



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 01:34 PM UTC

PDB ID : 7D1T / pdb_00007d1t
EMDB ID : EMD-30547
Title : Cryo-EM Structure of PSII at 1.95 angstrom resolution
Authors : Kato, K.; Miyazaki, N.; Hamaguchi, T.; Nakajima, Y.; Akita, F.; Yonekura, K.; Shen, J.R.
Deposited on : 2020-09-15
Resolution : 1.95 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

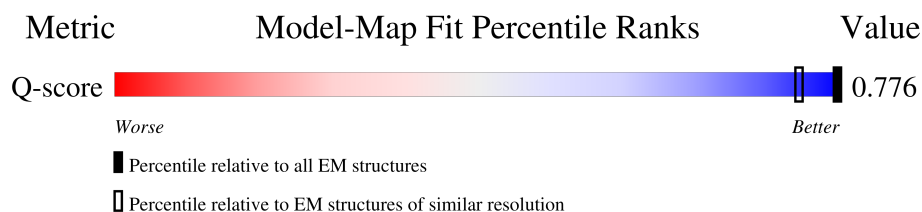
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.95 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	1316 (1.45 - 2.45)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
33	BCT	D	403	-	X	-	-
33	BCT	d	403	-	X	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 52994 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	2	0
			2634	1725	433	461	15		
1	a	334	Total	C	N	O	S	2	0
			2634	1725	433	461	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			

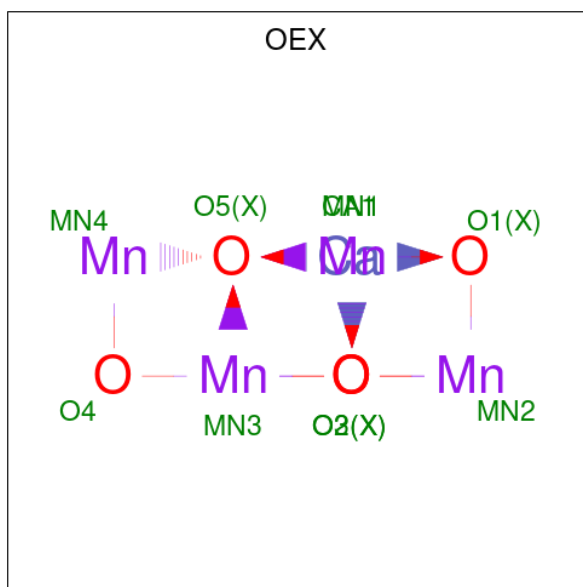
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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	

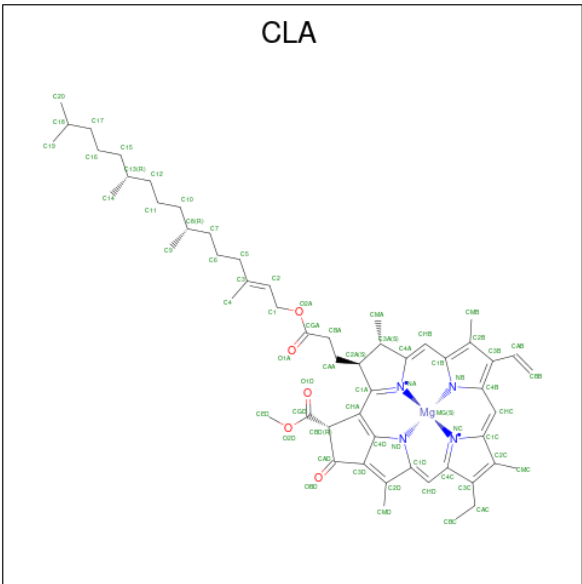
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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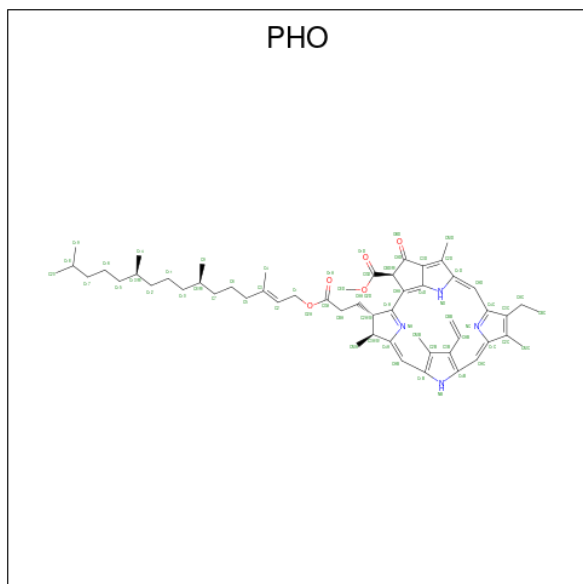
Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total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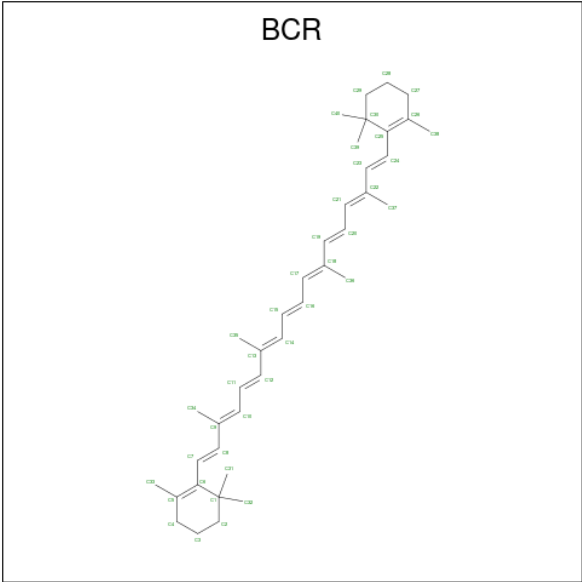
Mol	Chain	Residues	Atoms					AltConf
24	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- 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: $C_{40}H_{56}$).



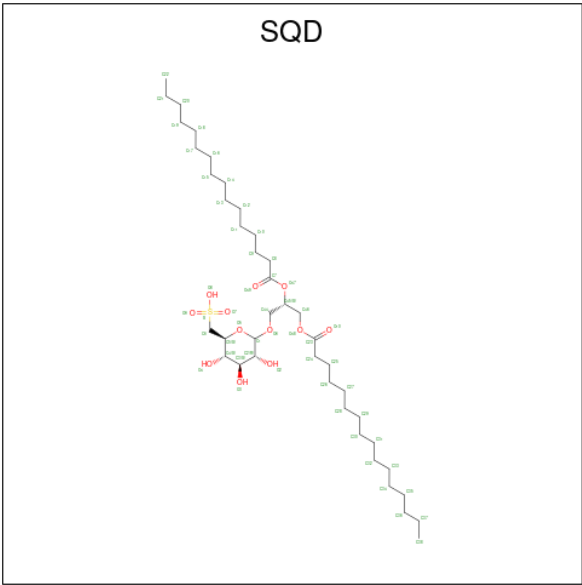
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	D	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	T	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	b	1	Total C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

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Mol	Chain	Residues	Atoms	AltConf
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	j	1	Total C 40 40	0
26	t	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).



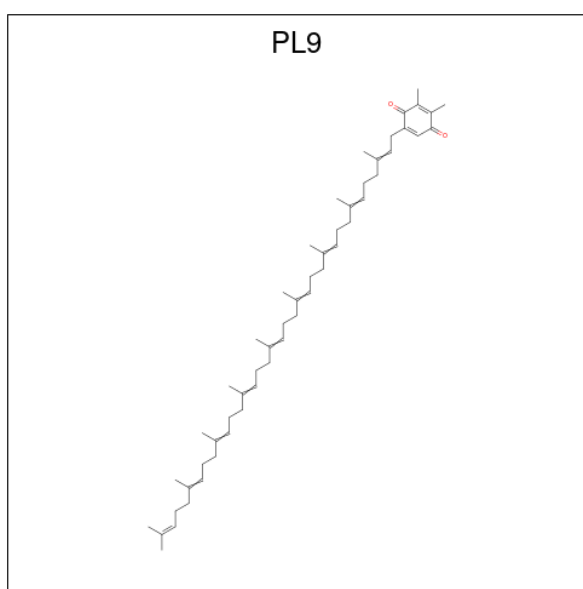
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C O S 54 41 12 1	0
27	A	1	Total C O S 54 41 12 1	0
27	B	1	Total C O S 54 41 12 1	0
27	F	1	Total C O S 45 32 12 1	0
27	L	1	Total C O S 54 41 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	C	O	S	0
			54	41	12	1	
27	a	1	Total	C	O	S	0
			54	41	12	1	
27	f	1	Total	C	O	S	0
			45	32	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:).

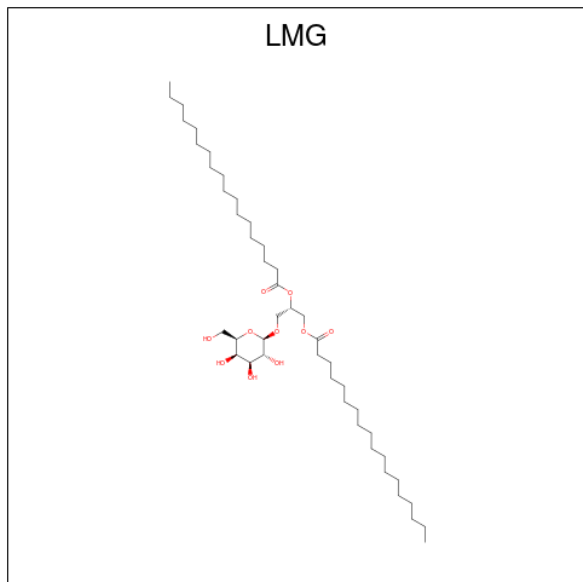
Mol	Chain	Residues	Atoms				AltConf
29	A	2	Total	C	O		0
			59	49	10		

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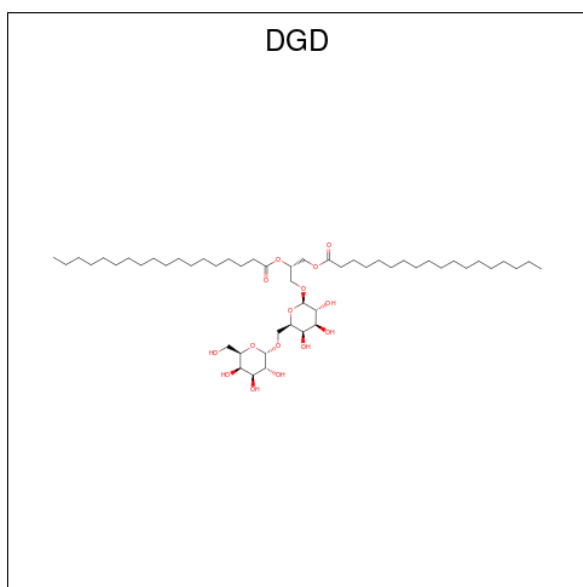
Mol	Chain	Residues	Atoms	AltConf
29	B	5	Total C 56 56	0
29	C	1	Total C 10 10	0
29	D	2	Total C O 56 51 5	0
29	E	1	Total C 10 10	0
29	I	2	Total C 17 17	0
29	J	1	Total C 10 10	0
29	K	1	Total C O 34 29 5	0
29	M	1	Total C 10 10	0
29	T	1	Total C 16 16	0
29	X	1	Total C 10 10	0
29	a	2	Total C O 59 49 10	0
29	b	5	Total C 56 56	0
29	c	1	Total C 10 10	0
29	d	2	Total C O 56 51 5	0
29	e	1	Total C 10 10	0
29	i	2	Total C 17 17	0
29	j	1	Total C 10 10	0
29	k	1	Total C O 34 29 5	0
29	m	1	Total C 10 10	0
29	t	1	Total C 16 16	0
29	x	1	Total C 10 10	0

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



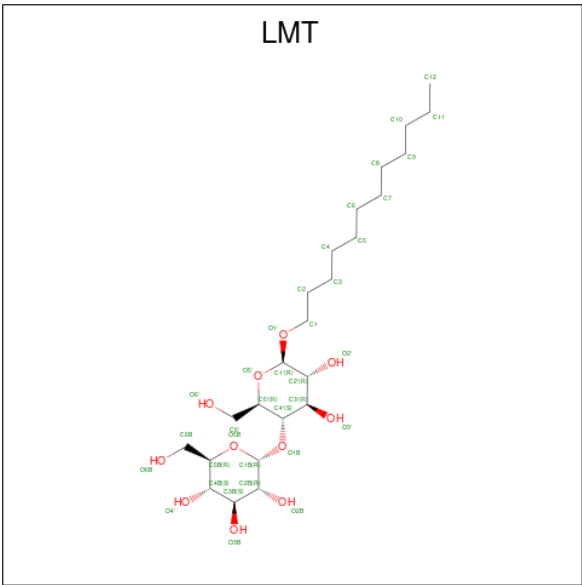
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	D	1	Total	C	O	0
			51	41	10	
30	b	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			51	41	10	
30	c	1	Total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

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



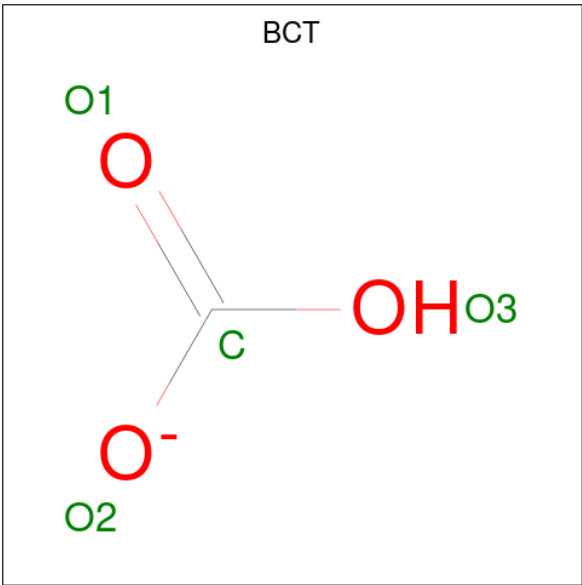
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	H	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			62	47	15	
31	h	1	Total	C	O	0
			62	47	15	

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



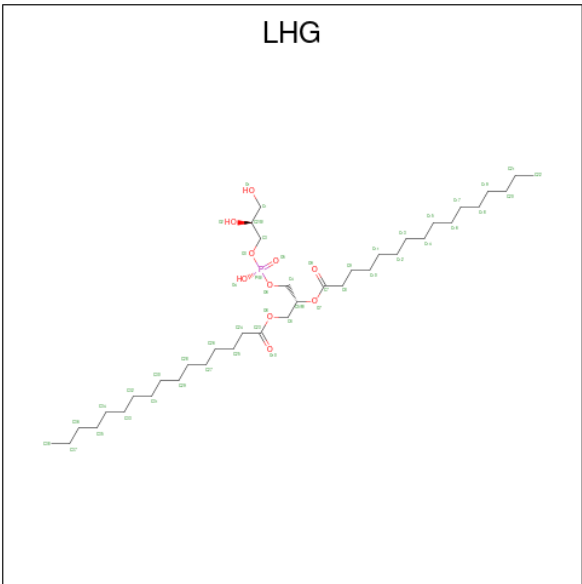
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			35	24	11	
32	J	1	Total	C	O	0
			24	18	6	
32	M	1	Total	C	O	0
			35	24	11	
32	Z	1	Total	C	O	0
			35	24	11	
32	c	1	Total	C	O	0
			35	24	11	
32	j	1	Total	C	O	0
			24	18	6	
32	m	1	Total	C	O	0
			35	24	11	
32	z	1	Total	C	O	0
			35	24	11	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			4	1	3	
33	d	1	Total	C	O	0
			4	1	3	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total	C	O	P	0
			49	38	10	1	

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

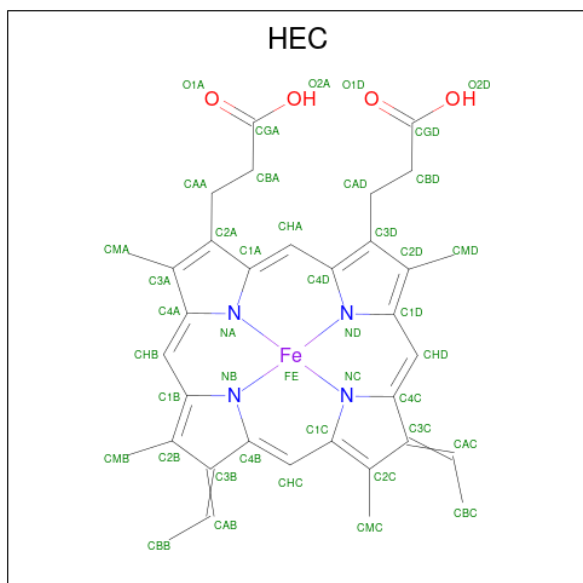
- # HEM



- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

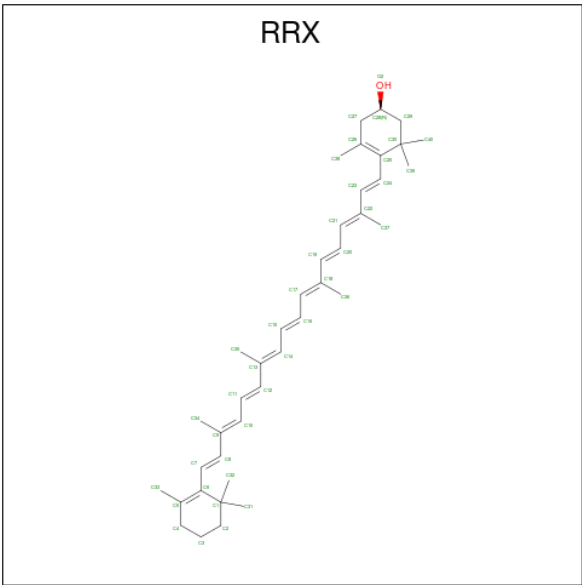
Mol	Chain	Residues	Atoms		AltConf
36	J	1	Total	Mg	0
			1	1	
36	j	1	Total	Mg	0
			1	1	

- Molecule 37 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



Mol	Chain	Residues	Atoms			AltConf
38	X	1	Total	C	O	0
			41	40	1	
38	x	1	Total	C	O	0
			41	40	1	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	152	Total	O	0
			152	152	
39	B	298	Total	O	0
			298	298	
39	C	220	Total	O	0
			220	220	
39	D	154	Total	O	0
			154	154	
39	E	26	Total	O	0
			26	26	
39	F	5	Total	O	0
			5	5	
39	H	38	Total	O	0
			38	38	
39	I	13	Total	O	0
			13	13	
39	J	11	Total	O	0
			11	11	
39	K	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
39	L	19	Total 19	O 19	0
39	M	8	Total 8	O 8	0
39	O	114	Total 114	O 114	0
39	T	9	Total 9	O 9	0
39	U	64	Total 64	O 64	0
39	V	78	Total 78	O 78	0
39	Y	2	Total 2	O 2	0
39	X	8	Total 8	O 8	0
39	a	152	Total 152	O 152	0
39	b	292	Total 292	O 292	0
39	c	220	Total 220	O 220	0
39	d	154	Total 154	O 154	0
39	e	26	Total 26	O 26	0
39	f	5	Total 5	O 5	0
39	h	38	Total 38	O 38	0
39	i	13	Total 13	O 13	0
39	j	11	Total 11	O 11	0
39	k	3	Total 3	O 3	0
39	l	13	Total 13	O 13	0
39	m	8	Total 8	O 8	0
39	o	114	Total 114	O 114	0

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Mol	Chain	Residues	Atoms		AltConf
39	t	9	Total 9	O 9	0
39	u	64	Total 64	O 64	0
39	v	78	Total 78	O 78	0
39	y	2	Total 2	O 2	0
39	x	8	Total 8	O 8	0

MolProbity failed to run properly - this section is therefore empty.

