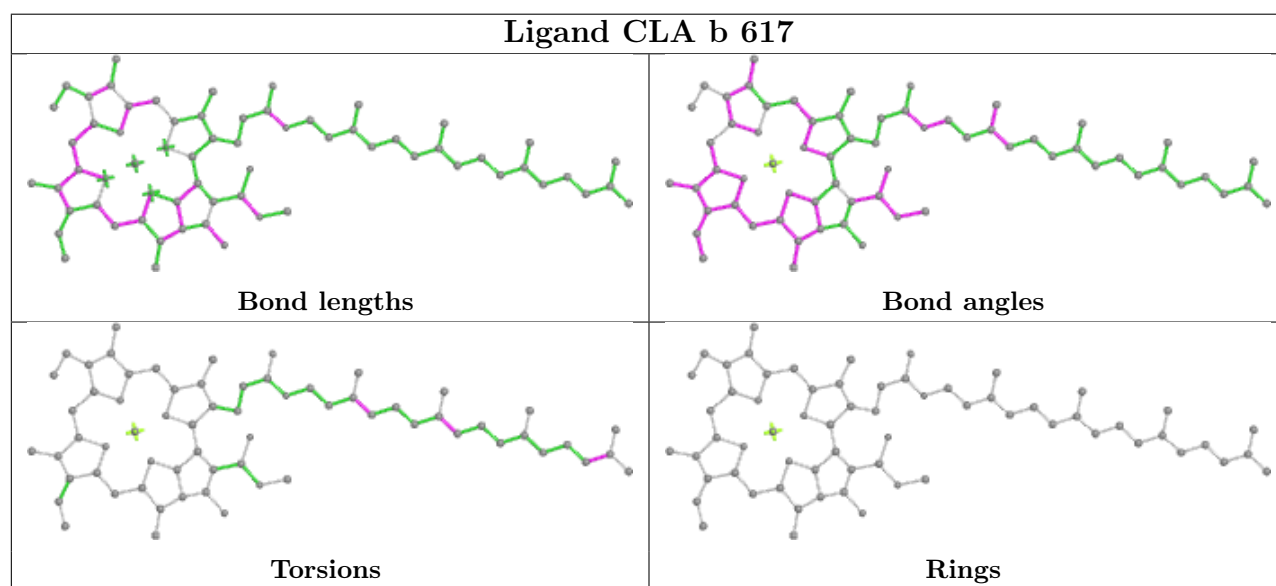
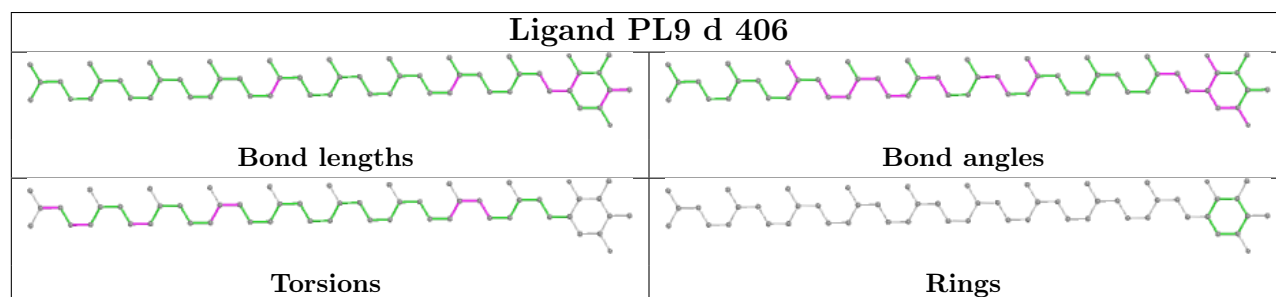
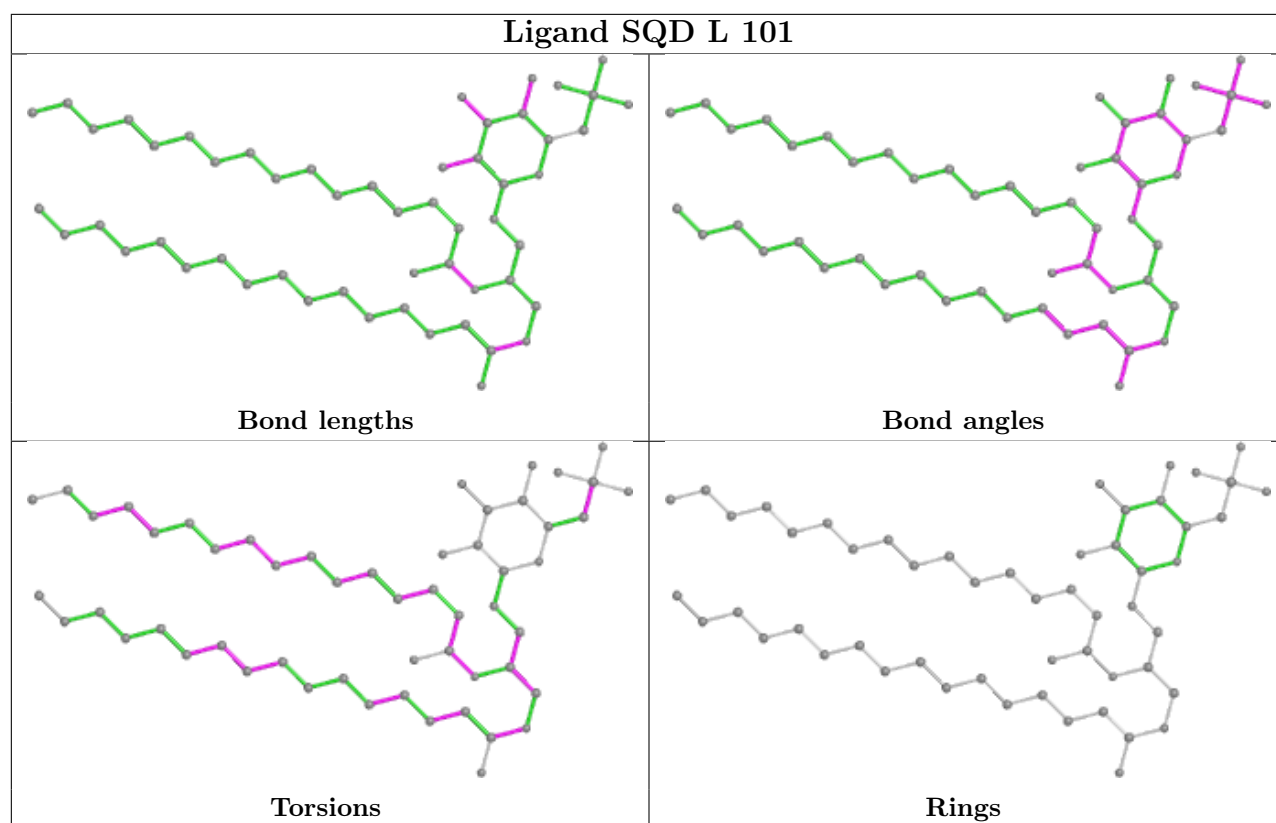
Ligand LMT J 102

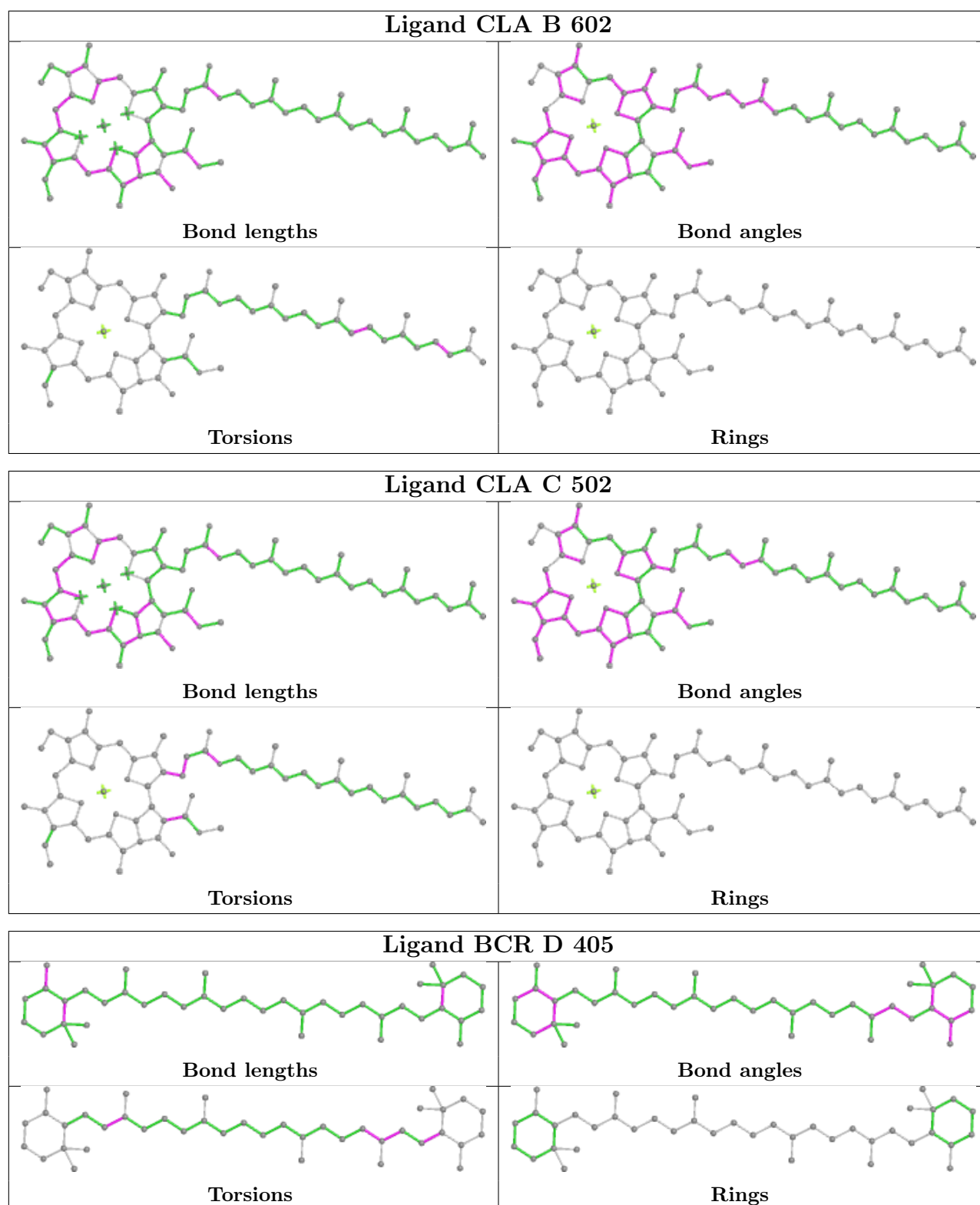


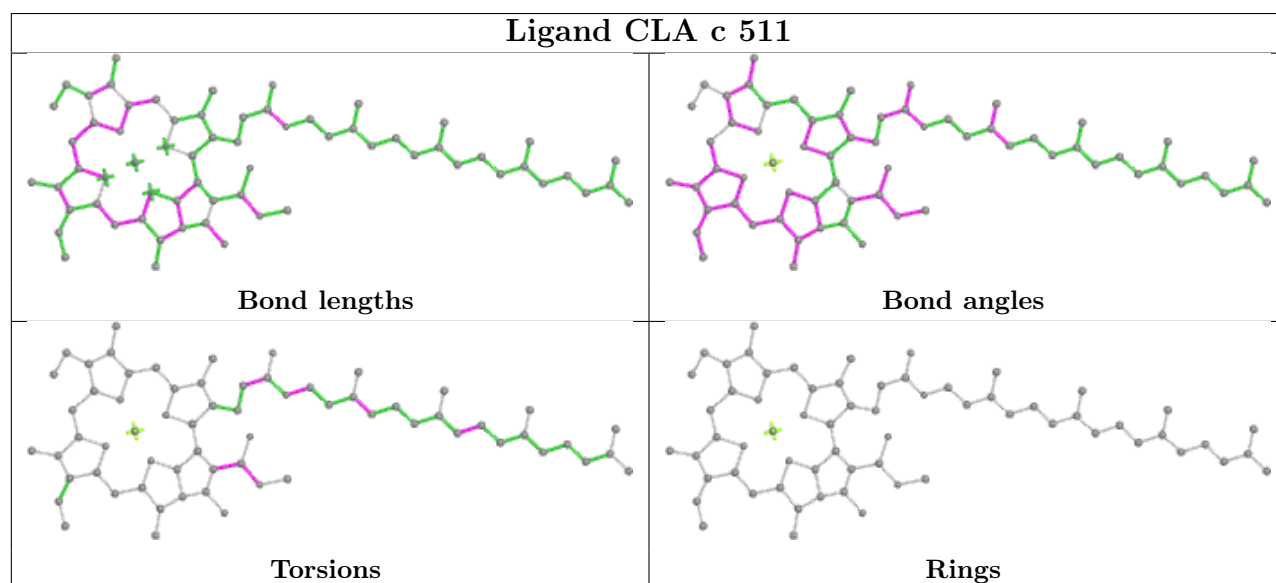
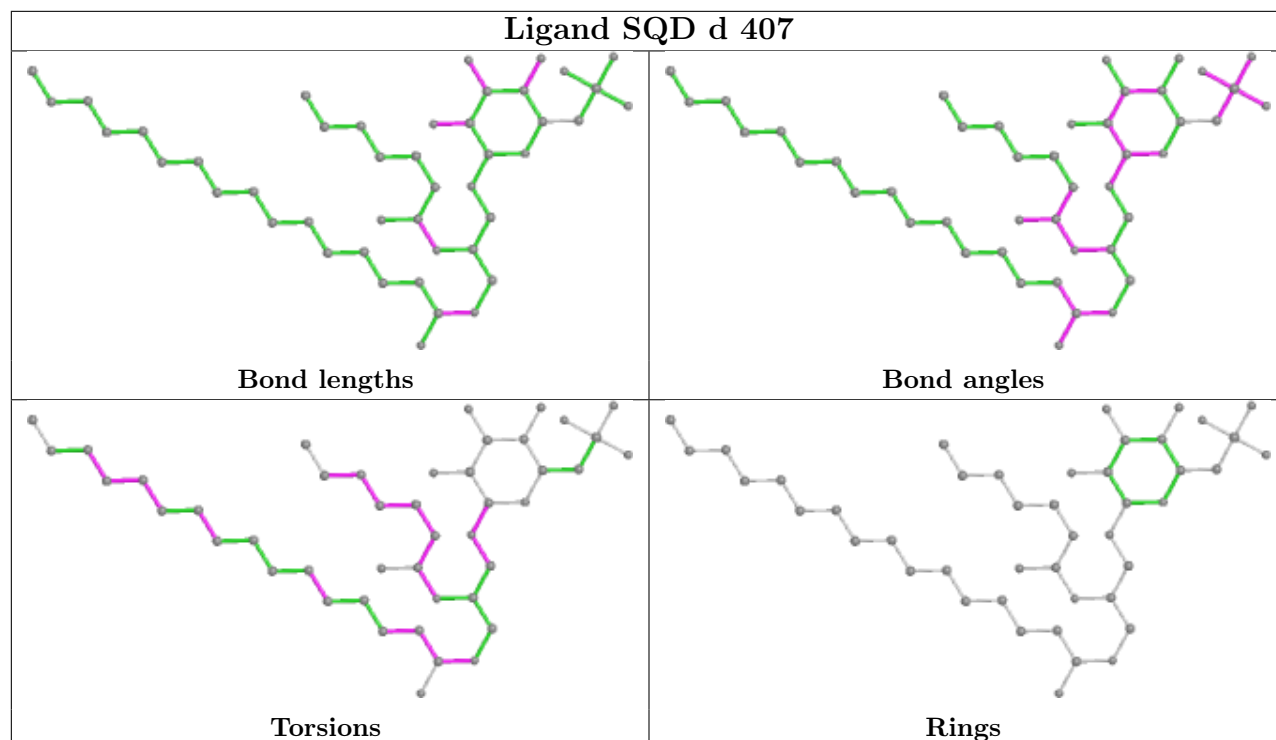
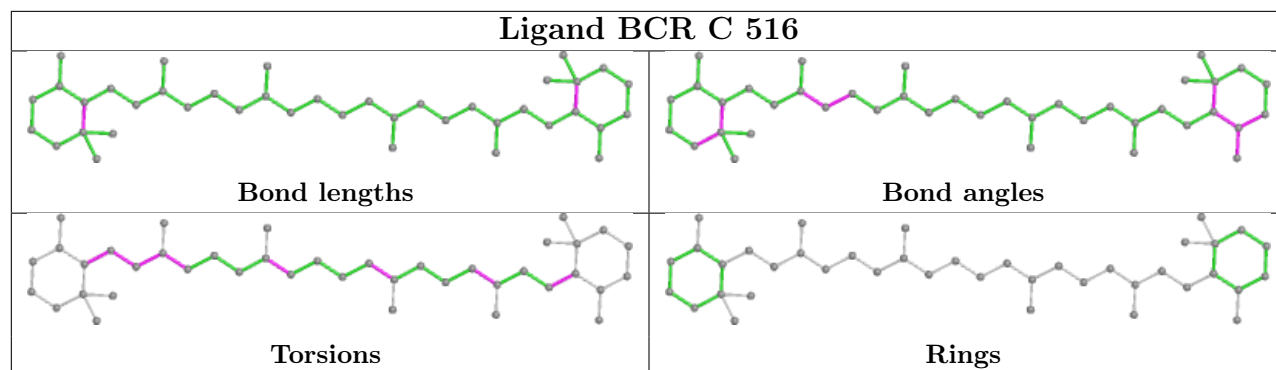
Ligand CLA a 405

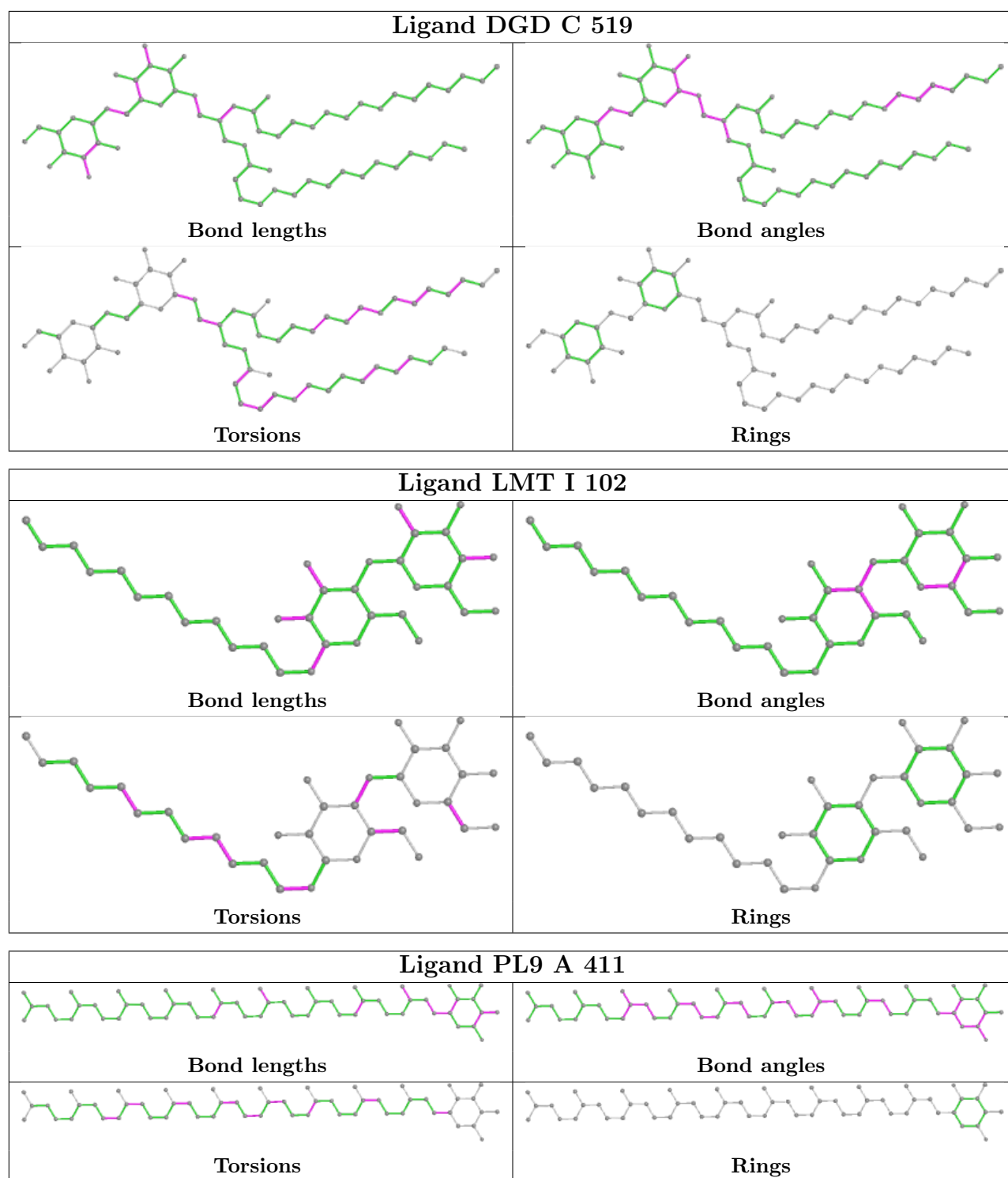


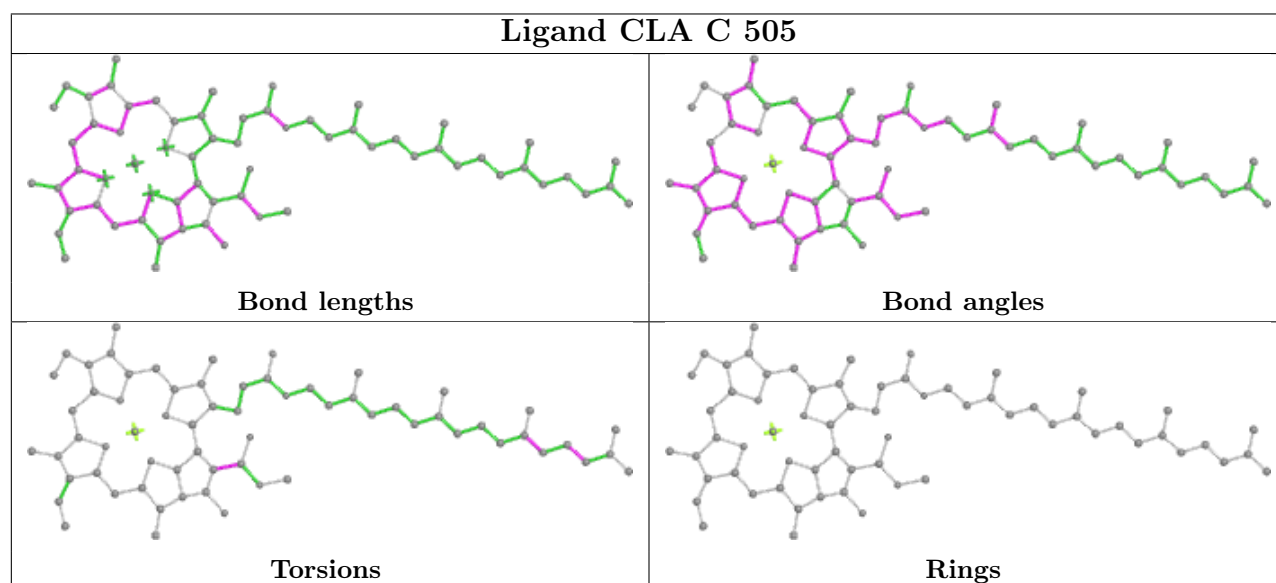
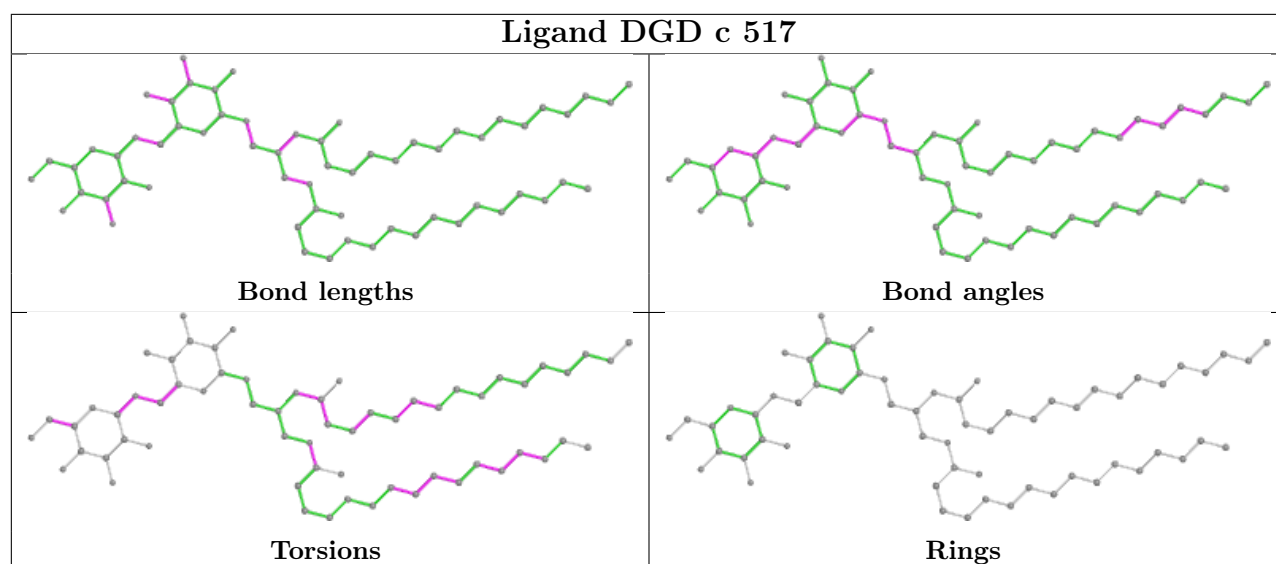


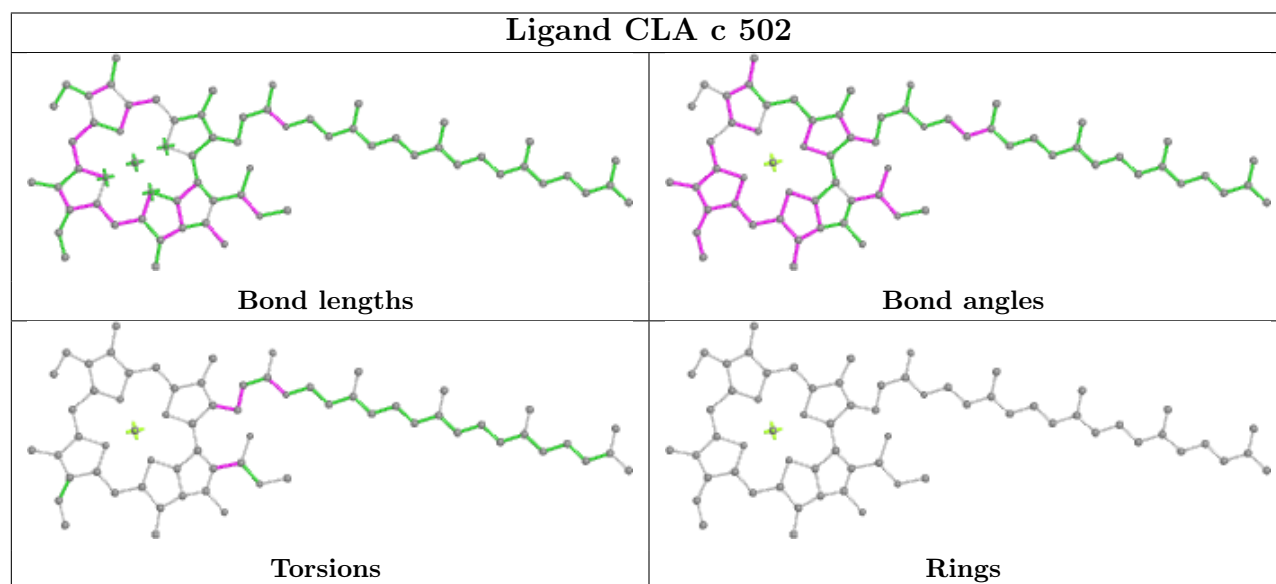
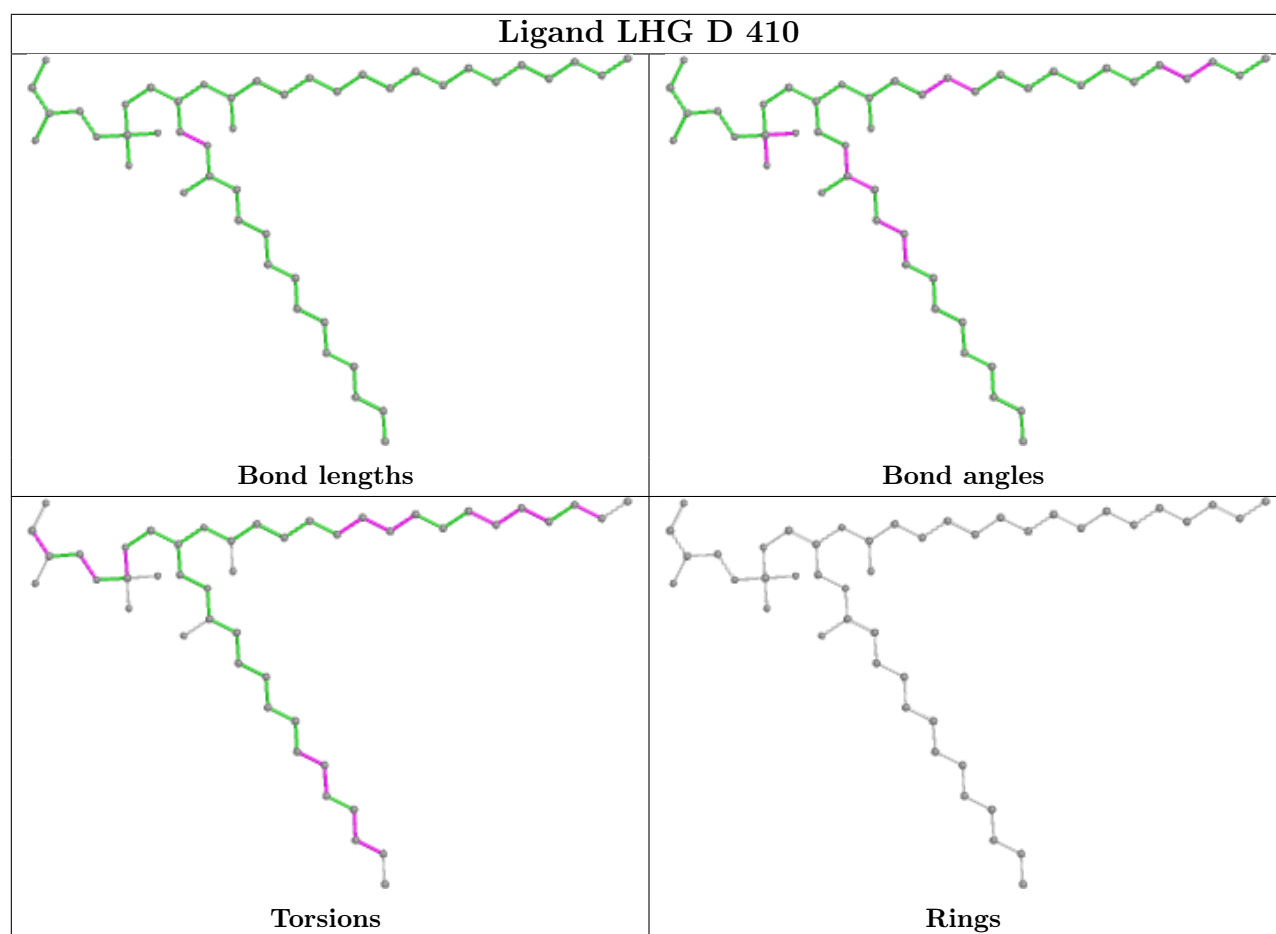


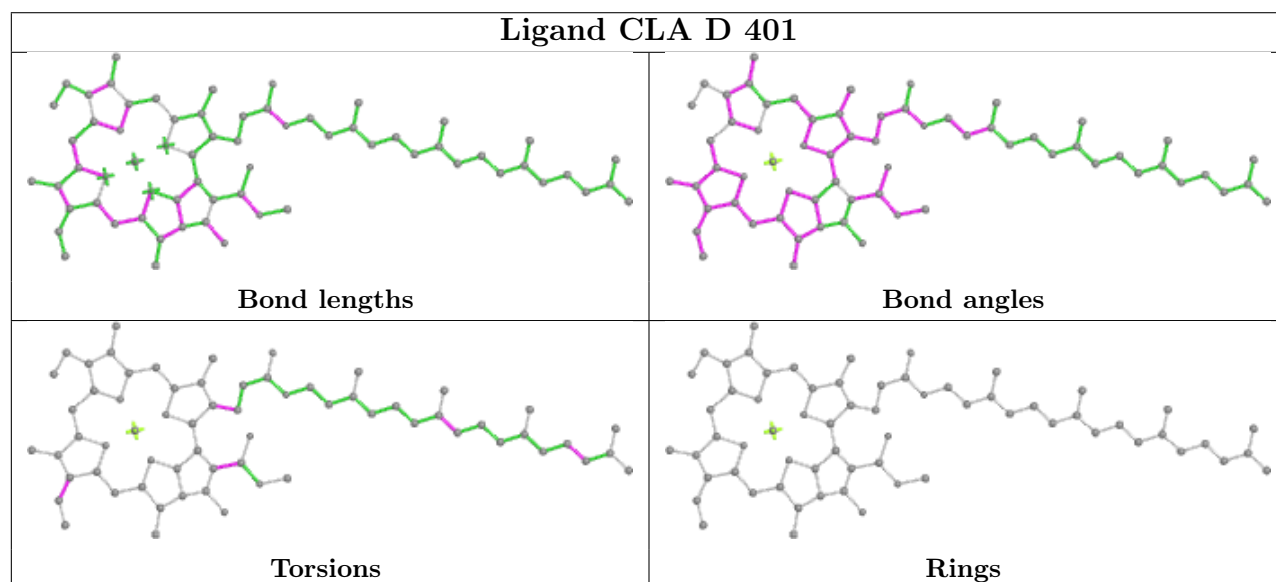
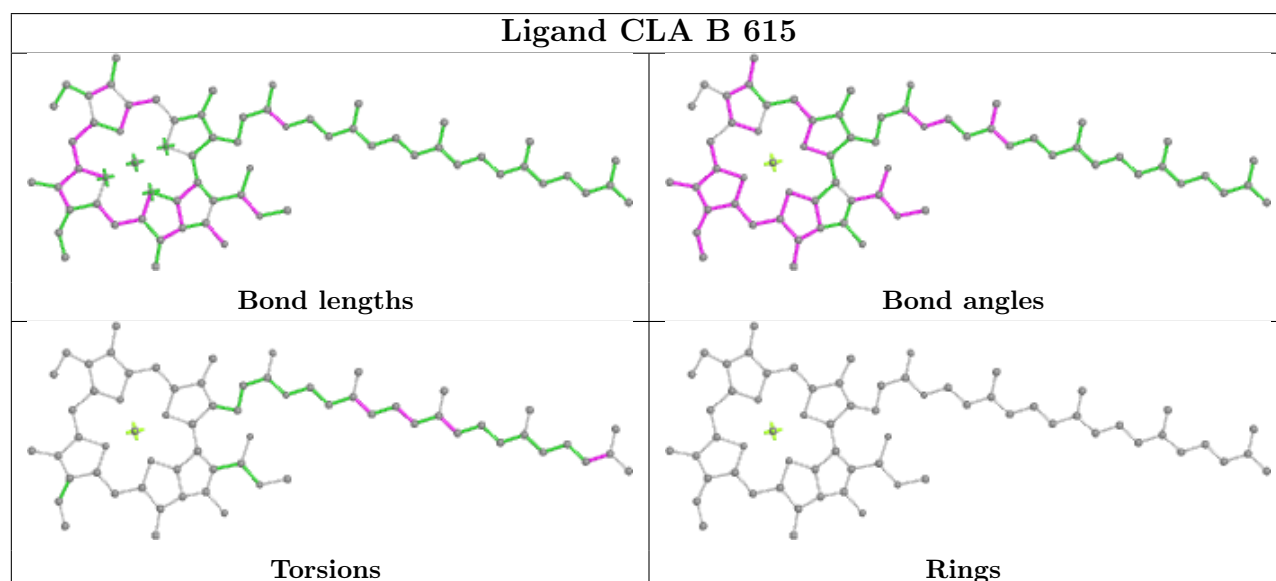
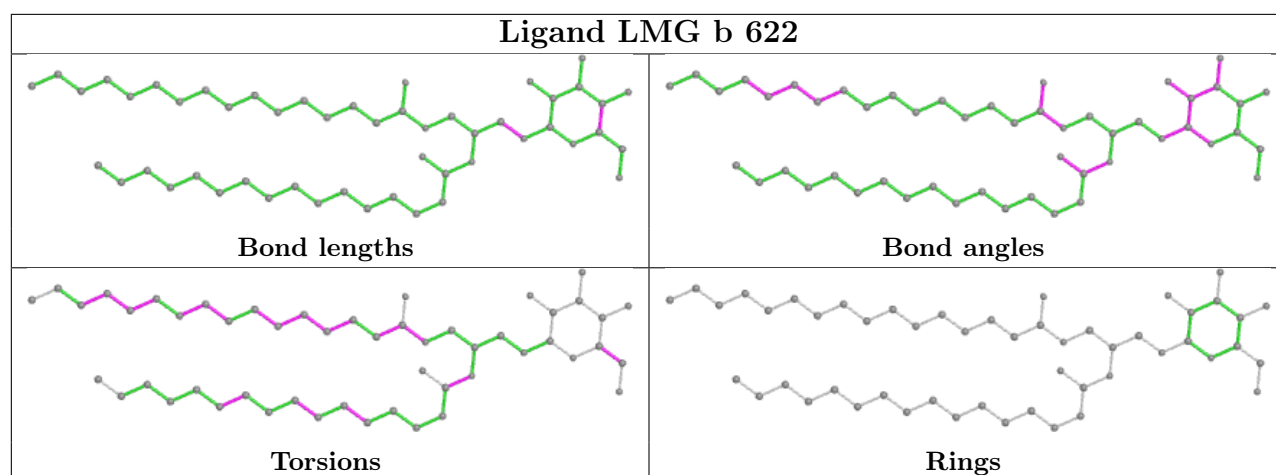