3 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	0.242	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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	$\# Z > 2$
8	FME	I	1	8	8,9,10	1.02	0	8,9,11	1.11	1 (12%)
14	FME	t	1	14	8,9,10	0.95	0	8,9,11	1.62	2 (25%)
14	FME	T	1	14	8,9,10	0.94	0	8,9,11	1.62	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HSK	D	336	4	10,11,12	1.78	2 (20%)	5,14,16	1.24	1 (20%)
8	FME	i	1	8	8,9,10	1.02	0	8,9,11	1.11	1 (12%)
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	1.02	1 (12%)
12	FME	M	1	12	8,9,10	0.97	0	8,9,11	1.02	1 (12%)
4	HSK	d	336	4	10,11,12	1.80	2 (20%)	5,14,16	1.19	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
8	FME	I	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
4	HSK	D	336	4	-	0/5/6/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
4	HSK	d	336	4	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	HSK	OM-ND1	-4.57	1.29	1.38
4	D	336	HSK	OM-ND1	-4.52	1.30	1.38
4	d	336	HSK	CD2-CG	2.33	1.39	1.36
4	D	336	HSK	CD2-CG	2.25	1.39	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CB-CA-N	3.11	116.19	110.52
14	T	1	FME	CB-CA-N	3.10	116.17	110.52
14	t	1	FME	C-CA-N	2.58	114.47	109.50
14	T	1	FME	C-CA-N	2.56	114.44	109.50
12	M	1	FME	CB-CA-N	2.47	115.02	110.52
12	m	1	FME	CB-CA-N	2.47	115.02	110.52
8	I	1	FME	CB-CA-N	2.36	114.81	110.52
8	i	1	FME	CB-CA-N	2.36	114.81	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	336	HSK	CB-CG-ND1	2.02	126.30	122.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN
12	M	1	FME	N-CA-CB-CG
12	m	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 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
27	SQD	B	620	-	52,54,54	0.92	5 (9%)	62,65,65	2.19	11 (17%)
25	PHO	D	402	-	58,69,69	2.09	9 (15%)	55,99,99	1.76	11 (20%)
24	CLA	B	605	2	69,73,73	1.85	19 (27%)	82,113,113	2.66	34 (41%)
24	CLA	B	615	2	69,73,73	1.83	19 (27%)	82,113,113	2.57	30 (36%)
30	LMG	D	411	36	51,51,55	1.06	6 (11%)	59,59,63	1.32	7 (11%)
30	LMG	C	520	-	51,51,55	0.95	4 (7%)	59,59,63	1.36	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PHO	A	407	-	58,69,69	2.32	14 (24%)	55,99,99	1.68	4 (7%)
30	LMG	d	411	36	51,51,55	1.06	6 (11%)	59,59,63	1.32	7 (11%)
27	SQD	A	410	-	52,54,54	1.06	6 (11%)	62,65,65	1.85	8 (12%)
38	RRX	X	101	-	42,42,42	1.86	9 (21%)	56,58,58	2.05	17 (30%)
28	PL9	D	407	-	55,55,55	1.92	11 (20%)	68,69,69	1.53	14 (20%)
34	LHG	d	408	-	48,48,48	0.88	1 (2%)	51,54,54	1.24	8 (15%)
24	CLA	c	507	3	69,73,73	1.89	18 (26%)	82,113,113	2.59	32 (39%)
24	CLA	a	408	1	69,73,73	1.88	16 (23%)	82,113,113	2.73	31 (37%)
28	PL9	d	407	-	55,55,55	1.91	11 (20%)	68,69,69	1.54	14 (20%)
24	CLA	c	502	3	69,73,73	1.86	18 (26%)	82,113,113	2.61	31 (37%)
24	CLA	C	509	3	69,73,73	1.86	17 (24%)	82,113,113	2.63	31 (37%)
38	RRX	x	101	-	42,42,42	1.86	9 (21%)	56,58,58	2.05	17 (30%)
30	LMG	B	621	-	51,51,55	1.05	3 (5%)	59,59,63	1.30	6 (10%)
31	DGD	C	519	-	63,63,67	1.20	7 (11%)	77,77,81	1.31	8 (10%)
24	CLA	B	610	39	69,73,73	1.85	19 (27%)	82,113,113	2.47	29 (35%)
26	BCR	b	620	-	41,41,41	1.12	3 (7%)	56,56,56	1.26	7 (12%)
30	LMG	C	501	-	51,51,55	1.21	6 (11%)	59,59,63	1.38	7 (11%)
24	CLA	d	401	39	69,73,73	1.97	18 (26%)	82,113,113	2.70	31 (37%)
24	CLA	c	512	3	69,73,73	1.91	20 (28%)	82,113,113	2.71	30 (36%)
21	OEX	A	401	3,1,39	0,15,15	-	-	-	-	-
30	LMG	c	501	-	51,51,55	1.21	6 (11%)	59,59,63	1.38	7 (11%)
26	BCR	b	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	3 (5%)
26	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.08	4 (7%)
32	LMT	z	101	-	36,36,36	1.26	6 (16%)	47,47,47	1.14	5 (10%)
24	CLA	b	609	39	69,73,73	1.85	18 (26%)	82,113,113	2.62	28 (34%)
24	CLA	C	513	3	69,73,73	1.83	18 (26%)	82,113,113	2.72	34 (41%)
24	CLA	B	604	2	69,73,73	1.90	22 (31%)	82,113,113	2.57	32 (39%)
24	CLA	b	608	2	69,73,73	1.95	21 (30%)	82,113,113	2.69	33 (40%)
30	LMG	c	520	-	51,51,55	0.95	4 (7%)	59,59,63	1.36	7 (11%)
26	BCR	c	522	-	41,41,41	1.02	2 (4%)	56,56,56	1.19	6 (10%)
24	CLA	B	609	2	69,73,73	1.84	17 (24%)	82,113,113	2.67	35 (42%)
35	HEM	E	103	5,6	50,50,50	1.54	6 (12%)	67,82,82	1.36	9 (13%)
31	DGD	H	101	-	63,63,67	1.27	6 (9%)	77,77,81	1.27	9 (11%)
24	CLA	A	408	1	69,73,73	1.88	16 (23%)	82,113,113	2.73	31 (37%)
34	LHG	D	409	-	48,48,48	0.88	1 (2%)	51,54,54	1.13	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	614	2	69,73,73	1.83	20 (28%)	82,113,113	2.72	32 (39%)
24	CLA	B	606	2	69,73,73	1.95	21 (30%)	82,113,113	2.69	33 (40%)
24	CLA	C	506	3	69,73,73	1.87	22 (31%)	82,113,113	2.47	28 (34%)
34	LHG	d	409	-	48,48,48	0.88	1 (2%)	51,54,54	1.13	3 (5%)
24	CLA	b	615	2	69,73,73	1.87	19 (27%)	82,113,113	2.49	31 (37%)
33	BCT	D	403	22	3,3,3	1.65	1 (33%)	2,3,3	3.97	2 (100%)
34	LHG	l	101	-	48,48,48	0.73	1 (2%)	51,54,54	1.14	4 (7%)
24	CLA	A	405	1	69,73,73	1.78	18 (26%)	82,113,113	2.36	25 (30%)
24	CLA	D	405	4	69,73,73	1.91	21 (30%)	82,113,113	2.62	31 (37%)
24	CLA	c	513	3	69,73,73	1.83	18 (26%)	82,113,113	2.72	35 (42%)
24	CLA	d	405	4	69,73,73	1.91	21 (30%)	82,113,113	2.62	30 (36%)
24	CLA	c	506	3	69,73,73	1.87	22 (31%)	82,113,113	2.47	28 (34%)
24	CLA	C	511	3	69,73,73	1.93	18 (26%)	82,113,113	2.54	32 (39%)
27	SQD	a	412	-	52,54,54	0.97	4 (7%)	62,65,65	1.68	10 (16%)
24	CLA	C	508	39	69,73,73	1.87	21 (30%)	82,113,113	2.67	30 (36%)
32	LMT	C	521	-	36,36,36	1.28	4 (11%)	47,47,47	1.31	4 (8%)
24	CLA	C	512	3	69,73,73	1.91	20 (28%)	82,113,113	2.71	30 (36%)
24	CLA	D	401	39	69,73,73	1.97	18 (26%)	82,113,113	2.70	31 (37%)
24	CLA	b	603	39	69,73,73	1.96	21 (30%)	82,113,113	2.56	30 (36%)
26	BCR	D	406	-	41,41,41	1.19	3 (7%)	56,56,56	1.43	9 (16%)
24	CLA	C	503	3	69,73,73	1.89	17 (24%)	82,113,113	2.50	26 (31%)
24	CLA	b	618	2	69,73,73	1.85	17 (24%)	82,113,113	2.63	35 (42%)
24	CLA	b	605	2	69,73,73	1.87	18 (26%)	82,113,113	2.56	33 (40%)
24	CLA	c	508	39	69,73,73	1.87	21 (30%)	82,113,113	2.67	30 (36%)
25	PHO	d	402	-	58,69,69	2.09	9 (15%)	55,99,99	1.76	11 (20%)
24	CLA	b	607	2	69,73,73	1.85	19 (27%)	82,113,113	2.66	34 (41%)
26	BCR	A	409	-	41,41,41	1.02	3 (7%)	56,56,56	1.28	8 (14%)
24	CLA	b	617	2	69,73,73	1.83	19 (27%)	82,113,113	2.57	30 (36%)
26	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.19	4 (7%)
30	LMG	c	523	-	51,51,55	0.85	2 (3%)	59,59,63	1.36	8 (13%)
24	CLA	B	603	2	69,73,73	1.87	18 (26%)	82,113,113	2.56	33 (40%)
32	LMT	Z	101	-	36,36,36	1.26	6 (16%)	47,47,47	1.13	5 (10%)
34	LHG	e	101	-	48,48,48	0.73	1 (2%)	51,54,54	1.29	7 (13%)
26	BCR	j	104	-	41,41,41	1.16	3 (7%)	56,56,56	1.15	4 (7%)
26	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.18	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	507	3	69,73,73	1.89	18 (26%)	82,113,113	2.59	32 (39%)
26	BCR	B	617	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	3 (5%)
30	LMG	C	523	-	51,51,55	0.85	2 (3%)	59,59,63	1.36	8 (13%)
26	BCR	J	104	-	41,41,41	1.16	3 (7%)	56,56,56	1.16	4 (7%)
26	BCR	B	618	-	41,41,41	1.12	3 (7%)	56,56,56	1.26	7 (12%)
34	LHG	E	101	-	48,48,48	0.73	1 (2%)	51,54,54	1.28	7 (13%)
32	LMT	M	101	-	36,36,36	1.37	4 (11%)	47,47,47	1.03	1 (2%)
31	DGD	c	517	-	63,63,67	1.12	5 (7%)	77,77,81	1.42	11 (14%)
24	CLA	C	505	39	69,73,73	1.86	18 (26%)	82,113,113	2.57	33 (40%)
24	CLA	B	602	2	69,73,73	1.85	17 (24%)	82,113,113	2.74	30 (36%)
24	CLA	B	611	2	69,73,73	1.76	18 (26%)	82,113,113	2.57	31 (37%)
26	BCR	C	515	-	41,41,41	1.13	4 (9%)	56,56,56	1.44	10 (17%)
31	DGD	C	518	-	63,63,67	1.54	13 (20%)	77,77,81	1.44	10 (12%)
24	CLA	c	503	3	69,73,73	1.89	17 (24%)	82,113,113	2.50	26 (31%)
34	LHG	L	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.14	4 (7%)
26	BCR	d	406	-	41,41,41	1.19	3 (7%)	56,56,56	1.43	9 (16%)
24	CLA	c	509	3	69,73,73	1.86	17 (24%)	82,113,113	2.64	31 (37%)
26	BCR	c	515	-	41,41,41	1.13	4 (9%)	56,56,56	1.44	10 (17%)
27	SQD	A	412	-	52,54,54	0.97	4 (7%)	62,65,65	1.67	10 (16%)
31	DGD	h	101	-	63,63,67	1.27	6 (9%)	77,77,81	1.27	9 (11%)
32	LMT	J	102	-	24,24,36	0.99	1 (4%)	29,29,47	1.51	3 (10%)
24	CLA	C	504	3	69,73,73	1.84	21 (30%)	82,113,113	2.58	25 (30%)
24	CLA	b	611	2	69,73,73	1.85	17 (24%)	82,113,113	2.67	35 (42%)
26	BCR	T	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.30	7 (12%)
24	CLA	B	612	2	69,73,73	1.83	17 (24%)	82,113,113	2.54	30 (36%)
24	CLA	B	607	39	69,73,73	1.86	18 (26%)	82,113,113	2.62	28 (34%)
27	SQD	f	101	-	43,45,54	1.10	5 (11%)	53,56,65	2.13	14 (26%)
31	DGD	c	519	-	63,63,67	1.20	7 (11%)	77,77,81	1.31	8 (10%)
24	CLA	c	504	3	69,73,73	1.84	21 (30%)	82,113,113	2.58	25 (30%)
24	CLA	B	613	2	69,73,73	1.87	19 (27%)	82,113,113	2.50	31 (37%)
26	BCR	C	522	-	41,41,41	1.02	2 (4%)	56,56,56	1.19	6 (10%)
24	CLA	b	612	39	69,73,73	1.84	20 (28%)	82,113,113	2.48	29 (35%)
34	LHG	D	410	-	45,45,48	0.81	1 (2%)	48,51,54	1.19	4 (8%)
24	CLA	D	404	4	69,73,73	1.81	20 (28%)	82,113,113	2.55	26 (31%)
34	LHG	d	410	-	45,45,48	0.81	1 (2%)	48,51,54	1.19	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	a	405	1	69,73,73	1.78	19 (27%)	82,113,113	2.36	25 (30%)
24	CLA	c	514	3	69,73,73	1.98	20 (28%)	82,113,113	2.71	34 (41%)
26	BCR	b	621	-	41,41,41	1.13	2 (4%)	56,56,56	1.08	4 (7%)
31	DGD	C	517	-	63,63,67	1.12	5 (7%)	77,77,81	1.42	11 (14%)
28	PL9	a	411	-	55,55,55	1.52	9 (16%)	68,69,69	1.53	11 (16%)
32	LMT	j	102	-	24,24,36	0.99	1 (4%)	29,29,47	1.51	3 (10%)
21	OEX	a	401	3,1,39	0,15,15	-	-	-	-	-
24	CLA	b	610	2	69,73,73	1.89	20 (28%)	82,113,113	2.41	29 (35%)
24	CLA	b	613	2	69,73,73	1.77	18 (26%)	82,113,113	2.57	31 (37%)
24	CLA	C	510	3	69,73,73	1.93	18 (26%)	82,113,113	2.55	33 (40%)
24	CLA	C	514	3	69,73,73	1.97	20 (28%)	82,113,113	2.71	34 (41%)
24	CLA	B	601	39	69,73,73	1.96	21 (30%)	82,113,113	2.56	30 (36%)
24	CLA	c	505	39	69,73,73	1.86	18 (26%)	82,113,113	2.58	33 (40%)
24	CLA	c	511	3	69,73,73	1.93	18 (26%)	82,113,113	2.54	32 (39%)
26	BCR	t	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.29	7 (12%)
27	SQD	F	101	-	43,45,54	1.10	5 (11%)	53,56,65	2.13	14 (26%)
24	CLA	C	502	3	69,73,73	1.86	18 (26%)	82,113,113	2.61	29 (35%)
26	BCR	a	409	-	41,41,41	1.01	3 (7%)	56,56,56	1.28	8 (14%)
34	LHG	D	408	-	48,48,48	0.88	1 (2%)	51,54,54	1.24	8 (15%)
24	CLA	B	608	2	69,73,73	1.89	19 (27%)	82,113,113	2.41	29 (35%)
24	CLA	b	614	2	69,73,73	1.83	17 (24%)	82,113,113	2.54	30 (36%)
37	HEC	v	201	16	46,50,50	2.01	8 (17%)	58,82,82	1.38	5 (8%)
30	LMG	b	622	-	51,51,55	1.05	3 (5%)	59,59,63	1.30	6 (10%)
32	LMT	c	521	-	36,36,36	1.28	4 (11%)	47,47,47	1.31	4 (8%)
24	CLA	b	616	2	69,73,73	1.82	20 (28%)	82,113,113	2.72	32 (39%)
31	DGD	c	518	-	63,63,67	1.54	13 (20%)	77,77,81	1.44	10 (12%)
37	HEC	V	201	16	46,50,50	2.01	9 (19%)	58,82,82	1.38	5 (8%)
27	SQD	a	410	-	52,54,54	1.06	6 (11%)	62,65,65	1.86	9 (14%)
33	BCT	d	403	22	3,3,3	1.64	1 (33%)	2,3,3	3.96	2 (100%)
25	PHO	a	407	-	58,69,69	2.32	14 (24%)	55,99,99	1.68	4 (7%)
24	CLA	d	404	4	69,73,73	1.81	20 (28%)	82,113,113	2.56	26 (31%)
24	CLA	A	406	39	69,73,73	1.90	21 (30%)	82,113,113	2.39	30 (36%)
24	CLA	b	606	2	69,73,73	1.90	22 (31%)	82,113,113	2.57	32 (39%)
24	CLA	a	406	39	69,73,73	1.90	20 (28%)	82,113,113	2.38	30 (36%)
32	LMT	m	102	-	36,36,36	1.36	4 (11%)	47,47,47	1.03	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	L	102	-	52,54,54	0.92	5 (9%)	62,65,65	2.19	11 (17%)
24	CLA	B	616	2	69,73,73	1.85	17 (24%)	82,113,113	2.63	35 (42%)
35	HEM	e	103	5,6	50,50,50	1.54	6 (12%)	67,82,82	1.36	9 (13%)
24	CLA	b	604	2	69,73,73	1.85	17 (24%)	82,113,113	2.74	31 (37%)
24	CLA	c	510	3	69,73,73	1.94	18 (26%)	82,113,113	2.55	33 (40%)
28	PL9	A	411	-	55,55,55	1.52	9 (16%)	68,69,69	1.53	11 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	B	620	-	-	25/49/69/69	0/1/1/1
25	PHO	D	402	-	-	3/37/103/103	0/5/6/6
24	CLA	B	605	2	1/1/15/20	5/39/115/115	-
24	CLA	B	615	2	1/1/15/20	14/39/115/115	-
30	LMG	D	411	36	-	16/46/66/70	0/1/1/1
30	LMG	C	520	-	-	21/46/66/70	0/1/1/1
25	PHO	A	407	-	-	5/37/103/103	0/5/6/6
30	LMG	d	411	36	-	16/46/66/70	0/1/1/1
27	SQD	A	410	-	-	12/49/69/69	0/1/1/1
38	RRX	X	101	-	-	3/29/65/65	0/2/2/2
28	PL9	D	407	-	-	10/53/73/73	0/1/1/1
34	LHG	d	408	-	-	15/53/53/53	-
24	CLA	c	507	3	1/1/15/20	6/39/115/115	-
24	CLA	a	408	1	-	13/39/115/115	-
28	PL9	d	407	-	-	10/53/73/73	0/1/1/1
24	CLA	c	502	3	1/1/15/20	4/39/115/115	-
24	CLA	C	509	3	1/1/15/20	4/39/115/115	-
38	RRX	x	101	-	-	3/29/65/65	0/2/2/2
30	LMG	B	621	-	-	15/46/66/70	0/1/1/1
31	DGD	C	519	-	-	13/51/91/95	0/2/2/2
24	CLA	B	610	39	1/1/15/20	4/39/115/115	-
26	BCR	b	620	-	-	3/29/63/63	0/2/2/2
30	LMG	C	501	-	-	27/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	401	39	1/1/15/20	5/39/115/115	-
24	CLA	c	512	3	1/1/15/20	11/39/115/115	-
30	LMG	c	501	-	-	27/46/66/70	0/1/1/1
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
26	BCR	B	619	-	-	10/29/63/63	0/2/2/2
32	LMT	z	101	-	-	13/21/61/61	0/2/2/2
24	CLA	b	609	39	1/1/15/20	8/39/115/115	-
24	CLA	C	513	3	1/1/15/20	12/39/115/115	-
24	CLA	B	604	2	1/1/15/20	6/39/115/115	-
24	CLA	b	608	2	1/1/15/20	3/39/115/115	-
30	LMG	c	520	-	-	21/46/66/70	0/1/1/1
26	BCR	c	522	-	-	10/29/63/63	0/2/2/2
24	CLA	B	609	2	1/1/15/20	4/39/115/115	-
35	HEM	E	103	5,6	-	1/14/54/54	-
31	DGD	H	101	-	-	11/51/91/95	0/2/2/2
24	CLA	A	408	1	-	13/39/115/115	-
34	LHG	D	409	-	-	19/53/53/53	-
24	CLA	B	614	2	1/1/15/20	14/39/115/115	-
24	CLA	B	606	2	1/1/15/20	3/39/115/115	-
24	CLA	C	506	3	1/1/15/20	8/39/115/115	-
34	LHG	d	409	-	-	19/53/53/53	-
24	CLA	b	615	2	1/1/15/20	6/39/115/115	-
34	LHG	l	101	-	-	16/53/53/53	-
24	CLA	A	405	1	1/1/15/20	5/39/115/115	-
24	CLA	D	405	4	-	11/39/115/115	-
24	CLA	c	513	3	1/1/15/20	12/39/115/115	-
24	CLA	d	405	4	-	11/39/115/115	-
24	CLA	c	506	3	1/1/15/20	8/39/115/115	-
24	CLA	C	511	3	1/1/15/20	5/39/115/115	-
27	SQD	a	412	-	-	19/49/69/69	0/1/1/1
24	CLA	C	508	39	1/1/15/20	10/39/115/115	-
32	LMT	C	521	-	-	10/21/61/61	0/2/2/2
24	CLA	C	512	3	1/1/15/20	11/39/115/115	-
24	CLA	D	401	39	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	603	39	1/1/15/20	12/39/115/115	-
26	BCR	D	406	-	-	5/29/63/63	0/2/2/2
24	CLA	b	618	2	1/1/15/20	9/39/115/115	-
24	CLA	C	503	3	-	9/39/115/115	-
24	CLA	b	605	2	1/1/15/20	7/39/115/115	-
24	CLA	c	508	39	1/1/15/20	10/39/115/115	-
25	PHO	d	402	-	-	3/37/103/103	0/5/6/6
24	CLA	b	607	2	1/1/15/20	5/39/115/115	-
26	BCR	A	409	-	-	7/29/63/63	0/2/2/2
24	CLA	b	617	2	1/1/15/20	14/39/115/115	-
26	BCR	C	516	-	-	7/29/63/63	0/2/2/2
30	LMG	c	523	-	-	27/46/66/70	0/1/1/1
24	CLA	B	603	2	1/1/15/20	7/39/115/115	-
32	LMT	Z	101	-	-	13/21/61/61	0/2/2/2
34	LHG	e	101	-	-	24/53/53/53	-
26	BCR	j	104	-	-	11/29/63/63	0/2/2/2
26	BCR	c	516	-	-	7/29/63/63	0/2/2/2
24	CLA	C	507	3	1/1/15/20	6/39/115/115	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
30	LMG	C	523	-	-	27/46/66/70	0/1/1/1
26	BCR	J	104	-	-	11/29/63/63	0/2/2/2
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
34	LHG	E	101	-	-	24/53/53/53	-
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
31	DGD	c	517	-	-	13/51/91/95	0/2/2/2
24	CLA	C	505	39	1/1/15/20	5/39/115/115	-
24	CLA	B	602	2	1/1/15/20	5/39/115/115	-
24	CLA	B	611	2	1/1/15/20	2/39/115/115	-
26	BCR	C	515	-	-	11/29/63/63	0/2/2/2
31	DGD	C	518	-	-	25/51/91/95	0/2/2/2
24	CLA	c	503	3	-	9/39/115/115	-
34	LHG	L	101	-	-	16/53/53/53	-
26	BCR	d	406	-	-	5/29/63/63	0/2/2/2
24	CLA	c	509	3	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	c	515	-	-	11/29/63/63	0/2/2/2
27	SQD	A	412	-	-	19/49/69/69	0/1/1/1
31	DGD	h	101	-	-	11/51/91/95	0/2/2/2
32	LMT	J	102	-	-	4/15/35/61	0/1/1/2
24	CLA	C	504	3	1/1/15/20	9/39/115/115	-
24	CLA	b	611	2	1/1/15/20	4/39/115/115	-
26	BCR	T	101	-	-	10/29/63/63	0/2/2/2
24	CLA	B	612	2	1/1/15/20	5/39/115/115	-
24	CLA	B	607	39	1/1/15/20	8/39/115/115	-
27	SQD	f	101	-	-	12/40/60/69	0/1/1/1
31	DGD	c	519	-	-	13/51/91/95	0/2/2/2
24	CLA	c	504	3	1/1/15/20	9/39/115/115	-
24	CLA	B	613	2	1/1/15/20	6/39/115/115	-
26	BCR	C	522	-	-	10/29/63/63	0/2/2/2
24	CLA	b	612	39	1/1/15/20	4/39/115/115	-
34	LHG	D	410	-	-	15/50/50/53	-
24	CLA	D	404	4	1/1/15/20	2/39/115/115	-
34	LHG	d	410	-	-	15/50/50/53	-
24	CLA	a	405	1	1/1/15/20	5/39/115/115	-
24	CLA	c	514	3	1/1/15/20	10/39/115/115	-
26	BCR	b	621	-	-	10/29/63/63	0/2/2/2
31	DGD	C	517	-	-	13/51/91/95	0/2/2/2
28	PL9	a	411	-	-	19/53/73/73	0/1/1/1
32	LMT	j	102	-	-	4/15/35/61	0/1/1/2
24	CLA	b	610	2	-	2/39/115/115	-
24	CLA	b	613	2	1/1/15/20	2/39/115/115	-
24	CLA	C	510	3	1/1/15/20	12/39/115/115	-
24	CLA	C	514	3	1/1/15/20	10/39/115/115	-
24	CLA	B	601	39	1/1/15/20	12/39/115/115	-
24	CLA	c	505	39	1/1/15/20	5/39/115/115	-
24	CLA	c	511	3	1/1/15/20	5/39/115/115	-
26	BCR	t	102	-	-	10/29/63/63	0/2/2/2
27	SQD	F	101	-	-	12/40/60/69	0/1/1/1
24	CLA	C	502	3	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	a	409	-	-	7/29/63/63	0/2/2/2
34	LHG	D	408	-	-	15/53/53/53	-
24	CLA	B	608	2	-	2/39/115/115	-
24	CLA	b	614	2	1/1/15/20	5/39/115/115	-
37	HEC	v	201	16	-	6/14/54/54	-
30	LMG	b	622	-	-	15/46/66/70	0/1/1/1
32	LMT	c	521	-	-	10/21/61/61	0/2/2/2
24	CLA	b	616	2	1/1/15/20	14/39/115/115	-
31	DGD	c	518	-	-	25/51/91/95	0/2/2/2
37	HEC	V	201	16	-	6/14/54/54	-
27	SQD	a	410	-	-	12/49/69/69	0/1/1/1
25	PHO	a	407	-	-	5/37/103/103	0/5/6/6
24	CLA	d	404	4	1/1/15/20	2/39/115/115	-
24	CLA	A	406	39	-	8/39/115/115	-
24	CLA	b	606	2	1/1/15/20	6/39/115/115	-
24	CLA	a	406	39	-	8/39/115/115	-
32	LMT	m	102	-	-	4/21/61/61	0/2/2/2
27	SQD	L	102	-	-	25/49/69/69	0/1/1/1
24	CLA	B	616	2	1/1/15/20	9/39/115/115	-
35	HEM	e	103	5,6	-	1/14/54/54	-
24	CLA	b	604	2	1/1/15/20	5/39/115/115	-
24	CLA	c	510	3	1/1/15/20	12/39/115/115	-
28	PL9	A	411	-	-	19/53/73/73	0/1/1/1

All (1691) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	407	PHO	C1B-C2B	10.25	1.50	1.39
25	a	407	PHO	C1B-C2B	10.25	1.50	1.39
25	A	407	PHO	C3B-C4B	9.12	1.50	1.41
25	a	407	PHO	C3B-C4B	9.12	1.50	1.41
25	D	402	PHO	C3B-C4B	9.09	1.50	1.41
25	d	402	PHO	C3B-C4B	9.09	1.50	1.41
25	D	402	PHO	C1B-C2B	8.68	1.49	1.39
25	d	402	PHO	C1B-C2B	8.68	1.49	1.39
28	D	407	PL9	C3-C4	-8.04	1.36	1.49
28	d	407	PL9	C3-C4	-8.04	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	V	201	HEC	CAC-C3C	6.54	1.56	1.35
37	v	201	HEC	CAC-C3C	6.54	1.56	1.35
37	V	201	HEC	CAB-C3B	6.06	1.54	1.35
37	v	201	HEC	CAB-C3B	6.06	1.54	1.35
24	B	606	CLA	C1B-NB	-5.84	1.30	1.37
24	b	608	CLA	C1B-NB	-5.84	1.30	1.37
24	D	401	CLA	C1B-NB	-5.66	1.30	1.37
24	d	401	CLA	C1B-NB	-5.66	1.30	1.37
24	C	508	CLA	C4B-NB	-5.32	1.30	1.37
24	c	508	CLA	C4B-NB	-5.32	1.30	1.37
24	B	601	CLA	C3C-C2C	5.29	1.48	1.36
24	b	603	CLA	C3C-C2C	5.29	1.48	1.36
24	b	611	CLA	O2D-CGD	5.24	1.46	1.33
24	B	609	CLA	O2D-CGD	5.24	1.46	1.33
24	B	607	CLA	C1B-NB	-5.15	1.31	1.37
24	b	609	CLA	C1B-NB	-5.15	1.31	1.37
24	c	514	CLA	C3C-C2C	5.12	1.47	1.36
24	D	401	CLA	C3C-C2C	5.11	1.47	1.36
24	d	401	CLA	C3C-C2C	5.11	1.47	1.36
24	C	514	CLA	C3C-C2C	5.09	1.47	1.36
24	B	608	CLA	C1B-NB	-5.06	1.31	1.37
24	b	612	CLA	C1B-NB	-5.04	1.31	1.37
24	A	406	CLA	C3C-C2C	5.04	1.47	1.36
24	a	406	CLA	C3C-C2C	5.02	1.47	1.36
24	B	610	CLA	C1B-NB	-5.01	1.31	1.37
24	c	514	CLA	CHC-C1C	5.00	1.48	1.38
24	C	513	CLA	C3C-C2C	4.99	1.47	1.36
24	c	513	CLA	C3C-C2C	4.99	1.47	1.36
24	C	507	CLA	C1B-NB	-4.99	1.31	1.37
24	c	507	CLA	C1B-NB	-4.99	1.31	1.37
24	b	610	CLA	C1B-NB	-4.98	1.31	1.37
24	C	514	CLA	CHC-C1C	4.96	1.48	1.38
24	B	602	CLA	C3C-C2C	4.91	1.47	1.36
24	b	604	CLA	C3C-C2C	4.91	1.47	1.36
28	A	411	PL9	C3-C4	-4.91	1.41	1.49
28	a	411	PL9	C3-C4	-4.91	1.41	1.49
24	B	603	CLA	C3C-C2C	4.90	1.47	1.36
24	b	605	CLA	C3C-C2C	4.90	1.47	1.36
24	C	509	CLA	C1B-NB	-4.89	1.31	1.37
24	c	509	CLA	C1B-NB	-4.89	1.31	1.37
24	D	405	CLA	C3C-C2C	4.87	1.47	1.36
24	C	505	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	C3C-C2C	4.85	1.47	1.36
24	C	507	CLA	C3C-C2C	4.85	1.47	1.36
24	c	507	CLA	C3C-C2C	4.85	1.47	1.36
24	B	604	CLA	C1B-NB	-4.84	1.31	1.37
24	b	606	CLA	C1B-NB	-4.84	1.31	1.37
24	d	405	CLA	C3C-C2C	4.83	1.47	1.36
24	C	508	CLA	C3C-C2C	4.82	1.47	1.36
24	c	508	CLA	C3C-C2C	4.82	1.47	1.36
24	C	511	CLA	C3C-C2C	4.82	1.47	1.36
24	c	511	CLA	C3C-C2C	4.82	1.47	1.36
24	B	613	CLA	O2D-CGD	4.80	1.45	1.33
24	b	615	CLA	O2D-CGD	4.80	1.45	1.33
24	a	408	CLA	C1B-NB	-4.80	1.31	1.37
24	C	504	CLA	C3C-C2C	4.79	1.47	1.36
24	c	504	CLA	C3C-C2C	4.79	1.47	1.36
24	A	408	CLA	C1B-NB	-4.79	1.31	1.37
24	C	510	CLA	C3C-C2C	4.78	1.47	1.36
24	c	510	CLA	C3C-C2C	4.78	1.47	1.36
24	B	612	CLA	C1B-NB	-4.76	1.31	1.37
24	C	508	CLA	C1B-NB	-4.74	1.31	1.37
24	c	508	CLA	C1B-NB	-4.74	1.31	1.37
24	b	614	CLA	C1B-NB	-4.71	1.31	1.37
24	C	510	CLA	O2D-CGD	4.70	1.44	1.33
24	c	510	CLA	O2D-CGD	4.70	1.44	1.33
24	C	502	CLA	O2D-CGD	4.70	1.44	1.33
24	c	502	CLA	O2D-CGD	4.70	1.44	1.33
24	A	406	CLA	CHC-C1C	4.67	1.47	1.38
24	A	408	CLA	C3C-C2C	4.66	1.46	1.36
24	a	408	CLA	C3C-C2C	4.66	1.46	1.36
24	a	406	CLA	CHC-C1C	4.65	1.47	1.38
24	A	406	CLA	C1B-NB	-4.65	1.31	1.37
24	b	608	CLA	C3C-C2C	4.64	1.46	1.36
24	B	601	CLA	O2D-CGD	4.63	1.44	1.33
24	C	509	CLA	C3C-C2C	4.61	1.46	1.36
24	c	509	CLA	C3C-C2C	4.61	1.46	1.36
24	C	514	CLA	O2D-CGD	4.61	1.44	1.33
24	c	514	CLA	O2D-CGD	4.61	1.44	1.33
24	b	603	CLA	O2D-CGD	4.61	1.44	1.33
24	B	606	CLA	C3C-C2C	4.61	1.46	1.36
24	a	406	CLA	C1B-NB	-4.61	1.31	1.37
24	C	503	CLA	O2D-CGD	4.60	1.44	1.33
24	c	503	CLA	O2D-CGD	4.60	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C4B-NB	-4.60	1.31	1.37
24	b	618	CLA	C4B-NB	-4.60	1.31	1.37
24	B	613	CLA	C3C-C2C	4.60	1.46	1.36
24	B	610	CLA	C3C-C2C	4.60	1.46	1.36
24	C	511	CLA	C1B-NB	-4.59	1.31	1.37
24	c	511	CLA	C1B-NB	-4.59	1.31	1.37
24	b	615	CLA	C3C-C2C	4.59	1.46	1.36
38	X	101	RRX	C8-C9	4.59	1.55	1.46
38	x	101	RRX	C8-C9	4.59	1.55	1.46
24	C	506	CLA	CHC-C1C	4.58	1.47	1.38
24	c	506	CLA	CHC-C1C	4.58	1.47	1.38
24	b	613	CLA	C1B-NB	-4.58	1.31	1.37
24	b	616	CLA	C3C-C2C	4.57	1.46	1.36
24	B	615	CLA	C1B-NB	-4.57	1.31	1.37
24	b	617	CLA	C1B-NB	-4.57	1.31	1.37
24	b	612	CLA	C3C-C2C	4.57	1.46	1.36
24	B	611	CLA	C1B-NB	-4.57	1.31	1.37
24	b	607	CLA	CHC-C1C	4.56	1.47	1.38
24	B	605	CLA	C3C-C2C	4.56	1.46	1.36
24	C	509	CLA	O2D-CGD	4.55	1.44	1.33
24	c	509	CLA	O2D-CGD	4.55	1.44	1.33
24	B	614	CLA	C3C-C2C	4.55	1.46	1.36
24	C	510	CLA	O2A-CGA	4.54	1.46	1.33
24	c	510	CLA	O2A-CGA	4.54	1.46	1.33
24	B	605	CLA	O2D-CGD	4.54	1.44	1.33
24	b	607	CLA	O2D-CGD	4.54	1.44	1.33
24	C	507	CLA	O2D-CGD	4.54	1.44	1.33
24	c	507	CLA	O2D-CGD	4.54	1.44	1.33
24	A	405	CLA	C3C-C2C	4.53	1.46	1.36
24	a	405	CLA	C3C-C2C	4.53	1.46	1.36
24	B	614	CLA	C4B-NB	-4.52	1.31	1.37
24	A	408	CLA	O2D-CGD	4.52	1.44	1.33
24	a	408	CLA	O2D-CGD	4.52	1.44	1.33
24	B	605	CLA	CHC-C1C	4.52	1.47	1.38
24	B	607	CLA	C3C-C2C	4.51	1.46	1.36
24	b	609	CLA	C3C-C2C	4.51	1.46	1.36
24	b	607	CLA	C3C-C2C	4.51	1.46	1.36
24	B	612	CLA	O2D-CGD	4.50	1.44	1.33
24	b	614	CLA	O2D-CGD	4.50	1.44	1.33
24	B	608	CLA	C4B-NB	-4.50	1.31	1.37
24	C	506	CLA	C3C-C2C	4.50	1.46	1.36
24	c	506	CLA	C3C-C2C	4.50	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C4B-NB	-4.50	1.32	1.37
24	c	503	CLA	C4B-NB	-4.50	1.32	1.37
24	C	512	CLA	C3C-C2C	4.49	1.46	1.36
24	c	512	CLA	C3C-C2C	4.49	1.46	1.36
24	b	610	CLA	C4B-NB	-4.48	1.32	1.37
24	b	604	CLA	C1B-NB	-4.45	1.32	1.37
24	B	615	CLA	C3C-C2C	4.45	1.46	1.36
24	b	617	CLA	C3C-C2C	4.45	1.46	1.36
35	E	103	HEM	FE-NA	4.45	2.09	1.95
35	e	103	HEM	FE-NA	4.45	2.09	1.95
24	b	611	CLA	C1B-NB	-4.44	1.32	1.37
24	C	510	CLA	C1B-NB	-4.43	1.32	1.37
24	c	510	CLA	C1B-NB	-4.43	1.32	1.37
24	B	603	CLA	C1B-NB	-4.42	1.32	1.37
24	b	605	CLA	C1B-NB	-4.42	1.32	1.37
24	B	612	CLA	C3C-C2C	4.42	1.46	1.36
24	b	614	CLA	C3C-C2C	4.42	1.46	1.36
24	D	401	CLA	O2A-CGA	4.42	1.46	1.33
24	d	401	CLA	O2A-CGA	4.42	1.46	1.33
24	C	506	CLA	O2D-CGD	4.41	1.44	1.33
24	c	506	CLA	O2D-CGD	4.41	1.44	1.33
24	C	513	CLA	O2A-CGA	4.40	1.46	1.33
24	c	513	CLA	O2A-CGA	4.40	1.46	1.33
24	B	602	CLA	C1B-NB	-4.38	1.32	1.37
24	b	616	CLA	C4B-NB	-4.38	1.32	1.37
24	D	405	CLA	O2A-CGA	4.38	1.46	1.33
24	d	405	CLA	O2A-CGA	4.38	1.46	1.33
24	D	401	CLA	O2D-CGD	4.35	1.43	1.33
24	d	401	CLA	O2D-CGD	4.35	1.43	1.33
24	b	618	CLA	O2D-CGD	4.34	1.43	1.33
24	c	512	CLA	O2D-CGD	4.34	1.43	1.33
24	c	502	CLA	C3C-C2C	4.33	1.46	1.36
24	D	404	CLA	C4B-NB	-4.33	1.32	1.37
24	d	404	CLA	C4B-NB	-4.33	1.32	1.37
37	V	201	HEC	CBB-CAB	-4.33	1.33	1.49
37	v	201	HEC	CBB-CAB	-4.33	1.33	1.49
24	B	609	CLA	C1B-NB	-4.33	1.32	1.37
24	C	512	CLA	O2D-CGD	4.33	1.43	1.33
24	B	613	CLA	C1B-NB	-4.32	1.32	1.37
24	B	616	CLA	O2D-CGD	4.32	1.43	1.33
24	b	603	CLA	C1B-NB	-4.31	1.32	1.37
24	B	608	CLA	C3C-C2C	4.31	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	CHC-C1C	4.31	1.47	1.38
24	b	604	CLA	CHC-C1C	4.31	1.47	1.38
24	C	509	CLA	C4B-NB	-4.31	1.32	1.37
24	c	509	CLA	C4B-NB	-4.31	1.32	1.37
24	b	607	CLA	C1B-NB	-4.30	1.32	1.37
24	B	604	CLA	O2D-CGD	4.30	1.43	1.33
24	b	610	CLA	C3C-C2C	4.29	1.46	1.36
24	B	605	CLA	C1B-NB	-4.29	1.32	1.37
24	C	502	CLA	C3C-C2C	4.29	1.46	1.36
24	B	613	CLA	C4B-NB	-4.29	1.32	1.37
24	b	615	CLA	C4B-NB	-4.29	1.32	1.37
24	C	512	CLA	C1B-NB	-4.29	1.32	1.37
24	c	512	CLA	C1B-NB	-4.29	1.32	1.37
24	c	503	CLA	C3C-C2C	4.27	1.46	1.36
24	b	606	CLA	O2D-CGD	4.27	1.43	1.33
24	b	615	CLA	C1B-NB	-4.27	1.32	1.37
24	A	406	CLA	O2D-CGD	4.26	1.43	1.33
24	a	406	CLA	O2D-CGD	4.26	1.43	1.33
24	B	601	CLA	C1B-NB	-4.26	1.32	1.37
24	b	603	CLA	CHC-C1C	4.26	1.47	1.38
24	D	404	CLA	C1B-NB	-4.25	1.32	1.37
24	d	404	CLA	C1B-NB	-4.25	1.32	1.37
24	C	513	CLA	O2D-CGD	4.25	1.43	1.33
24	B	616	CLA	O2A-CGA	4.25	1.45	1.33
24	C	503	CLA	C1B-NB	-4.24	1.32	1.37
24	c	503	CLA	C1B-NB	-4.24	1.32	1.37
24	A	408	CLA	CHC-C1C	4.24	1.47	1.38
24	a	408	CLA	CHC-C1C	4.24	1.47	1.38
24	C	503	CLA	C3C-C2C	4.24	1.45	1.36
24	B	611	CLA	O2D-CGD	4.24	1.43	1.33
24	b	613	CLA	O2D-CGD	4.24	1.43	1.33
24	b	618	CLA	O2A-CGA	4.24	1.45	1.33
24	b	611	CLA	C3C-C2C	4.24	1.45	1.36
24	C	502	CLA	C1B-NB	-4.23	1.32	1.37
24	B	601	CLA	O2A-CGA	4.23	1.45	1.33
24	C	514	CLA	O2A-CGA	4.22	1.45	1.33
24	c	514	CLA	O2A-CGA	4.22	1.45	1.33
37	V	201	HEC	CBC-CAC	-4.21	1.33	1.49
37	v	201	HEC	CBC-CAC	-4.21	1.33	1.49
24	c	513	CLA	O2D-CGD	4.21	1.43	1.33
24	b	603	CLA	O2A-CGA	4.21	1.45	1.33
28	D	407	PL9	C7-C8	-4.20	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	407	PL9	C7-C8	-4.20	1.44	1.50
24	D	401	CLA	C4B-NB	-4.20	1.32	1.37
24	d	401	CLA	C4B-NB	-4.20	1.32	1.37
24	C	505	CLA	O2D-CGD	4.20	1.43	1.33
24	C	512	CLA	CHC-C1C	4.20	1.46	1.38
24	B	606	CLA	C4B-NB	-4.19	1.32	1.37
24	b	608	CLA	C4B-NB	-4.19	1.32	1.37
24	B	607	CLA	O2D-CGD	4.19	1.43	1.33
24	b	609	CLA	O2D-CGD	4.19	1.43	1.33
24	b	616	CLA	CHC-C1C	4.19	1.46	1.38
24	B	606	CLA	O2D-CGD	4.19	1.43	1.33
24	b	608	CLA	O2D-CGD	4.19	1.43	1.33
24	c	502	CLA	C1B-NB	-4.19	1.32	1.37
24	B	601	CLA	CHC-C1C	4.18	1.46	1.38
24	D	405	CLA	CHD-C1D	4.18	1.46	1.38
24	d	405	CLA	CHD-C1D	4.18	1.46	1.38
24	C	511	CLA	C4B-NB	-4.18	1.32	1.37
24	c	511	CLA	C4B-NB	-4.18	1.32	1.37
24	d	404	CLA	C3C-C2C	4.18	1.45	1.36
24	C	502	CLA	CHC-C1C	4.18	1.46	1.38
24	c	502	CLA	CHC-C1C	4.18	1.46	1.38
24	B	615	CLA	O2D-CGD	4.18	1.43	1.33
24	b	617	CLA	O2D-CGD	4.18	1.43	1.33
24	B	609	CLA	C3C-C2C	4.18	1.45	1.36
24	b	610	CLA	O2D-CGD	4.18	1.43	1.33
24	c	505	CLA	O2D-CGD	4.17	1.43	1.33
24	C	511	CLA	O2D-CGD	4.17	1.43	1.33
24	c	511	CLA	O2D-CGD	4.17	1.43	1.33
24	B	608	CLA	O2D-CGD	4.17	1.43	1.33
24	c	512	CLA	CHC-C1C	4.16	1.46	1.38
24	B	604	CLA	C3C-C2C	4.14	1.45	1.36
24	b	606	CLA	C3C-C2C	4.14	1.45	1.36
24	D	404	CLA	C3C-C2C	4.14	1.45	1.36
24	B	614	CLA	CHC-C1C	4.14	1.46	1.38
30	C	501	LMG	O1-C7	-4.14	1.36	1.43
30	c	501	LMG	O1-C7	-4.14	1.36	1.43
24	b	616	CLA	C1B-NB	-4.13	1.32	1.37
24	C	511	CLA	CHD-C1D	4.13	1.46	1.38
24	c	511	CLA	CHD-C1D	4.13	1.46	1.38
24	A	408	CLA	O2A-CGA	4.12	1.45	1.33
24	a	408	CLA	O2A-CGA	4.12	1.45	1.33
24	C	513	CLA	CHC-C1C	4.11	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	CHC-C1C	4.11	1.46	1.38
24	B	603	CLA	O2D-CGD	4.10	1.43	1.33
24	b	605	CLA	O2D-CGD	4.10	1.43	1.33
24	B	616	CLA	C1B-NB	-4.09	1.32	1.37
24	b	618	CLA	C1B-NB	-4.09	1.32	1.37
24	B	615	CLA	O2A-CGA	4.08	1.45	1.33
24	C	514	CLA	C1B-NB	-4.07	1.32	1.37
24	c	514	CLA	C1B-NB	-4.07	1.32	1.37
24	b	617	CLA	O2A-CGA	4.07	1.45	1.33
24	C	514	CLA	CHD-C1D	4.05	1.46	1.38
24	B	612	CLA	C4B-NB	-4.04	1.32	1.37
24	B	614	CLA	C1B-NB	-4.04	1.32	1.37
26	D	406	BCR	C1-C6	-4.04	1.48	1.53
26	d	406	BCR	C1-C6	-4.04	1.48	1.53
24	C	504	CLA	CHC-C1C	4.03	1.46	1.38
24	c	504	CLA	CHC-C1C	4.03	1.46	1.38
24	c	514	CLA	CHD-C1D	4.03	1.46	1.38
24	B	602	CLA	O2D-CGD	4.03	1.43	1.33
24	b	604	CLA	O2D-CGD	4.03	1.43	1.33
24	C	513	CLA	C3D-C2D	4.02	1.50	1.39
24	c	513	CLA	C3D-C2D	4.02	1.50	1.39
24	A	405	CLA	C1B-NB	-4.02	1.32	1.37
24	a	405	CLA	C1B-NB	-4.02	1.32	1.37
24	b	614	CLA	C4B-NB	-4.01	1.32	1.37
24	c	510	CLA	C4B-NB	-4.01	1.32	1.37
24	b	617	CLA	CHD-C1D	4.01	1.46	1.38
24	D	405	CLA	C1B-NB	-4.00	1.32	1.37
24	d	405	CLA	C1B-NB	-4.00	1.32	1.37
24	C	508	CLA	O2A-CGA	4.00	1.45	1.33
24	c	508	CLA	O2A-CGA	4.00	1.45	1.33
24	C	505	CLA	O2A-CGA	4.00	1.45	1.33
24	c	505	CLA	O2A-CGA	4.00	1.45	1.33
24	C	505	CLA	C1B-NB	-4.00	1.32	1.37
24	c	505	CLA	C1B-NB	-4.00	1.32	1.37
24	B	609	CLA	O2A-CGA	3.99	1.45	1.33
24	b	611	CLA	O2A-CGA	3.99	1.45	1.33
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	B	615	CLA	CHD-C1D	3.98	1.46	1.38
24	B	603	CLA	CHC-C1C	3.98	1.46	1.38
24	b	605	CLA	CHC-C1C	3.98	1.46	1.38
24	B	610	CLA	CHC-C1C	3.98	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	CLA	O2A-CGA	3.98	1.44	1.33
24	C	505	CLA	CHC-C1C	3.97	1.46	1.38
24	c	505	CLA	CHC-C1C	3.97	1.46	1.38
24	C	506	CLA	C1B-NB	-3.97	1.32	1.37
24	c	506	CLA	C1B-NB	-3.97	1.32	1.37
24	C	510	CLA	C4B-NB	-3.97	1.32	1.37
24	D	405	CLA	CHC-C1C	3.97	1.46	1.38
24	d	405	CLA	CHC-C1C	3.97	1.46	1.38
24	C	510	CLA	CHC-C1C	3.96	1.46	1.38
24	c	510	CLA	CHC-C1C	3.96	1.46	1.38
38	X	101	RRX	C12-C13	3.95	1.54	1.46
38	x	101	RRX	C12-C13	3.95	1.54	1.46
24	C	514	CLA	C1D-ND	3.95	1.43	1.37
24	c	514	CLA	C1D-ND	3.95	1.43	1.37
24	A	406	CLA	O2A-CGA	3.95	1.44	1.33
28	D	407	PL9	C31-C29	-3.95	1.43	1.51
24	D	404	CLA	O2A-CGA	3.95	1.44	1.33
24	d	404	CLA	O2A-CGA	3.95	1.44	1.33
24	C	512	CLA	O2A-CGA	3.94	1.44	1.33
24	c	512	CLA	O2A-CGA	3.94	1.44	1.33
24	b	612	CLA	CHC-C1C	3.94	1.46	1.38
24	C	507	CLA	CHC-C1C	3.93	1.46	1.38
24	c	507	CLA	CHC-C1C	3.93	1.46	1.38
24	B	611	CLA	C3C-C2C	3.93	1.45	1.36
24	C	511	CLA	CHB-C1B	3.93	1.48	1.39
24	c	511	CLA	CHB-C1B	3.93	1.48	1.39
38	X	101	RRX	C19-C18	3.92	1.54	1.46
38	x	101	RRX	C19-C18	3.92	1.54	1.46
24	B	611	CLA	CHC-C1C	3.92	1.46	1.38
24	b	613	CLA	CHC-C1C	3.92	1.46	1.38
24	b	616	CLA	O2A-CGA	3.92	1.44	1.33
28	d	407	PL9	C31-C29	-3.92	1.43	1.51
25	D	402	PHO	C4D-ND	-3.91	1.32	1.38
25	d	402	PHO	C4D-ND	-3.91	1.32	1.38