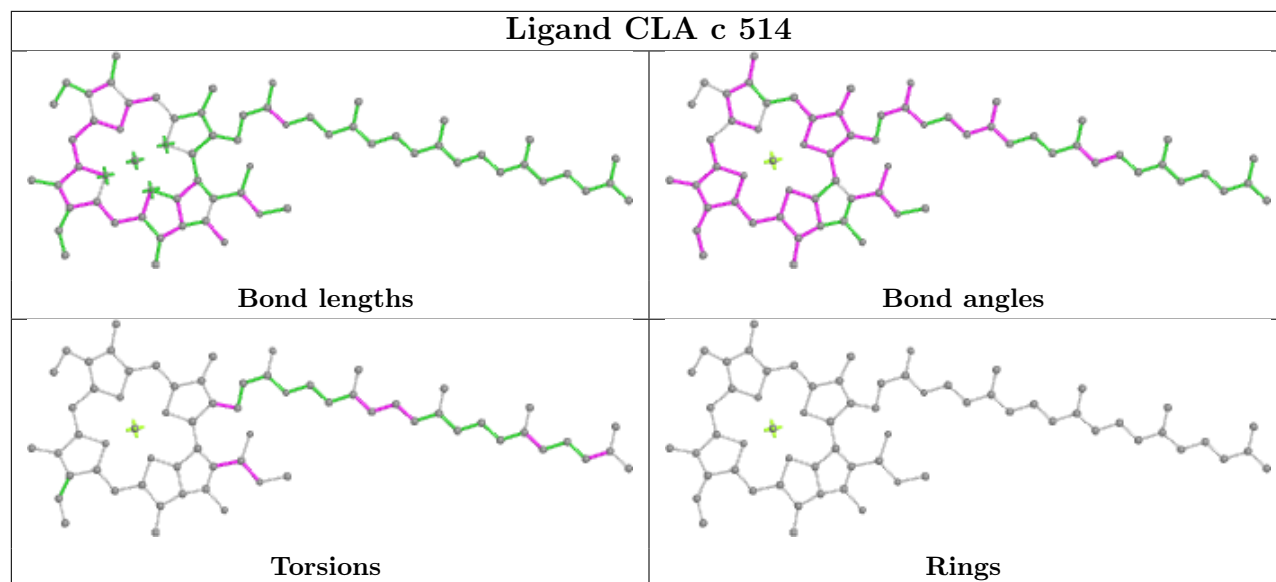




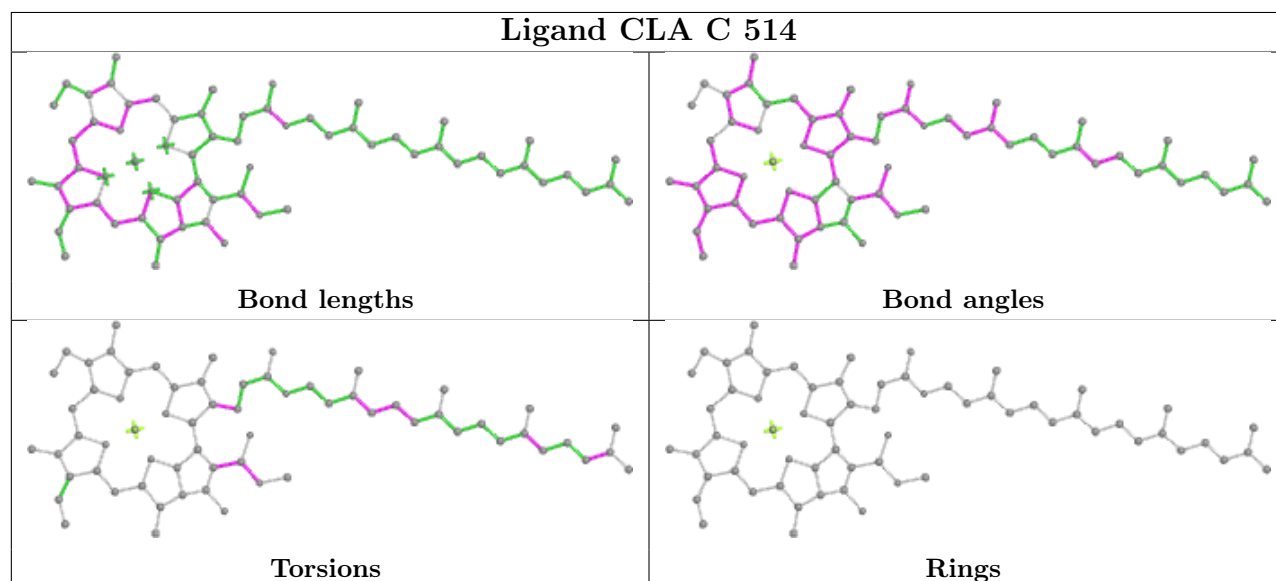




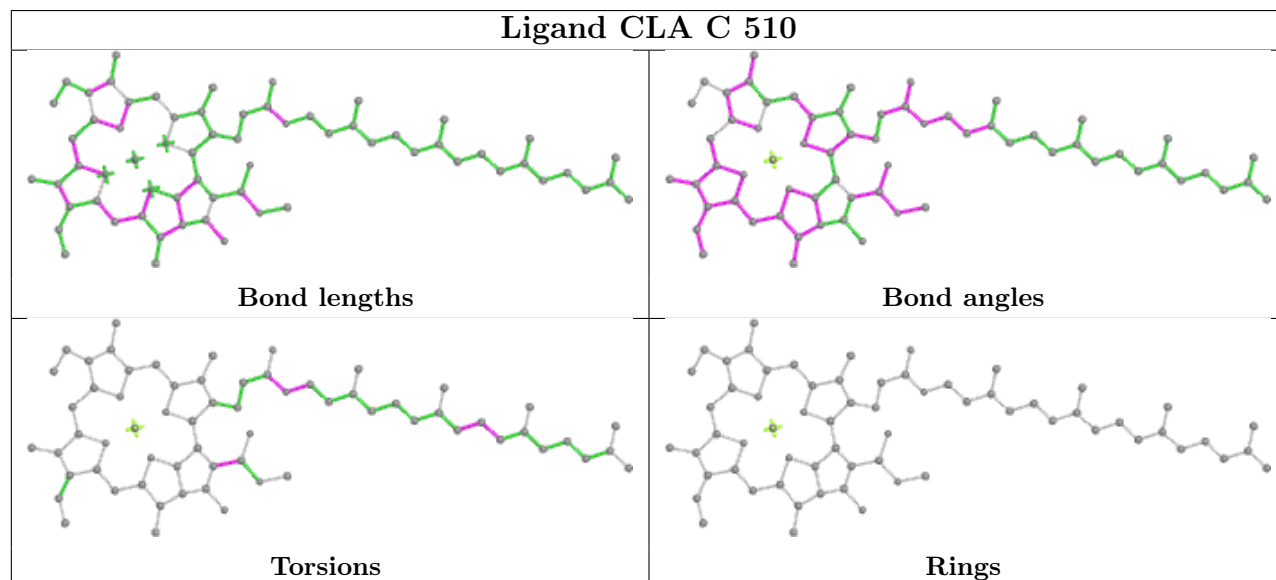
Ligand CLA c 514



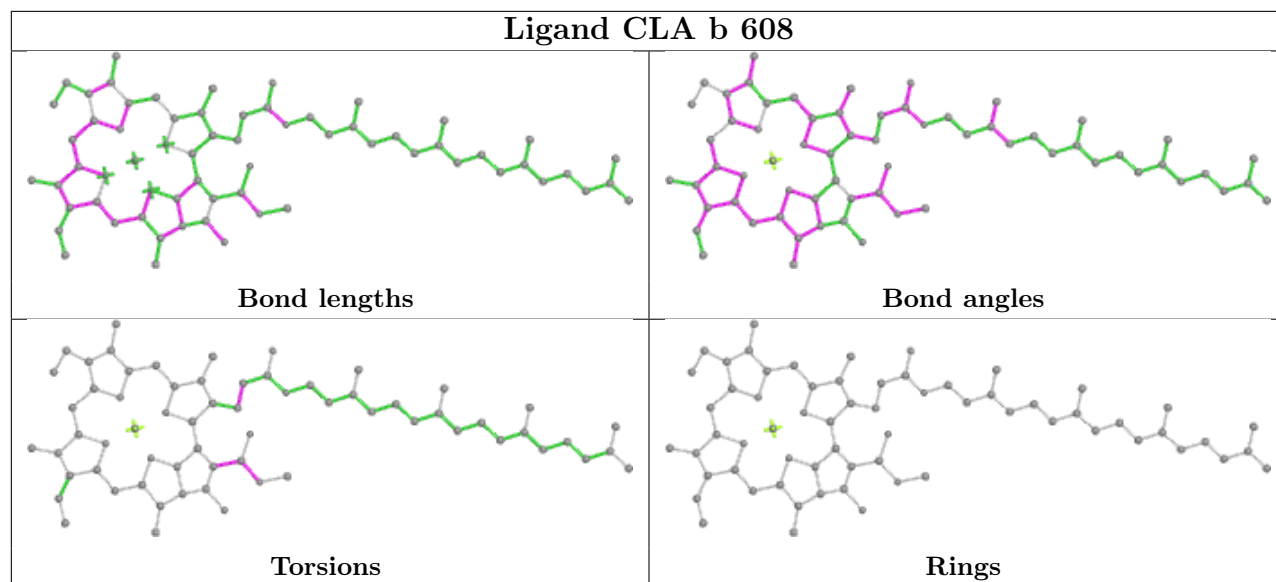
Ligand CLA C 514



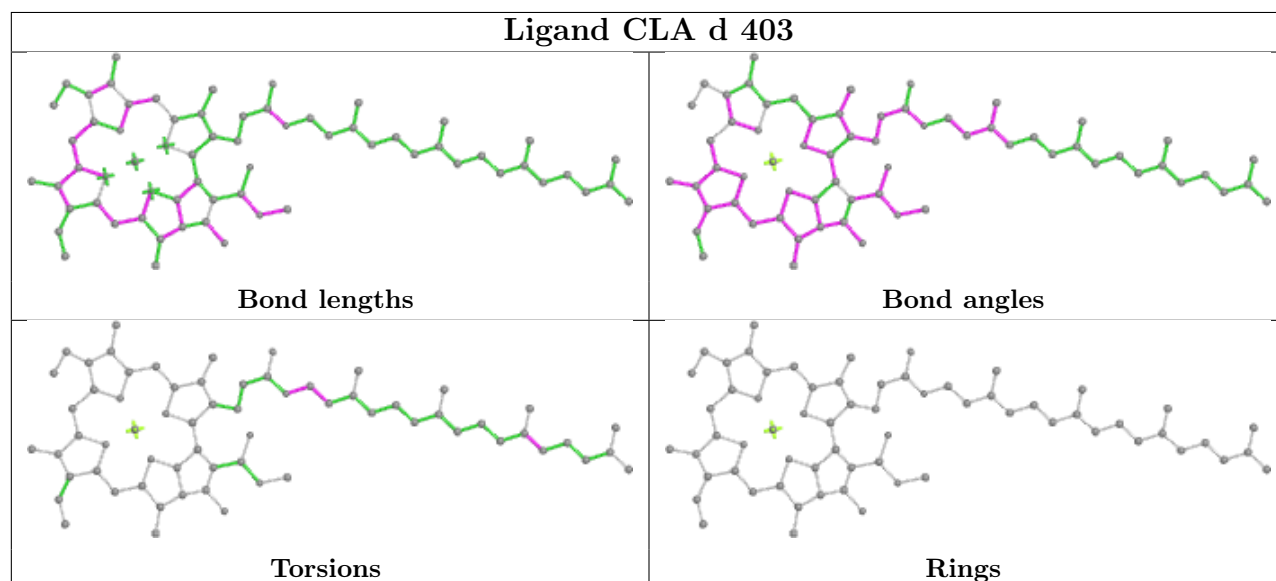
Ligand CLA C 510



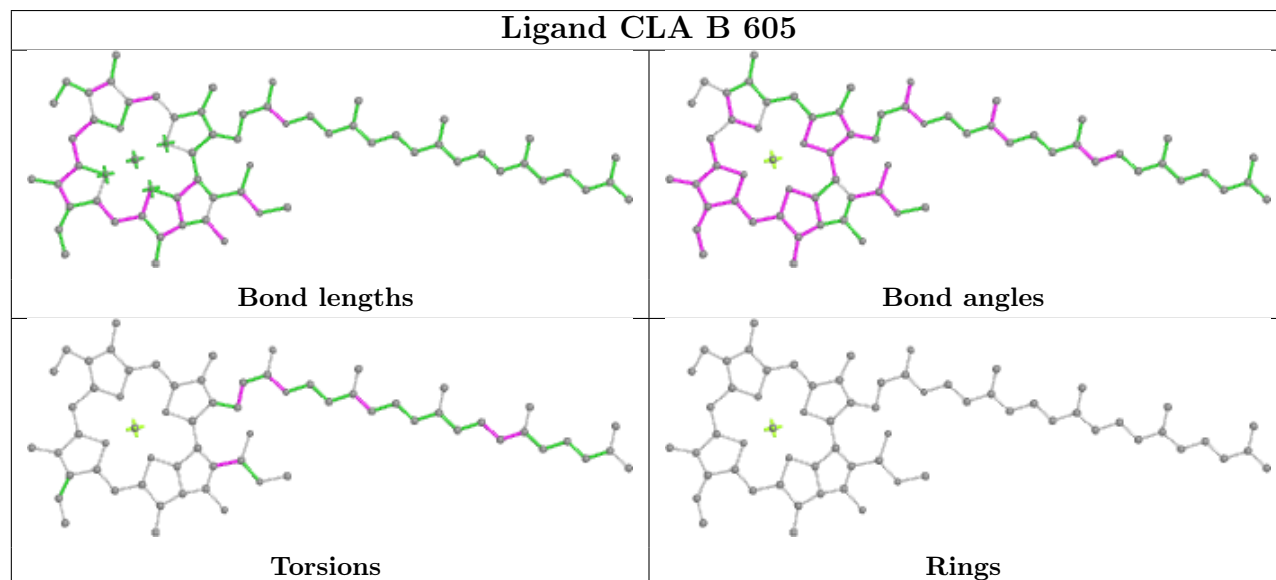
Ligand CLA b 608

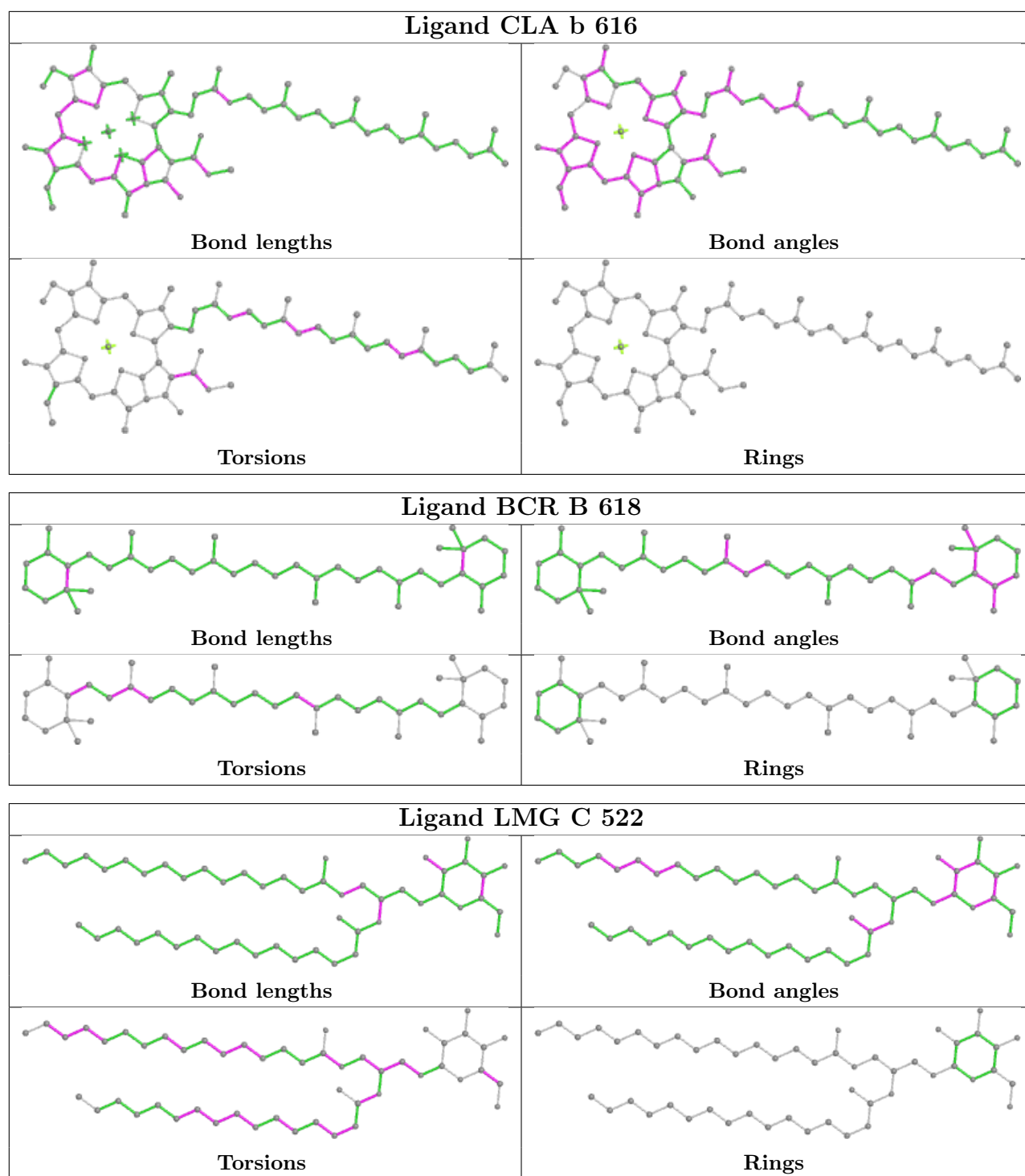


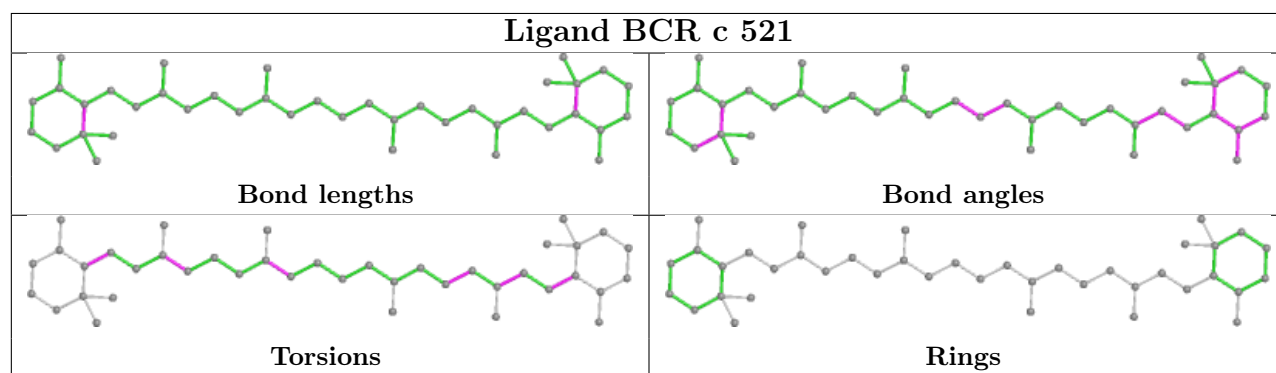
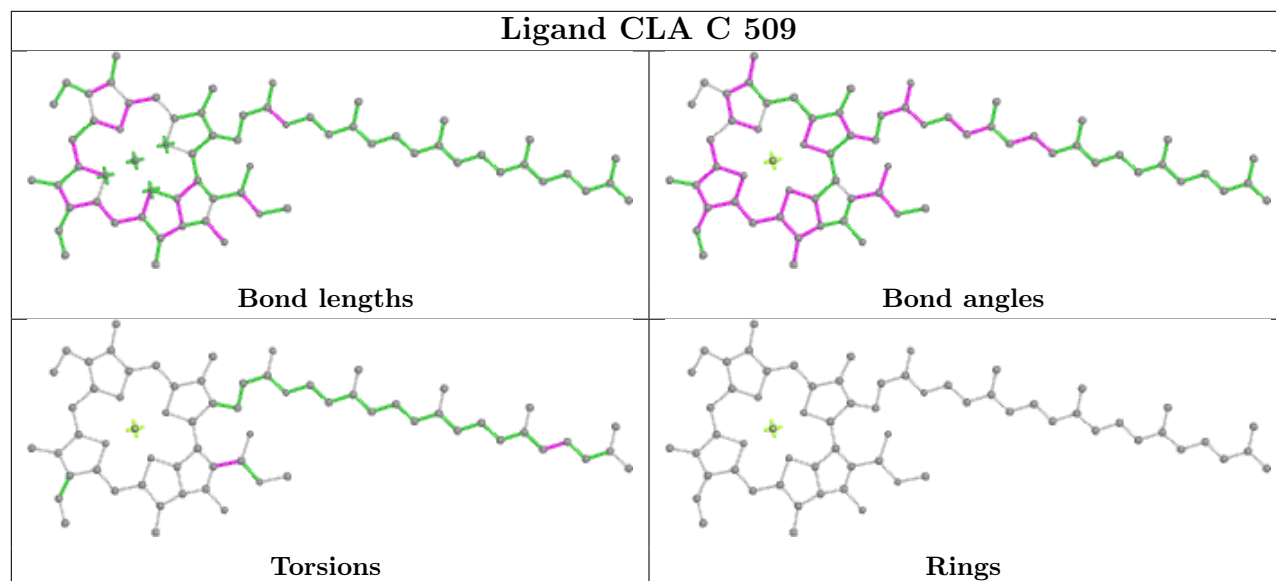
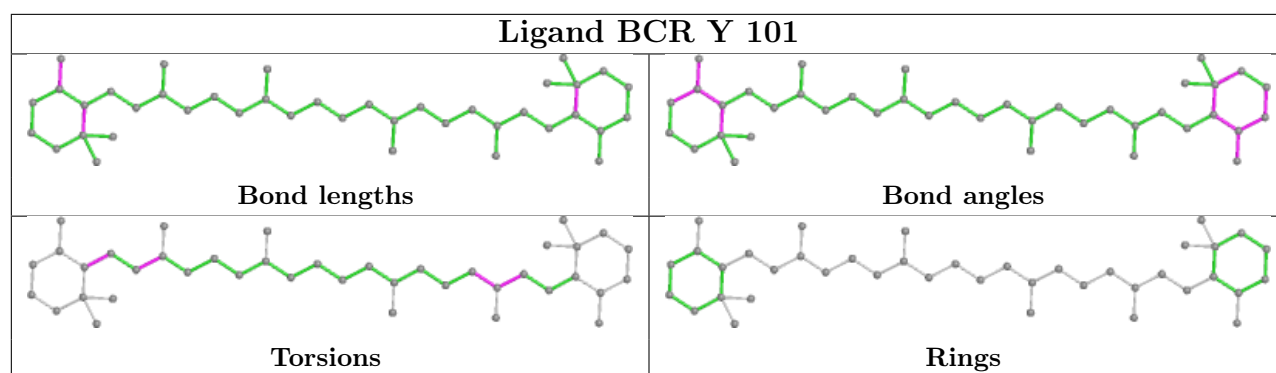
Ligand CLA d 403



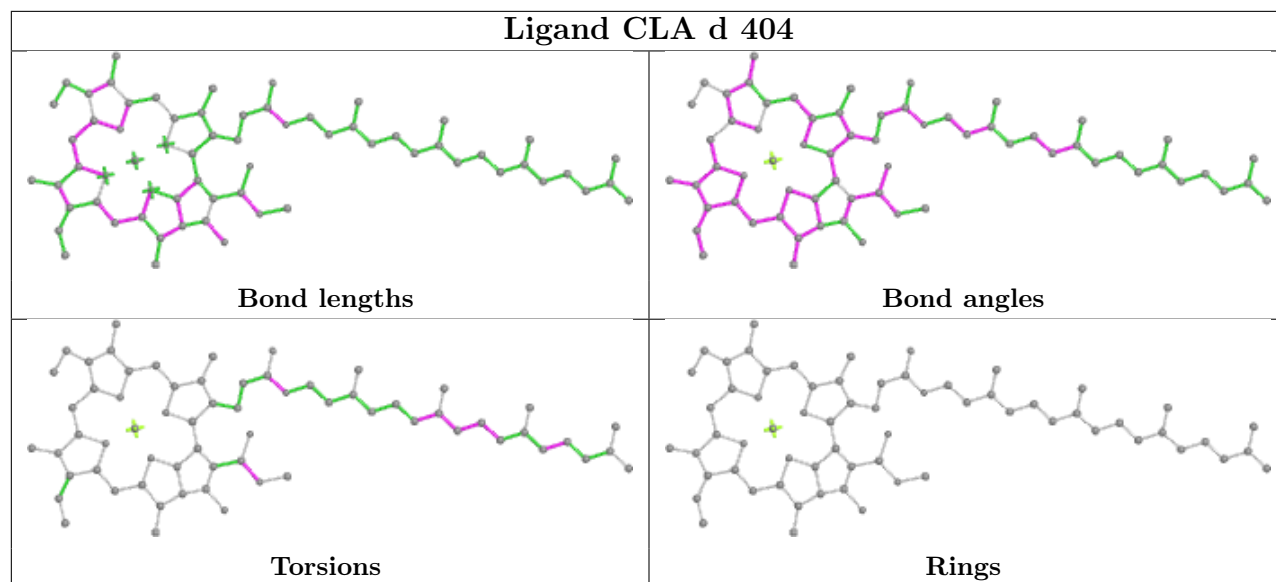
Ligand CLA B 605



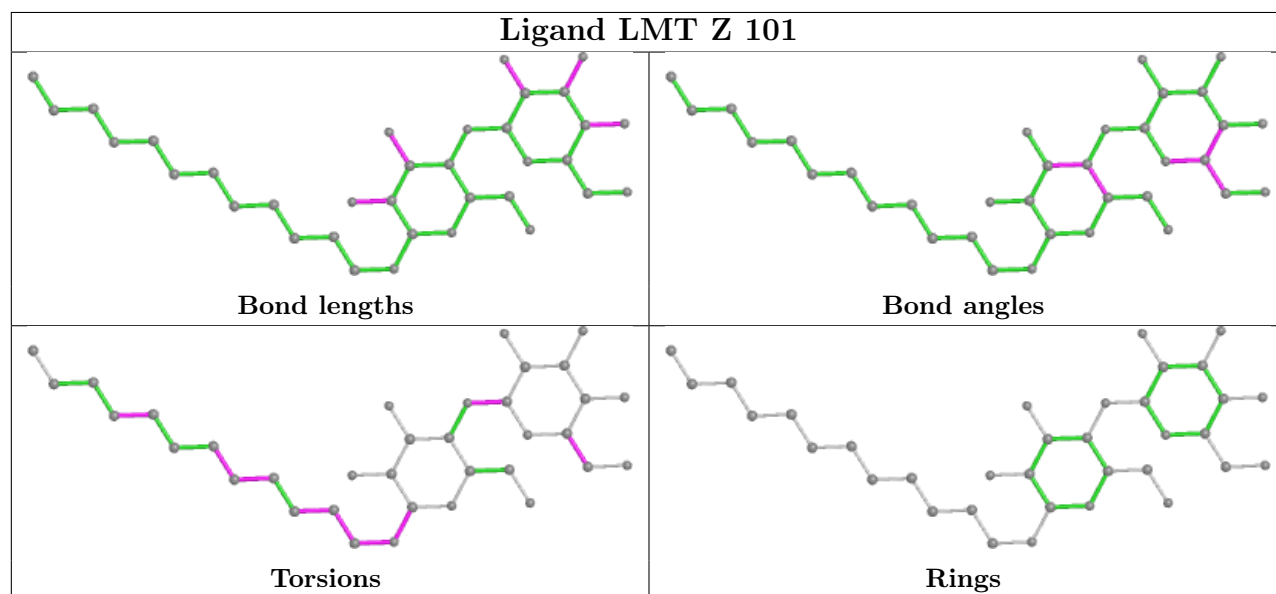


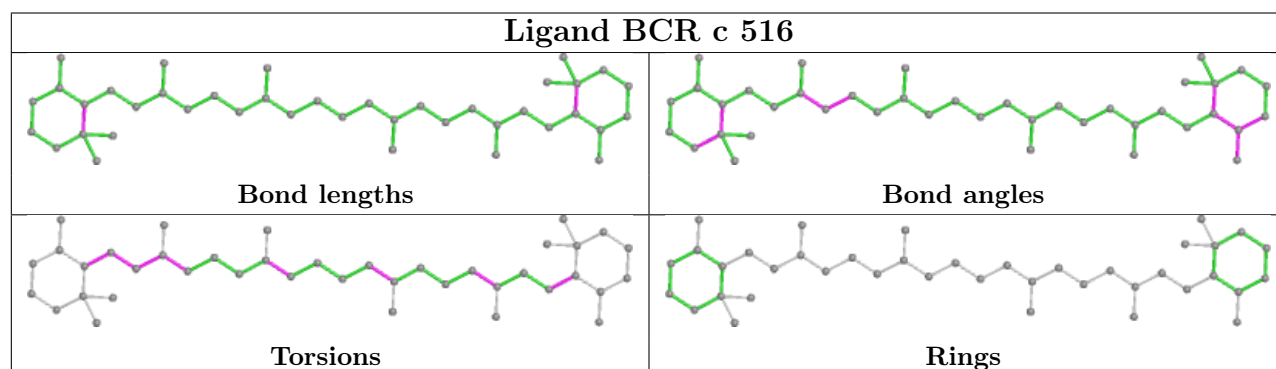
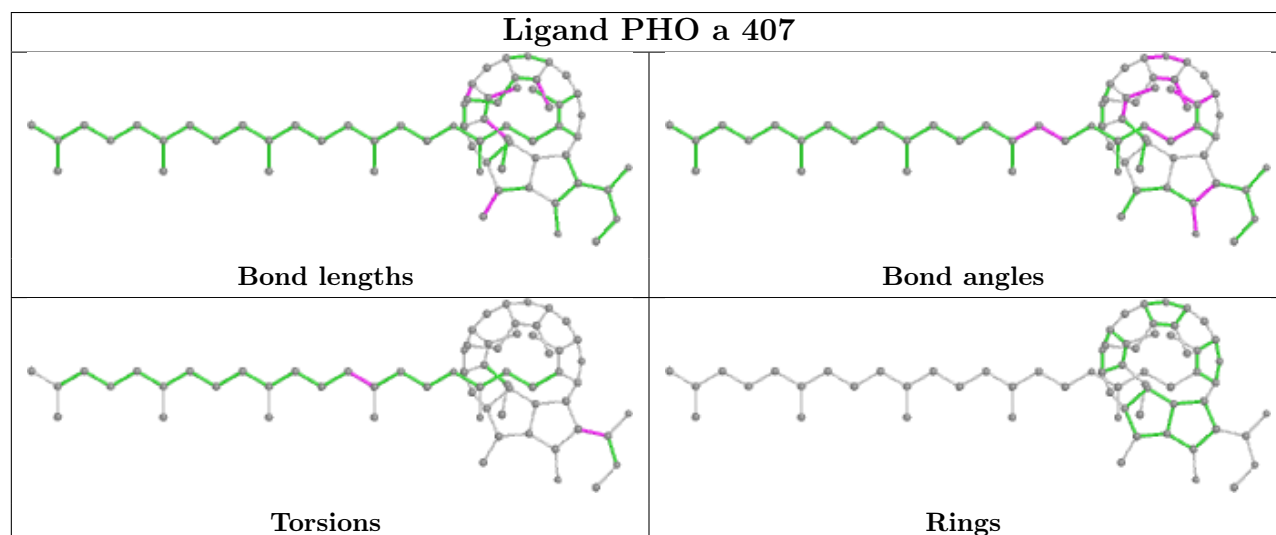
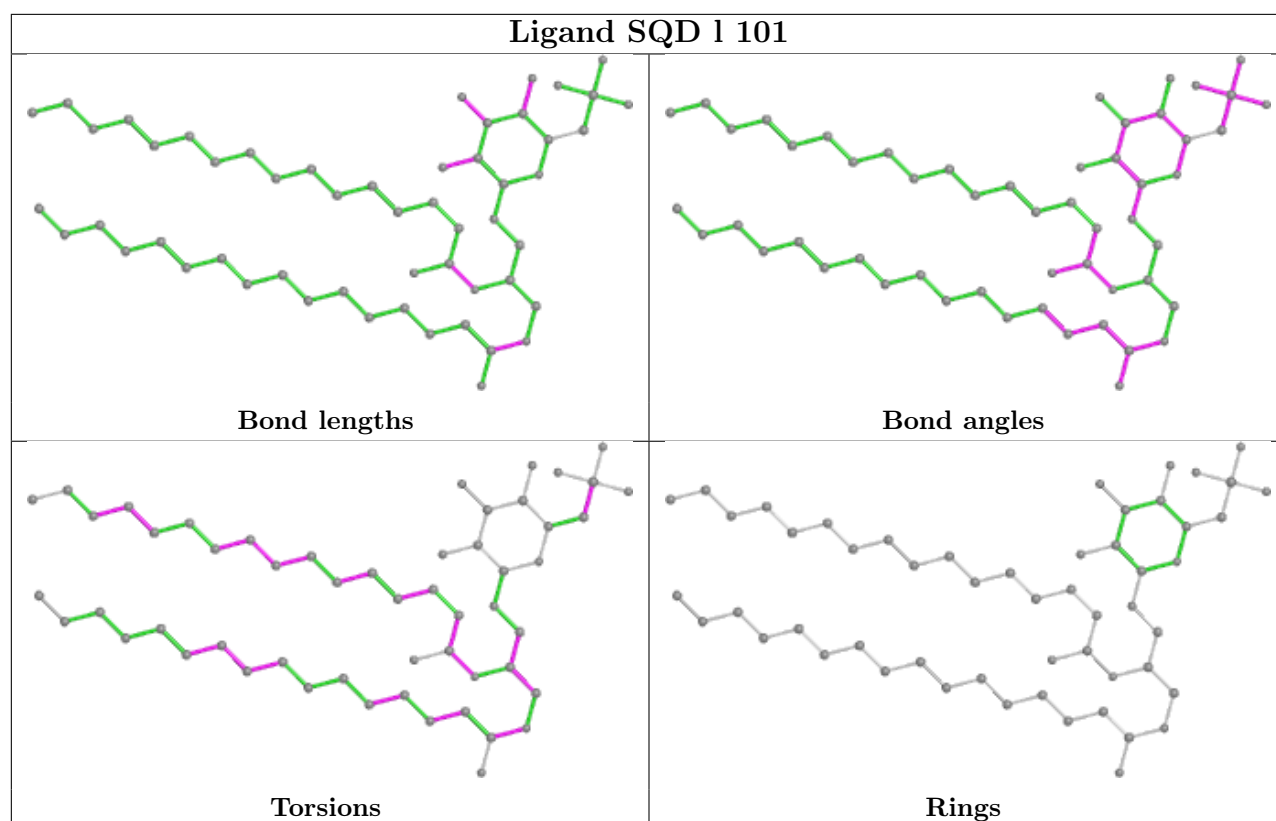


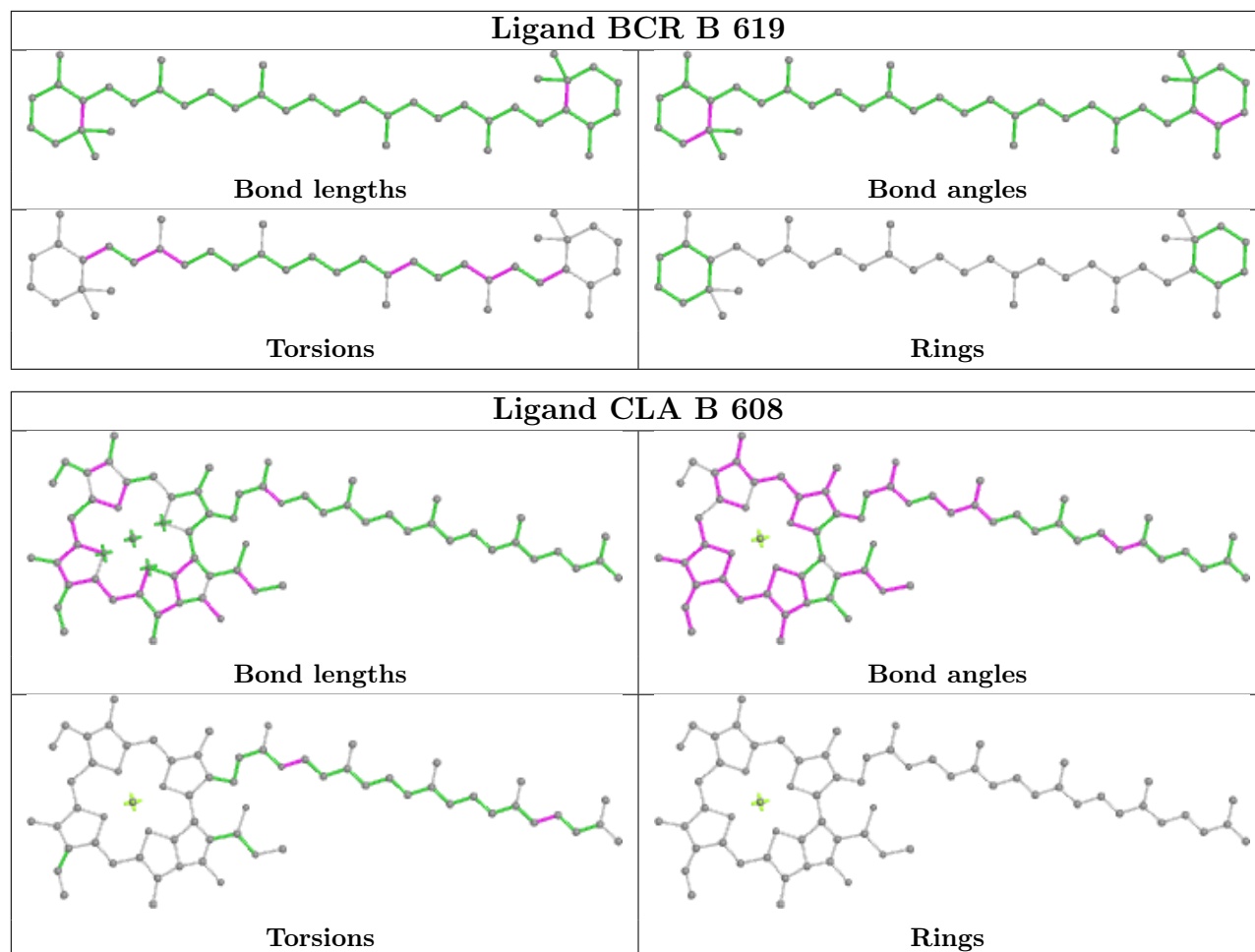
Ligand CLA d 404

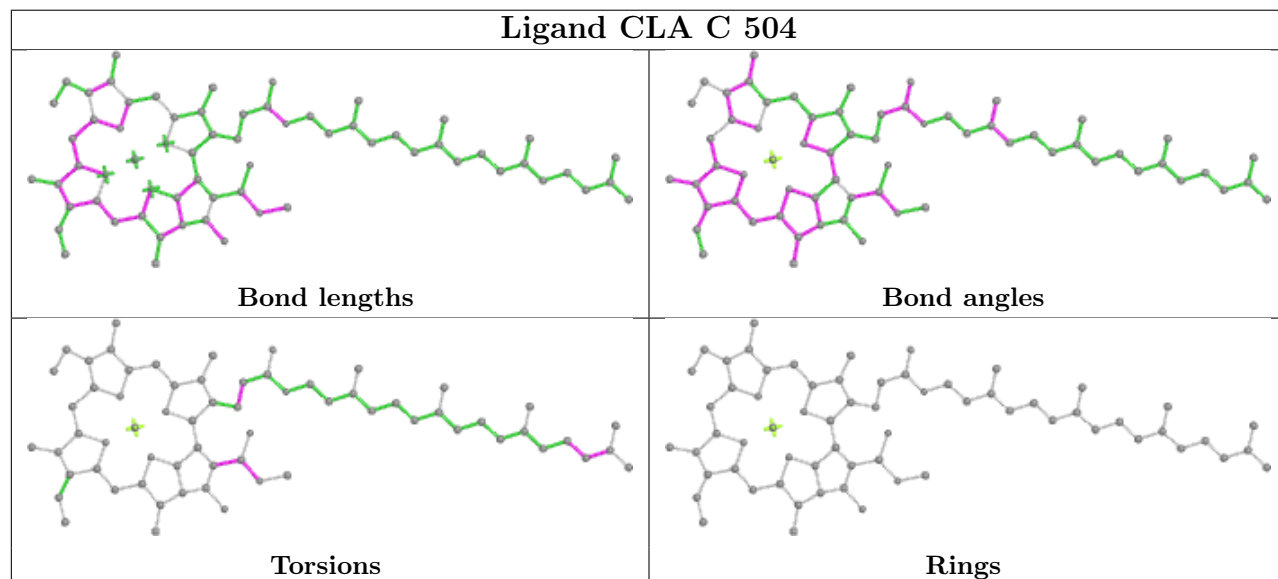
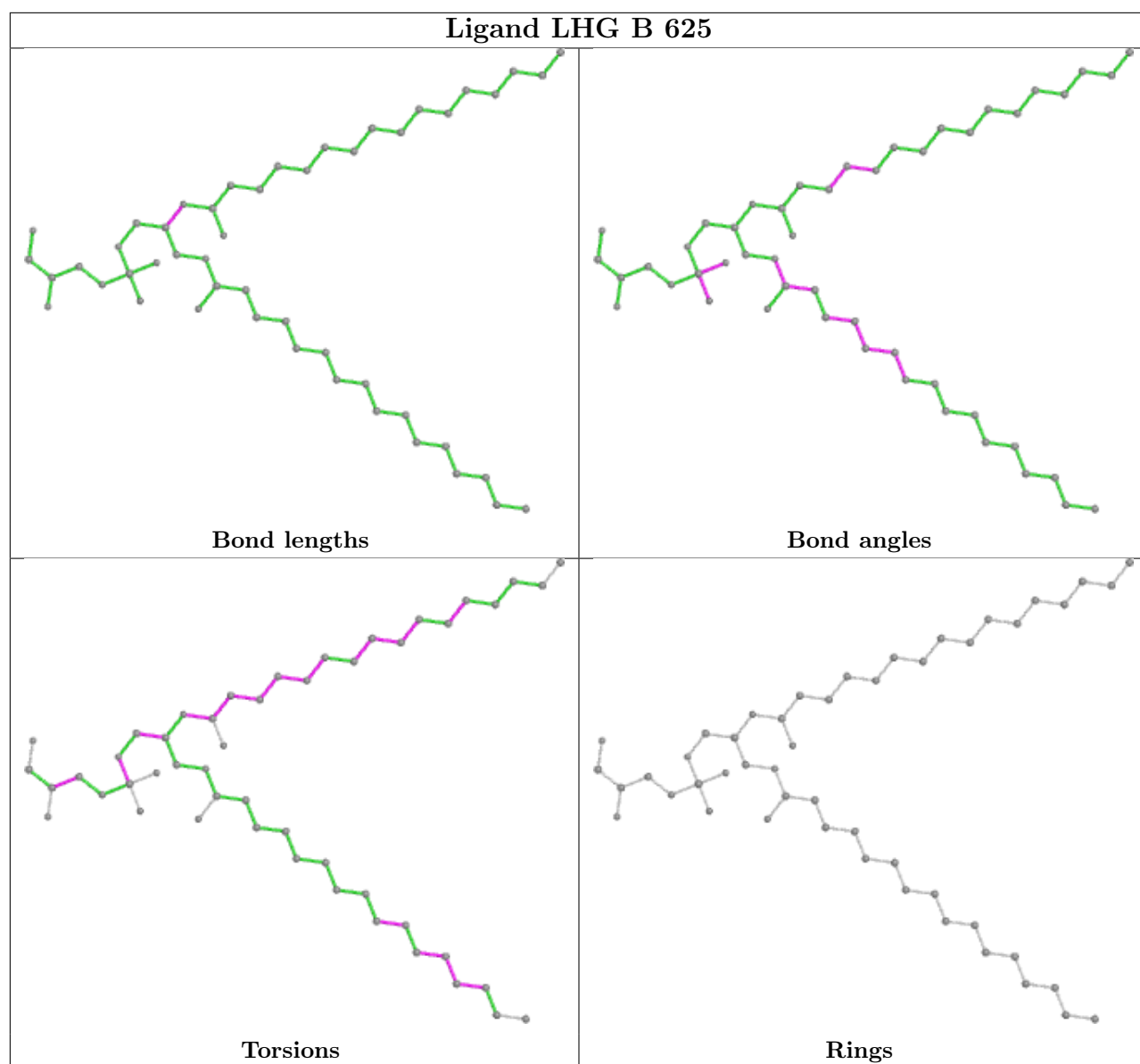


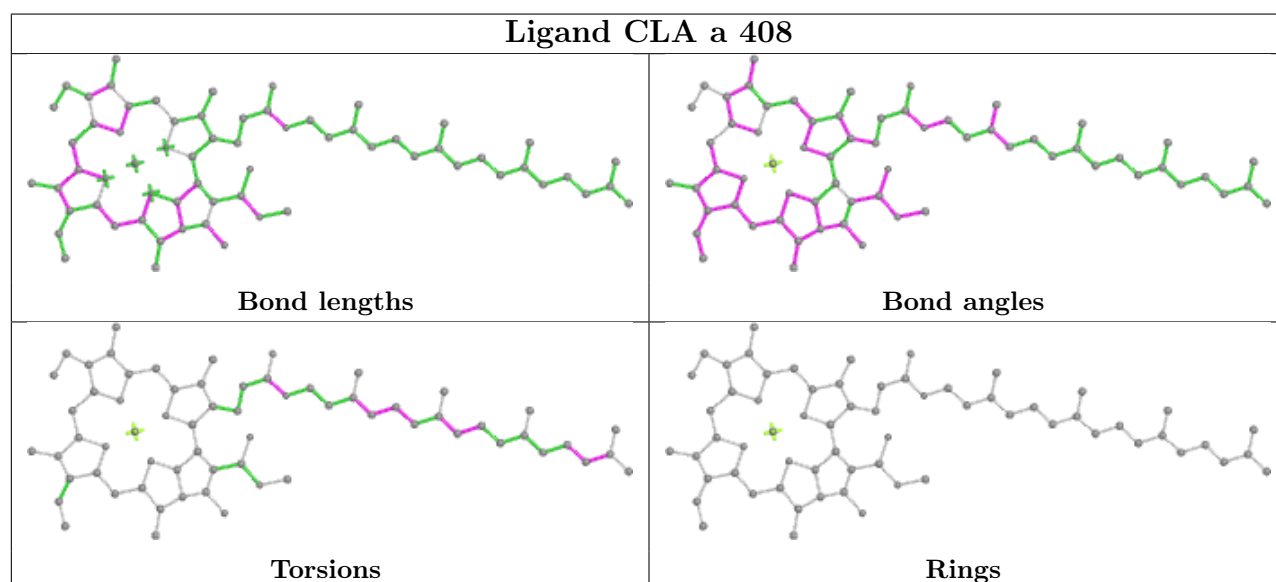
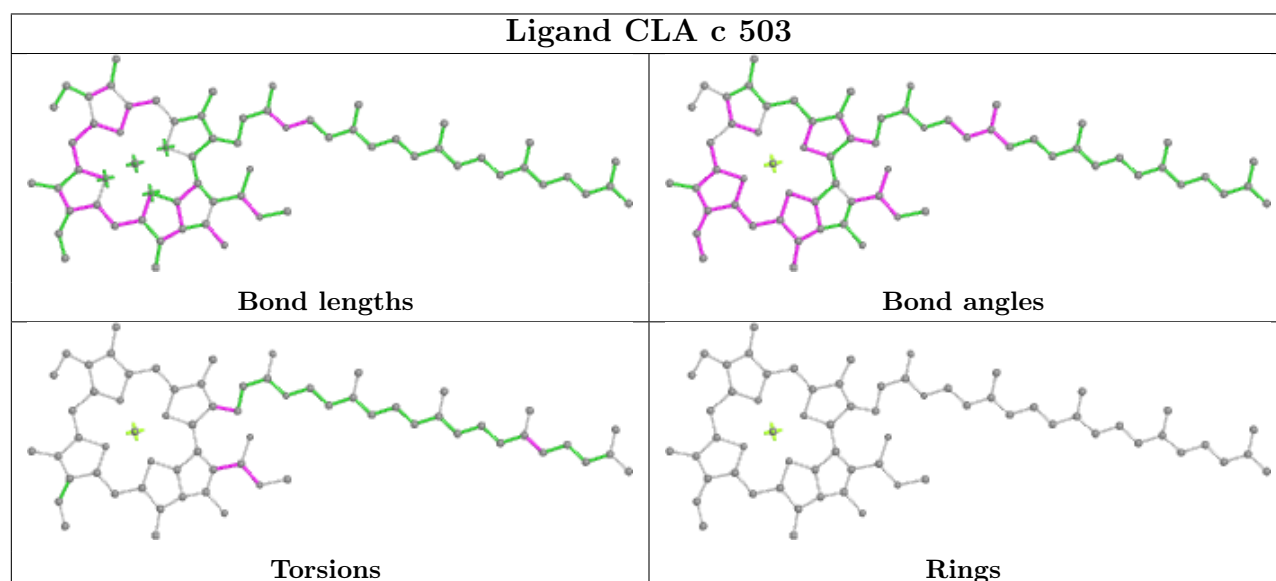
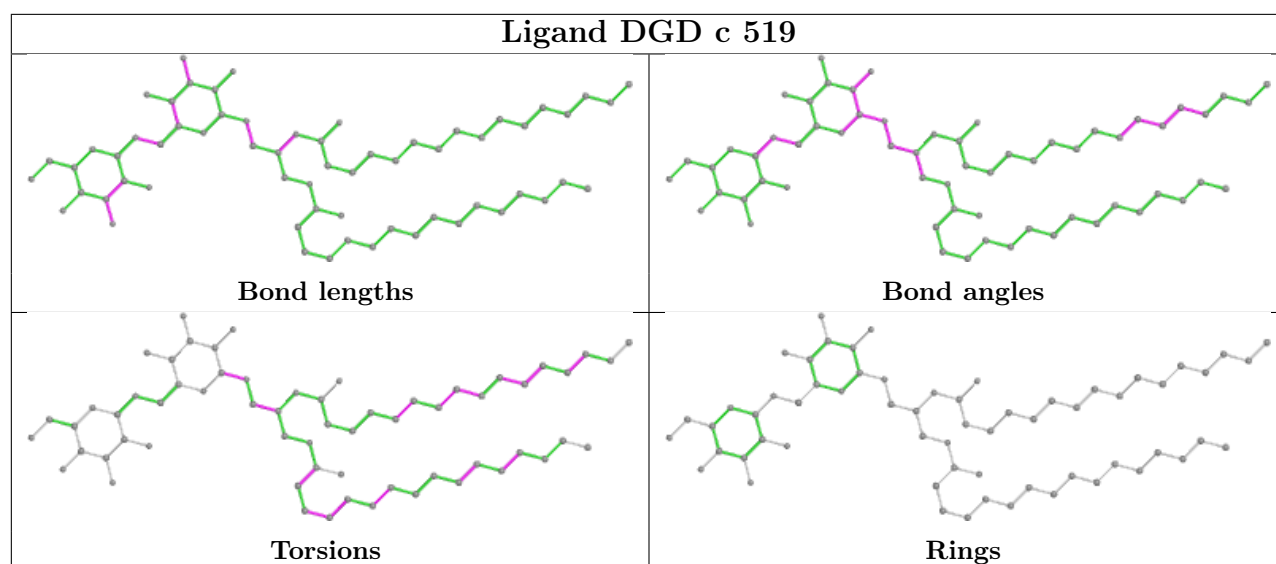
Ligand LMT Z 101

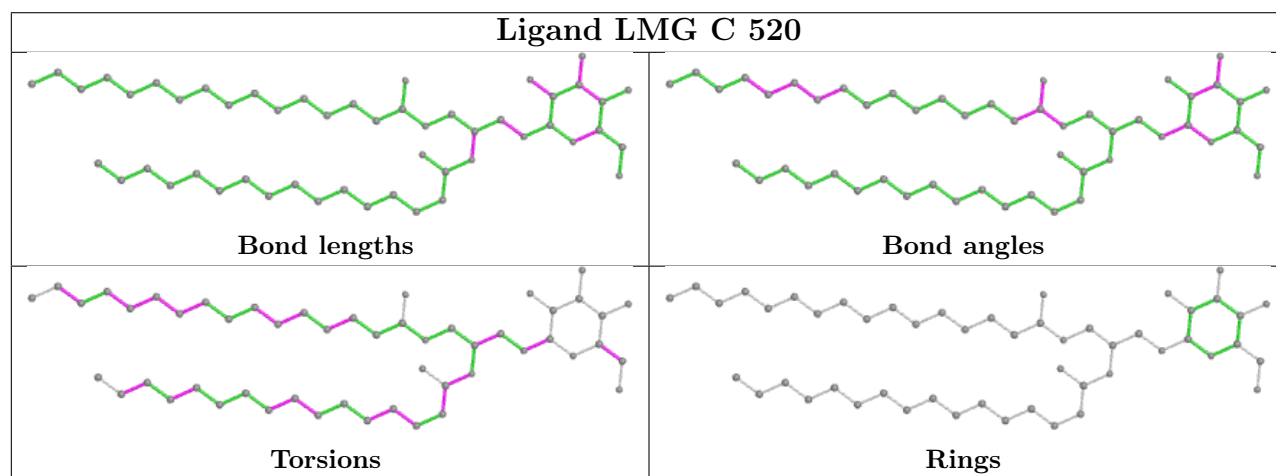
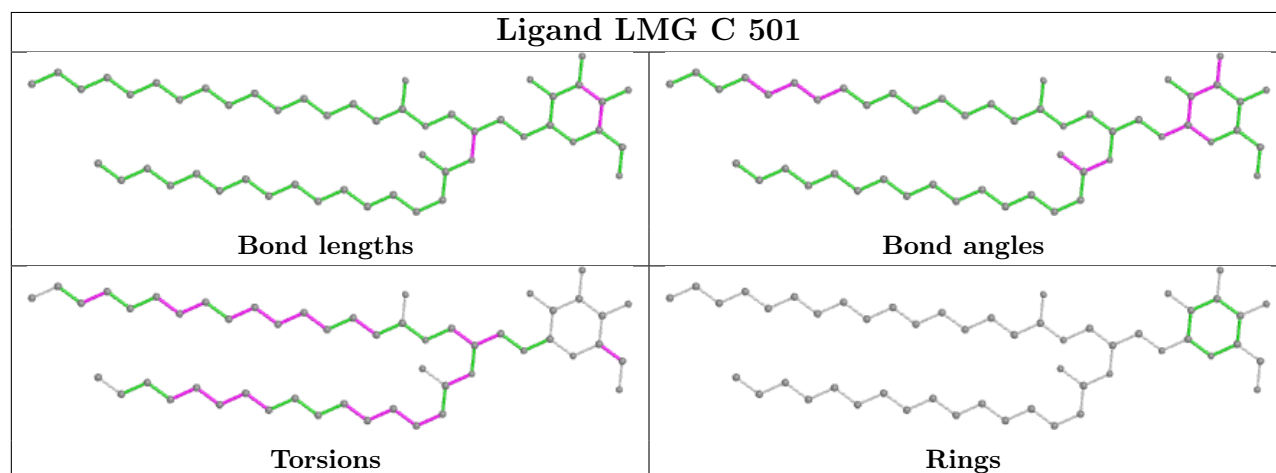
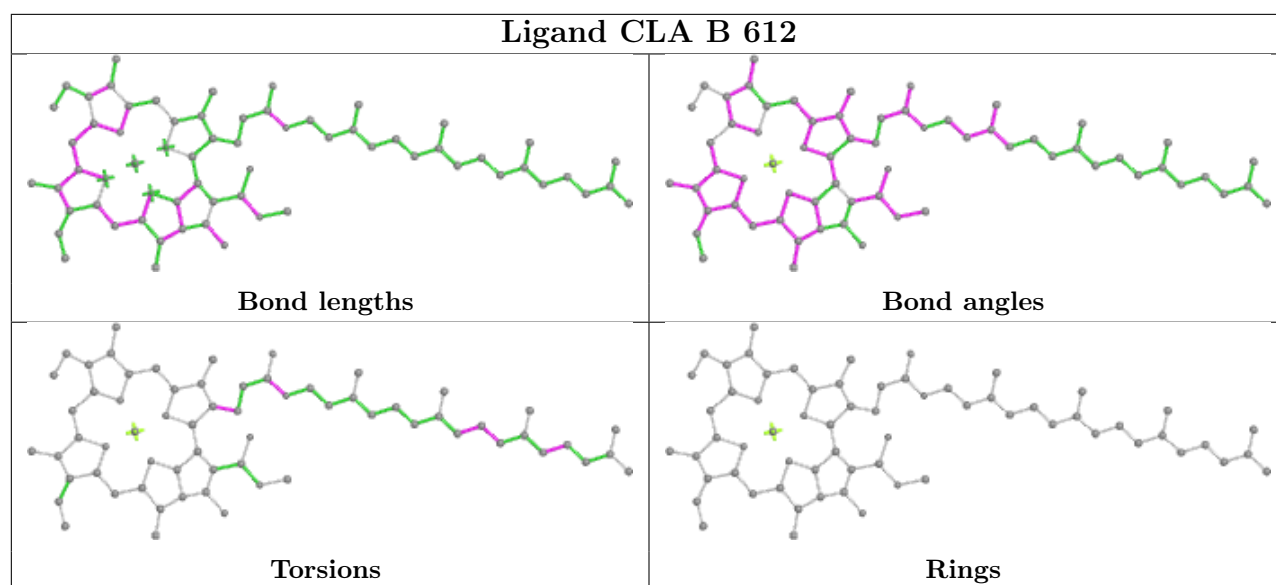


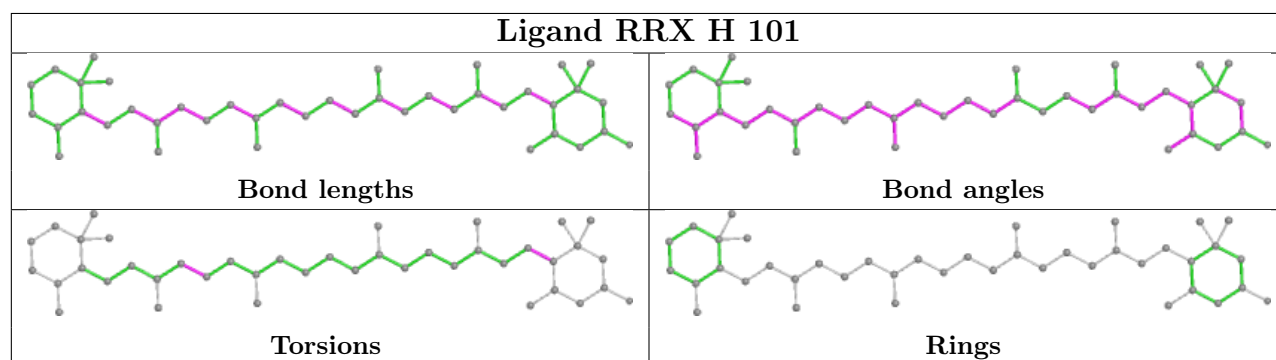
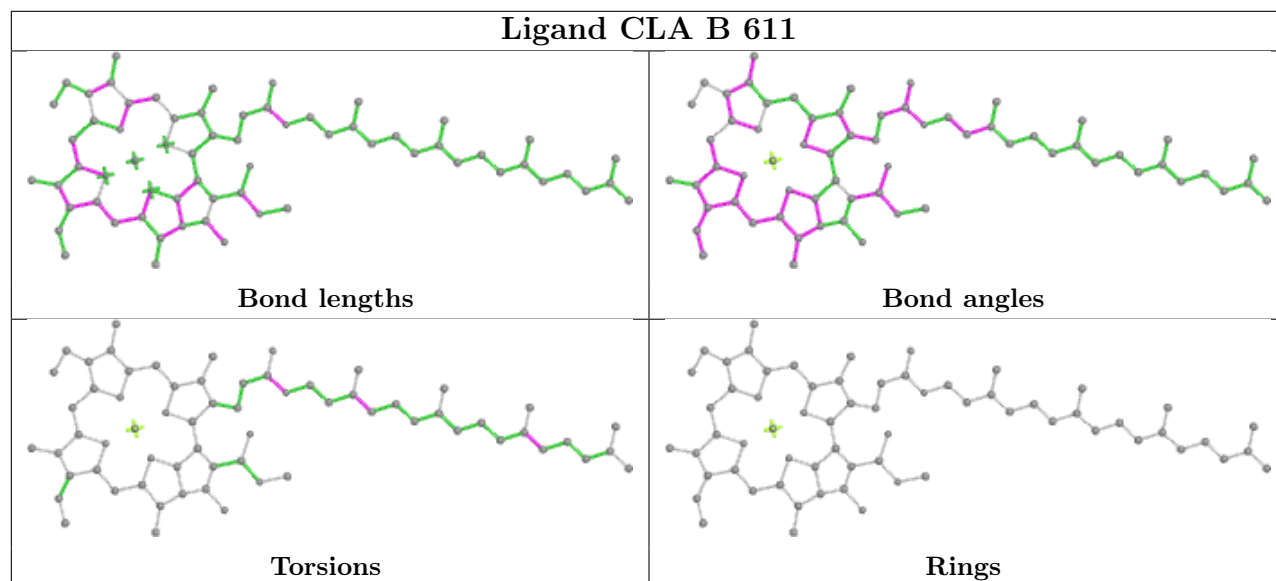
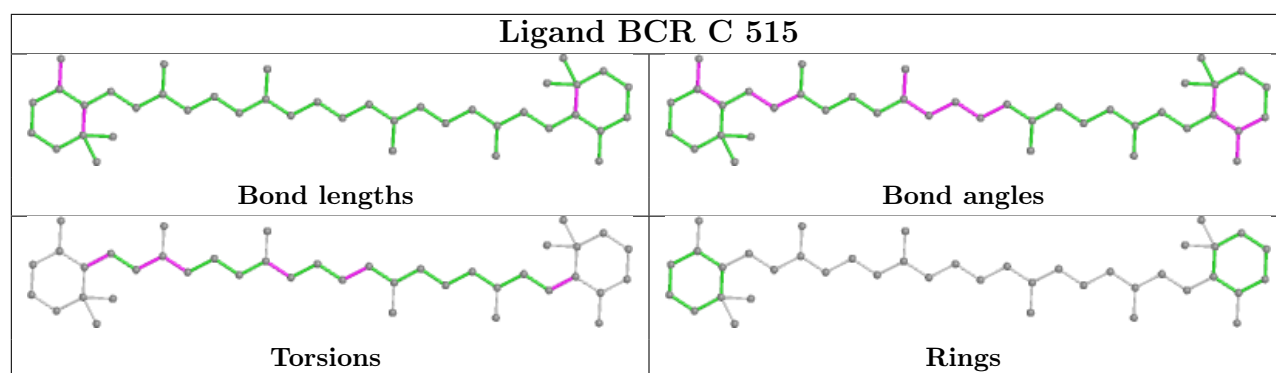


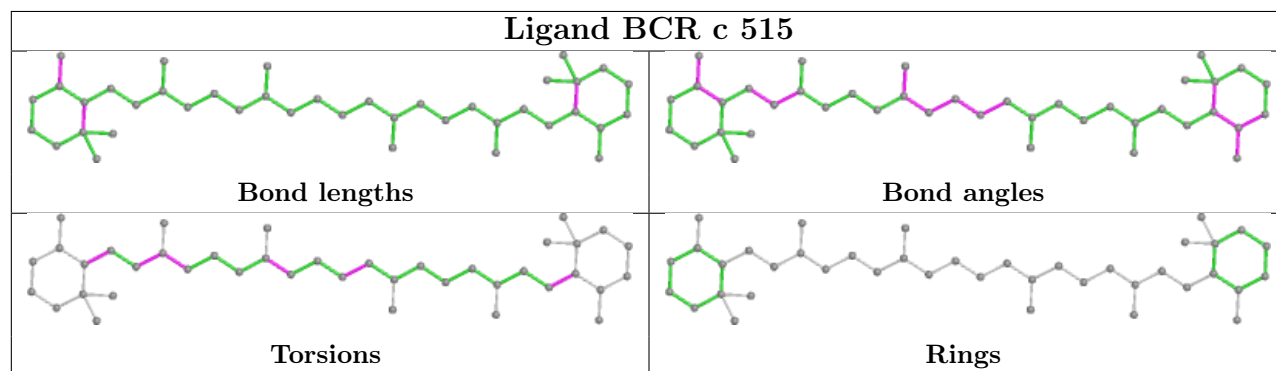
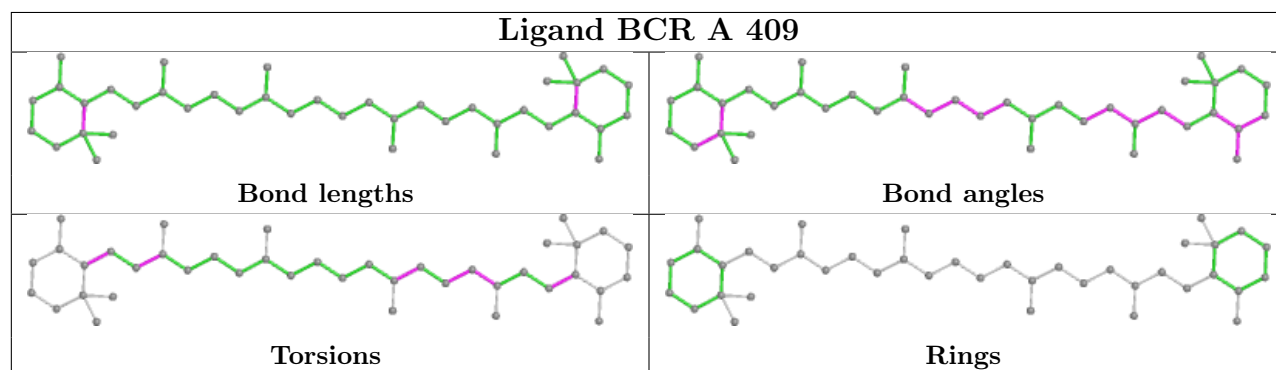
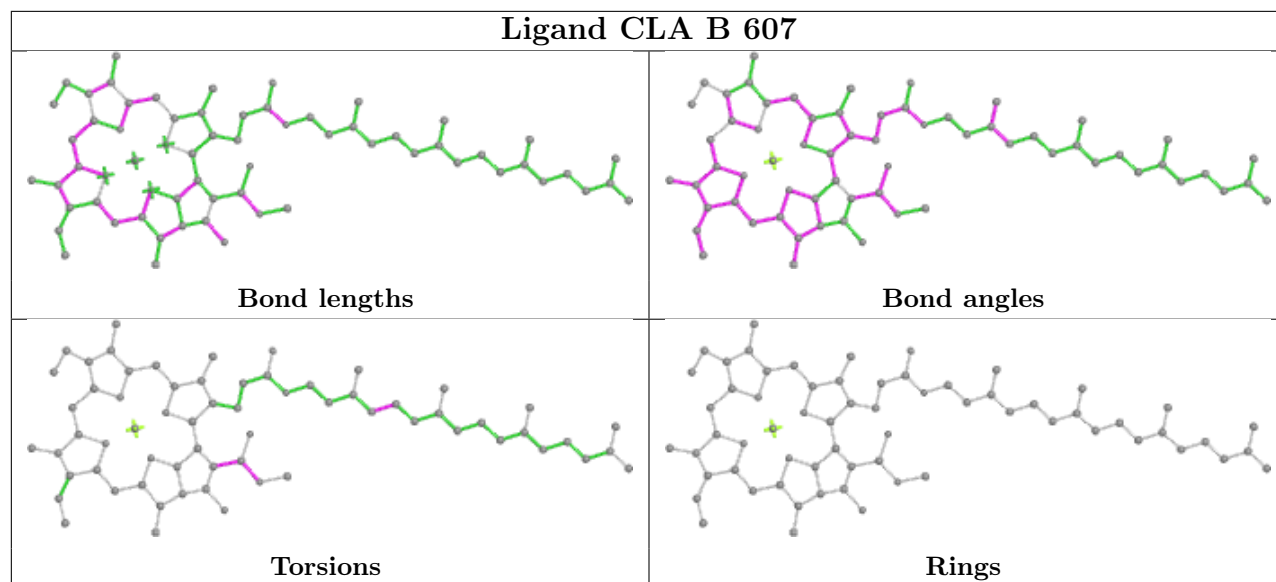