24	B	614	CLA	O2A-CGA	3.91	1.44	1.33
24	B	607	CLA	C4B-NB	-3.90	1.32	1.37
24	b	609	CLA	C4B-NB	-3.90	1.32	1.37
24	C	503	CLA	O2A-CGA	3.90	1.44	1.33
24	c	503	CLA	O2A-CGA	3.90	1.44	1.33
24	B	614	CLA	O2D-CGD	3.88	1.42	1.33
24	b	616	CLA	O2D-CGD	3.88	1.42	1.33
24	B	616	CLA	C3C-C2C	3.88	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C3C-C2C	3.88	1.45	1.36
24	b	613	CLA	C3C-C2C	3.87	1.45	1.36
24	A	405	CLA	O2D-CGD	3.87	1.42	1.33
24	a	405	CLA	O2D-CGD	3.87	1.42	1.33
24	D	405	CLA	O2D-CGD	3.87	1.42	1.33
24	d	405	CLA	O2D-CGD	3.87	1.42	1.33
24	A	405	CLA	C4B-NB	-3.86	1.32	1.37
24	a	405	CLA	C4B-NB	-3.86	1.32	1.37
30	C	501	LMG	C4-C5	3.86	1.61	1.53
30	c	501	LMG	C4-C5	3.86	1.61	1.53
25	A	407	PHO	CMC-C2C	-3.86	1.44	1.50
25	a	407	PHO	CMC-C2C	-3.86	1.44	1.50
24	C	504	CLA	C1B-NB	-3.85	1.32	1.37
24	c	504	CLA	C1B-NB	-3.85	1.32	1.37
24	D	401	CLA	CHD-C4C	3.83	1.47	1.39
24	d	401	CLA	CHD-C4C	3.83	1.47	1.39
24	B	610	CLA	O2D-CGD	3.82	1.42	1.33
24	C	508	CLA	O2D-CGD	3.81	1.42	1.33
24	c	508	CLA	O2D-CGD	3.81	1.42	1.33
24	B	612	CLA	CHC-C1C	3.80	1.46	1.38
24	b	612	CLA	O2D-CGD	3.79	1.42	1.33
24	b	604	CLA	O2A-CGA	3.79	1.44	1.33
24	c	503	CLA	CHC-C1C	3.79	1.46	1.38
24	B	601	CLA	C4B-NB	-3.78	1.32	1.37
24	b	603	CLA	C4B-NB	-3.78	1.32	1.37
24	B	602	CLA	CHD-C4C	3.78	1.47	1.39
24	b	604	CLA	CHD-C4C	3.78	1.47	1.39
24	B	612	CLA	C1C-NC	-3.77	1.31	1.37
24	b	614	CLA	C1C-NC	-3.77	1.31	1.37
24	b	614	CLA	CHC-C1C	3.77	1.46	1.38
24	B	602	CLA	O2A-CGA	3.77	1.44	1.33
24	B	604	CLA	C4B-NB	-3.76	1.32	1.37
24	b	606	CLA	C4B-NB	-3.76	1.32	1.37
24	C	503	CLA	CHC-C1C	3.76	1.46	1.38
24	B	613	CLA	O2A-CGA	3.75	1.44	1.33
24	C	508	CLA	CHC-C1C	3.75	1.46	1.38
24	c	508	CLA	CHC-C1C	3.75	1.46	1.38
24	B	615	CLA	CHC-C1C	3.74	1.46	1.38
24	b	617	CLA	CHC-C1C	3.74	1.46	1.38
24	C	511	CLA	C1D-ND	3.74	1.42	1.37
24	c	511	CLA	C1D-ND	3.74	1.42	1.37
24	C	503	CLA	CHB-C1B	3.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	CHB-C1B	3.73	1.47	1.39
24	a	408	CLA	CHD-C1D	3.73	1.45	1.38
24	B	606	CLA	CHC-C1C	3.73	1.46	1.38
38	x	101	RRX	C23-C22	3.73	1.53	1.46
24	b	615	CLA	O2A-CGA	3.73	1.44	1.33
24	C	502	CLA	C4B-NB	-3.72	1.33	1.37
24	D	404	CLA	O2D-CGD	3.72	1.42	1.33
24	d	404	CLA	O2D-CGD	3.72	1.42	1.33
24	b	608	CLA	CHC-C1C	3.71	1.45	1.38
38	X	101	RRX	C23-C22	3.70	1.53	1.46
24	D	404	CLA	CHB-C1B	3.70	1.47	1.39
24	d	404	CLA	CHB-C1B	3.70	1.47	1.39
24	C	509	CLA	CHB-C1B	3.70	1.47	1.39
24	c	509	CLA	CHB-C1B	3.70	1.47	1.39
24	C	510	CLA	CHD-C1D	3.70	1.45	1.38
24	c	510	CLA	CHD-C1D	3.70	1.45	1.38
24	B	610	CLA	C3D-C2D	3.70	1.49	1.39
24	A	408	CLA	CHD-C1D	3.69	1.45	1.38
24	C	512	CLA	C1D-ND	3.69	1.42	1.37
24	c	512	CLA	C1D-ND	3.69	1.42	1.37
24	B	610	CLA	C4B-NB	-3.69	1.33	1.37
24	B	604	CLA	O2A-CGA	3.69	1.44	1.33
24	b	612	CLA	C3D-C2D	3.68	1.49	1.39
24	C	511	CLA	O2A-CGA	3.68	1.44	1.33
24	B	607	CLA	CHC-C1C	3.68	1.45	1.38
24	b	609	CLA	CHC-C1C	3.68	1.45	1.38
24	B	610	CLA	O2A-CGA	3.68	1.44	1.33
24	C	502	CLA	CHD-C1D	3.68	1.45	1.38
24	C	510	CLA	C3D-C2D	3.68	1.49	1.39
24	c	510	CLA	C3D-C2D	3.68	1.49	1.39
24	B	616	CLA	CHC-C1C	3.68	1.45	1.38
24	b	618	CLA	CHC-C1C	3.68	1.45	1.38
24	c	502	CLA	CHD-C1D	3.68	1.45	1.38
24	b	606	CLA	O2A-CGA	3.67	1.44	1.33
24	c	511	CLA	O2A-CGA	3.67	1.44	1.33
24	C	512	CLA	CHD-C4C	3.67	1.47	1.39
24	c	502	CLA	C4B-NB	-3.67	1.33	1.37
24	C	505	CLA	C4B-NB	-3.67	1.33	1.37
24	c	505	CLA	C4B-NB	-3.67	1.33	1.37
24	c	512	CLA	CHD-C4C	3.67	1.47	1.39
24	b	610	CLA	CHD-C1D	3.66	1.45	1.38
24	D	405	CLA	C4B-NB	-3.66	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	C4B-NB	-3.66	1.33	1.37
24	C	514	CLA	C4B-NB	-3.65	1.33	1.37
24	b	612	CLA	O2A-CGA	3.65	1.44	1.33
24	B	605	CLA	C4B-NB	-3.65	1.33	1.37
24	b	607	CLA	C4B-NB	-3.65	1.33	1.37
34	D	408	LHG	O7-C5	-3.64	1.38	1.46
34	d	408	LHG	O7-C5	-3.64	1.38	1.46
24	B	616	CLA	CHD-C4C	3.64	1.47	1.39
24	b	618	CLA	CHD-C4C	3.64	1.47	1.39
24	B	608	CLA	CHC-C1C	3.64	1.45	1.38
24	b	610	CLA	CHC-C1C	3.64	1.45	1.38
24	c	507	CLA	CHD-C1D	3.64	1.45	1.38
24	C	503	CLA	CHD-C1D	3.63	1.45	1.38
24	c	503	CLA	CHD-C1D	3.63	1.45	1.38
24	a	408	CLA	C4B-NB	-3.63	1.33	1.37
24	C	504	CLA	C4B-NB	-3.63	1.33	1.37
24	c	504	CLA	C4B-NB	-3.63	1.33	1.37
24	c	514	CLA	C4B-NB	-3.63	1.33	1.37
24	A	408	CLA	C4B-NB	-3.63	1.33	1.37
24	C	504	CLA	O2A-CGA	3.62	1.43	1.33
24	c	504	CLA	O2A-CGA	3.62	1.43	1.33
24	B	608	CLA	CHD-C1D	3.61	1.45	1.38
24	b	612	CLA	C4B-NB	-3.60	1.33	1.37
24	C	505	CLA	CHD-C4C	3.60	1.47	1.39
24	c	505	CLA	CHD-C4C	3.60	1.47	1.39
24	B	604	CLA	CHD-C1D	3.60	1.45	1.38
24	b	606	CLA	CHD-C1D	3.60	1.45	1.38
24	a	405	CLA	CHC-C1C	3.60	1.45	1.38
24	C	507	CLA	CHD-C1D	3.60	1.45	1.38
24	A	405	CLA	CHC-C1C	3.59	1.45	1.38
24	b	610	CLA	O2A-CGA	3.59	1.43	1.33
24	C	511	CLA	CHD-C4C	3.59	1.47	1.39
24	c	511	CLA	CHD-C4C	3.59	1.47	1.39
38	X	101	RRX	C15-C14	3.58	1.54	1.43
24	D	401	CLA	CHC-C1C	3.58	1.45	1.38
24	d	401	CLA	CHC-C1C	3.58	1.45	1.38
24	C	513	CLA	CHC-C4B	3.58	1.47	1.39
24	c	513	CLA	CHC-C4B	3.58	1.47	1.39
24	B	616	CLA	C1D-ND	3.58	1.42	1.37
24	b	618	CLA	C1D-ND	3.58	1.42	1.37
24	D	405	CLA	CHB-C1B	3.57	1.47	1.39
24	d	405	CLA	CHB-C1B	3.57	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	O2A-CGA	3.57	1.43	1.33
24	a	405	CLA	O2A-CGA	3.57	1.43	1.33
24	C	506	CLA	O2A-CGA	3.56	1.43	1.33
24	c	506	CLA	O2A-CGA	3.56	1.43	1.33
24	B	608	CLA	O2A-CGA	3.56	1.43	1.33
31	C	518	DGD	O6D-C5D	-3.56	1.35	1.44
31	c	518	DGD	O6D-C5D	-3.56	1.35	1.44
38	x	101	RRX	C15-C14	3.56	1.54	1.43
24	D	401	CLA	CHD-C1D	3.55	1.45	1.38
24	d	401	CLA	CHD-C1D	3.55	1.45	1.38
24	b	611	CLA	C3D-C2D	3.55	1.48	1.39
24	B	604	CLA	CHD-C4C	3.55	1.47	1.39
24	b	606	CLA	CHD-C4C	3.55	1.47	1.39
24	B	615	CLA	C3D-C2D	3.54	1.48	1.39
24	b	617	CLA	C3D-C2D	3.54	1.48	1.39
24	C	506	CLA	CHB-C1B	3.54	1.47	1.39
24	c	506	CLA	CHB-C1B	3.54	1.47	1.39
24	B	614	CLA	CHD-C4C	3.54	1.47	1.39
24	b	616	CLA	CHD-C4C	3.54	1.47	1.39
24	B	602	CLA	C4B-NB	-3.54	1.33	1.37
24	B	609	CLA	C3D-C2D	3.54	1.48	1.39
24	d	405	CLA	C3D-C2D	3.53	1.48	1.39
24	B	609	CLA	CHC-C1C	3.53	1.45	1.38
31	C	519	DGD	O1G-C1G	-3.53	1.37	1.45
31	c	519	DGD	O1G-C1G	-3.53	1.37	1.45
24	B	610	CLA	CHB-C1B	3.53	1.47	1.39
24	A	408	CLA	CHD-C4C	3.53	1.47	1.39
24	a	408	CLA	CHD-C4C	3.53	1.47	1.39
30	B	621	LMG	C4-C5	3.52	1.60	1.53
30	b	622	LMG	C4-C5	3.52	1.60	1.53
24	D	405	CLA	C3D-C2D	3.52	1.48	1.39
26	J	104	BCR	C1-C6	-3.52	1.49	1.53
24	C	513	CLA	CHB-C1B	3.52	1.47	1.39
24	c	513	CLA	CHB-C1B	3.52	1.47	1.39
25	A	407	PHO	C1D-C2D	3.52	1.43	1.39
25	a	407	PHO	C1D-C2D	3.52	1.43	1.39
24	C	506	CLA	CHD-C4C	3.52	1.47	1.39
24	c	506	CLA	CHD-C4C	3.52	1.47	1.39
25	A	407	PHO	C4D-ND	-3.52	1.33	1.38
25	a	407	PHO	C4D-ND	-3.52	1.33	1.38
24	b	611	CLA	CHC-C1C	3.52	1.45	1.38
24	c	502	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C1C-NC	-3.51	1.32	1.37
24	c	509	CLA	C1C-NC	-3.51	1.32	1.37
24	C	509	CLA	C3D-C2D	3.51	1.48	1.39
24	c	509	CLA	C3D-C2D	3.51	1.48	1.39
26	j	104	BCR	C1-C6	-3.51	1.49	1.53
24	B	607	CLA	CHD-C4C	3.50	1.47	1.39
24	b	609	CLA	CHD-C4C	3.50	1.47	1.39
24	C	504	CLA	CHD-C4C	3.50	1.47	1.39
24	c	504	CLA	CHD-C4C	3.50	1.47	1.39
24	b	612	CLA	CHB-C1B	3.50	1.47	1.39
24	B	601	CLA	CHD-C1D	3.50	1.45	1.38
24	b	603	CLA	CHD-C1D	3.50	1.45	1.38
24	b	604	CLA	C4B-NB	-3.50	1.33	1.37
24	A	406	CLA	C1D-ND	3.49	1.42	1.37
24	a	406	CLA	C1D-ND	3.49	1.42	1.37
24	B	606	CLA	O2A-CGA	3.48	1.43	1.33
24	b	608	CLA	O2A-CGA	3.48	1.43	1.33
24	C	504	CLA	CHB-C1B	3.48	1.47	1.39
24	c	504	CLA	CHB-C1B	3.48	1.47	1.39
24	B	601	CLA	CHD-C4C	3.47	1.47	1.39
24	b	603	CLA	CHD-C4C	3.47	1.47	1.39
24	b	613	CLA	C3D-C2D	3.47	1.48	1.39
24	D	404	CLA	CHC-C1C	3.47	1.45	1.38
24	d	404	CLA	CHC-C1C	3.47	1.45	1.38
24	b	608	CLA	CHD-C1D	3.47	1.45	1.38
24	A	408	CLA	C3D-C2D	3.47	1.48	1.39
24	B	611	CLA	C3D-C2D	3.47	1.48	1.39
24	a	408	CLA	C3D-C2D	3.47	1.48	1.39
24	B	613	CLA	CHD-C1D	3.46	1.45	1.38
24	b	615	CLA	CHD-C1D	3.46	1.45	1.38
24	b	611	CLA	C1C-NC	-3.46	1.32	1.37
24	B	601	CLA	C3D-C2D	3.46	1.48	1.39
24	b	603	CLA	C3D-C2D	3.46	1.48	1.39
38	X	101	RRX	C16-C17	3.46	1.53	1.43
38	x	101	RRX	C16-C17	3.46	1.53	1.43
24	b	610	CLA	CHD-C4C	3.46	1.47	1.39
24	D	401	CLA	C3D-C2D	3.46	1.48	1.39
24	d	401	CLA	C3D-C2D	3.46	1.48	1.39
24	B	608	CLA	CHD-C4C	3.46	1.47	1.39
24	B	604	CLA	CHB-C1B	3.46	1.47	1.39
24	b	606	CLA	CHB-C1B	3.46	1.47	1.39
24	D	405	CLA	CHD-C4C	3.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	CHD-C4C	3.46	1.47	1.39
24	C	514	CLA	C3D-C2D	3.45	1.48	1.39
24	c	514	CLA	C3D-C2D	3.45	1.48	1.39
24	C	502	CLA	C1D-ND	3.45	1.42	1.37
24	B	603	CLA	C4B-NB	-3.44	1.33	1.37
24	b	605	CLA	C4B-NB	-3.44	1.33	1.37
32	M	101	LMT	O1'-C1'	-3.44	1.34	1.40
32	m	102	LMT	O1'-C1'	-3.44	1.34	1.40
24	B	609	CLA	C1C-NC	-3.44	1.32	1.37
24	B	602	CLA	C1D-ND	3.44	1.42	1.37
24	b	604	CLA	C1D-ND	3.44	1.42	1.37
24	B	616	CLA	CHD-C1D	3.44	1.45	1.38
24	b	618	CLA	CHD-C1D	3.44	1.45	1.38
24	C	505	CLA	CHD-C1D	3.44	1.45	1.38
24	c	505	CLA	CHD-C1D	3.44	1.45	1.38
24	B	601	CLA	CHC-C4B	3.44	1.47	1.39
24	b	603	CLA	CHC-C4B	3.44	1.47	1.39
24	B	606	CLA	CHD-C1D	3.44	1.45	1.38
24	C	503	CLA	C3D-C2D	3.43	1.48	1.39
24	c	503	CLA	C3D-C2D	3.43	1.48	1.39
24	C	504	CLA	O2D-CGD	3.43	1.41	1.33
24	c	504	CLA	O2D-CGD	3.43	1.41	1.33
24	B	603	CLA	CHB-C1B	3.42	1.47	1.39
24	b	605	CLA	CHB-C1B	3.42	1.47	1.39
31	c	518	DGD	O2G-C2G	-3.42	1.38	1.46
24	B	607	CLA	O2A-CGA	3.41	1.43	1.33
24	b	609	CLA	O2A-CGA	3.41	1.43	1.33
24	C	502	CLA	C3D-C2D	3.41	1.48	1.39
24	B	613	CLA	CHB-C1B	3.41	1.47	1.39
32	Z	101	LMT	O2B-C2B	-3.41	1.34	1.43
32	z	101	LMT	O2B-C2B	-3.41	1.34	1.43
38	X	101	RRX	C11-C10	3.41	1.53	1.43
38	x	101	RRX	C11-C10	3.41	1.53	1.43
31	C	518	DGD	O2G-C2G	-3.40	1.38	1.46
24	C	509	CLA	O2A-CGA	3.40	1.43	1.33
24	c	509	CLA	O2A-CGA	3.40	1.43	1.33
24	B	609	CLA	CHD-C1D	3.40	1.45	1.38
24	b	613	CLA	O2A-CGA	3.40	1.43	1.33
24	b	611	CLA	CHD-C1D	3.40	1.45	1.38
24	B	611	CLA	O2A-CGA	3.39	1.43	1.33
24	c	502	CLA	C3D-C2D	3.39	1.48	1.39
24	c	512	CLA	C3D-C2D	3.39	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C4B-NB	-3.38	1.33	1.37
24	c	507	CLA	C4B-NB	-3.38	1.33	1.37
24	C	507	CLA	O2A-CGA	3.38	1.43	1.33
24	c	507	CLA	O2A-CGA	3.38	1.43	1.33
24	b	615	CLA	CHC-C1C	3.38	1.45	1.38
31	C	518	DGD	C4D-C3D	3.38	1.61	1.52
31	c	518	DGD	C4D-C3D	3.38	1.61	1.52
24	C	502	CLA	O2A-CGA	3.37	1.43	1.33
24	B	613	CLA	CHC-C1C	3.37	1.45	1.38
24	C	512	CLA	CHB-C1B	3.37	1.47	1.39
24	c	512	CLA	CHB-C1B	3.37	1.47	1.39
24	B	606	CLA	C3D-C2D	3.37	1.48	1.39
24	b	608	CLA	C3D-C2D	3.37	1.48	1.39
24	b	615	CLA	CHB-C1B	3.37	1.47	1.39
24	B	606	CLA	CHD-C4C	3.37	1.46	1.39
24	C	506	CLA	CHC-C4B	3.37	1.47	1.39
24	c	506	CLA	CHC-C4B	3.37	1.47	1.39
24	b	608	CLA	CHD-C4C	3.37	1.46	1.39
24	C	512	CLA	C3D-C2D	3.36	1.48	1.39
24	C	505	CLA	C3D-C2D	3.35	1.48	1.39
24	c	505	CLA	C3D-C2D	3.35	1.48	1.39
31	C	518	DGD	O3D-C3D	-3.35	1.34	1.43
31	c	518	DGD	O3D-C3D	-3.35	1.34	1.43
24	B	608	CLA	C3D-C2D	3.35	1.48	1.39
24	D	401	CLA	C1D-ND	3.35	1.42	1.37
24	d	401	CLA	C1D-ND	3.35	1.42	1.37
26	B	617	BCR	C1-C6	-3.35	1.49	1.53
26	b	619	BCR	C1-C6	-3.35	1.49	1.53
24	c	502	CLA	O2A-CGA	3.34	1.43	1.33
24	b	610	CLA	C3D-C2D	3.34	1.48	1.39
24	C	507	CLA	CHB-C1B	3.33	1.46	1.39
24	c	507	CLA	CHB-C1B	3.33	1.46	1.39
24	C	513	CLA	CHD-C4C	3.32	1.46	1.39
24	c	513	CLA	CHD-C4C	3.32	1.46	1.39
24	C	506	CLA	C4B-NB	-3.32	1.33	1.37
24	c	506	CLA	C4B-NB	-3.32	1.33	1.37
24	C	506	CLA	CHD-C1D	3.32	1.44	1.38
24	c	506	CLA	CHD-C1D	3.32	1.44	1.38
24	C	507	CLA	C1D-ND	3.32	1.42	1.37
24	c	507	CLA	C1D-ND	3.32	1.42	1.37
24	b	604	CLA	CHB-C1B	3.32	1.46	1.39
31	H	101	DGD	O4D-C4D	-3.32	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	h	101	DGD	O4D-C4D	-3.32	1.34	1.43
24	B	612	CLA	O2A-CGA	3.31	1.43	1.33
24	A	408	CLA	OBD-CAD	3.31	1.28	1.22
24	a	408	CLA	OBD-CAD	3.31	1.28	1.22
24	D	405	CLA	C1D-ND	3.31	1.42	1.37
24	d	405	CLA	C1D-ND	3.31	1.42	1.37
24	C	510	CLA	CHB-C1B	3.31	1.46	1.39
24	c	510	CLA	CHB-C1B	3.31	1.46	1.39
24	B	605	CLA	C3D-C2D	3.30	1.48	1.39
24	b	607	CLA	C3D-C2D	3.30	1.48	1.39
24	C	514	CLA	CHC-C4B	3.30	1.46	1.39
24	c	514	CLA	CHC-C4B	3.30	1.46	1.39
24	b	613	CLA	C4B-NB	-3.30	1.33	1.37
24	B	605	CLA	CHC-C4B	3.30	1.46	1.39
24	b	607	CLA	CHC-C4B	3.30	1.46	1.39
24	b	614	CLA	O2A-CGA	3.29	1.42	1.33
24	C	509	CLA	CHC-C1C	3.29	1.45	1.38
24	c	509	CLA	CHC-C1C	3.29	1.45	1.38
24	B	602	CLA	CHB-C1B	3.29	1.46	1.39
24	B	605	CLA	CHD-C1D	3.28	1.44	1.38
24	b	607	CLA	CHD-C1D	3.28	1.44	1.38
28	A	411	PL9	C7-C3	-3.28	1.46	1.51
24	A	406	CLA	C3D-C4D	-3.28	1.36	1.44
24	a	406	CLA	C3D-C4D	-3.28	1.36	1.44
25	D	402	PHO	CMD-C2D	-3.28	1.45	1.51
38	X	101	RRX	C20-C21	3.27	1.53	1.43
38	x	101	RRX	C20-C21	3.27	1.53	1.43
25	d	402	PHO	CMD-C2D	-3.27	1.45	1.51
31	C	518	DGD	O4D-C4D	-3.27	1.34	1.43
31	c	518	DGD	O4D-C4D	-3.27	1.34	1.43
27	f	101	SQD	O48-C23	3.27	1.42	1.33
24	b	607	CLA	CHB-C1B	3.27	1.46	1.39
24	C	507	CLA	CHD-C4C	3.27	1.46	1.39
28	D	407	PL9	C6-C1	-3.26	1.43	1.48
24	C	502	CLA	CHB-C1B	3.26	1.46	1.39
24	B	605	CLA	CHB-C1B	3.26	1.46	1.39
24	a	406	CLA	CHB-C1B	3.26	1.46	1.39
28	a	411	PL9	C7-C3	-3.25	1.46	1.51
24	c	507	CLA	CHD-C4C	3.25	1.46	1.39
24	b	614	CLA	CHC-C4B	3.25	1.46	1.39
31	C	517	DGD	O5D-C6D	-3.24	1.38	1.43
24	B	609	CLA	C1D-ND	3.24	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C4B-NB	-3.24	1.33	1.37
27	F	101	SQD	O48-C23	3.24	1.42	1.33
24	C	510	CLA	CHD-C4C	3.23	1.46	1.39
24	A	406	CLA	CHB-C1B	3.23	1.46	1.39
24	C	510	CLA	C3D-C4D	-3.23	1.36	1.44
24	c	510	CLA	C3D-C4D	-3.23	1.36	1.44
24	B	615	CLA	CHB-C1B	3.23	1.46	1.39
24	b	617	CLA	CHB-C1B	3.23	1.46	1.39
35	E	103	HEM	FE-ND	3.23	2.04	1.94
35	e	103	HEM	FE-ND	3.23	2.04	1.94
24	B	612	CLA	CHC-C4B	3.23	1.46	1.39
28	d	407	PL9	C6-C1	-3.23	1.43	1.48
24	c	510	CLA	CHD-C4C	3.22	1.46	1.39
24	c	502	CLA	CHB-C1B	3.22	1.46	1.39
24	B	607	CLA	C3D-C2D	3.22	1.47	1.39
24	b	609	CLA	C3D-C2D	3.22	1.47	1.39
24	B	605	CLA	C1D-ND	3.22	1.42	1.37
24	b	607	CLA	C1D-ND	3.22	1.42	1.37
24	B	615	CLA	CHD-C4C	3.22	1.46	1.39
24	b	614	CLA	CHD-C1D	3.21	1.44	1.38
24	b	608	CLA	CHB-C1B	3.21	1.46	1.39
26	B	619	BCR	C30-C25	-3.21	1.49	1.53
26	b	621	BCR	C30-C25	-3.21	1.49	1.53
24	B	602	CLA	CHC-C4B	3.21	1.46	1.39
24	b	603	CLA	CHB-C1B	3.21	1.46	1.39
24	B	612	CLA	CHD-C1D	3.21	1.44	1.38
24	B	613	CLA	C3D-C2D	3.20	1.47	1.39
24	b	615	CLA	C3D-C2D	3.20	1.47	1.39
24	b	612	CLA	CHD-C1D	3.20	1.44	1.38
24	C	507	CLA	C3D-C2D	3.20	1.47	1.39
24	c	507	CLA	C3D-C2D	3.20	1.47	1.39
31	H	101	DGD	C4D-C5D	3.20	1.59	1.53
31	h	101	DGD	C4D-C5D	3.20	1.59	1.53
24	b	611	CLA	C1D-ND	3.20	1.42	1.37
24	B	601	CLA	CHB-C1B	3.20	1.46	1.39
31	c	517	DGD	O5D-C6D	-3.19	1.38	1.43
24	B	601	CLA	C1D-ND	3.19	1.42	1.37
24	b	603	CLA	C1D-ND	3.19	1.42	1.37
24	B	606	CLA	CHB-C1B	3.19	1.46	1.39
24	C	505	CLA	CHB-C1B	3.19	1.46	1.39
24	c	505	CLA	CHB-C1B	3.19	1.46	1.39
24	C	512	CLA	CHD-C1D	3.18	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	CHD-C1D	3.18	1.44	1.38
24	C	510	CLA	C1D-ND	3.18	1.42	1.37
24	c	510	CLA	C1D-ND	3.18	1.42	1.37
31	C	518	DGD	O3G-C3G	-3.18	1.38	1.43
31	c	518	DGD	O3G-C3G	-3.18	1.38	1.43
24	B	603	CLA	O2A-CGA	3.18	1.42	1.33
24	B	603	CLA	CHD-C1D	3.18	1.44	1.38
24	b	603	CLA	C1C-NC	-3.18	1.32	1.37
24	B	603	CLA	C3D-C4D	-3.18	1.37	1.44
27	A	410	SQD	O47-C45	-3.17	1.39	1.46
24	b	617	CLA	CHD-C4C	3.17	1.46	1.39
24	B	610	CLA	C1C-NC	-3.17	1.32	1.37
24	C	504	CLA	C1D-ND	3.17	1.42	1.37
24	c	504	CLA	C1D-ND	3.17	1.42	1.37
24	B	610	CLA	CHD-C1D	3.17	1.44	1.38
24	C	512	CLA	C4B-NB	-3.17	1.33	1.37
24	c	512	CLA	C4B-NB	-3.17	1.33	1.37
24	b	604	CLA	CHC-C4B	3.16	1.46	1.39
24	C	511	CLA	C3D-C2D	3.16	1.47	1.39
24	c	511	CLA	C3D-C2D	3.16	1.47	1.39
24	b	605	CLA	C3D-C4D	-3.16	1.37	1.44
24	B	608	CLA	CHB-C1B	3.16	1.46	1.39
24	C	508	CLA	CHD-C1D	3.16	1.44	1.38
24	b	605	CLA	CHD-C1D	3.16	1.44	1.38
24	c	508	CLA	CHD-C1D	3.16	1.44	1.38
24	C	504	CLA	CHC-C4B	3.15	1.46	1.39
24	c	504	CLA	CHC-C4B	3.15	1.46	1.39
24	B	606	CLA	CHC-C4B	3.15	1.46	1.39
24	b	608	CLA	CHC-C4B	3.15	1.46	1.39
24	D	405	CLA	CHC-C4B	3.15	1.46	1.39
24	d	405	CLA	CHC-C4B	3.15	1.46	1.39
34	D	409	LHG	O7-C5	-3.15	1.39	1.46
34	d	409	LHG	O7-C5	-3.15	1.39	1.46
24	b	605	CLA	O2A-CGA	3.15	1.42	1.33
24	C	505	CLA	CHC-C4B	3.14	1.46	1.39
24	c	505	CLA	CHC-C4B	3.14	1.46	1.39
27	a	410	SQD	O47-C45	-3.14	1.39	1.46
24	A	408	CLA	CHC-C4B	3.14	1.46	1.39
24	a	408	CLA	CHC-C4B	3.14	1.46	1.39
24	b	612	CLA	C1C-NC	-3.14	1.32	1.37
26	C	516	BCR	C1-C6	-3.14	1.49	1.53
26	c	516	BCR	C1-C6	-3.14	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C3D-C2D	3.13	1.47	1.39
24	b	618	CLA	C3D-C2D	3.13	1.47	1.39
24	B	609	CLA	C4B-NB	-3.13	1.33	1.37
24	B	601	CLA	C1C-NC	-3.13	1.33	1.37
24	B	605	CLA	CHD-C4C	3.12	1.46	1.39
24	b	607	CLA	CHD-C4C	3.12	1.46	1.39
24	C	502	CLA	CHD-C4C	3.12	1.46	1.39
24	c	502	CLA	CHD-C4C	3.12	1.46	1.39
24	b	610	CLA	CHB-C1B	3.12	1.46	1.39
24	B	611	CLA	CHD-C1D	3.11	1.44	1.38
24	b	613	CLA	CHD-C1D	3.11	1.44	1.38
24	B	612	CLA	CHB-C1B	3.11	1.46	1.39
24	b	614	CLA	CHB-C1B	3.11	1.46	1.39
32	z	101	LMT	O2'-C2'	-3.11	1.35	1.43
24	D	404	CLA	CHD-C4C	3.11	1.46	1.39
24	c	503	CLA	CHD-C4C	3.11	1.46	1.39
24	d	404	CLA	CHD-C4C	3.11	1.46	1.39
32	Z	101	LMT	O2'-C2'	-3.10	1.35	1.43
24	C	504	CLA	CHD-C1D	3.10	1.44	1.38
24	c	504	CLA	CHD-C1D	3.10	1.44	1.38
24	B	616	CLA	CHB-C1B	3.09	1.46	1.39
24	b	618	CLA	CHB-C1B	3.09	1.46	1.39
24	A	406	CLA	CHC-C4B	3.09	1.46	1.39
24	a	406	CLA	CHC-C4B	3.09	1.46	1.39
24	B	613	CLA	C3D-C4D	-3.09	1.37	1.44
24	b	615	CLA	C3D-C4D	-3.09	1.37	1.44
24	C	512	CLA	C1B-C2B	3.09	1.50	1.43
24	c	512	CLA	C1B-C2B	3.09	1.50	1.43
24	B	602	CLA	CHD-C1D	3.09	1.44	1.38
24	b	604	CLA	CHD-C1D	3.09	1.44	1.38
24	B	615	CLA	C4B-NB	-3.08	1.33	1.37
24	b	617	CLA	C4B-NB	-3.08	1.33	1.37
24	C	503	CLA	C3D-C4D	-3.08	1.37	1.44
24	C	507	CLA	C3D-C4D	-3.08	1.37	1.44
24	c	503	CLA	C3D-C4D	-3.08	1.37	1.44
24	c	507	CLA	C3D-C4D	-3.08	1.37	1.44
24	B	603	CLA	C1C-NC	-3.07	1.33	1.37
24	b	605	CLA	C1C-NC	-3.07	1.33	1.37
28	a	411	PL9	C7-C8	-3.07	1.45	1.50
24	A	406	CLA	C4B-NB	-3.06	1.33	1.37
24	a	406	CLA	C4B-NB	-3.06	1.33	1.37
24	b	610	CLA	C3D-C4D	-3.06	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	CHD-C4C	3.06	1.46	1.39
24	C	507	CLA	CHC-C4B	3.06	1.46	1.39
24	c	507	CLA	CHC-C4B	3.06	1.46	1.39
24	D	401	CLA	C1C-NC	-3.06	1.33	1.37
24	d	401	CLA	C1C-NC	-3.06	1.33	1.37
24	C	505	CLA	C3D-C4D	-3.06	1.37	1.44
24	c	505	CLA	C3D-C4D	-3.06	1.37	1.44
24	b	611	CLA	C4B-NB	-3.06	1.33	1.37
24	C	503	CLA	CHD-C4C	3.06	1.46	1.39
24	c	503	CLA	C1C-NC	-3.06	1.33	1.37
24	C	512	CLA	OBD-CAD	3.06	1.27	1.22
24	c	512	CLA	OBD-CAD	3.06	1.27	1.22
31	C	518	DGD	C4E-C3E	3.05	1.60	1.52
31	c	518	DGD	C4E-C3E	3.05	1.60	1.52
24	B	614	CLA	C1C-NC	-3.05	1.33	1.37
24	b	616	CLA	C1C-NC	-3.05	1.33	1.37
24	C	512	CLA	CHC-C4B	3.05	1.46	1.39
28	A	411	PL9	C7-C8	-3.05	1.45	1.50
24	A	405	CLA	C3D-C4D	-3.05	1.37	1.44
24	a	405	CLA	C3D-C4D	-3.05	1.37	1.44
24	c	512	CLA	CHC-C4B	3.04	1.46	1.39
24	C	511	CLA	C3D-C4D	-3.03	1.37	1.44
24	c	511	CLA	C3D-C4D	-3.03	1.37	1.44
24	C	502	CLA	CHC-C4B	3.03	1.46	1.39
24	c	502	CLA	CHC-C4B	3.03	1.46	1.39
24	b	612	CLA	CHD-C4C	3.03	1.46	1.39
24	C	509	CLA	CHD-C1D	3.03	1.44	1.38
24	c	509	CLA	CHD-C1D	3.03	1.44	1.38
24	B	609	CLA	CHD-C4C	3.03	1.46	1.39
31	C	517	DGD	O1G-C1G	-3.02	1.38	1.45
31	c	517	DGD	O1G-C1G	-3.02	1.38	1.45
24	C	503	CLA	C1D-ND	3.02	1.41	1.37
24	c	503	CLA	C1D-ND	3.02	1.41	1.37
24	B	604	CLA	CHC-C1C	3.02	1.44	1.38
24	b	606	CLA	CHC-C1C	3.02	1.44	1.38
31	C	518	DGD	O4E-C4E	-3.02	1.35	1.43
31	c	518	DGD	O4E-C4E	-3.02	1.35	1.43
24	C	513	CLA	CHD-C1D	3.01	1.44	1.38
24	c	513	CLA	CHD-C1D	3.01	1.44	1.38
35	E	103	HEM	CAB-C3B	3.01	1.55	1.47
35	e	103	HEM	CAB-C3B	3.01	1.55	1.47
24	A	406	CLA	CHD-C4C	3.01	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	CLA	CHD-C4C	3.01	1.46	1.39
24	C	503	CLA	C1C-NC	-3.01	1.33	1.37
31	c	519	DGD	O3E-C3E	-3.01	1.35	1.43
31	C	519	DGD	O3E-C3E	-3.01	1.35	1.43
35	E	103	HEM	CAC-C3C	3.01	1.55	1.47
35	e	103	HEM	CAC-C3C	3.01	1.55	1.47
24	b	611	CLA	CHD-C4C	3.01	1.46	1.39
24	B	608	CLA	C3D-C4D	-3.01	1.37	1.44
24	B	607	CLA	CHD-C1D	3.00	1.44	1.38
24	b	609	CLA	CHD-C1D	3.00	1.44	1.38
24	B	614	CLA	C3D-C4D	-3.00	1.37	1.44
28	D	407	PL9	C7-C3	-3.00	1.47	1.51
28	d	407	PL9	C7-C3	-3.00	1.47	1.51
32	C	521	LMT	O3'-C3'	-3.00	1.35	1.43
32	c	521	LMT	O3'-C3'	-3.00	1.35	1.43
24	C	508	CLA	CHD-C4C	2.99	1.46	1.39
24	c	508	CLA	CHD-C4C	2.99	1.46	1.39
24	B	606	CLA	C1D-ND	2.99	1.41	1.37
24	b	608	CLA	C1D-ND	2.99	1.41	1.37
28	A	411	PL9	C53-C6	-2.99	1.44	1.50
25	A	407	PHO	C4D-CHA	2.99	1.44	1.39
25	a	407	PHO	C4D-CHA	2.99	1.44	1.39
24	A	405	CLA	O2D-CED	-2.99	1.38	1.45
24	a	405	CLA	O2D-CED	-2.99	1.38	1.45
24	b	616	CLA	C3D-C4D	-2.98	1.37	1.44
26	D	406	BCR	C30-C25	-2.98	1.50	1.53
26	d	406	BCR	C30-C25	-2.98	1.50	1.53
26	B	619	BCR	C1-C6	-2.98	1.50	1.53
26	b	621	BCR	C1-C6	-2.98	1.50	1.53
25	d	402	PHO	C1D-C2D	2.98	1.42	1.39
24	B	605	CLA	O2A-CGA	2.98	1.42	1.33
24	b	607	CLA	O2A-CGA	2.98	1.42	1.33
28	d	407	PL9	C51-C49	-2.98	1.42	1.50
24	B	613	CLA	CHD-C4C	2.98	1.46	1.39
24	b	615	CLA	CHD-C4C	2.98	1.46	1.39
24	B	604	CLA	CHC-C4B	2.98	1.46	1.39
24	b	606	CLA	CHC-C4B	2.98	1.46	1.39
24	C	508	CLA	C3D-C2D	2.98	1.47	1.39
24	c	508	CLA	C3D-C2D	2.98	1.47	1.39
24	b	605	CLA	CHD-C4C	2.97	1.46	1.39
28	D	407	PL9	C51-C49	-2.97	1.42	1.50
24	B	607	CLA	CHC-C4B	2.97	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	CHC-C4B	2.97	1.46	1.39
24	B	603	CLA	CHD-C4C	2.97	1.46	1.39
24	C	510	CLA	CHC-C4B	2.97	1.46	1.39
24	B	610	CLA	C1D-ND	2.97	1.41	1.37
24	C	513	CLA	C1B-NB	-2.97	1.34	1.37
24	c	513	CLA	C1B-NB	-2.97	1.34	1.37
24	c	510	CLA	CHC-C4B	2.96	1.46	1.39
24	B	611	CLA	C1D-ND	2.96	1.41	1.37
24	b	613	CLA	C1D-ND	2.96	1.41	1.37
24	B	611	CLA	CHB-C1B	2.95	1.46	1.39
24	b	606	CLA	C3D-C2D	2.95	1.47	1.39
25	D	402	PHO	C1D-C2D	2.95	1.42	1.39
31	C	519	DGD	O3G-C3G	-2.95	1.38	1.43
31	c	519	DGD	O3G-C3G	-2.95	1.38	1.43
24	b	614	CLA	C3D-C2D	2.95	1.47	1.39
28	a	411	PL9	C53-C6	-2.94	1.44	1.50
24	b	613	CLA	CHB-C1B	2.94	1.46	1.39
24	C	513	CLA	C4B-NB	-2.94	1.34	1.37
24	c	513	CLA	C4B-NB	-2.94	1.34	1.37
24	d	404	CLA	C3D-C4D	-2.94	1.37	1.44
24	B	607	CLA	CHB-C1B	2.94	1.46	1.39
24	b	609	CLA	CHB-C1B	2.94	1.46	1.39
24	B	609	CLA	CHC-C4B	2.93	1.46	1.39
24	b	611	CLA	CHC-C4B	2.93	1.46	1.39
24	B	604	CLA	C3D-C2D	2.93	1.47	1.39
24	D	404	CLA	C3D-C4D	-2.93	1.37	1.44
24	B	607	CLA	C1C-NC	-2.93	1.33	1.37
24	b	609	CLA	C1C-NC	-2.93	1.33	1.37
24	B	604	CLA	C1C-NC	-2.93	1.33	1.37
24	b	606	CLA	C1C-NC	-2.93	1.33	1.37
24	b	605	CLA	OBD-CAD	2.93	1.27	1.22
24	B	616	CLA	C3D-C4D	-2.92	1.37	1.44
24	b	618	CLA	C3D-C4D	-2.92	1.37	1.44
24	b	605	CLA	C3D-C2D	2.91	1.46	1.39
24	C	508	CLA	C1D-ND	2.91	1.41	1.37
24	c	508	CLA	C1D-ND	2.91	1.41	1.37
24	B	601	CLA	OBD-CAD	2.91	1.27	1.22
24	b	603	CLA	OBD-CAD	2.91	1.27	1.22
24	C	508	CLA	CHB-C1B	2.91	1.45	1.39
24	c	508	CLA	CHB-C1B	2.91	1.45	1.39
24	D	401	CLA	CHC-C4B	2.91	1.45	1.39
24	d	401	CLA	CHC-C4B	2.91	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C3D-C2D	2.90	1.46	1.39
24	B	606	CLA	OBD-CAD	2.90	1.27	1.22
24	D	404	CLA	C1C-NC	-2.90	1.33	1.37
24	d	404	CLA	C1C-NC	-2.90	1.33	1.37
24	C	506	CLA	C1D-ND	2.90	1.41	1.37
24	c	506	CLA	C1D-ND	2.90	1.41	1.37
24	b	611	CLA	CHB-C1B	2.90	1.45	1.39
24	A	406	CLA	CHD-C1D	2.90	1.44	1.38
24	a	406	CLA	CHD-C1D	2.90	1.44	1.38
24	B	615	CLA	C1B-C2B	2.89	1.49	1.43
24	b	617	CLA	C1B-C2B	2.89	1.49	1.43
24	A	405	CLA	CHD-C4C	2.89	1.45	1.39
24	a	405	CLA	CHD-C4C	2.89	1.45	1.39
24	B	603	CLA	C3D-C2D	2.88	1.46	1.39
27	B	620	SQD	O48-C23	2.88	1.41	1.33
27	L	102	SQD	O48-C23	2.88	1.41	1.33
24	C	511	CLA	CHC-C1C	2.87	1.44	1.38
24	c	511	CLA	CHC-C1C	2.87	1.44	1.38
24	B	609	CLA	CHB-C1B	2.86	1.45	1.39
24	B	603	CLA	OBD-CAD	2.86	1.27	1.22
24	B	603	CLA	CHC-C4B	2.86	1.45	1.39
24	B	613	CLA	CHC-C4B	2.86	1.45	1.39
24	b	605	CLA	CHC-C4B	2.86	1.45	1.39
24	b	614	CLA	C3D-C4D	-2.86	1.37	1.44
24	C	503	CLA	CHC-C4B	2.86	1.45	1.39
24	D	404	CLA	CHC-C4B	2.86	1.45	1.39
24	c	503	CLA	CHC-C4B	2.86	1.45	1.39
24	d	404	CLA	CHC-C4B	2.86	1.45	1.39
25	A	407	PHO	CMD-C2D	-2.86	1.45	1.51
25	a	407	PHO	CMD-C2D	-2.86	1.45	1.51
24	B	602	CLA	C3D-C2D	2.86	1.46	1.39
24	b	604	CLA	C3D-C2D	2.86	1.46	1.39
27	A	412	SQD	O48-C23	2.85	1.41	1.33
27	a	412	SQD	O48-C23	2.85	1.41	1.33
24	C	509	CLA	CHC-C4B	2.85	1.45	1.39
24	c	509	CLA	CHC-C4B	2.85	1.45	1.39
26	B	618	BCR	C30-C25	-2.85	1.50	1.53
26	b	620	BCR	C30-C25	-2.85	1.50	1.53
24	B	612	CLA	C3D-C4D	-2.85	1.37	1.44
35	E	103	HEM	FE-NB	2.85	2.03	1.94
35	e	103	HEM	FE-NB	2.85	2.03	1.94
24	C	514	CLA	OBD-CAD	2.85	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	OBD-CAD	2.85	1.27	1.22
24	B	608	CLA	CHC-C4B	2.85	1.45	1.39
24	b	610	CLA	CHC-C4B	2.85	1.45	1.39
24	B	608	CLA	C1C-NC	-2.84	1.33	1.37
31	h	101	DGD	O5D-C6D	-2.84	1.38	1.43
26	C	522	BCR	C1-C6	-2.83	1.50	1.53
26	c	522	BCR	C1-C6	-2.83	1.50	1.53
24	b	608	CLA	OBD-CAD	2.83	1.27	1.22
24	C	514	CLA	CHB-C1B	2.83	1.45	1.39
24	b	615	CLA	CHC-C4B	2.83	1.45	1.39
24	c	514	CLA	CHB-C1B	2.83	1.45	1.39
27	a	412	SQD	O47-C7	2.83	1.42	1.34
24	D	405	CLA	C1B-C2B	2.82	1.49	1.43
24	d	405	CLA	C1B-C2B	2.82	1.49	1.43
24	b	612	CLA	C1D-ND	2.82	1.41	1.37
27	A	412	SQD	O47-C7	2.82	1.42	1.34
24	B	615	CLA	C1C-NC	-2.82	1.33	1.37
24	b	617	CLA	C1C-NC	-2.82	1.33	1.37
31	C	518	DGD	C3E-C2E	2.82	1.59	1.52
31	c	518	DGD	C3E-C2E	2.82	1.59	1.52
24	D	404	CLA	C1B-C2B	2.82	1.49	1.43
24	d	404	CLA	C1B-C2B	2.82	1.49	1.43
24	B	614	CLA	CHC-C4B	2.82	1.45	1.39
24	B	612	CLA	CHD-C4C	2.82	1.45	1.39
24	b	614	CLA	CHD-C4C	2.82	1.45	1.39
24	B	604	CLA	C3D-C4D	-2.81	1.37	1.44
24	b	610	CLA	C1C-NC	-2.81	1.33	1.37
24	A	405	CLA	C1C-NC	-2.81	1.33	1.37
24	a	405	CLA	C1C-NC	-2.81	1.33	1.37
24	B	611	CLA	CHD-C4C	2.81	1.45	1.39
24	b	613	CLA	CHD-C4C	2.81	1.45	1.39
24	a	408	CLA	C1D-ND	2.80	1.41	1.37
24	C	508	CLA	C1B-C2B	2.80	1.49	1.43
24	c	508	CLA	C1B-C2B	2.80	1.49	1.43
24	C	511	CLA	CHC-C4B	2.80	1.45	1.39
24	c	511	CLA	CHC-C4B	2.80	1.45	1.39
31	H	101	DGD	O5D-C6D	-2.79	1.38	1.43
24	b	611	CLA	OBD-CAD	2.79	1.27	1.22
24	b	606	CLA	C3D-C4D	-2.78	1.37	1.44
28	a	411	PL9	C16-C14	-2.78	1.45	1.51