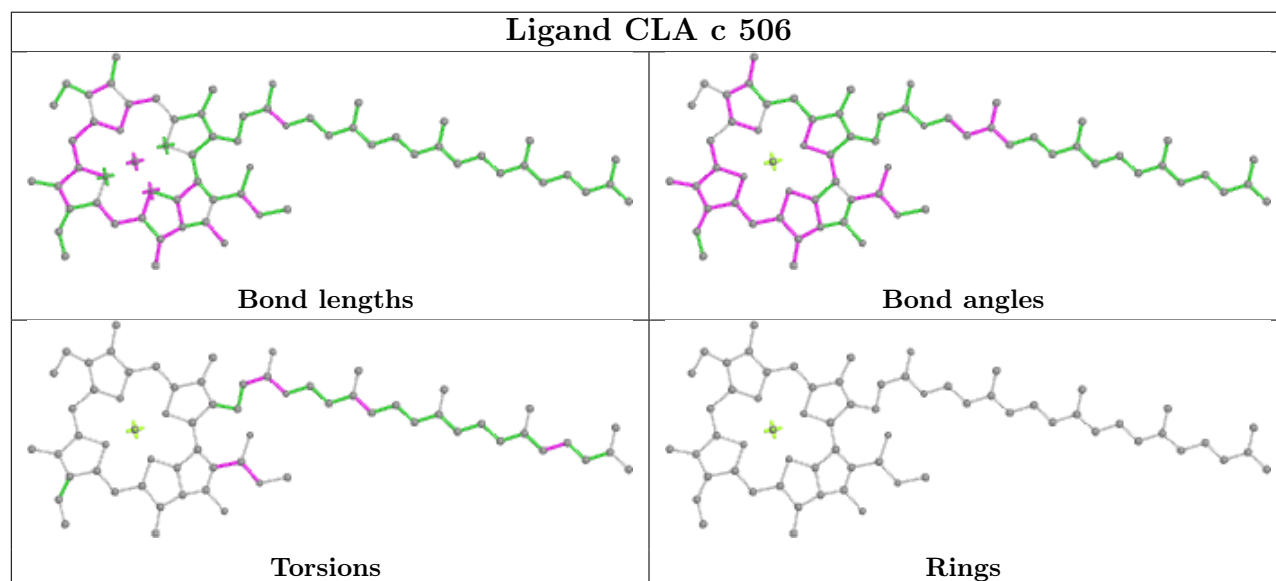
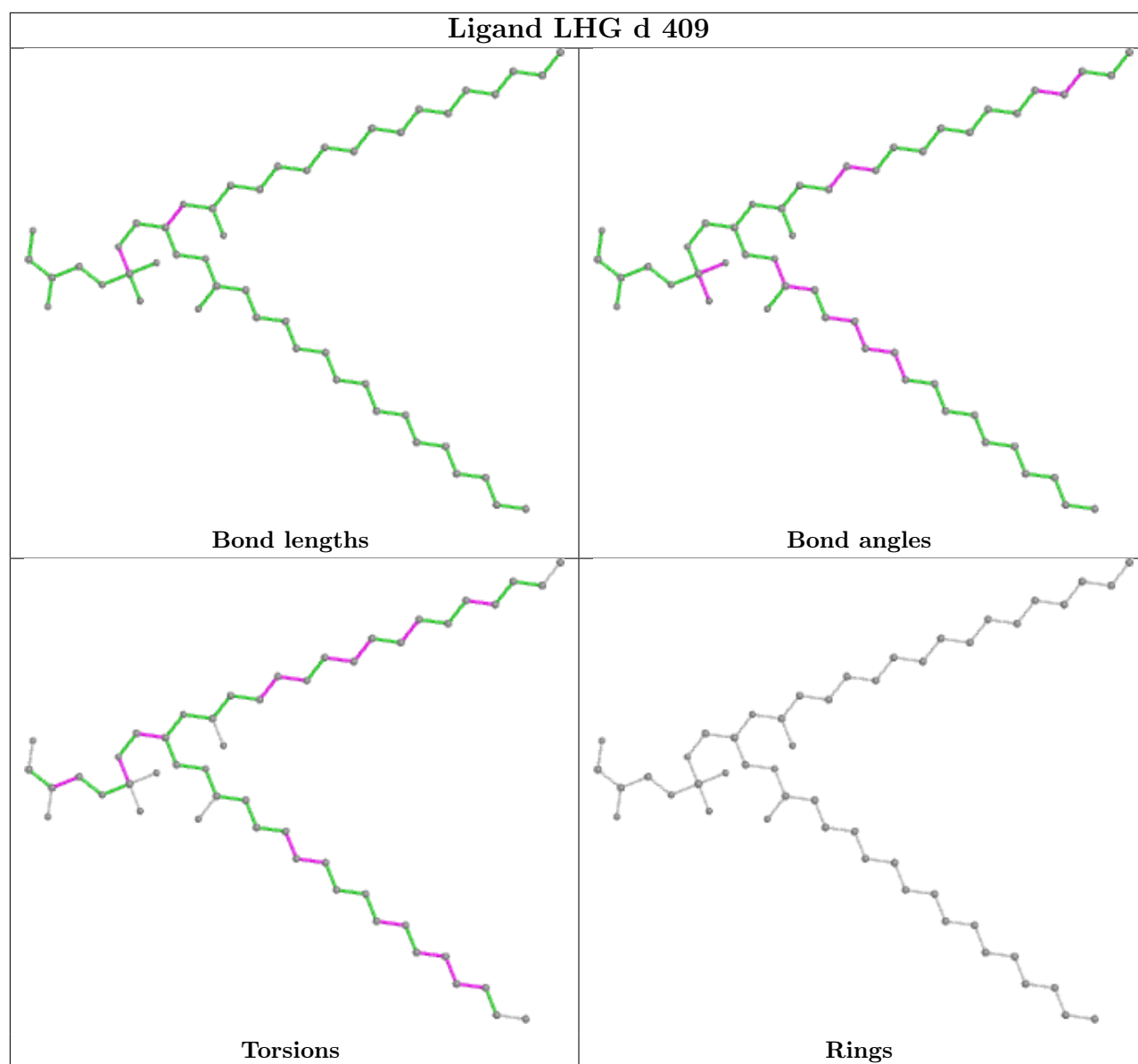


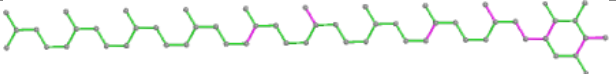
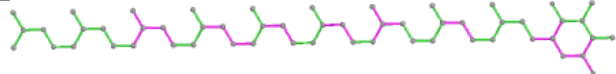
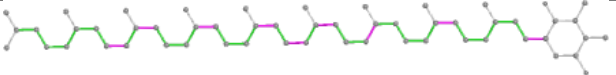
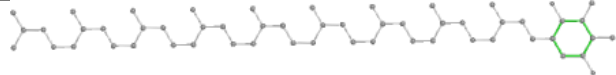


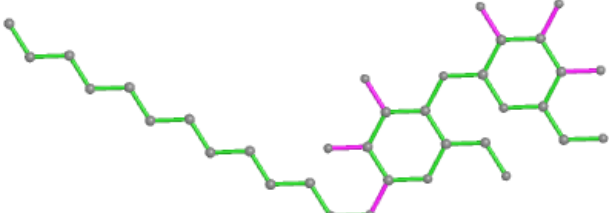
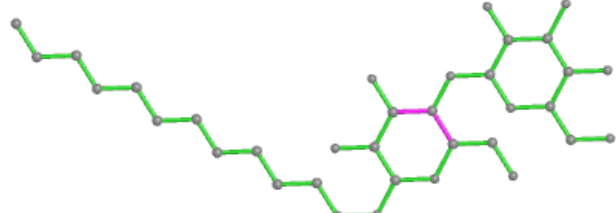
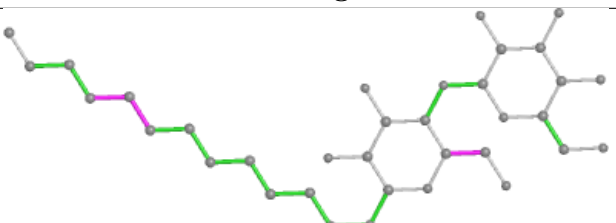
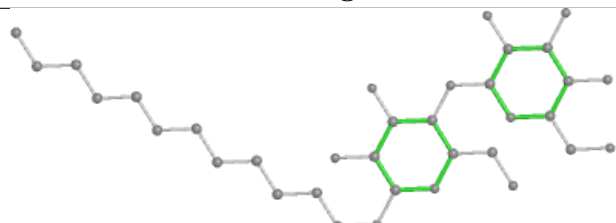


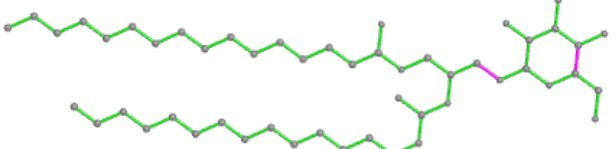
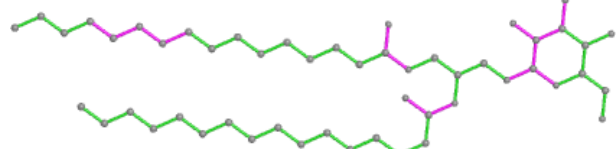
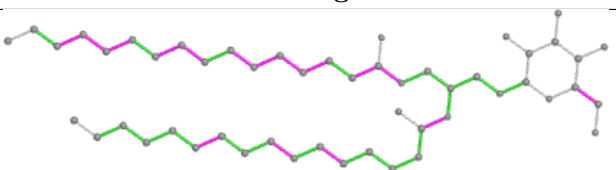



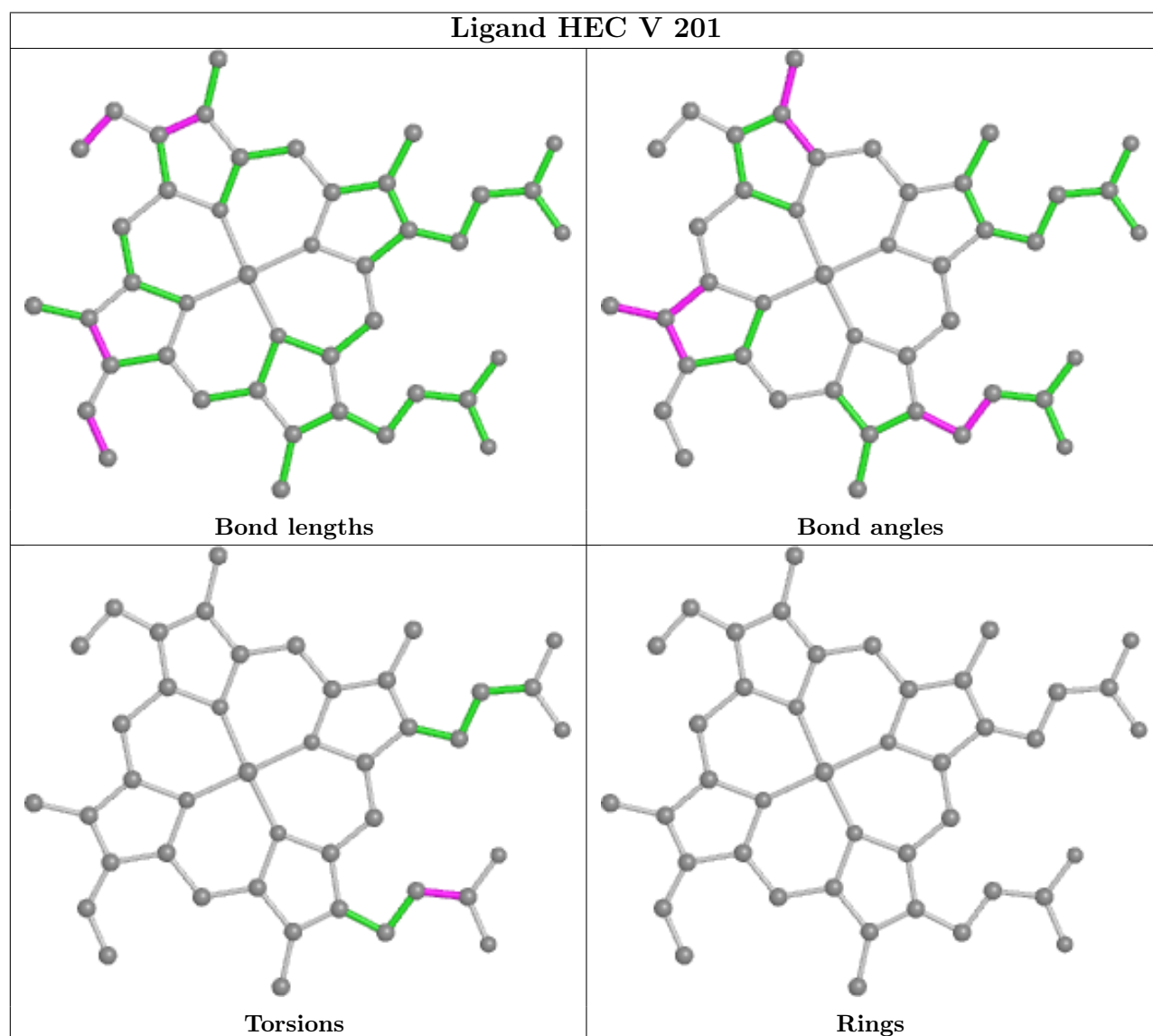
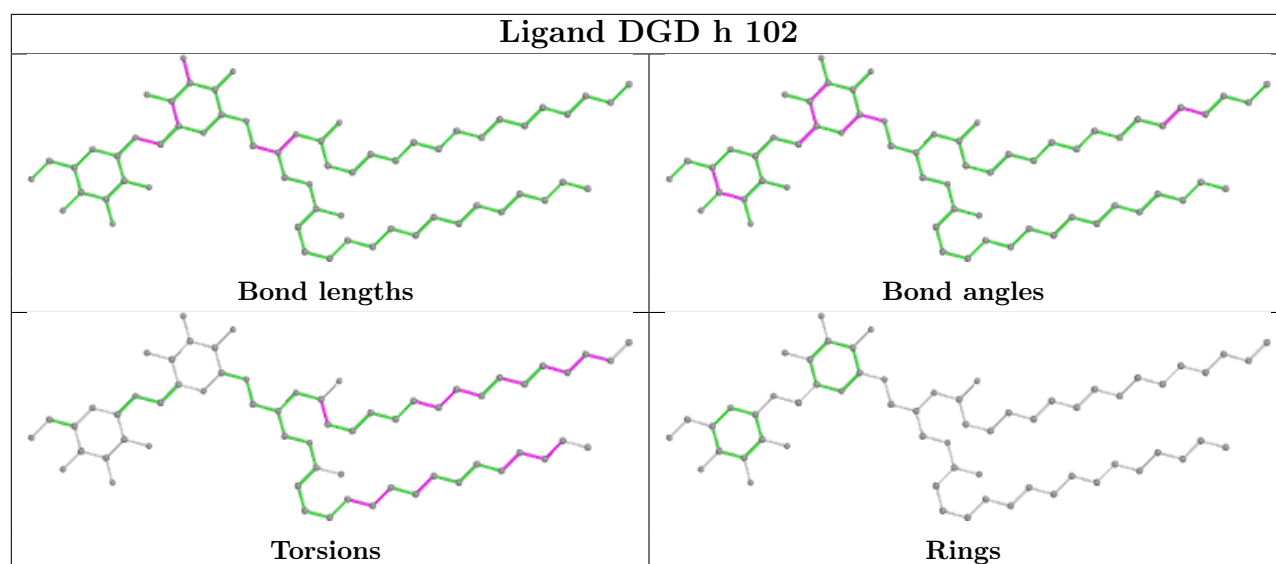


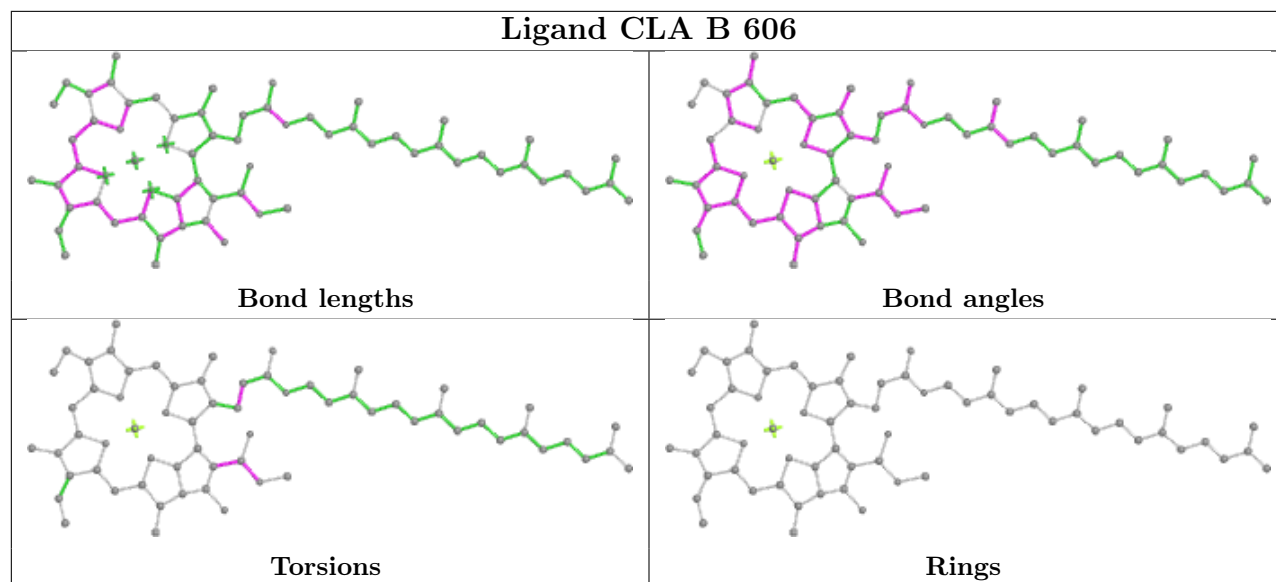
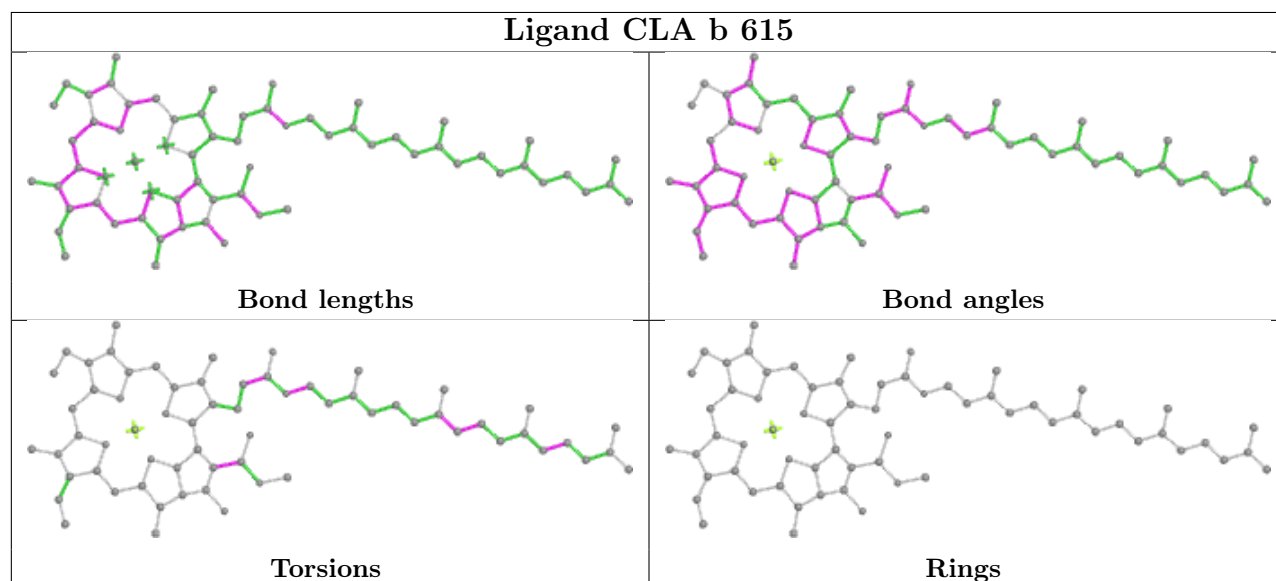
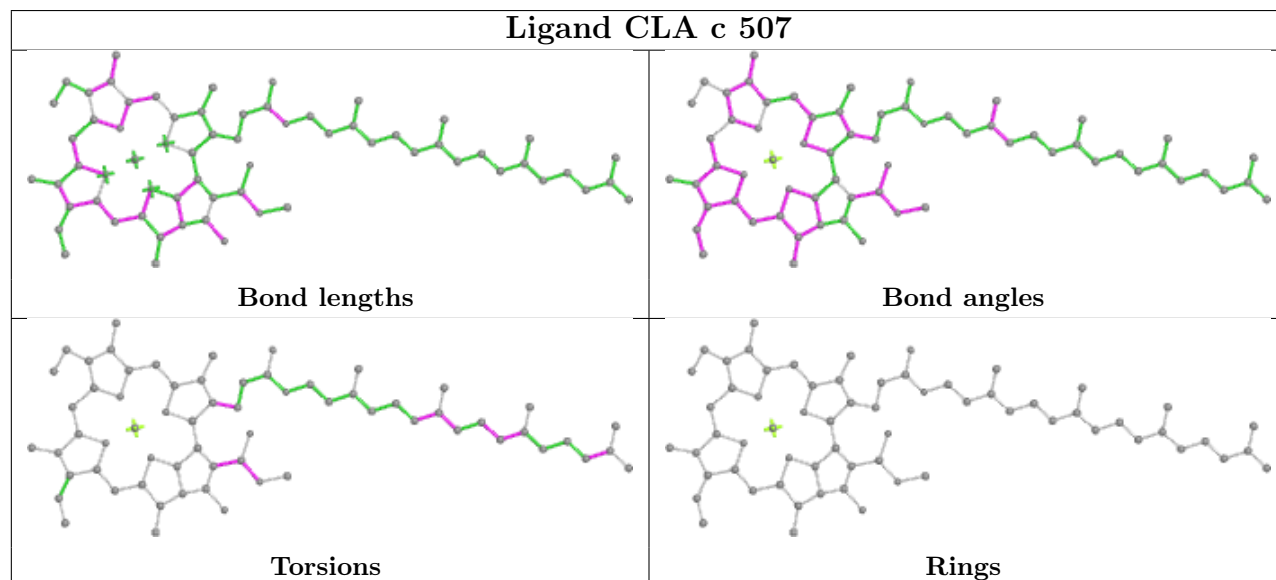


Ligand PL9 a 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

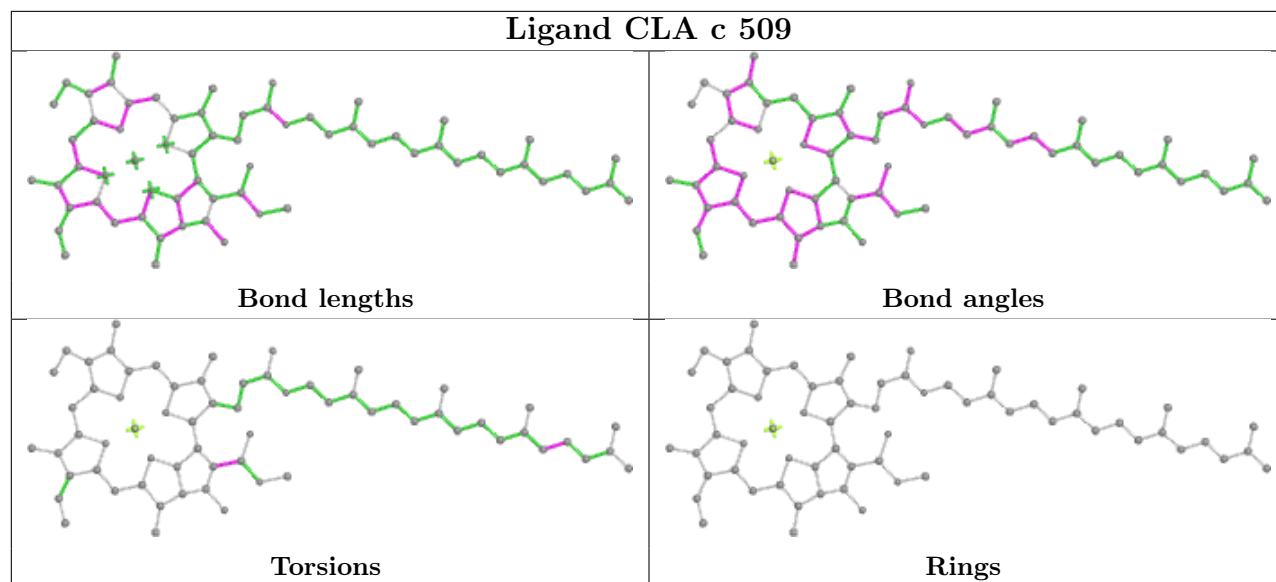
Ligand LMT M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