24	A	408	CLA	C1D-ND	2.78	1.41	1.37
24	b	616	CLA	CHC-C4B	2.78	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	405	CLA	CHC-C4B	2.78	1.45	1.39
24	A	405	CLA	CHC-C4B	2.78	1.45	1.39
28	A	411	PL9	C16-C14	-2.78	1.45	1.51
24	C	505	CLA	C1D-ND	2.78	1.41	1.37
24	c	505	CLA	C1D-ND	2.78	1.41	1.37
24	B	609	CLA	OBD-CAD	2.78	1.27	1.22
24	A	408	CLA	CHB-C1B	2.77	1.45	1.39
24	a	408	CLA	CHB-C1B	2.77	1.45	1.39
27	F	101	SQD	O47-C7	2.77	1.42	1.34
27	f	101	SQD	O47-C7	2.77	1.42	1.34
24	A	405	CLA	CHB-C1B	2.77	1.45	1.39
24	a	405	CLA	CHB-C1B	2.77	1.45	1.39
24	C	507	CLA	C1C-NC	-2.77	1.33	1.37
24	c	507	CLA	C1C-NC	-2.77	1.33	1.37
24	C	512	CLA	C1C-NC	-2.76	1.33	1.37
24	c	512	CLA	C1C-NC	-2.76	1.33	1.37
30	c	501	LMG	O7-C8	-2.76	1.40	1.46
26	C	515	BCR	C30-C25	-2.76	1.50	1.53
26	c	515	BCR	C30-C25	-2.76	1.50	1.53
24	B	616	CLA	C1C-NC	-2.76	1.33	1.37
24	b	618	CLA	C1C-NC	-2.76	1.33	1.37
24	C	504	CLA	C3D-C2D	2.76	1.46	1.39
24	c	504	CLA	C3D-C2D	2.76	1.46	1.39
24	C	508	CLA	CHC-C4B	2.75	1.45	1.39
24	c	508	CLA	CHC-C4B	2.75	1.45	1.39
24	B	606	CLA	C1C-NC	-2.75	1.33	1.37
24	B	614	CLA	CHB-C1B	2.75	1.45	1.39
28	d	407	PL9	C41-C39	-2.74	1.45	1.51
24	C	502	CLA	C3D-C4D	-2.74	1.38	1.44
24	B	616	CLA	CHC-C4B	2.74	1.45	1.39
24	b	618	CLA	CHC-C4B	2.74	1.45	1.39
30	C	501	LMG	O7-C8	-2.74	1.40	1.46
25	A	407	PHO	CAC-C3C	-2.74	1.46	1.51
25	a	407	PHO	CAC-C3C	-2.74	1.46	1.51
26	B	618	BCR	C1-C6	-2.73	1.50	1.53
26	b	620	BCR	C1-C6	-2.73	1.50	1.53
24	B	616	CLA	C1B-C2B	2.73	1.49	1.43
24	b	618	CLA	C1B-C2B	2.73	1.49	1.43
31	C	517	DGD	O3E-C3E	-2.73	1.36	1.43
31	c	517	DGD	O3E-C3E	-2.73	1.36	1.43
26	T	101	BCR	C30-C25	-2.73	1.50	1.53
26	t	102	BCR	C30-C25	-2.73	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	523	LMG	O7-C8	-2.73	1.40	1.46
30	c	523	LMG	O7-C8	-2.73	1.40	1.46
28	D	407	PL9	C41-C39	-2.72	1.45	1.51
24	B	609	CLA	C4D-CHA	2.72	1.47	1.38
24	b	611	CLA	C4D-CHA	2.72	1.47	1.38
24	D	401	CLA	CHB-C1B	2.72	1.45	1.39
24	d	401	CLA	CHB-C1B	2.72	1.45	1.39
24	B	603	CLA	CMD-C2D	-2.72	1.45	1.50
24	b	605	CLA	CMD-C2D	-2.72	1.45	1.50
31	C	517	DGD	O2D-C2D	-2.72	1.36	1.43
31	c	517	DGD	O2D-C2D	-2.72	1.36	1.43
24	C	509	CLA	CHD-C4C	2.72	1.45	1.39
24	c	509	CLA	CHD-C4C	2.72	1.45	1.39
24	b	608	CLA	C1C-NC	-2.71	1.33	1.37
31	C	519	DGD	O3D-C3D	-2.71	1.36	1.43
31	c	519	DGD	O3D-C3D	-2.71	1.36	1.43
26	D	406	BCR	C33-C5	-2.71	1.46	1.50
26	d	406	BCR	C33-C5	-2.71	1.46	1.50
24	B	607	CLA	C3D-C4D	-2.71	1.38	1.44
24	b	609	CLA	C3D-C4D	-2.71	1.38	1.44
24	b	616	CLA	CHB-C1B	2.70	1.45	1.39
24	B	614	CLA	C3D-C2D	2.70	1.46	1.39
24	c	502	CLA	C3D-C4D	-2.70	1.38	1.44
24	b	616	CLA	C1B-C2B	2.70	1.49	1.43
24	B	603	CLA	C1B-C2B	2.70	1.49	1.43
24	b	605	CLA	C1B-C2B	2.70	1.49	1.43
24	C	502	CLA	OBD-CAD	2.69	1.27	1.22
24	b	616	CLA	C3D-C2D	2.69	1.46	1.39
26	C	515	BCR	C1-C6	-2.69	1.50	1.53
26	c	515	BCR	C1-C6	-2.69	1.50	1.53
24	D	404	CLA	O2D-CED	-2.69	1.39	1.45
24	d	404	CLA	O2D-CED	-2.69	1.39	1.45
24	C	503	CLA	OBD-CAD	2.68	1.27	1.22
24	c	503	CLA	OBD-CAD	2.68	1.27	1.22
27	A	410	SQD	O2-C2	-2.68	1.36	1.43
27	a	410	SQD	O2-C2	-2.68	1.36	1.43
24	B	604	CLA	C1D-ND	2.68	1.41	1.37
24	b	606	CLA	C1D-ND	2.68	1.41	1.37
24	D	401	CLA	C4D-CHA	2.67	1.47	1.38
24	d	401	CLA	C4D-CHA	2.67	1.47	1.38
24	d	404	CLA	CHD-C1D	2.67	1.43	1.38
24	C	513	CLA	OBD-CAD	2.67	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	OBD-CAD	2.67	1.27	1.22
24	D	404	CLA	CHD-C1D	2.67	1.43	1.38
24	C	508	CLA	C1C-NC	-2.67	1.33	1.37
24	c	508	CLA	C1C-NC	-2.67	1.33	1.37
24	b	613	CLA	C1C-NC	-2.67	1.33	1.37
31	C	518	DGD	O5D-C6D	-2.67	1.39	1.43
31	c	518	DGD	O5D-C6D	-2.67	1.39	1.43
24	B	611	CLA	C1C-NC	-2.67	1.33	1.37
24	B	614	CLA	C1B-C2B	2.67	1.49	1.43
26	J	104	BCR	C33-C5	-2.66	1.46	1.50
24	b	612	CLA	CHC-C4B	2.66	1.45	1.39
24	D	401	CLA	CHB-C4A	-2.65	1.31	1.37
24	d	401	CLA	CHB-C4A	-2.65	1.31	1.37
26	j	104	BCR	C33-C5	-2.65	1.46	1.50
24	B	610	CLA	CHC-C4B	2.65	1.45	1.39
24	B	602	CLA	C3D-C4D	-2.65	1.38	1.44
24	b	604	CLA	C3D-C4D	-2.65	1.38	1.44
24	c	502	CLA	OBD-CAD	2.64	1.27	1.22
24	C	506	CLA	C3D-C2D	2.64	1.46	1.39
24	c	506	CLA	C3D-C2D	2.64	1.46	1.39
24	C	513	CLA	C1D-ND	2.62	1.41	1.37
24	c	513	CLA	C1D-ND	2.62	1.41	1.37
28	A	411	PL9	C36-C34	-2.62	1.45	1.51
28	a	411	PL9	C36-C34	-2.62	1.45	1.51
24	C	513	CLA	C4D-CHA	2.62	1.47	1.38
24	c	513	CLA	C4D-CHA	2.62	1.47	1.38
24	D	405	CLA	C3D-C4D	-2.62	1.38	1.44
24	d	405	CLA	C3D-C4D	-2.62	1.38	1.44
24	C	506	CLA	CMD-C2D	-2.62	1.45	1.50
24	c	506	CLA	CMD-C2D	-2.62	1.45	1.50
24	B	615	CLA	C1D-ND	2.62	1.41	1.37
24	b	617	CLA	C1D-ND	2.62	1.41	1.37
24	A	405	CLA	CHD-C1D	2.61	1.43	1.38
24	a	405	CLA	CHD-C1D	2.61	1.43	1.38
24	B	601	CLA	C3D-C4D	-2.61	1.38	1.44
24	b	603	CLA	C3D-C4D	-2.61	1.38	1.44
24	D	404	CLA	C3D-C2D	2.61	1.46	1.39
24	d	404	CLA	C3D-C2D	2.61	1.46	1.39
24	C	511	CLA	C4D-CHA	2.61	1.47	1.38
24	c	511	CLA	C4D-CHA	2.61	1.47	1.38
24	C	508	CLA	OBD-CAD	2.61	1.27	1.22
24	c	508	CLA	OBD-CAD	2.61	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	C4D-CHA	2.61	1.47	1.38
24	C	508	CLA	C3D-C4D	-2.60	1.38	1.44
24	c	508	CLA	C3D-C4D	-2.60	1.38	1.44
24	B	611	CLA	CHC-C4B	2.60	1.45	1.39
24	b	613	CLA	CHC-C4B	2.60	1.45	1.39
24	B	607	CLA	C1B-C2B	2.60	1.49	1.43
30	D	411	LMG	O7-C8	-2.60	1.40	1.46
24	b	609	CLA	C1B-C2B	2.59	1.49	1.43
32	M	101	LMT	O3'-C3'	-2.59	1.36	1.43
32	m	102	LMT	O3'-C3'	-2.59	1.36	1.43
24	b	609	CLA	C4D-CHA	2.58	1.47	1.38
24	C	511	CLA	OBD-CAD	2.58	1.26	1.22
28	D	407	PL9	C52-C5	-2.57	1.45	1.50
24	B	615	CLA	C4D-CHA	2.57	1.47	1.38
24	b	617	CLA	C4D-CHA	2.57	1.47	1.38
24	B	605	CLA	C3D-C4D	-2.57	1.38	1.44
24	b	607	CLA	C3D-C4D	-2.57	1.38	1.44
32	M	101	LMT	O3B-C3B	-2.57	1.36	1.43
32	m	102	LMT	O3B-C3B	-2.57	1.36	1.43
24	C	510	CLA	C1B-C2B	2.56	1.49	1.43
24	c	510	CLA	C1B-C2B	2.56	1.49	1.43
24	C	513	CLA	C1B-C2B	2.56	1.49	1.43
24	c	513	CLA	C1B-C2B	2.56	1.49	1.43
24	c	509	CLA	C1D-ND	2.56	1.41	1.37
30	d	411	LMG	O7-C8	-2.56	1.40	1.46
24	C	504	CLA	O2D-CED	-2.56	1.39	1.45
24	c	504	CLA	O2D-CED	-2.56	1.39	1.45
24	C	506	CLA	C3D-C4D	-2.55	1.38	1.44
24	c	506	CLA	C3D-C4D	-2.55	1.38	1.44
27	A	410	SQD	O48-C23	2.54	1.40	1.33
27	a	410	SQD	O48-C23	2.54	1.40	1.33
28	A	411	PL9	C12-C13	-2.54	1.42	1.50
28	a	411	PL9	C12-C13	-2.54	1.42	1.50
31	C	519	DGD	O2D-C2D	-2.54	1.36	1.43
31	c	519	DGD	O2D-C2D	-2.54	1.36	1.43
28	d	407	PL9	C52-C5	-2.54	1.45	1.50
25	D	402	PHO	CMC-C2C	-2.54	1.46	1.50
25	d	402	PHO	CMC-C2C	-2.54	1.46	1.50
24	A	406	CLA	C3D-C2D	2.54	1.45	1.39
24	a	406	CLA	C3D-C2D	2.54	1.45	1.39
24	c	511	CLA	OBD-CAD	2.53	1.26	1.22
24	B	613	CLA	C1D-ND	2.53	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	C1D-ND	2.53	1.41	1.37
24	B	606	CLA	C3D-C4D	-2.53	1.38	1.44
24	b	608	CLA	C3D-C4D	-2.53	1.38	1.44
24	B	611	CLA	C3D-C4D	-2.52	1.38	1.44
24	b	613	CLA	C3D-C4D	-2.52	1.38	1.44
26	A	409	BCR	C1-C6	-2.52	1.50	1.53
26	a	409	BCR	C1-C6	-2.52	1.50	1.53
24	B	602	CLA	OBD-CAD	2.52	1.26	1.22
24	b	604	CLA	OBD-CAD	2.52	1.26	1.22
25	d	402	PHO	CAC-C3C	-2.52	1.47	1.51
24	C	504	CLA	C1C-NC	-2.52	1.33	1.37
24	c	504	CLA	C1C-NC	-2.52	1.33	1.37
24	C	514	CLA	C3D-C4D	-2.51	1.38	1.44
24	c	514	CLA	C3D-C4D	-2.51	1.38	1.44
24	C	510	CLA	C4D-CHA	2.51	1.47	1.38
24	c	510	CLA	C4D-CHA	2.51	1.47	1.38
24	C	506	CLA	C1B-C2B	2.51	1.49	1.43
24	c	506	CLA	C1B-C2B	2.51	1.49	1.43
24	B	615	CLA	C3D-C4D	-2.51	1.38	1.44
24	b	617	CLA	C3D-C4D	-2.51	1.38	1.44
24	C	506	CLA	CBD-CAD	-2.51	1.45	1.56
24	c	506	CLA	CBD-CAD	-2.51	1.45	1.56
32	z	101	LMT	O3'-C3'	-2.51	1.36	1.43
24	C	509	CLA	C1D-ND	2.51	1.41	1.37
32	Z	101	LMT	O3'-C3'	-2.51	1.36	1.43
24	A	405	CLA	C3D-C2D	2.51	1.45	1.39
24	a	405	CLA	C3D-C2D	2.51	1.45	1.39
31	C	518	DGD	O3E-C3E	-2.50	1.36	1.43
31	c	518	DGD	O3E-C3E	-2.50	1.36	1.43
25	D	402	PHO	CAC-C3C	-2.50	1.47	1.51
24	b	606	CLA	OBD-CAD	2.50	1.26	1.22
24	B	604	CLA	C1C-C2C	2.50	1.49	1.44
24	b	606	CLA	C1C-C2C	2.50	1.49	1.44
26	B	618	BCR	C38-C26	-2.50	1.47	1.50
26	b	620	BCR	C38-C26	-2.50	1.47	1.50
24	B	615	CLA	CHC-C4B	2.49	1.45	1.39
24	b	617	CLA	CHC-C4B	2.49	1.45	1.39
24	b	608	CLA	C4D-CHA	2.49	1.46	1.38
24	B	601	CLA	C4D-CHA	2.49	1.46	1.38
24	b	603	CLA	C4D-CHA	2.49	1.46	1.38
24	B	609	CLA	C3D-C4D	-2.48	1.38	1.44
24	C	505	CLA	C4D-CHA	2.48	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	C4D-CHA	2.48	1.46	1.38
24	b	611	CLA	C3D-C4D	-2.48	1.38	1.44
24	B	608	CLA	C4D-CHA	2.48	1.46	1.38
24	B	606	CLA	C4D-CHA	2.48	1.46	1.38
33	D	403	BCT	O2-C	-2.48	1.12	1.33
24	B	616	CLA	C4D-CHA	2.47	1.46	1.38
24	b	618	CLA	C4D-CHA	2.47	1.46	1.38
30	d	411	LMG	O4-C4	-2.47	1.36	1.43
27	B	620	SQD	O47-C7	2.47	1.41	1.34
27	L	102	SQD	O47-C7	2.47	1.41	1.34
33	d	403	BCT	O2-C	-2.47	1.12	1.33
37	V	201	HEC	C3D-C2D	-2.47	1.32	1.38
37	v	201	HEC	C3D-C2D	-2.47	1.32	1.38
24	B	604	CLA	OBD-CAD	2.46	1.26	1.22
27	A	410	SQD	O3-C3	-2.46	1.36	1.43
27	a	410	SQD	O3-C3	-2.46	1.36	1.43
32	C	521	LMT	O4'-C4B	-2.46	1.36	1.43
32	c	521	LMT	O4'-C4B	-2.46	1.36	1.43
24	b	610	CLA	C4D-CHA	2.46	1.46	1.38
24	a	406	CLA	C1C-C2C	2.46	1.49	1.44
24	C	505	CLA	C1C-NC	-2.46	1.34	1.37
24	c	505	CLA	C1C-NC	-2.46	1.34	1.37
24	b	607	CLA	C1C-NC	-2.46	1.34	1.37
30	D	411	LMG	O4-C4	-2.46	1.36	1.43
28	d	407	PL9	C53-C6	-2.46	1.45	1.50
24	B	604	CLA	C1B-C2B	2.45	1.48	1.43
24	b	606	CLA	C1B-C2B	2.45	1.48	1.43
27	A	412	SQD	O2-C2	-2.45	1.36	1.43
27	a	412	SQD	O2-C2	-2.45	1.36	1.43
32	J	102	LMT	O3'-C3'	-2.45	1.36	1.43
27	F	101	SQD	O3-C3	-2.45	1.36	1.43
27	f	101	SQD	O3-C3	-2.45	1.36	1.43
32	j	102	LMT	O3'-C3'	-2.45	1.36	1.43
24	A	408	CLA	C1B-C2B	2.45	1.48	1.43
24	a	408	CLA	C1B-C2B	2.45	1.48	1.43
30	C	523	LMG	O2-C2	-2.45	1.36	1.43
30	c	523	LMG	O2-C2	-2.45	1.36	1.43
34	e	101	LHG	O8-C6	-2.44	1.39	1.45
24	A	406	CLA	C1C-C2C	2.44	1.49	1.44
24	B	606	CLA	C1C-C2C	2.44	1.49	1.44
26	J	104	BCR	C30-C25	-2.44	1.50	1.53
26	j	104	BCR	C30-C25	-2.44	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	521	LMT	O2'-C2'	-2.44	1.36	1.43
32	c	521	LMT	O2'-C2'	-2.44	1.36	1.43
28	D	407	PL9	C53-C6	-2.44	1.45	1.50
24	B	605	CLA	C4D-CHA	2.44	1.46	1.38
24	b	607	CLA	C4D-CHA	2.44	1.46	1.38
24	C	514	CLA	C4D-CHA	2.42	1.46	1.38
24	c	514	CLA	C4D-CHA	2.42	1.46	1.38
24	B	603	CLA	C3B-C2B	2.42	1.49	1.41
24	b	605	CLA	C3B-C2B	2.42	1.49	1.41
24	b	612	CLA	C3D-C4D	-2.42	1.38	1.44
24	B	605	CLA	C1C-NC	-2.42	1.34	1.37
24	C	505	CLA	C1B-C2B	2.42	1.48	1.43
24	c	505	CLA	C1B-C2B	2.42	1.48	1.43
27	F	101	SQD	O4-C4	-2.42	1.37	1.43
27	f	101	SQD	O4-C4	-2.42	1.37	1.43
24	C	503	CLA	C4D-CHA	2.41	1.46	1.38
24	c	503	CLA	C4D-CHA	2.41	1.46	1.38
24	B	614	CLA	CHD-C1D	2.41	1.43	1.38
24	b	616	CLA	CHD-C1D	2.41	1.43	1.38
31	C	517	DGD	C1D-C2D	2.41	1.59	1.52
31	c	517	DGD	C1D-C2D	2.41	1.59	1.52
34	E	101	LHG	O8-C6	-2.40	1.39	1.45
24	B	610	CLA	OBD-CAD	2.40	1.26	1.22
24	B	616	CLA	CBD-CAD	-2.40	1.45	1.56
24	b	618	CLA	CBD-CAD	-2.40	1.45	1.56
24	C	504	CLA	CBD-CAD	-2.40	1.45	1.56
24	c	504	CLA	CBD-CAD	-2.40	1.45	1.56
24	B	610	CLA	C3D-C4D	-2.40	1.38	1.44
24	b	608	CLA	C1C-C2C	2.39	1.49	1.44
24	B	610	CLA	O2D-CED	-2.39	1.40	1.45
24	A	406	CLA	C1B-C2B	2.39	1.48	1.43
25	A	407	PHO	CBD-CGD	-2.39	1.49	1.52
25	a	407	PHO	CBD-CGD	-2.39	1.49	1.52
31	C	518	DGD	O3G-C1D	-2.39	1.36	1.40
31	c	518	DGD	O3G-C1D	-2.39	1.36	1.40
30	B	621	LMG	O7-C8	-2.38	1.41	1.46
24	a	406	CLA	C1B-C2B	2.38	1.48	1.43
24	B	609	CLA	C1B-C2B	2.38	1.48	1.43
24	b	612	CLA	OBD-CAD	2.38	1.26	1.22
24	C	509	CLA	C3D-C4D	-2.37	1.38	1.44
24	c	509	CLA	C3D-C4D	-2.37	1.38	1.44
24	C	504	CLA	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	C1B-C2B	2.37	1.48	1.43
24	C	502	CLA	C4D-CHA	2.37	1.46	1.38
24	c	502	CLA	C4D-CHA	2.37	1.46	1.38
24	B	607	CLA	C4C-C3C	2.37	1.49	1.45
24	b	609	CLA	C4C-C3C	2.37	1.49	1.45
28	A	411	PL9	C10-C9	-2.37	1.44	1.50
24	B	602	CLA	C4D-CHA	2.37	1.46	1.38
24	b	604	CLA	C4D-CHA	2.37	1.46	1.38
24	C	512	CLA	C3B-C4B	2.37	1.49	1.42
24	c	512	CLA	C3B-C4B	2.37	1.49	1.42
24	C	511	CLA	C1B-C2B	2.37	1.48	1.43
24	c	511	CLA	C1B-C2B	2.37	1.48	1.43
32	Z	101	LMT	O1'-C1'	-2.37	1.36	1.40
32	z	101	LMT	O1'-C1'	-2.37	1.36	1.40
24	B	613	CLA	C4D-CHA	2.37	1.46	1.38
24	b	615	CLA	C4D-CHA	2.37	1.46	1.38
24	C	506	CLA	C1C-NC	-2.36	1.34	1.37
24	c	506	CLA	C1C-NC	-2.36	1.34	1.37
24	b	612	CLA	O2D-CED	-2.36	1.40	1.45
24	D	404	CLA	C4C-C3C	2.36	1.49	1.45
30	b	622	LMG	O7-C8	-2.35	1.41	1.46
31	H	101	DGD	O2G-C2G	-2.35	1.41	1.46
31	h	101	DGD	O2G-C2G	-2.35	1.41	1.46
24	B	614	CLA	C4D-CHA	2.35	1.46	1.38
24	b	616	CLA	C4D-CHA	2.35	1.46	1.38
24	D	401	CLA	C3D-C4D	-2.35	1.38	1.44
24	d	401	CLA	C3D-C4D	-2.35	1.38	1.44
24	A	406	CLA	OBD-CAD	2.34	1.26	1.22
24	a	406	CLA	OBD-CAD	2.34	1.26	1.22
30	C	501	LMG	O1-C1	-2.34	1.36	1.40
30	c	501	LMG	O1-C1	-2.34	1.36	1.40
28	a	411	PL9	C10-C9	-2.34	1.45	1.50
32	M	101	LMT	O2B-C2B	-2.34	1.37	1.43
32	m	102	LMT	O2B-C2B	-2.34	1.37	1.43
30	C	501	LMG	C4-C3	2.34	1.58	1.52
30	c	501	LMG	C4-C3	2.34	1.58	1.52
32	Z	101	LMT	O4'-C4B	-2.34	1.37	1.43
32	z	101	LMT	O4'-C4B	-2.34	1.37	1.43
24	b	611	CLA	C1B-C2B	2.33	1.48	1.43
35	E	103	HEM	C4D-ND	-2.33	1.36	1.40
35	e	103	HEM	C4D-ND	-2.33	1.36	1.40