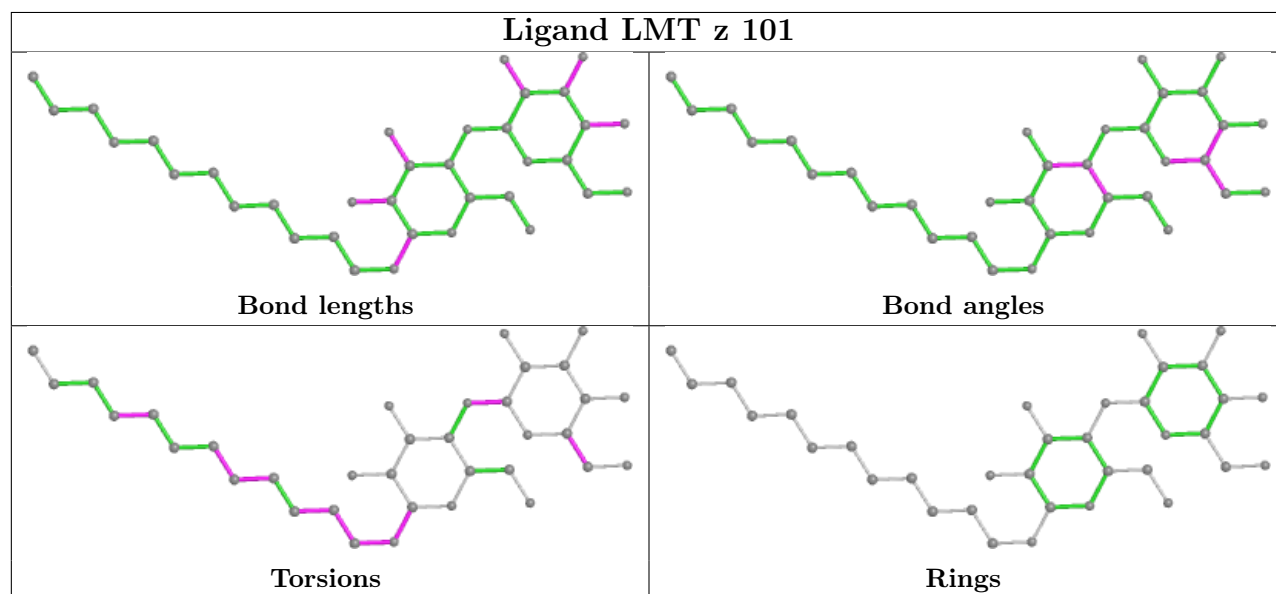


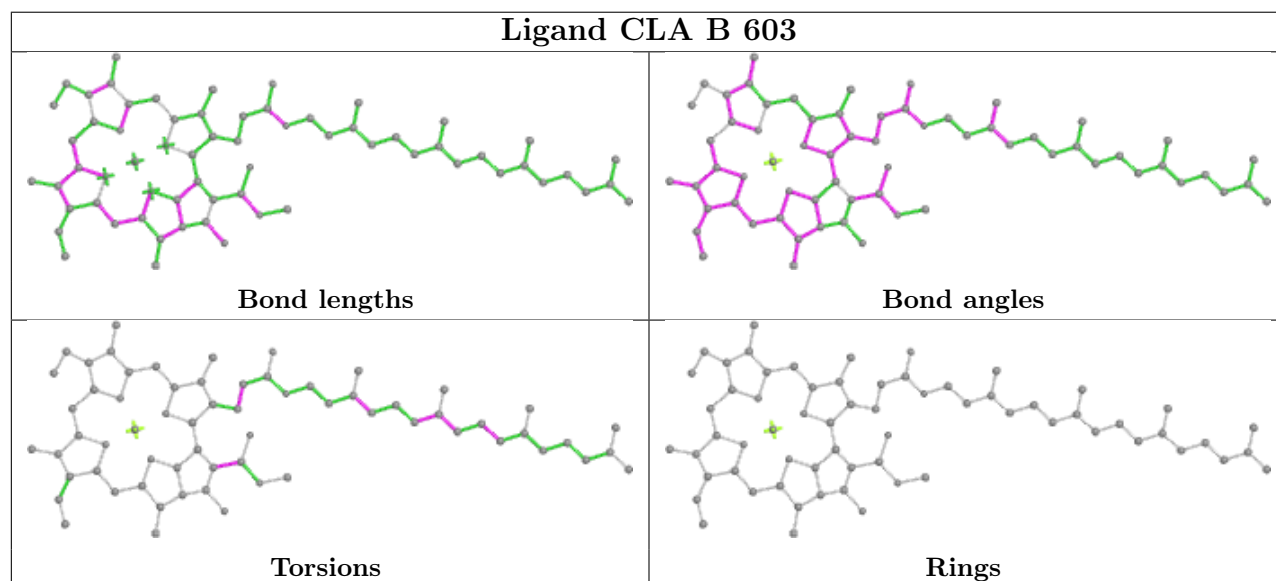
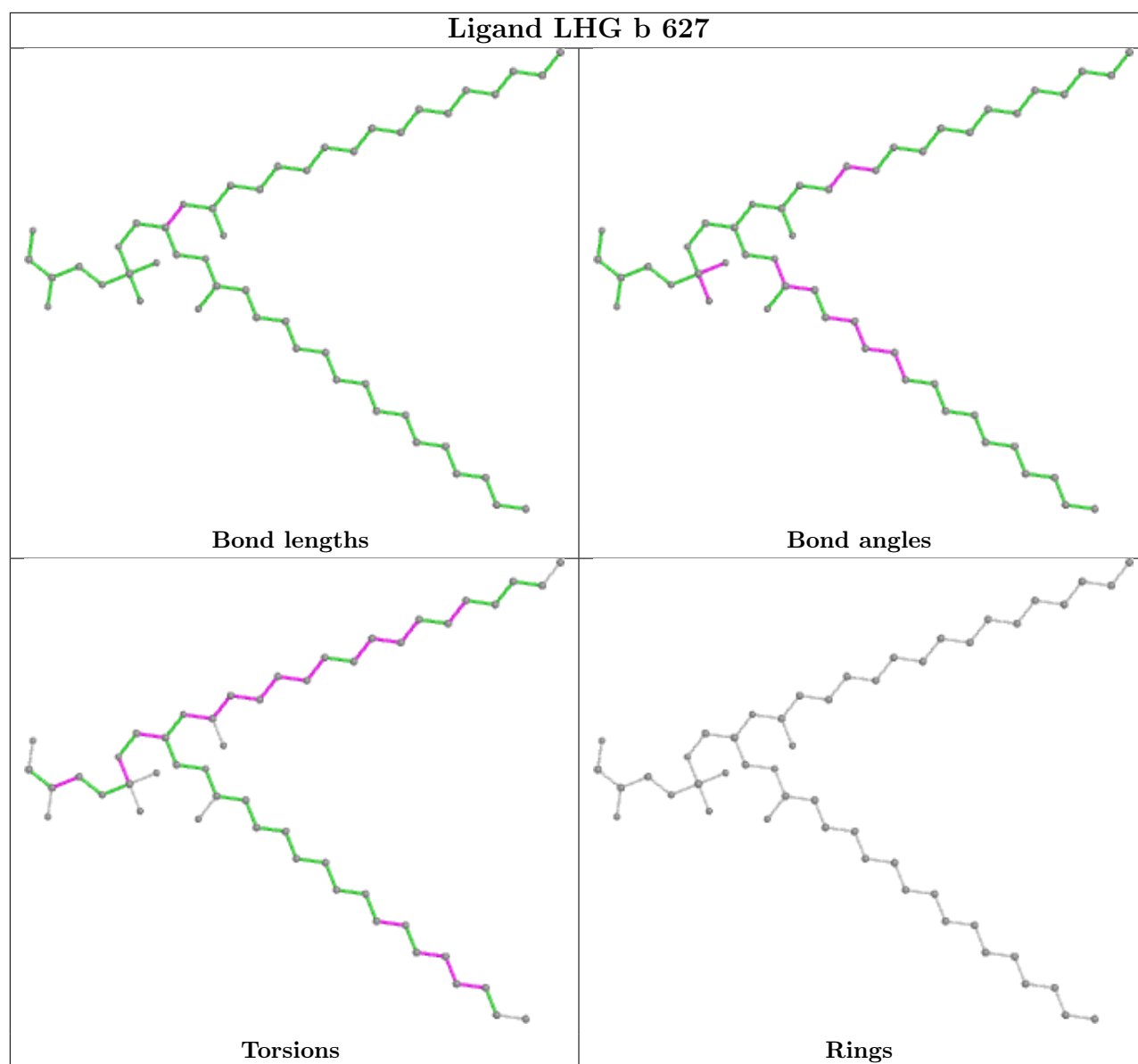
Ligand CLA B 606**Ligand CLA b 615****Ligand CLA c 507**

Ligand CLA c 509

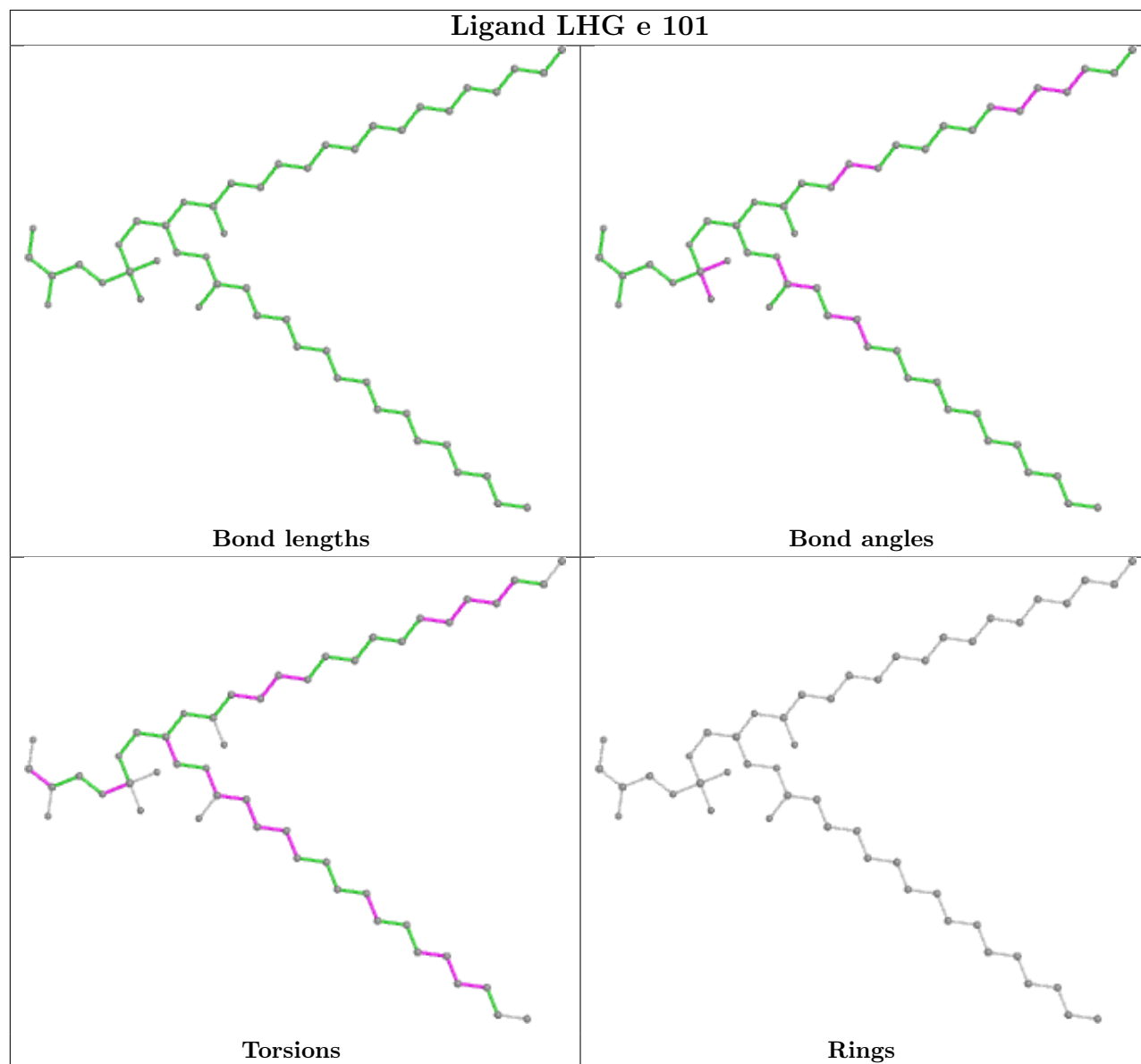


Ligand LMT z 101

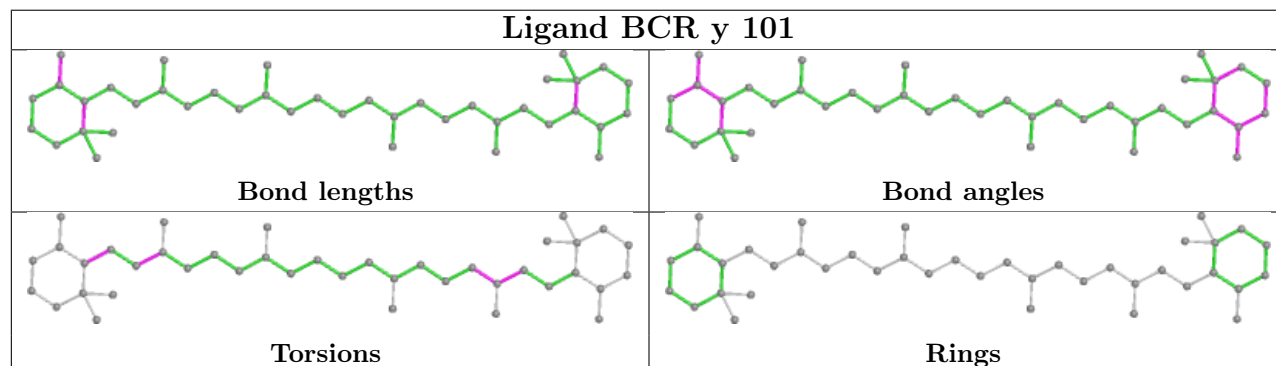


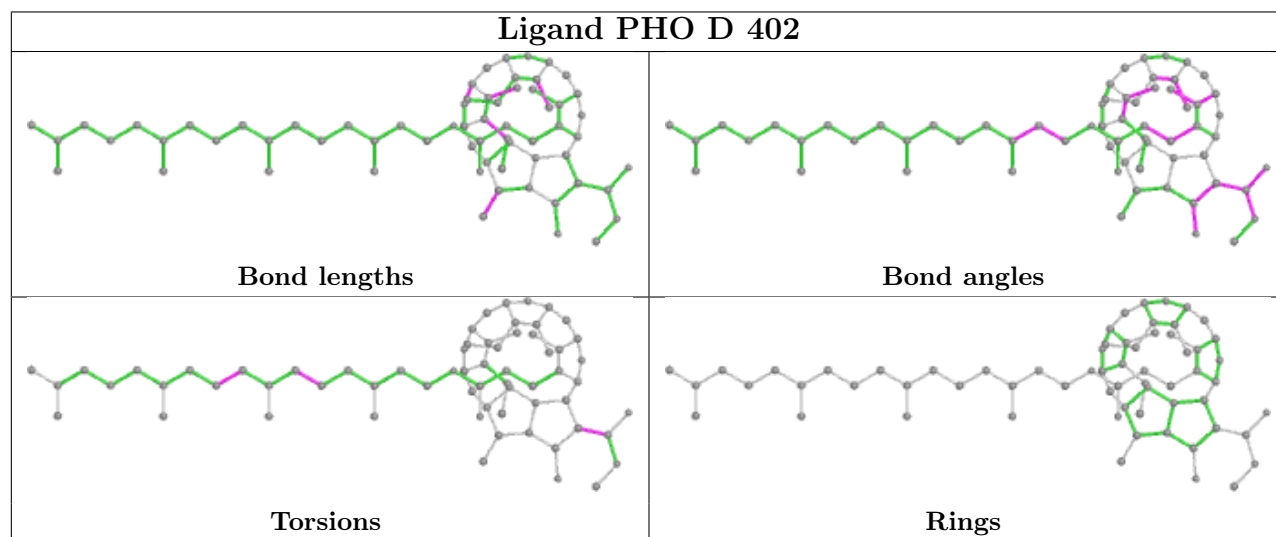
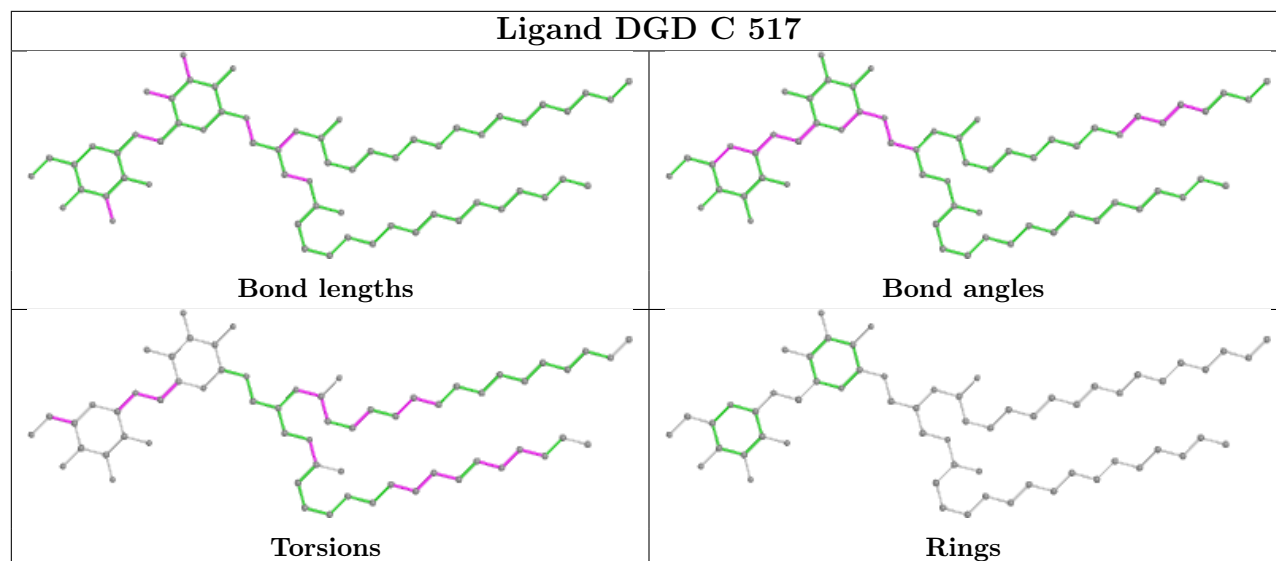


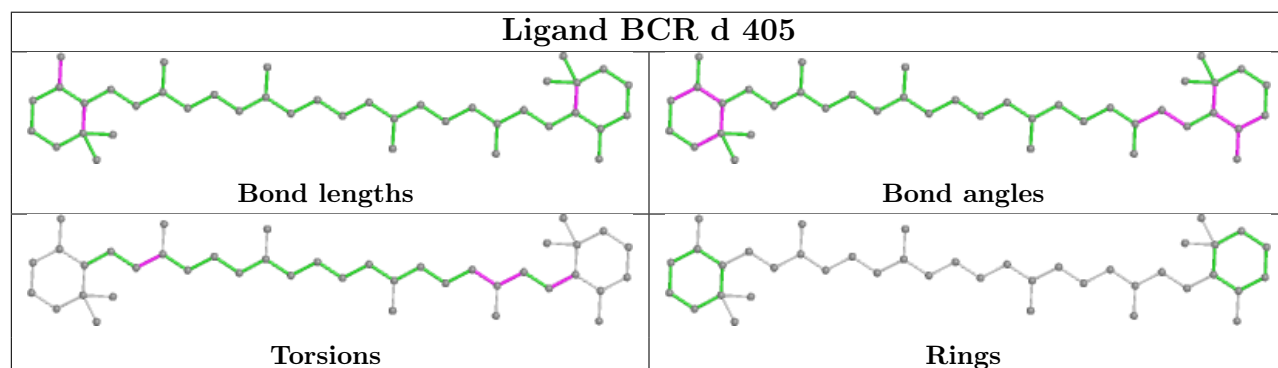
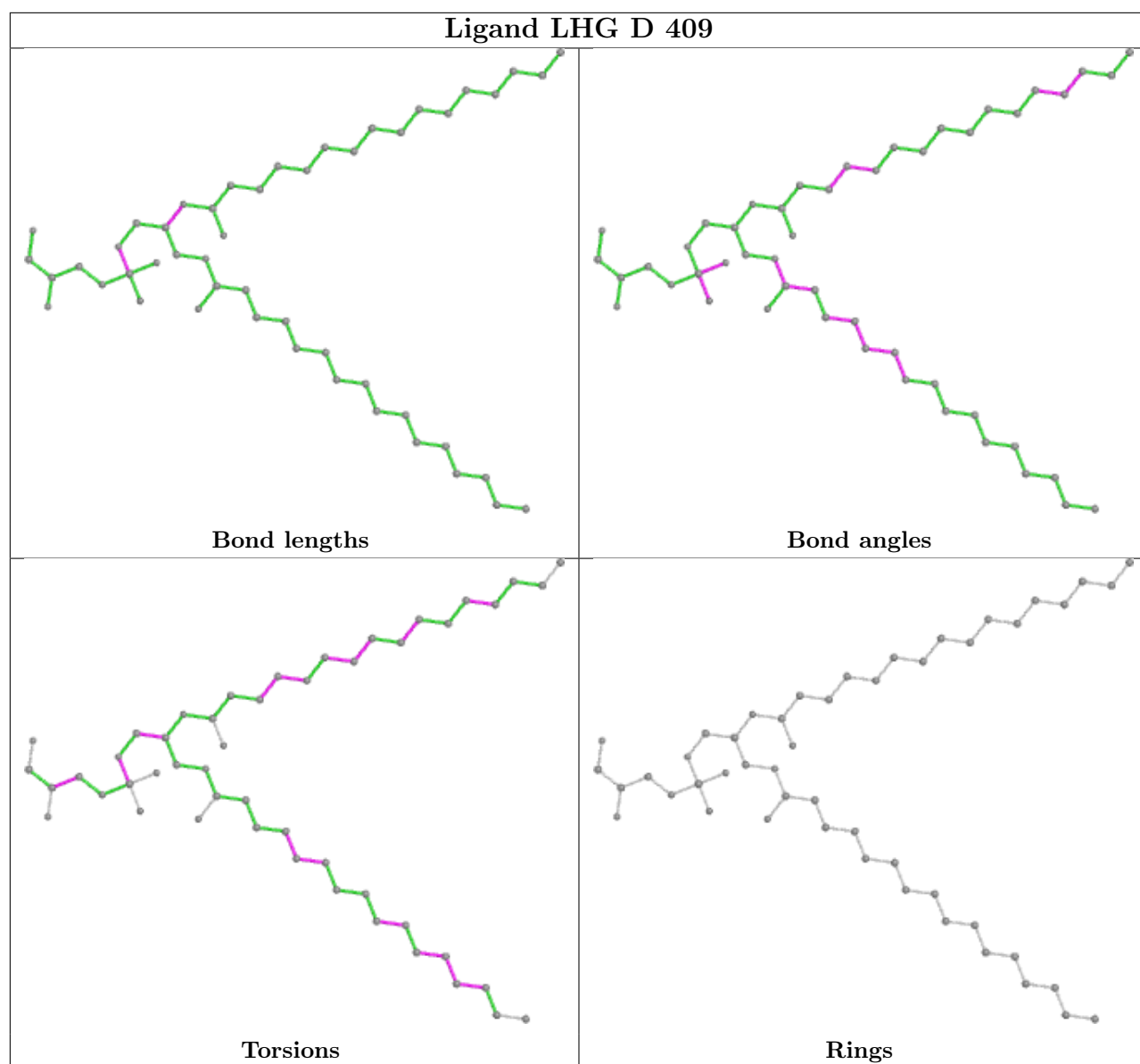
Ligand LHG e 101



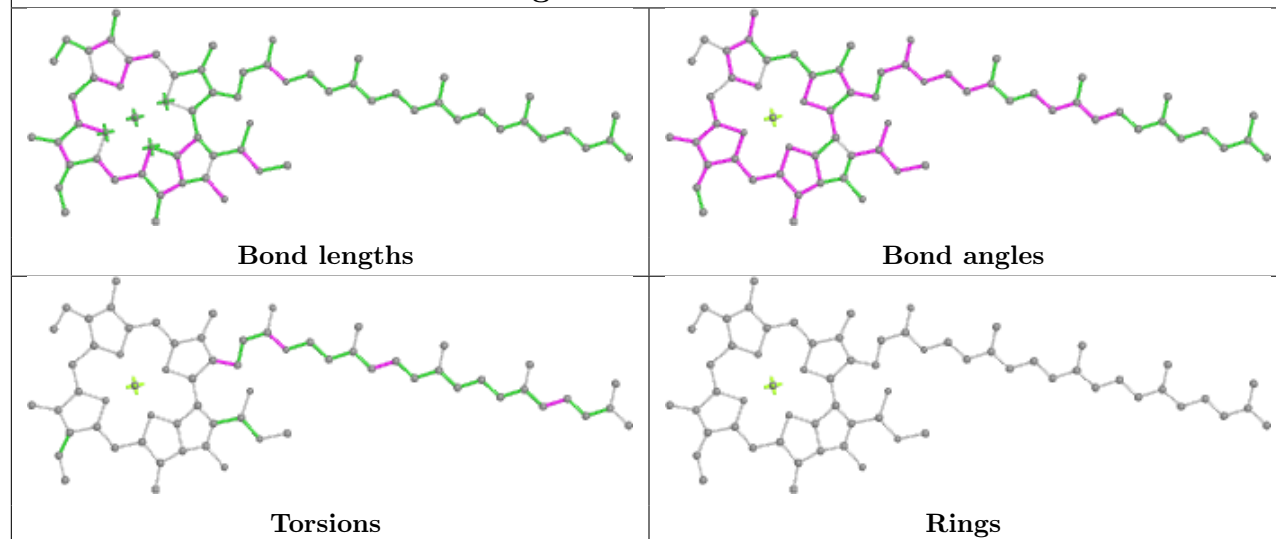
Ligand BCR y 101



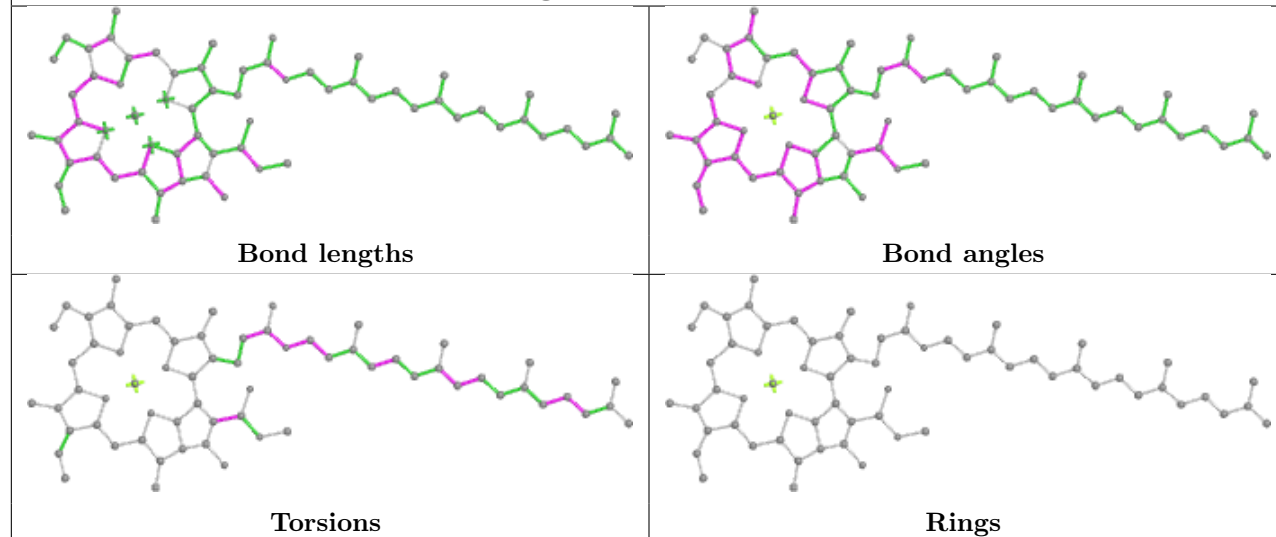




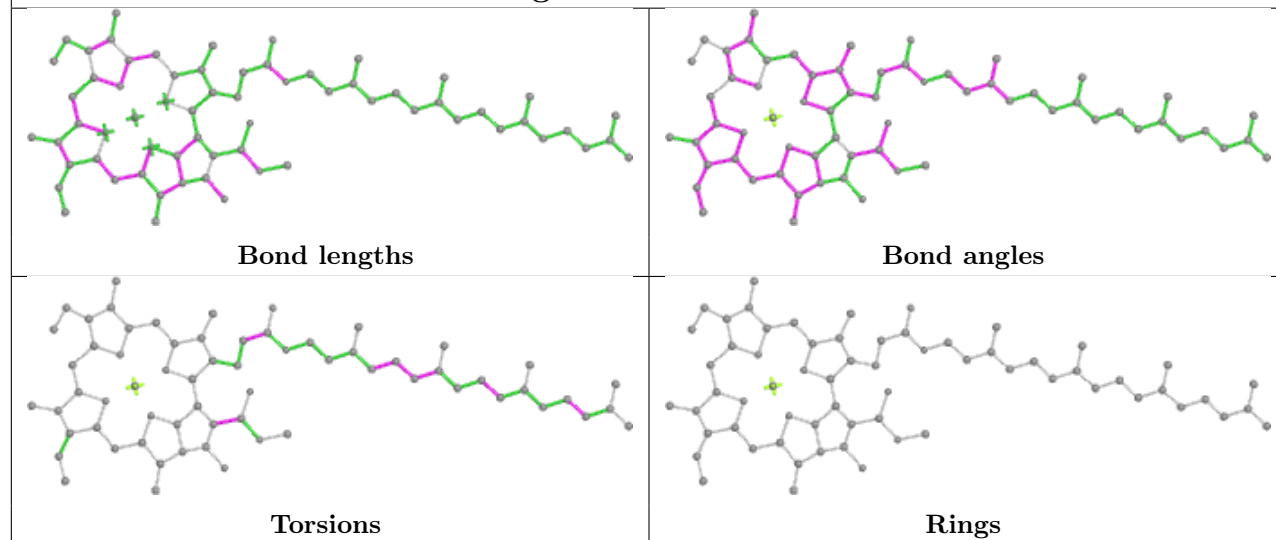
Ligand CLA B 604

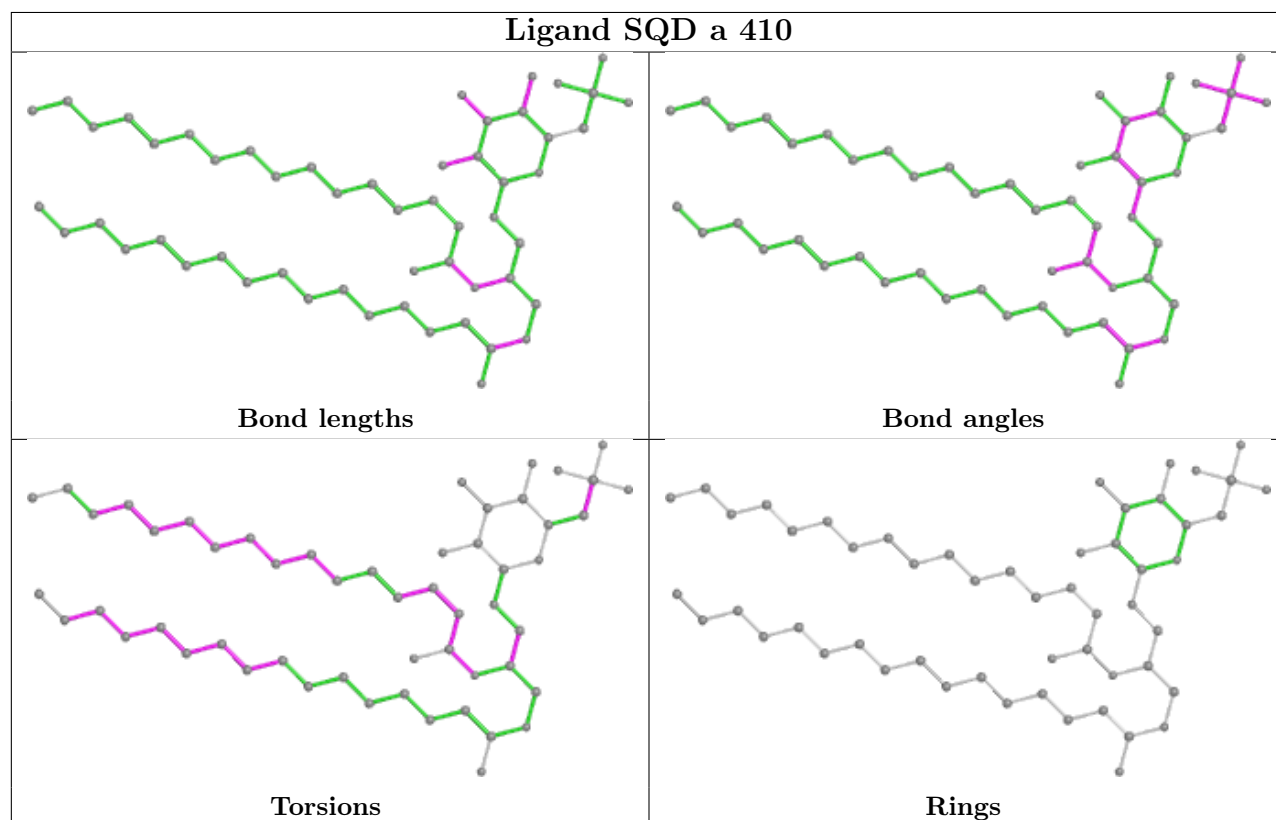
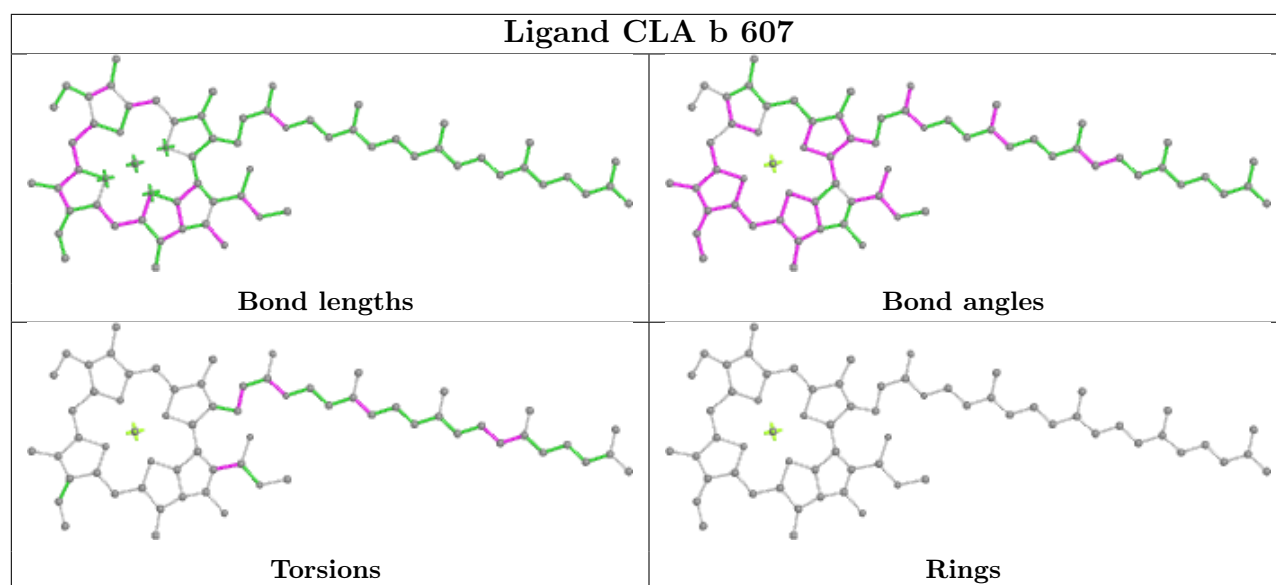


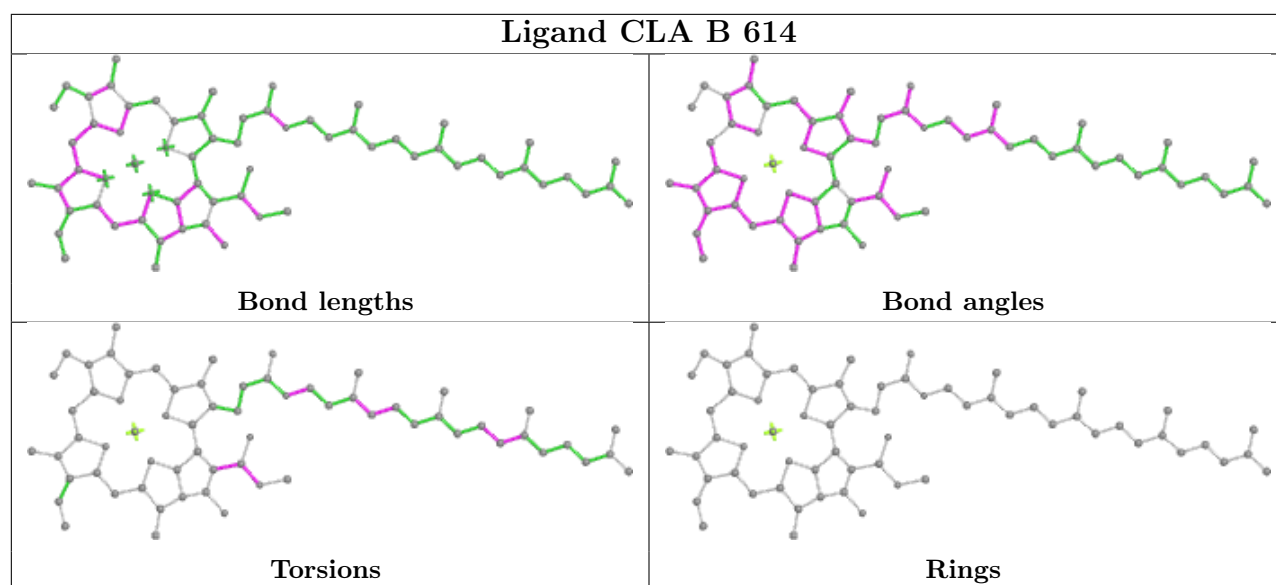
Ligand CLA c 513



Ligand CLA B 616







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.

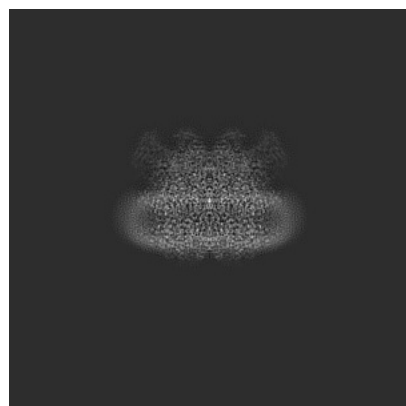
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30548. These allow visual inspection of the internal detail of the map and identification of artifacts.

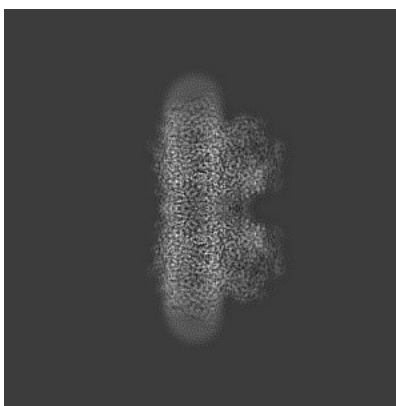
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

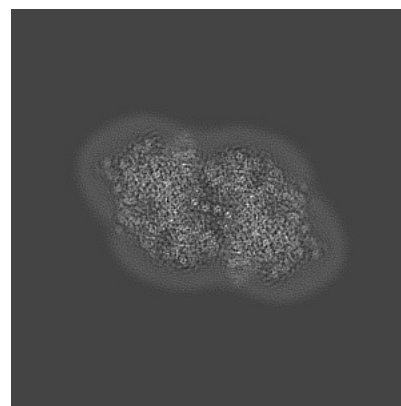
6.1.1 Primary map



X

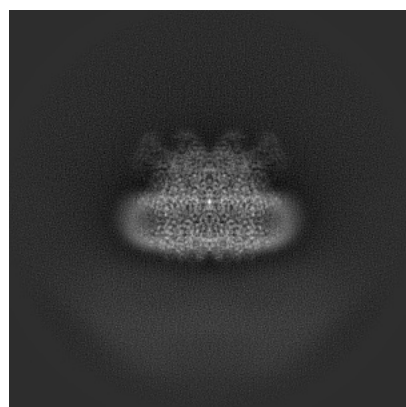


Y

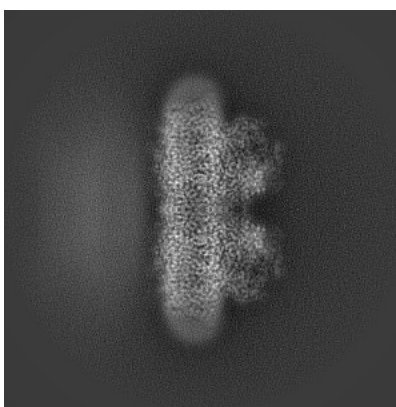


Z

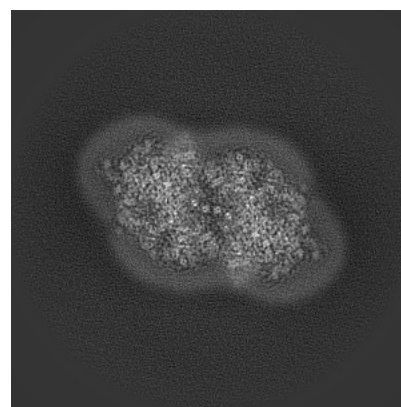
6.1.2 Raw map



X



Y

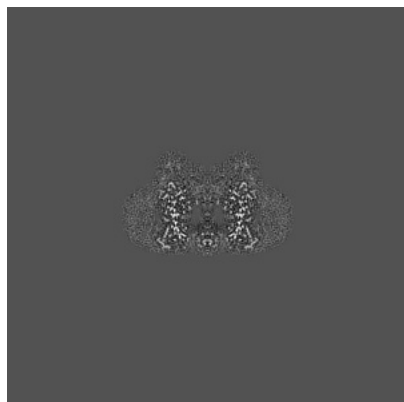


Z

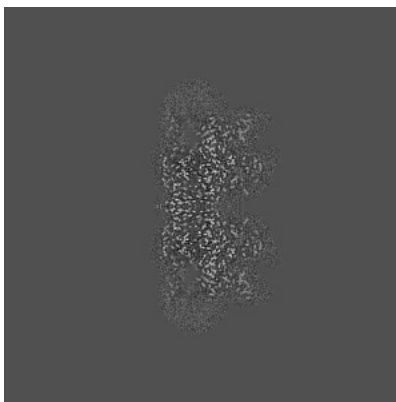
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

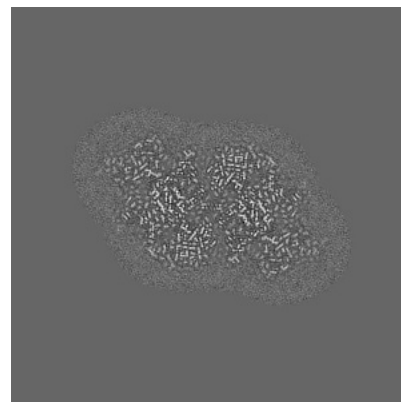
6.2.1 Primary map



X Index: 200

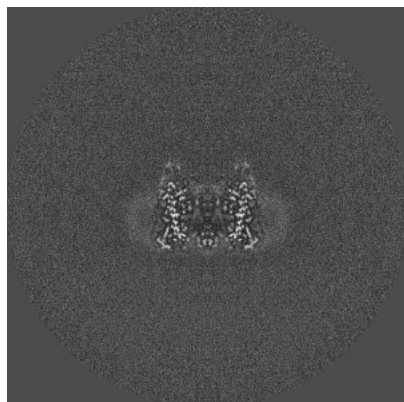


Y Index: 200

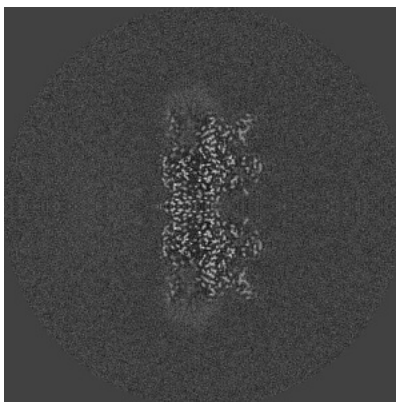


Z Index: 200

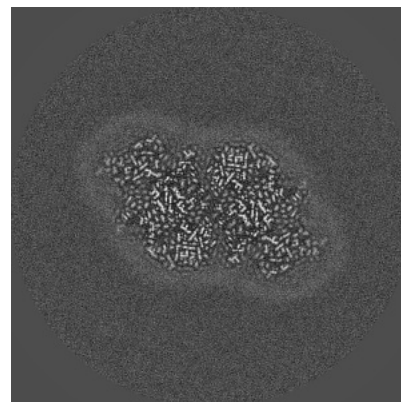
6.2.2 Raw map



X Index: 200



Y Index: 200

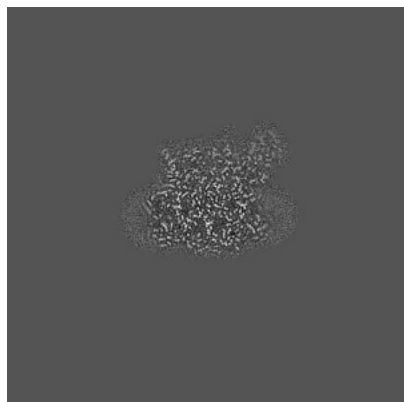


Z Index: 200

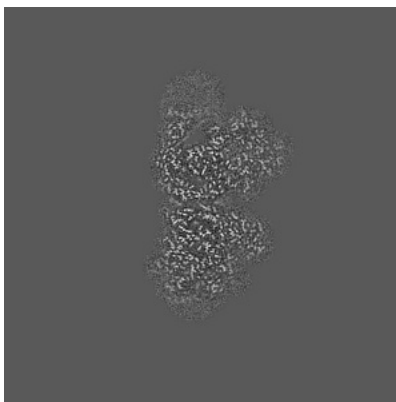
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

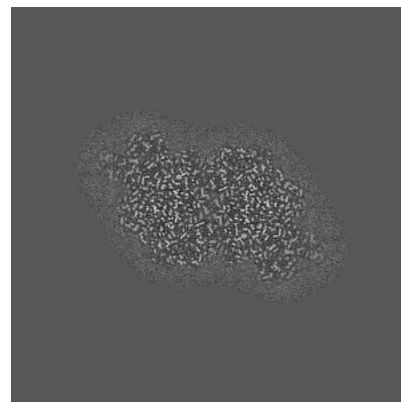
6.3.1 Primary map



X Index: 167

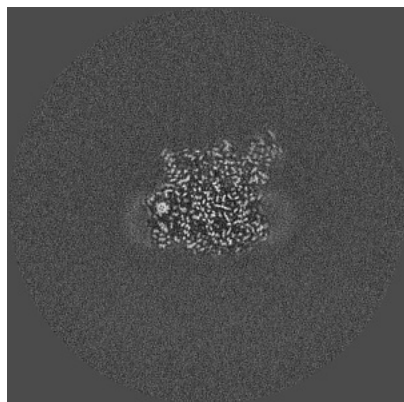


Y Index: 182

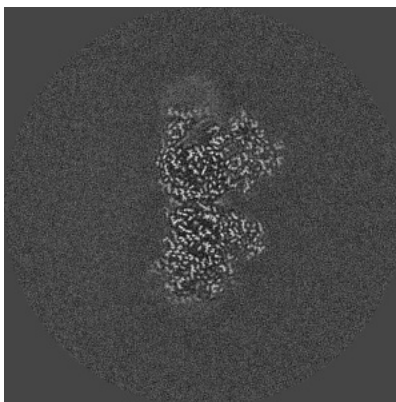


Z Index: 209

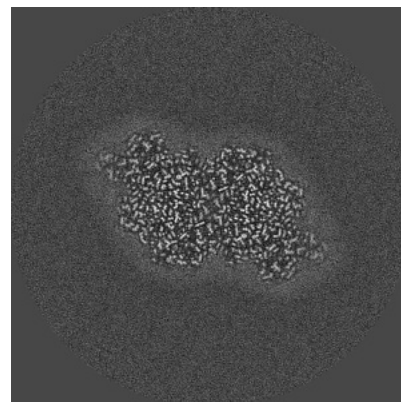
6.3.2 Raw map



X Index: 166



Y Index: 182

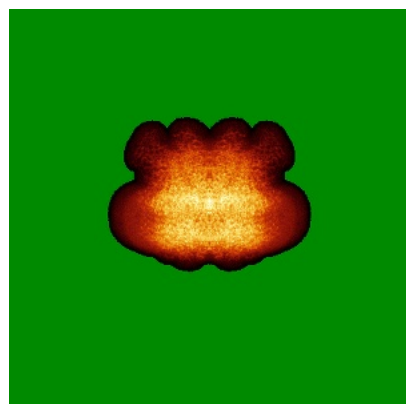


Z Index: 209

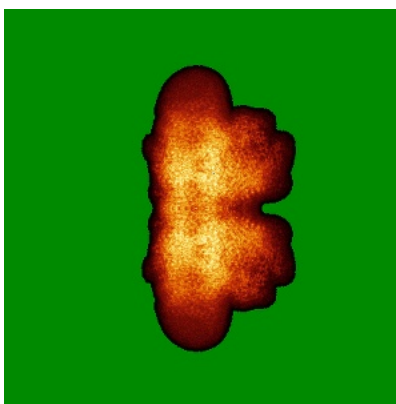
The images above show the largest variance slices of the map in three orthogonal directions.

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

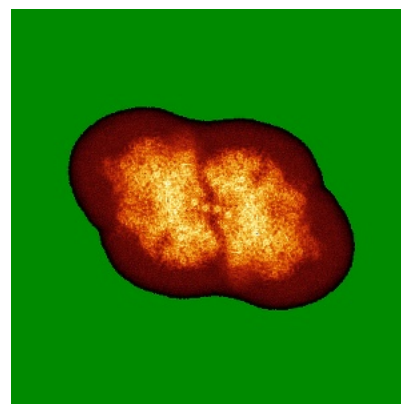
6.4.1 Primary map



X

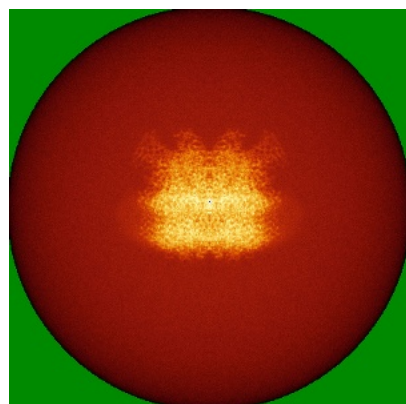


Y

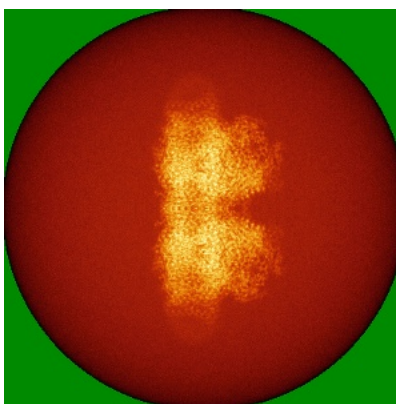


Z

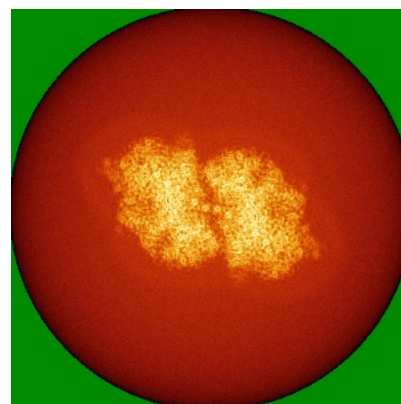
6.4.2 Raw map



X



Y

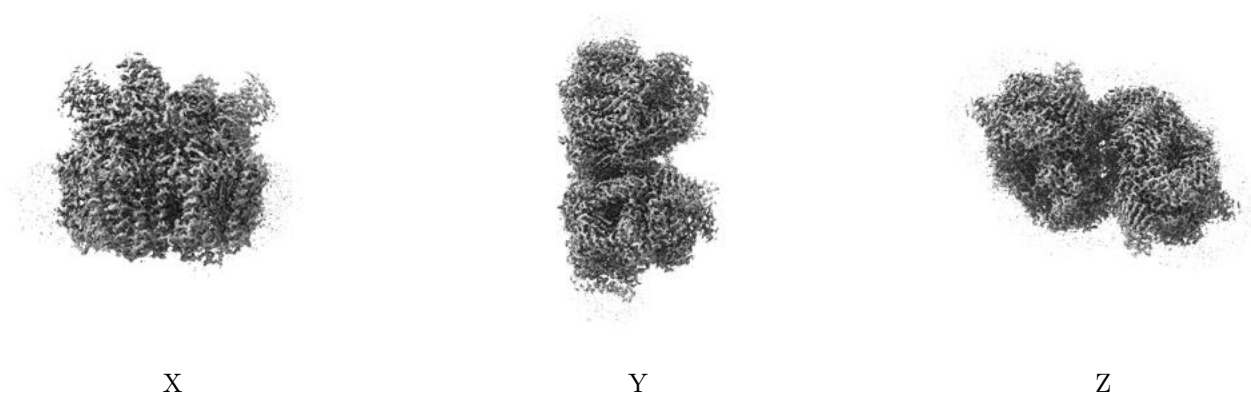


Z

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.