24	D	405	CLA	C4D-CHA	2.33	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	C4D-CHA	2.33	1.46	1.38
32	Z	101	LMT	O3B-C3B	-2.33	1.37	1.43
32	z	101	LMT	O3B-C3B	-2.33	1.37	1.43
30	c	520	LMG	C7-C8	2.32	1.58	1.50
24	c	502	CLA	C3B-C2B	2.32	1.49	1.41
24	d	404	CLA	C4C-C3C	2.32	1.49	1.45
25	a	407	PHO	C3D-CAD	-2.32	1.43	1.47
27	B	620	SQD	O4-C4	-2.32	1.37	1.43
24	C	512	CLA	C4D-CHA	2.31	1.46	1.38
24	c	512	CLA	C4D-CHA	2.31	1.46	1.38
24	B	615	CLA	CBD-CAD	-2.31	1.46	1.56
24	b	617	CLA	CBD-CAD	-2.31	1.46	1.56
24	D	405	CLA	C1C-NC	-2.31	1.34	1.37
24	d	405	CLA	C1C-NC	-2.31	1.34	1.37
27	L	102	SQD	O4-C4	-2.31	1.37	1.43
24	C	502	CLA	C3B-C2B	2.31	1.49	1.41
24	C	504	CLA	OBD-CAD	2.31	1.26	1.22
24	c	504	CLA	OBD-CAD	2.31	1.26	1.22
30	D	411	LMG	O3-C3	-2.30	1.37	1.43
30	d	411	LMG	O3-C3	-2.30	1.37	1.43
24	A	406	CLA	C1C-NC	-2.30	1.34	1.37
30	C	520	LMG	C7-C8	2.30	1.58	1.50
24	C	508	CLA	CBD-CAD	-2.30	1.46	1.56
24	c	508	CLA	CBD-CAD	-2.30	1.46	1.56
25	D	402	PHO	CMB-C2B	-2.30	1.47	1.51
25	d	402	PHO	CMB-C2B	-2.30	1.47	1.51
24	B	601	CLA	C3B-C4B	2.30	1.49	1.42
24	b	603	CLA	C3B-C4B	2.30	1.49	1.42
24	B	613	CLA	C1C-NC	-2.29	1.34	1.37
24	b	615	CLA	C1C-NC	-2.29	1.34	1.37
24	a	406	CLA	C1C-NC	-2.29	1.34	1.37
37	V	201	HEC	C4A-NA	-2.29	1.35	1.39
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	D	401	CLA	C4C-C3C	2.29	1.48	1.45
24	d	401	CLA	C4C-C3C	2.29	1.48	1.45
24	C	507	CLA	C4D-CHA	2.29	1.46	1.38
24	c	507	CLA	C4D-CHA	2.29	1.46	1.38
24	B	605	CLA	C1B-C2B	2.29	1.48	1.43
37	v	201	HEC	C4A-NA	-2.29	1.35	1.39
25	A	407	PHO	C3D-CAD	-2.29	1.43	1.47
30	b	622	LMG	C9-C8	2.28	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C1D-ND	2.28	1.40	1.37
24	b	607	CLA	C1B-C2B	2.28	1.48	1.43
30	B	621	LMG	C9-C8	2.28	1.57	1.50
24	B	606	CLA	C1B-C2B	2.28	1.48	1.43
24	b	608	CLA	C1B-C2B	2.28	1.48	1.43
24	A	406	CLA	C4D-CHA	2.28	1.46	1.38
24	a	406	CLA	C4D-CHA	2.28	1.46	1.38
24	C	506	CLA	C3B-C4B	2.27	1.49	1.42
24	c	506	CLA	C3B-C4B	2.27	1.49	1.42
24	C	514	CLA	C1C-NC	-2.27	1.34	1.37
24	c	514	CLA	C1C-NC	-2.27	1.34	1.37
24	B	612	CLA	C3B-C2B	2.27	1.48	1.41
24	b	614	CLA	C3B-C2B	2.27	1.48	1.41
30	C	520	LMG	C4-C5	2.27	1.57	1.53
30	c	520	LMG	C4-C5	2.27	1.57	1.53
24	b	606	CLA	CBD-CAD	-2.27	1.46	1.56
37	V	201	HEC	C3B-C2B	-2.26	1.33	1.41
37	v	201	HEC	C3B-C2B	-2.26	1.33	1.41
24	C	513	CLA	C3D-C4D	-2.26	1.39	1.44
24	c	513	CLA	C3D-C4D	-2.26	1.39	1.44
24	C	513	CLA	C1C-C2C	2.26	1.49	1.44
24	c	513	CLA	C1C-C2C	2.26	1.49	1.44
24	B	604	CLA	C4C-C3C	2.25	1.48	1.45
24	b	606	CLA	C4C-C3C	2.25	1.48	1.45
24	b	603	CLA	C1B-C2B	2.25	1.48	1.43
25	a	407	PHO	CAA-C2A	-2.25	1.49	1.54
25	A	407	PHO	CAA-C2A	-2.25	1.49	1.54
24	C	512	CLA	C3D-C4D	-2.25	1.39	1.44
24	c	512	CLA	C3D-C4D	-2.25	1.39	1.44
24	D	404	CLA	CBD-CAD	-2.25	1.46	1.56
24	d	404	CLA	CBD-CAD	-2.25	1.46	1.56
27	a	410	SQD	O4-C4	-2.25	1.37	1.43
30	C	520	LMG	O7-C8	-2.25	1.41	1.46
30	c	520	LMG	O7-C8	-2.25	1.41	1.46
24	b	610	CLA	C1D-ND	2.25	1.40	1.37
24	C	509	CLA	OBD-CAD	2.24	1.26	1.22
24	c	509	CLA	OBD-CAD	2.24	1.26	1.22
24	C	505	CLA	C3B-C2B	2.24	1.48	1.41
24	c	505	CLA	C3B-C2B	2.24	1.48	1.41
24	C	504	CLA	C3D-C4D	-2.24	1.39	1.44
24	c	504	CLA	C3D-C4D	-2.24	1.39	1.44
24	C	510	CLA	C1C-NC	-2.24	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	C1C-NC	-2.24	1.34	1.37
26	B	617	BCR	C33-C5	-2.24	1.47	1.50
26	b	619	BCR	C33-C5	-2.24	1.47	1.50
24	B	604	CLA	C4D-CHA	2.24	1.46	1.38
24	b	606	CLA	C4D-CHA	2.24	1.46	1.38
24	B	601	CLA	C1B-C2B	2.24	1.48	1.43
24	D	405	CLA	C1C-C2C	2.23	1.49	1.44
24	d	405	CLA	C1C-C2C	2.23	1.49	1.44
24	b	612	CLA	C1B-C2B	2.23	1.48	1.43
24	B	605	CLA	C1C-C2C	2.23	1.49	1.44
24	b	607	CLA	C1C-C2C	2.23	1.49	1.44
24	B	610	CLA	C1B-C2B	2.23	1.48	1.43
31	C	519	DGD	O2G-C2G	-2.23	1.41	1.46
31	c	519	DGD	O2G-C2G	-2.23	1.41	1.46
38	X	101	RRX	C24-C25	2.22	1.52	1.45
24	B	604	CLA	MG-NA	2.22	2.11	2.06
24	b	606	CLA	MG-NA	2.22	2.11	2.06
24	A	405	CLA	C1B-C2B	2.22	1.48	1.43
24	a	405	CLA	C1B-C2B	2.22	1.48	1.43
38	x	101	RRX	C24-C25	2.22	1.52	1.45
27	B	620	SQD	O3-C3	-2.22	1.37	1.43
27	L	102	SQD	O3-C3	-2.22	1.37	1.43
27	A	410	SQD	O4-C4	-2.22	1.37	1.43
24	C	510	CLA	C3B-C2B	2.22	1.48	1.41
24	c	510	CLA	C3B-C2B	2.22	1.48	1.41
24	B	604	CLA	CBD-CAD	-2.21	1.46	1.56
24	C	502	CLA	C1B-C2B	2.21	1.48	1.43
24	c	502	CLA	C1B-C2B	2.21	1.48	1.43
24	B	608	CLA	OBD-CAD	2.21	1.26	1.22
24	c	509	CLA	C4D-CHA	2.21	1.46	1.38
24	D	405	CLA	C3B-C2B	2.21	1.48	1.41
24	d	405	CLA	C3B-C2B	2.21	1.48	1.41
24	C	506	CLA	C1C-C2C	2.21	1.49	1.44
24	c	506	CLA	C1C-C2C	2.21	1.49	1.44
30	D	411	LMG	C3-C2	2.21	1.58	1.52
30	d	411	LMG	C3-C2	2.21	1.58	1.52
37	v	201	HEC	CMC-C2C	2.20	1.55	1.50
24	a	408	CLA	C4D-CHA	2.20	1.46	1.38
24	B	614	CLA	C3B-C4B	2.20	1.49	1.42
24	b	616	CLA	C3B-C4B	2.20	1.49	1.42
24	A	408	CLA	C4D-CHA	2.20	1.46	1.38
24	c	514	CLA	C4C-C3C	2.20	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C4D-CHA	2.20	1.46	1.38
24	b	610	CLA	OBD-CAD	2.20	1.26	1.22
24	b	607	CLA	CHB-C4A	-2.20	1.32	1.37
24	b	614	CLA	CBD-CAD	-2.20	1.46	1.56
25	A	407	PHO	CMB-C2B	-2.19	1.47	1.51
25	a	407	PHO	CMB-C2B	-2.19	1.47	1.51
31	H	101	DGD	C4D-C3D	2.19	1.58	1.52
31	h	101	DGD	C4D-C3D	2.19	1.58	1.52
24	b	612	CLA	C4D-CHA	2.19	1.45	1.38
32	C	521	LMT	O1'-C1'	-2.19	1.36	1.40
32	c	521	LMT	O1'-C1'	-2.19	1.36	1.40
24	C	509	CLA	C4D-CHA	2.19	1.45	1.38
24	B	605	CLA	CHB-C4A	-2.18	1.32	1.37
24	B	612	CLA	CBD-CAD	-2.18	1.46	1.56
24	B	601	CLA	C4C-C3C	2.18	1.48	1.45
24	b	603	CLA	C4C-C3C	2.18	1.48	1.45
30	C	520	LMG	O2-C2	-2.18	1.37	1.43
30	c	520	LMG	O2-C2	-2.18	1.37	1.43
24	D	404	CLA	C1C-C2C	2.17	1.48	1.44
24	d	404	CLA	C1C-C2C	2.17	1.48	1.44
24	C	508	CLA	C4D-CHA	2.17	1.45	1.38
24	c	508	CLA	C4D-CHA	2.17	1.45	1.38
24	B	607	CLA	C1D-ND	2.17	1.40	1.37
24	b	609	CLA	C1D-ND	2.17	1.40	1.37
24	b	610	CLA	CBD-CAD	-2.17	1.46	1.56
37	V	201	HEC	CMC-C2C	2.17	1.55	1.50
24	C	506	CLA	C4D-CHA	2.16	1.45	1.38
24	c	506	CLA	C4D-CHA	2.16	1.45	1.38
24	B	604	CLA	CMB-C2B	-2.16	1.46	1.50
24	b	606	CLA	CMB-C2B	-2.16	1.46	1.50
24	b	613	CLA	O2A-C1	-2.16	1.40	1.46
24	B	607	CLA	OBD-CAD	2.16	1.26	1.22
24	b	609	CLA	OBD-CAD	2.16	1.26	1.22
24	c	514	CLA	C3B-C2B	2.15	1.48	1.41
34	D	410	LHG	C4-C5	2.15	1.57	1.50
34	d	410	LHG	C4-C5	2.15	1.57	1.50
24	B	608	CLA	CBD-CAD	-2.15	1.46	1.56
24	b	604	CLA	C1B-C2B	2.15	1.48	1.43
24	b	608	CLA	C4C-C3C	2.15	1.48	1.45
24	c	508	CLA	O2D-CED	-2.14	1.40	1.45
24	B	613	CLA	CBD-CAD	-2.14	1.46	1.56
24	b	615	CLA	CBD-CAD	-2.14	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	407	PL9	C50-C49	-2.14	1.44	1.50
28	d	407	PL9	C50-C49	-2.14	1.44	1.50
24	b	610	CLA	O2A-C1	-2.14	1.40	1.46
27	A	412	SQD	O3-C3	-2.14	1.37	1.43
27	a	412	SQD	O3-C3	-2.14	1.37	1.43
31	H	101	DGD	O2E-C2E	-2.14	1.37	1.43
31	h	101	DGD	O2E-C2E	-2.14	1.37	1.43
24	B	608	CLA	O2A-C1	-2.14	1.40	1.46
24	B	602	CLA	C1B-C2B	2.13	1.48	1.43
24	B	614	CLA	CBD-CAD	-2.13	1.46	1.56
24	b	616	CLA	CBD-CAD	-2.13	1.46	1.56
24	B	603	CLA	C4C-C3C	2.13	1.48	1.45
24	b	605	CLA	C4C-C3C	2.13	1.48	1.45
24	B	611	CLA	C4D-CHA	2.13	1.45	1.38
24	b	613	CLA	C4D-CHA	2.13	1.45	1.38
24	C	513	CLA	C3B-C2B	2.13	1.48	1.41
24	c	513	CLA	C3B-C2B	2.13	1.48	1.41
24	C	514	CLA	C4C-C3C	2.13	1.48	1.45
24	B	611	CLA	O2A-C1	-2.13	1.40	1.46
24	C	514	CLA	C3B-C2B	2.13	1.48	1.41
24	C	506	CLA	C4C-C3C	2.13	1.48	1.45
24	c	506	CLA	C4C-C3C	2.13	1.48	1.45
24	a	408	CLA	C3D-C4D	-2.12	1.39	1.44
24	d	405	CLA	C4C-C3C	2.12	1.48	1.45
24	C	509	CLA	C3B-C2B	2.12	1.48	1.41
24	c	509	CLA	C3B-C2B	2.12	1.48	1.41
27	f	101	SQD	O2-C2	-2.12	1.37	1.43
24	B	602	CLA	C1C-C2C	2.12	1.48	1.44
24	b	604	CLA	C1C-C2C	2.12	1.48	1.44
24	C	508	CLA	O2D-CED	-2.12	1.40	1.45
24	A	408	CLA	C3D-C4D	-2.12	1.39	1.44
24	B	606	CLA	C3B-C2B	2.12	1.48	1.41
24	b	608	CLA	C3B-C2B	2.12	1.48	1.41
24	B	606	CLA	C4C-C3C	2.12	1.48	1.45
24	C	506	CLA	OBD-CAD	2.11	1.26	1.22
24	D	405	CLA	OBD-CAD	2.11	1.26	1.22
24	c	506	CLA	OBD-CAD	2.11	1.26	1.22
24	d	405	CLA	OBD-CAD	2.11	1.26	1.22
26	a	409	BCR	C30-C25	-2.11	1.51	1.53
25	A	407	PHO	OBD-CAD	-2.11	1.19	1.22
25	a	407	PHO	OBD-CAD	-2.11	1.19	1.22
24	C	512	CLA	CBD-CAD	-2.11	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	CBD-CAD	-2.11	1.47	1.56
27	B	620	SQD	O2-C2	-2.11	1.37	1.43
27	L	102	SQD	O2-C2	-2.11	1.37	1.43
26	C	515	BCR	C33-C5	-2.11	1.47	1.50
26	c	515	BCR	C33-C5	-2.11	1.47	1.50
24	B	611	CLA	C3B-C4B	2.11	1.48	1.42
25	A	407	PHO	C1C-NC	-2.11	1.31	1.37
25	a	407	PHO	C1C-NC	-2.11	1.31	1.37
31	C	519	DGD	O4E-C4E	-2.11	1.37	1.43
24	B	614	CLA	C3B-C2B	2.11	1.48	1.41
24	b	616	CLA	C3B-C2B	2.11	1.48	1.41
24	C	514	CLA	C3B-C4B	2.11	1.48	1.42
24	C	507	CLA	C3B-C2B	2.11	1.48	1.41
24	c	507	CLA	C3B-C2B	2.11	1.48	1.41
24	C	503	CLA	O2A-C1	-2.11	1.40	1.46
24	c	503	CLA	O2A-C1	-2.11	1.40	1.46
24	C	504	CLA	C4D-CHA	2.11	1.45	1.38
24	c	504	CLA	C4D-CHA	2.11	1.45	1.38
27	a	410	SQD	O5-C5	-2.10	1.39	1.44
31	C	518	DGD	O2E-C2E	-2.10	1.37	1.43
31	c	518	DGD	O2E-C2E	-2.10	1.37	1.43
24	A	406	CLA	MG-ND	-2.10	2.01	2.05
24	a	406	CLA	MG-ND	-2.10	2.01	2.05
24	D	401	CLA	OBD-CAD	2.10	1.26	1.22
24	d	401	CLA	OBD-CAD	2.10	1.26	1.22
24	C	512	CLA	C3B-C2B	2.10	1.48	1.41
24	c	512	CLA	C3B-C2B	2.10	1.48	1.41
24	B	601	CLA	C1C-C2C	2.10	1.48	1.44
24	B	605	CLA	C3B-C2B	2.10	1.48	1.41
24	b	607	CLA	C3B-C2B	2.10	1.48	1.41
24	B	610	CLA	C3B-C4B	2.10	1.48	1.42
24	B	601	CLA	CBD-CAD	-2.09	1.47	1.56
24	b	603	CLA	CBD-CAD	-2.09	1.47	1.56
28	d	407	PL9	C36-C34	-2.09	1.47	1.51
27	F	101	SQD	O2-C2	-2.09	1.37	1.43
31	c	519	DGD	O4E-C4E	-2.09	1.37	1.43
24	b	613	CLA	C3B-C4B	2.09	1.48	1.42
25	D	402	PHO	C4D-CHA	2.09	1.42	1.39
25	d	402	PHO	C4D-CHA	2.09	1.42	1.39
24	C	510	CLA	C1C-C2C	2.09	1.48	1.44
24	c	510	CLA	C1C-C2C	2.09	1.48	1.44
24	A	406	CLA	C3B-C4B	2.09	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	CLA	C3B-C4B	2.09	1.48	1.42
24	d	404	CLA	C3B-C2B	2.09	1.48	1.41
24	B	606	CLA	CBD-CAD	-2.09	1.47	1.56
24	b	608	CLA	CBD-CAD	-2.09	1.47	1.56
24	D	405	CLA	C4C-C3C	2.08	1.48	1.45
24	B	614	CLA	C1C-C2C	2.08	1.48	1.44
24	b	616	CLA	C1C-C2C	2.08	1.48	1.44
24	b	612	CLA	CHB-C4A	-2.08	1.32	1.37
24	b	613	CLA	C1B-C2B	2.08	1.48	1.43
24	C	507	CLA	CHB-C4A	-2.08	1.32	1.37
24	c	514	CLA	C3B-C4B	2.08	1.48	1.42
24	C	502	CLA	C1C-NC	-2.07	1.34	1.37
24	c	502	CLA	C1C-NC	-2.07	1.34	1.37
24	B	608	CLA	C4C-C3C	2.07	1.48	1.45
24	b	610	CLA	C4C-C3C	2.07	1.48	1.45
30	D	411	LMG	C7-C8	2.07	1.57	1.50
24	B	612	CLA	C4D-CHA	2.07	1.45	1.38
24	b	614	CLA	C4D-CHA	2.07	1.45	1.38
28	D	407	PL9	C36-C34	-2.07	1.47	1.51
30	d	411	LMG	C7-C8	2.07	1.57	1.50
24	b	612	CLA	C3B-C4B	2.07	1.48	1.42
24	d	404	CLA	C1D-ND	2.07	1.40	1.37
27	A	410	SQD	O5-C5	-2.07	1.39	1.44
24	A	405	CLA	CBD-CAD	-2.07	1.47	1.56
24	a	405	CLA	CBD-CAD	-2.07	1.47	1.56
24	B	615	CLA	C3B-C2B	2.07	1.48	1.41
24	b	617	CLA	C3B-C2B	2.07	1.48	1.41
24	b	603	CLA	C1C-C2C	2.07	1.48	1.44
24	b	615	CLA	C1B-C2B	2.06	1.48	1.43
24	B	613	CLA	MG-ND	-2.06	2.01	2.05
24	b	615	CLA	MG-ND	-2.06	2.01	2.05
24	B	611	CLA	C1B-C2B	2.06	1.48	1.43
24	D	404	CLA	C3B-C2B	2.06	1.48	1.41
26	C	515	BCR	C38-C26	-2.06	1.47	1.50
26	c	515	BCR	C38-C26	-2.06	1.47	1.50
30	D	411	LMG	C4-C5	2.06	1.57	1.53
30	d	411	LMG	C4-C5	2.06	1.57	1.53
24	B	613	CLA	C1C-C2C	2.06	1.48	1.44
24	C	505	CLA	CHB-C4A	-2.06	1.32	1.37
24	c	505	CLA	CHB-C4A	-2.06	1.32	1.37
24	C	511	CLA	C4C-C3C	2.05	1.48	1.45
24	c	511	CLA	C4C-C3C	2.05	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	409	BCR	C30-C25	-2.05	1.51	1.53
24	D	404	CLA	C1D-ND	2.05	1.40	1.37
24	C	514	CLA	C1C-C2C	2.05	1.48	1.44
24	c	507	CLA	CHB-C4A	-2.05	1.32	1.37
24	B	613	CLA	C1B-C2B	2.05	1.47	1.43
26	A	409	BCR	C38-C26	-2.05	1.47	1.50
30	C	501	LMG	O4-C4	-2.05	1.37	1.43
24	C	504	CLA	C3B-C4B	2.04	1.48	1.42
24	c	504	CLA	C3B-C4B	2.04	1.48	1.42
24	B	612	CLA	C1C-C2C	2.04	1.48	1.44
24	b	614	CLA	C1C-C2C	2.04	1.48	1.44
24	B	614	CLA	C1D-ND	2.04	1.40	1.37
24	b	616	CLA	C1D-ND	2.04	1.40	1.37
30	c	501	LMG	O4-C4	-2.04	1.37	1.43
24	A	405	CLA	MG-ND	-2.04	2.01	2.05
24	a	405	CLA	MG-ND	-2.04	2.01	2.05
37	V	201	HEC	C2A-C3A	-2.04	1.32	1.36
24	C	507	CLA	CBD-CAD	-2.04	1.47	1.56
24	c	507	CLA	CBD-CAD	-2.04	1.47	1.56
34	L	101	LHG	O7-C5	-2.03	1.41	1.46
34	l	101	LHG	O7-C5	-2.03	1.41	1.46
26	C	522	BCR	C33-C5	-2.03	1.47	1.50
26	c	522	BCR	C33-C5	-2.03	1.47	1.50
24	B	615	CLA	OBD-CAD	2.03	1.26	1.22
24	b	617	CLA	OBD-CAD	2.03	1.26	1.22
24	D	405	CLA	C3B-C4B	2.02	1.48	1.42
24	d	405	CLA	C3B-C4B	2.02	1.48	1.42
24	C	508	CLA	C3B-C2B	2.02	1.48	1.41
24	c	508	CLA	C3B-C2B	2.02	1.48	1.41
24	A	406	CLA	C4C-C3C	2.02	1.48	1.45
26	a	409	BCR	C38-C26	-2.02	1.47	1.50
24	b	615	CLA	C1C-C2C	2.02	1.48	1.44
24	C	508	CLA	C1C-C2C	2.02	1.48	1.44
24	c	508	CLA	C1C-C2C	2.02	1.48	1.44
24	a	405	CLA	C1C-C2C	2.01	1.48	1.44
24	A	405	CLA	C1C-C2C	2.01	1.48	1.44
24	c	514	CLA	C1C-C2C	2.01	1.48	1.44
28	A	411	PL9	C41-C39	-2.01	1.47	1.51
28	a	411	PL9	C41-C39	-2.01	1.47	1.51
24	C	504	CLA	C1C-C2C	2.01	1.48	1.44
24	c	504	CLA	C1C-C2C	2.01	1.48	1.44
24	b	610	CLA	CHB-C4A	-2.00	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	405	CLA	CBD-CGD	-2.00	1.46	1.52