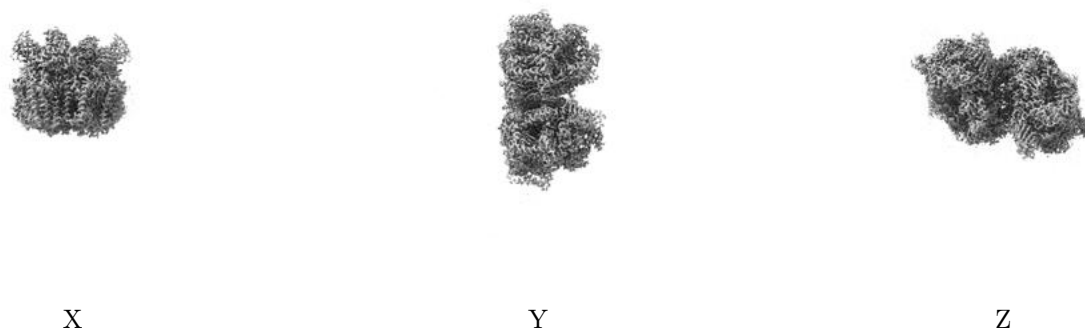
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



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.

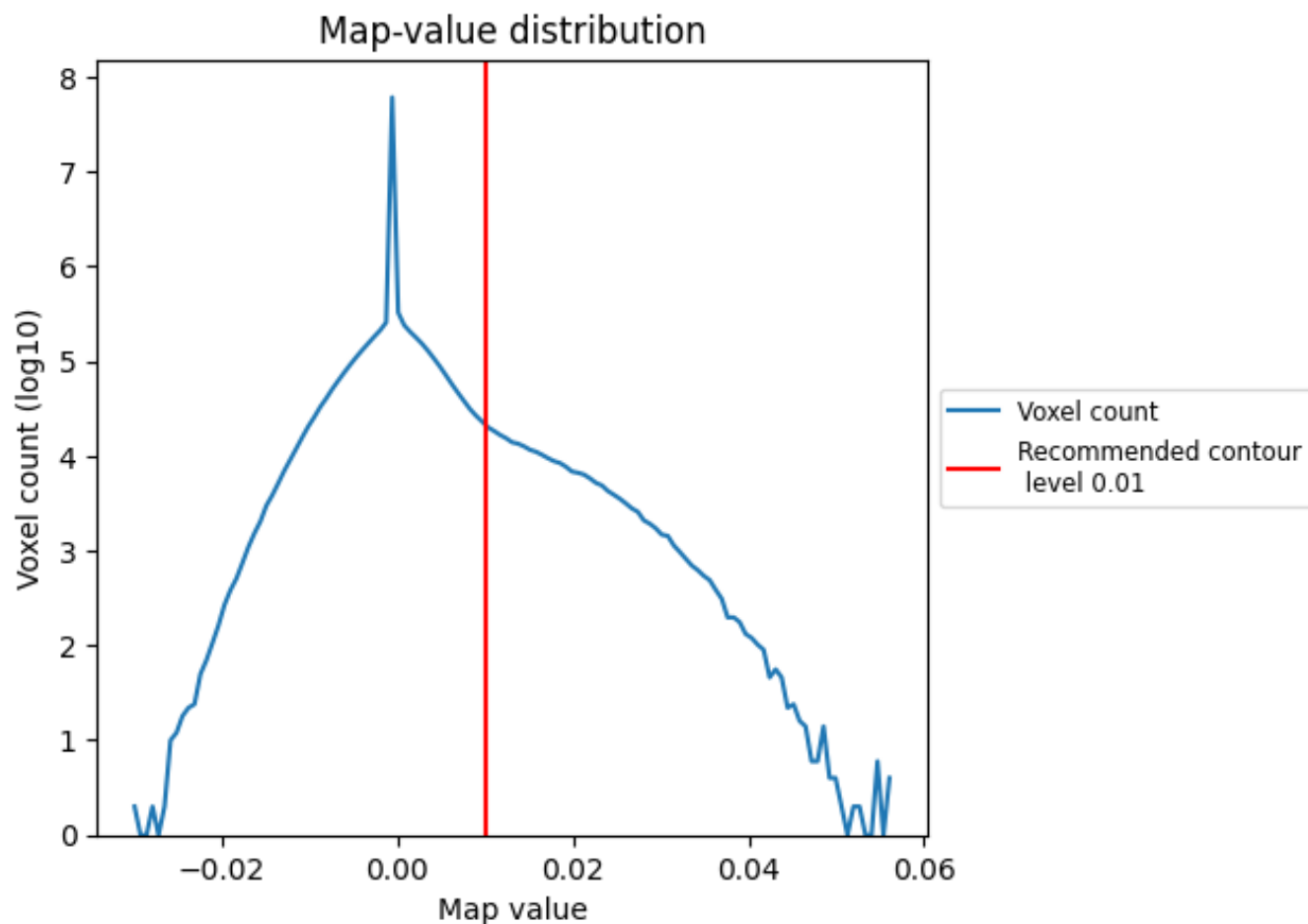
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

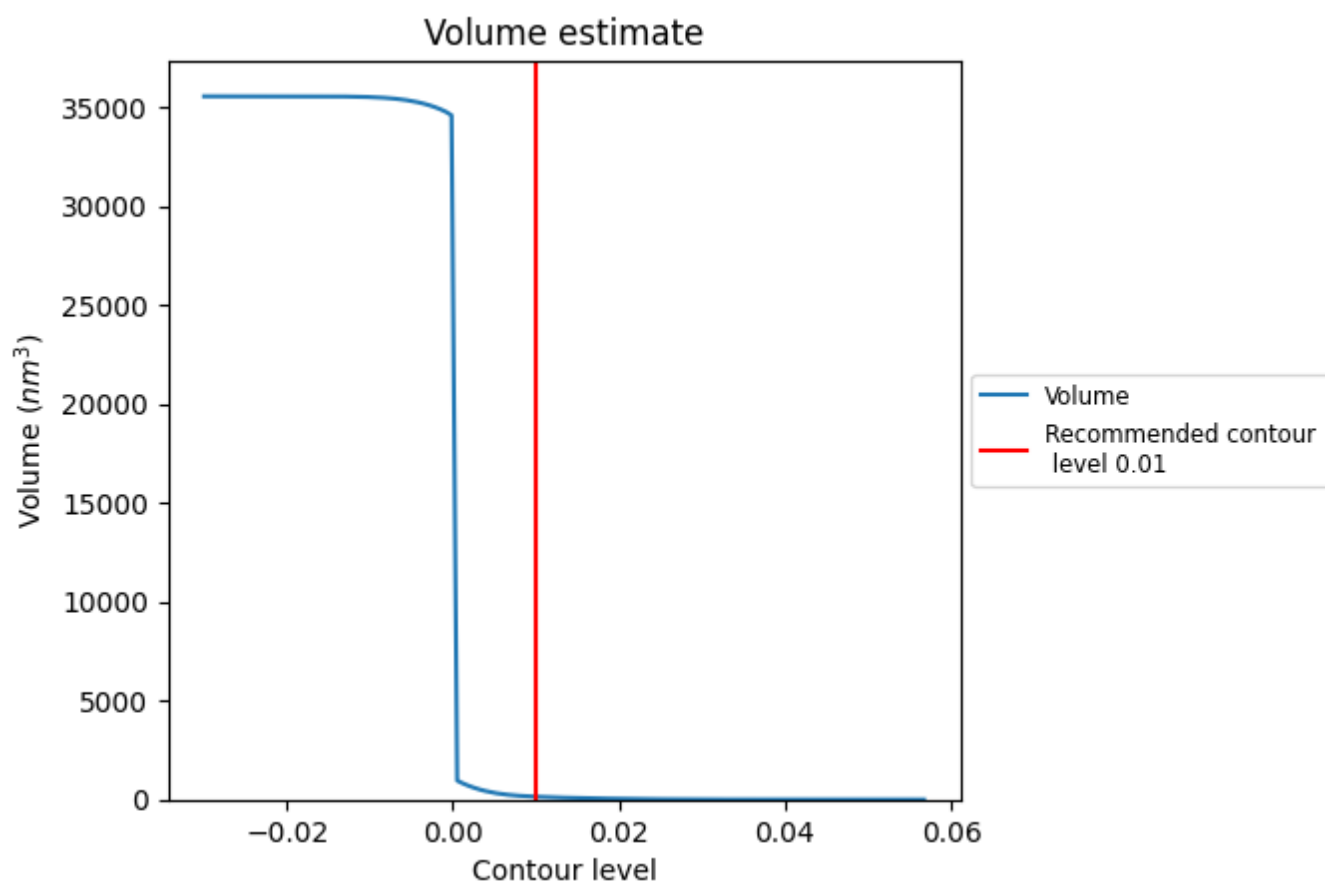
This section contains the results of statistical analysis of the map.

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.

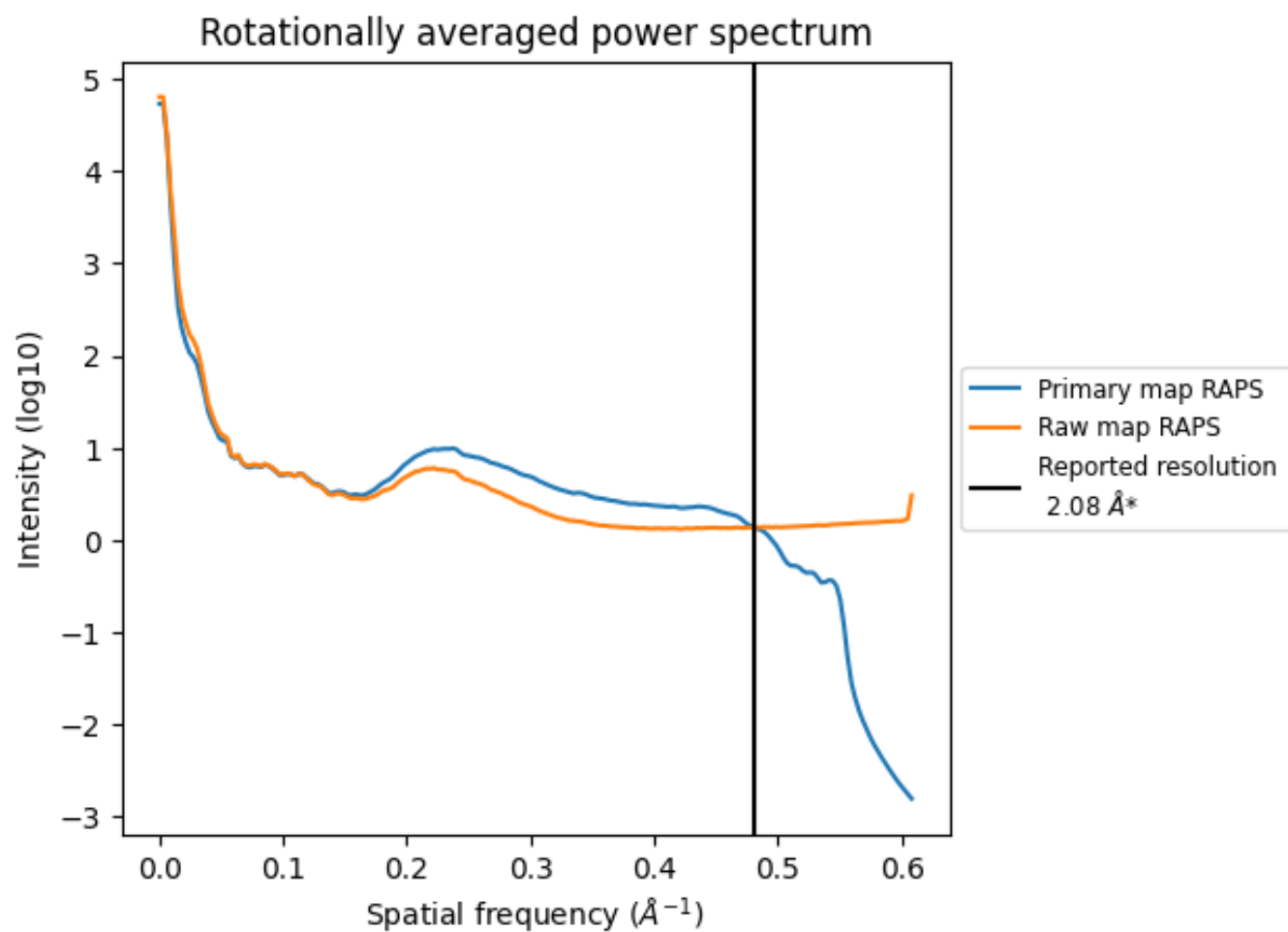
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm^3 ; this corresponds to an approximate mass of 130 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 ⓘ

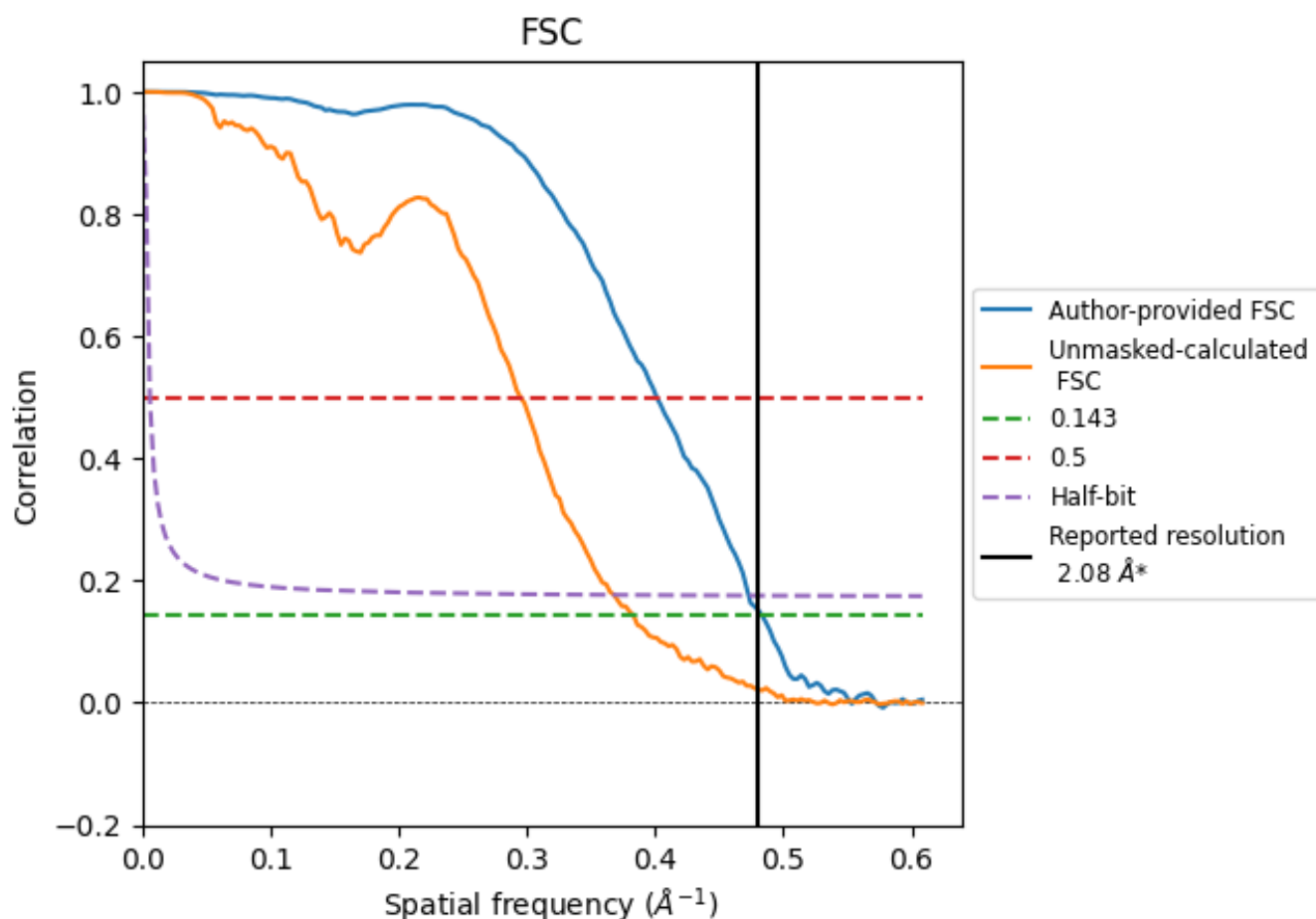


*Reported resolution corresponds to spatial frequency of 0.481 Å⁻¹

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 0.481 \AA^{-1}

8.2 Resolution estimates [i](#)

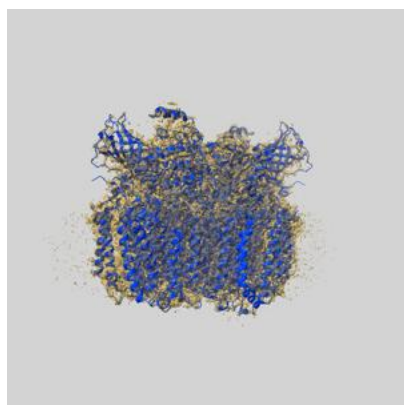
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.07	2.49	2.11
Unmasked-calculated*	2.61	3.39	2.72

*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 2.61 differs from the reported value 2.08 by more than 10 %

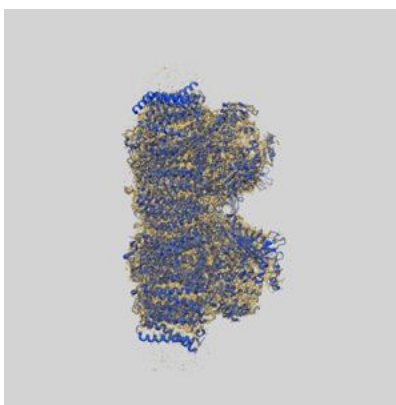
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30548 and PDB model 7D1U. Per-residue inclusion information can be found in [section 3](#) on [page 28](#).

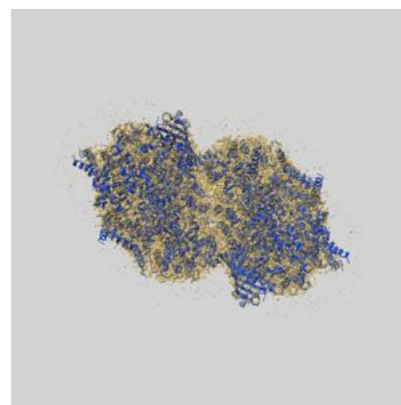
9.1 Map-model overlay [i](#)



X



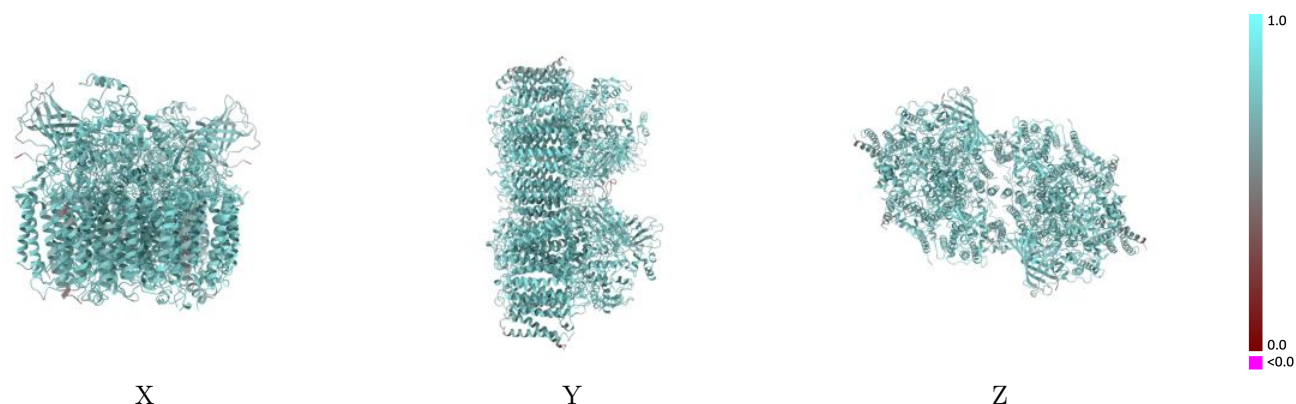
Y



Z

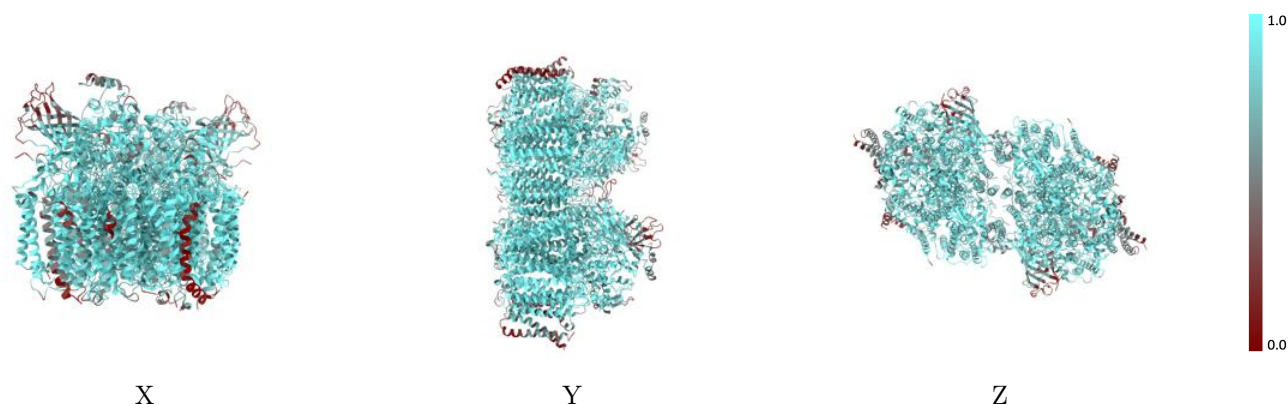
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



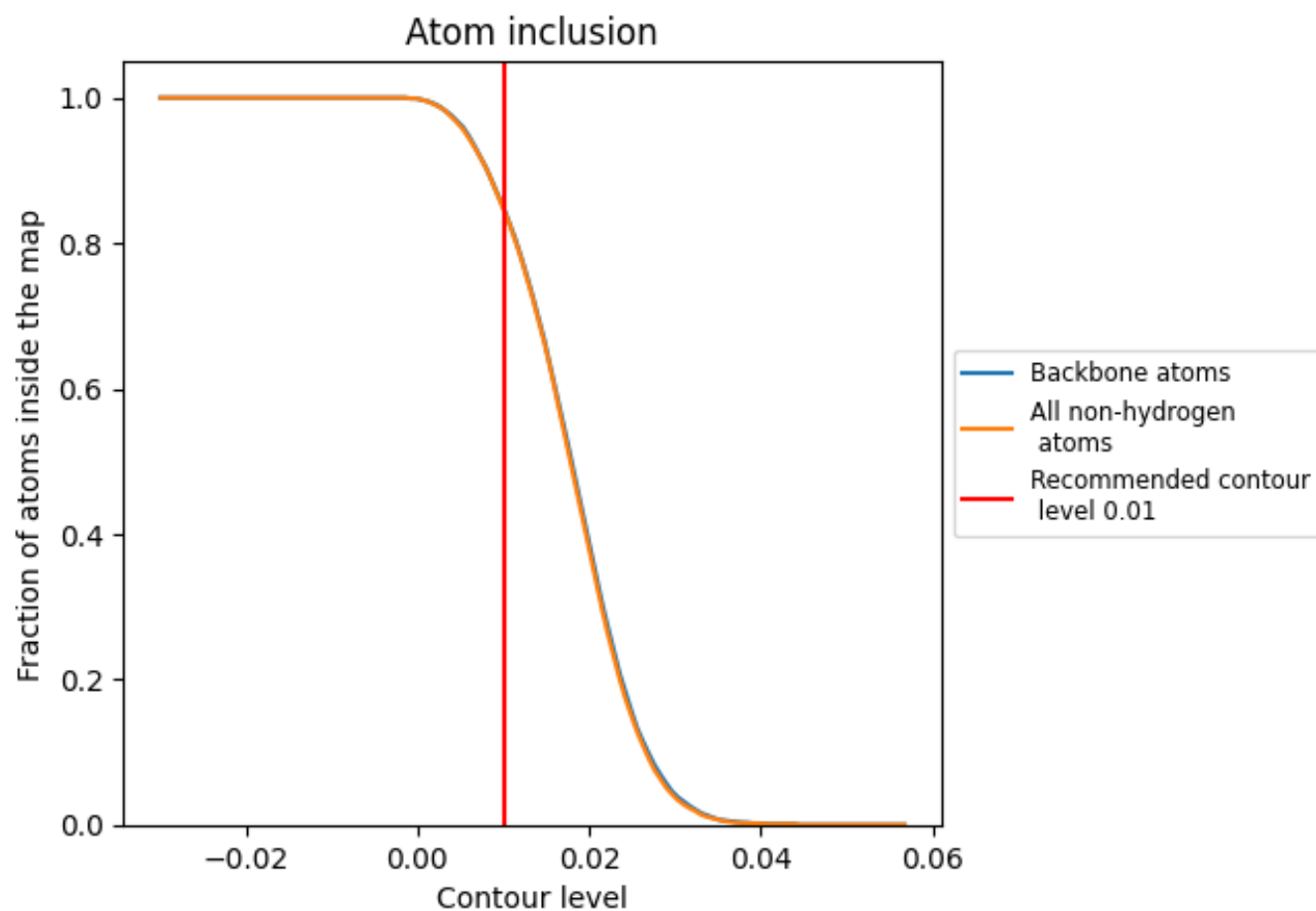
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.7570
A	 0.9260	 0.7880
B	 0.9070	 0.7750
C	 0.8830	 0.7580
D	 0.9350	 0.7890
E	 0.7720	 0.7350
F	 0.8770	 0.7660
H	 0.9050	 0.7620
I	 0.8190	 0.7350
J	 0.7980	 0.7450
K	 0.7680	 0.7150
L	 0.8380	 0.7630
M	 0.8520	 0.7760
O	 0.6800	 0.7040
R	 0.0940	 0.5780
T	 0.8750	 0.7760
U	 0.7700	 0.7360
V	 0.8080	 0.7400
X	 0.8030	 0.7360
Y	 0.5980	 0.6790
Z	 0.4130	 0.6240
a	 0.9260	 0.7880
b	 0.9060	 0.7750
c	 0.8830	 0.7580
d	 0.9350	 0.7890
e	 0.7720	 0.7360
f	 0.8770	 0.7650
h	 0.9050	 0.7610
i	 0.8190	 0.7390
j	 0.7980	 0.7420
k	 0.7680	 0.7160
l	 0.8380	 0.7690
m	 0.8490	 0.7750
o	 0.6800	 0.7040
r	 0.0940	 0.5770



Continued on next page...

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Chain	Atom inclusion	Q-score
t	 0.8600	 0.7780
u	 0.7700	 0.7390
v	 0.8080	 0.7410
x	 0.8030	 0.7380
y	 0.5980	 0.6750
z	 0.4110	 0.6210