All (2730) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	102	SQD	O6-C1-C2	10.89	124.81	108.27
27	B	620	SQD	O6-C1-C2	10.89	124.81	108.27
24	B	614	CLA	C1D-ND-C4D	-10.10	99.23	106.31
24	b	616	CLA	C1D-ND-C4D	-10.10	99.23	106.31
24	D	401	CLA	C1D-ND-C4D	-9.99	99.30	106.31
24	d	401	CLA	C1D-ND-C4D	-9.99	99.30	106.31
24	a	408	CLA	C1D-ND-C4D	-9.84	99.41	106.31
24	A	408	CLA	C1D-ND-C4D	-9.79	99.44	106.31
27	a	410	SQD	O6-C1-C2	9.78	123.13	108.27
27	A	410	SQD	O6-C1-C2	9.75	123.08	108.27
24	B	602	CLA	C1D-ND-C4D	-9.60	99.57	106.31
24	b	604	CLA	C1D-ND-C4D	-9.60	99.57	106.31
24	C	512	CLA	C1D-ND-C4D	-9.51	99.64	106.31
24	c	512	CLA	C1D-ND-C4D	-9.51	99.64	106.31
24	c	509	CLA	C1D-ND-C4D	-9.39	99.72	106.31
24	C	504	CLA	C1D-ND-C4D	-9.39	99.72	106.31
24	c	504	CLA	C1D-ND-C4D	-9.39	99.72	106.31
24	d	404	CLA	C1D-ND-C4D	-9.33	99.76	106.31
24	C	509	CLA	C1D-ND-C4D	-9.32	99.77	106.31
24	D	404	CLA	C1D-ND-C4D	-9.31	99.78	106.31
24	C	513	CLA	C1D-ND-C4D	-9.24	99.83	106.31
24	c	513	CLA	C1D-ND-C4D	-9.24	99.83	106.31
24	B	611	CLA	C1D-ND-C4D	-9.16	99.89	106.31
24	b	613	CLA	C1D-ND-C4D	-9.16	99.89	106.31
24	C	508	CLA	C1D-ND-C4D	-9.12	99.91	106.31
24	c	508	CLA	C1D-ND-C4D	-9.12	99.91	106.31
24	D	405	CLA	C1D-ND-C4D	-8.75	100.17	106.31
24	d	405	CLA	C1D-ND-C4D	-8.75	100.17	106.31
24	B	605	CLA	C1D-ND-C4D	-8.75	100.17	106.31
24	b	607	CLA	C1D-ND-C4D	-8.75	100.17	106.31
25	A	407	PHO	C4D-CHA-CBD	-8.71	104.28	108.45
25	a	407	PHO	C4D-CHA-CBD	-8.71	104.28	108.45
24	C	514	CLA	C1D-ND-C4D	-8.47	100.37	106.31
24	c	514	CLA	C1D-ND-C4D	-8.47	100.37	106.31
24	C	503	CLA	C1D-ND-C4D	-8.46	100.37	106.31
24	c	503	CLA	C1D-ND-C4D	-8.46	100.37	106.31
27	f	101	SQD	O6-C1-C2	8.36	120.96	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C1D-ND-C4D	-8.35	100.45	106.31
27	F	101	SQD	O6-C1-C2	8.35	120.96	108.27
24	c	502	CLA	C1D-ND-C4D	-8.33	100.46	106.31
24	C	502	CLA	C1D-ND-C4D	-8.31	100.48	106.31
24	B	606	CLA	C1D-ND-C4D	-8.25	100.52	106.31
24	b	608	CLA	C1D-ND-C4D	-8.24	100.53	106.31
24	B	607	CLA	C1D-ND-C4D	-8.22	100.54	106.31
24	b	609	CLA	C1D-ND-C4D	-8.22	100.54	106.31
24	b	611	CLA	C1D-ND-C4D	-8.21	100.55	106.31
24	B	601	CLA	C1D-ND-C4D	-8.07	100.65	106.31
24	b	603	CLA	C1D-ND-C4D	-8.07	100.65	106.31
24	B	615	CLA	C1D-ND-C4D	-8.00	100.70	106.31
24	b	617	CLA	C1D-ND-C4D	-8.00	100.70	106.31
24	C	506	CLA	C1D-ND-C4D	-7.92	100.76	106.31
24	c	506	CLA	C1D-ND-C4D	-7.92	100.76	106.31
24	b	612	CLA	C1D-ND-C4D	-7.88	100.79	106.31
24	C	505	CLA	C1D-ND-C4D	-7.87	100.79	106.31
24	c	505	CLA	C1D-ND-C4D	-7.87	100.79	106.31
24	B	610	CLA	C1D-ND-C4D	-7.86	100.80	106.31
24	b	614	CLA	C1D-ND-C4D	-7.67	100.93	106.31
24	B	612	CLA	C1D-ND-C4D	-7.64	100.95	106.31
24	C	513	CLA	C2D-C1D-ND	7.64	117.69	110.13
24	c	513	CLA	C2D-C1D-ND	7.64	117.69	110.13
24	C	507	CLA	C1D-ND-C4D	-7.60	100.98	106.31
24	c	507	CLA	C1D-ND-C4D	-7.60	100.98	106.31
24	B	616	CLA	C1D-ND-C4D	-7.54	101.02	106.31
24	b	618	CLA	C1D-ND-C4D	-7.54	101.02	106.31
24	C	510	CLA	C1D-ND-C4D	-7.53	101.03	106.31
24	c	510	CLA	C1D-ND-C4D	-7.53	101.03	106.31
24	B	613	CLA	C1D-ND-C4D	-7.51	101.04	106.31
24	b	615	CLA	C1D-ND-C4D	-7.51	101.04	106.31
24	B	605	CLA	O2D-CGD-CBD	7.38	124.12	111.23
24	b	607	CLA	O2D-CGD-CBD	7.38	124.12	111.23
24	c	509	CLA	C2D-C1D-ND	7.33	117.38	110.13
24	C	509	CLA	C2D-C1D-ND	7.31	117.36	110.13
24	C	511	CLA	C2C-C1C-NC	7.30	117.65	109.98
24	c	511	CLA	C2C-C1C-NC	7.30	117.65	109.98
24	C	511	CLA	CMD-C2D-C1D	7.28	137.56	124.73
24	c	511	CLA	CMD-C2D-C1D	7.28	137.56	124.73
24	a	408	CLA	C2D-C1D-ND	7.27	117.33	110.13
24	B	612	CLA	O2D-CGD-CBD	7.27	123.94	111.23
24	b	614	CLA	O2D-CGD-CBD	7.26	123.93	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	408	CLA	C2D-C1D-ND	7.23	117.28	110.13
24	B	602	CLA	CMD-C2D-C1D	7.18	137.38	124.73
24	b	604	CLA	CMD-C2D-C1D	7.18	137.38	124.73
24	B	603	CLA	C1D-ND-C4D	-7.12	101.32	106.31
24	D	401	CLA	C2D-C1D-ND	7.10	117.15	110.13
24	d	401	CLA	C2D-C1D-ND	7.10	117.15	110.13
24	b	605	CLA	C1D-ND-C4D	-7.04	101.37	106.31
24	b	610	CLA	C1D-ND-C4D	-6.86	101.50	106.31
24	A	405	CLA	CMD-C2D-C1D	6.85	136.80	124.73
24	a	405	CLA	CMD-C2D-C1D	6.85	136.80	124.73
24	B	613	CLA	CMD-C2D-C1D	6.83	136.76	124.73
24	b	615	CLA	CMD-C2D-C1D	6.83	136.76	124.73
24	B	606	CLA	CMD-C2D-C1D	6.83	136.75	124.73
24	b	608	CLA	CMD-C2D-C1D	6.82	136.74	124.73
24	C	508	CLA	CMD-C2D-C1D	6.81	136.73	124.73
24	c	508	CLA	CMD-C2D-C1D	6.81	136.73	124.73
24	B	608	CLA	C1D-ND-C4D	-6.81	101.54	106.31
24	D	404	CLA	CMD-C2D-C1D	6.80	136.71	124.73
24	d	404	CLA	CMD-C2D-C1D	6.80	136.70	124.73
24	B	604	CLA	O2D-CGD-CBD	6.71	122.96	111.23
24	C	504	CLA	CMD-C2D-C1D	6.69	136.51	124.73
24	c	504	CLA	CMD-C2D-C1D	6.69	136.51	124.73
24	b	606	CLA	O2D-CGD-CBD	6.68	122.90	111.23
24	b	611	CLA	CHD-C4C-C3C	-6.64	115.10	124.77
24	B	609	CLA	CHD-C4C-C3C	-6.63	115.10	124.77
24	C	514	CLA	O2D-CGD-CBD	6.60	122.77	111.23
24	c	514	CLA	O2D-CGD-CBD	6.60	122.77	111.23
24	A	406	CLA	C1D-ND-C4D	-6.57	101.70	106.31
24	a	406	CLA	C1D-ND-C4D	-6.57	101.70	106.31
24	A	406	CLA	CMD-C2D-C1D	6.54	136.25	124.73
24	C	514	CLA	CMD-C2D-C1D	6.54	136.25	124.73
24	a	406	CLA	CMD-C2D-C1D	6.54	136.25	124.73
24	c	514	CLA	CMD-C2D-C1D	6.54	136.25	124.73
24	c	512	CLA	CMD-C2D-C1D	6.54	136.24	124.73
24	b	603	CLA	O2D-CGD-CBD	6.53	122.65	111.23
24	b	613	CLA	C2D-C1D-ND	6.53	116.58	110.13
24	B	607	CLA	CMD-C2D-C1D	6.52	136.20	124.73
24	b	609	CLA	CMD-C2D-C1D	6.52	136.20	124.73
24	B	611	CLA	C2D-C1D-ND	6.51	116.57	110.13
24	C	512	CLA	CMD-C2D-C1D	6.51	136.19	124.73
24	B	601	CLA	O2D-CGD-CBD	6.50	122.59	111.23
24	A	405	CLA	C1D-ND-C4D	-6.44	101.79	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	405	CLA	C1D-ND-C4D	-6.44	101.79	106.31
24	d	405	CLA	CMD-C2D-C1D	6.43	136.05	124.73
24	C	511	CLA	C1D-ND-C4D	-6.41	101.81	106.31
24	c	511	CLA	C1D-ND-C4D	-6.41	101.81	106.31
24	D	405	CLA	CMD-C2D-C1D	6.41	136.01	124.73
24	C	507	CLA	CMD-C2D-C1D	6.40	136.00	124.73
24	c	507	CLA	CMD-C2D-C1D	6.40	136.00	124.73
24	B	614	CLA	C2D-C1D-ND	6.39	116.45	110.13
24	A	406	CLA	CHD-C4C-C3C	-6.36	115.50	124.77
24	B	604	CLA	C1D-ND-C4D	-6.36	101.85	106.31
24	b	606	CLA	C1D-ND-C4D	-6.36	101.85	106.31
24	b	616	CLA	C2D-C1D-ND	6.35	116.42	110.13
24	c	512	CLA	C2D-C1D-ND	6.35	116.42	110.13
24	a	406	CLA	CHD-C4C-C3C	-6.35	115.51	124.77
24	B	612	CLA	CHD-C4C-C3C	-6.34	115.53	124.77
24	b	614	CLA	CHD-C4C-C3C	-6.34	115.53	124.77
24	B	602	CLA	C2D-C1D-ND	6.33	116.39	110.13
24	b	604	CLA	C2D-C1D-ND	6.33	116.39	110.13
24	C	504	CLA	C2D-C1D-ND	6.32	116.38	110.13
24	C	512	CLA	C2D-C1D-ND	6.32	116.38	110.13
24	c	504	CLA	C2D-C1D-ND	6.32	116.38	110.13
24	B	604	CLA	C2C-C1C-NC	6.29	116.59	109.98
24	b	606	CLA	C2C-C1C-NC	6.29	116.59	109.98
24	B	616	CLA	CHD-C4C-C3C	-6.28	115.61	124.77
24	b	618	CLA	CHD-C4C-C3C	-6.28	115.61	124.77
24	C	505	CLA	CMD-C2D-C1D	6.25	135.74	124.73
24	c	505	CLA	CMD-C2D-C1D	6.25	135.74	124.73
24	C	506	CLA	O2D-CGD-CBD	6.23	122.13	111.23
24	c	506	CLA	O2D-CGD-CBD	6.23	122.13	111.23
24	B	605	CLA	C2D-C1D-ND	6.23	116.29	110.13
24	b	607	CLA	C2D-C1D-ND	6.23	116.29	110.13
24	C	508	CLA	C2D-C1D-ND	6.20	116.26	110.13
24	c	508	CLA	C2D-C1D-ND	6.20	116.26	110.13
24	C	513	CLA	CHD-C4C-C3C	-6.19	115.74	124.77
24	c	513	CLA	CHD-C4C-C3C	-6.19	115.74	124.77
24	c	514	CLA	C2B-C1B-NB	6.15	116.70	110.33
24	b	612	CLA	C2D-C1D-ND	6.12	116.19	110.13
24	C	514	CLA	C2B-C1B-NB	6.12	116.67	110.33
24	C	504	CLA	CHD-C4C-C3C	-6.11	115.87	124.77
24	c	504	CLA	CHD-C4C-C3C	-6.11	115.87	124.77
24	d	404	CLA	C2D-C1D-ND	6.09	116.15	110.13
24	D	404	CLA	C2D-C1D-ND	6.09	116.15	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	402	PHO	C4D-CHA-CBD	-6.08	105.54	108.45
25	d	402	PHO	C4D-CHA-CBD	-6.08	105.54	108.45
24	C	502	CLA	CMD-C2D-C1D	6.08	135.43	124.73
24	B	610	CLA	C2D-C1D-ND	6.07	116.14	110.13
24	c	502	CLA	CMD-C2D-C1D	6.06	135.41	124.73
24	b	611	CLA	O2D-CGD-CBD	6.05	121.80	111.23
24	c	513	CLA	O2D-CGD-CBD	6.03	121.77	111.23
24	B	609	CLA	O2D-CGD-CBD	6.03	121.77	111.23
24	C	513	CLA	O2D-CGD-CBD	6.03	121.77	111.23
24	D	401	CLA	C2C-C1C-NC	6.02	116.30	109.98
24	d	401	CLA	C2C-C1C-NC	6.02	116.30	109.98
24	B	609	CLA	CMD-C2D-C1D	6.00	135.29	124.73
24	C	508	CLA	CHD-C4C-C3C	-5.99	116.03	124.77
24	c	508	CLA	CHD-C4C-C3C	-5.99	116.03	124.77
24	b	608	CLA	CHD-C4C-C3C	-5.98	116.06	124.77
24	B	604	CLA	CMD-C2D-C1D	5.97	135.24	124.73
24	b	606	CLA	CMD-C2D-C1D	5.97	135.24	124.73
24	C	506	CLA	CMD-C2D-C1D	5.96	135.23	124.73
24	c	506	CLA	CMD-C2D-C1D	5.96	135.23	124.73
24	b	611	CLA	CMD-C2D-C1D	5.95	135.21	124.73
24	b	609	CLA	O2D-CGD-CBD	5.94	121.61	111.23
24	C	508	CLA	C3B-C2B-C1B	-5.94	100.17	107.17
24	c	508	CLA	C3B-C2B-C1B	-5.94	100.17	107.17
24	B	606	CLA	CHD-C4C-C3C	-5.93	116.13	124.77
24	B	607	CLA	O2D-CGD-CBD	5.92	121.59	111.23
24	B	609	CLA	C2D-C1D-ND	5.91	115.98	110.13
24	C	510	CLA	CMD-C2D-C1D	5.90	135.11	124.73
24	c	510	CLA	CMD-C2D-C1D	5.90	135.11	124.73
24	B	615	CLA	C2D-C1D-ND	5.88	115.94	110.13
24	b	617	CLA	C2D-C1D-ND	5.88	115.94	110.13
24	b	611	CLA	C2D-C1D-ND	5.85	115.91	110.13
24	C	509	CLA	O2D-CGD-CBD	5.84	121.44	111.23
24	c	509	CLA	O2D-CGD-CBD	5.84	121.44	111.23
24	B	601	CLA	CMD-C2D-C1D	5.83	134.99	124.73
24	b	603	CLA	CMD-C2D-C1D	5.82	134.98	124.73
24	B	608	CLA	C2C-C1C-NC	5.82	116.09	109.98
24	c	505	CLA	O2D-CGD-CBD	5.81	121.38	111.23
24	C	505	CLA	O2D-CGD-CBD	5.79	121.36	111.23
24	B	607	CLA	C2C-C1C-NC	5.79	116.07	109.98
24	b	609	CLA	C2C-C1C-NC	5.79	116.07	109.98
24	b	610	CLA	C2C-C1C-NC	5.77	116.04	109.98
24	C	502	CLA	C2D-C1D-ND	5.75	115.81	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	CHD-C4C-C3C	-5.74	116.40	124.77
24	b	604	CLA	CHD-C4C-C3C	-5.74	116.40	124.77
24	c	503	CLA	C2C-C1C-NC	5.74	116.02	109.98
24	c	502	CLA	C2D-C1D-ND	5.74	115.81	110.13
24	B	616	CLA	C3B-C2B-C1B	-5.73	100.41	107.17
24	b	618	CLA	C3B-C2B-C1B	-5.73	100.41	107.17
24	C	512	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
24	C	509	CLA	CHD-C4C-C3C	-5.72	116.44	124.77
24	c	509	CLA	CHD-C4C-C3C	-5.72	116.44	124.77
24	B	611	CLA	CHD-C4C-C3C	-5.71	116.44	124.77
24	b	613	CLA	CHD-C4C-C3C	-5.71	116.44	124.77
24	c	512	CLA	CHD-C4C-C3C	-5.71	116.44	124.77
24	C	503	CLA	C2C-C1C-NC	5.70	115.97	109.98
24	c	514	CLA	C3B-C2B-C1B	-5.70	100.44	107.17
24	C	514	CLA	C3B-C2B-C1B	-5.69	100.46	107.17
24	C	514	CLA	C2D-C1D-ND	5.69	115.75	110.13
24	c	514	CLA	C2D-C1D-ND	5.69	115.75	110.13
24	B	603	CLA	C2C-C1C-NC	5.67	115.93	109.98
24	b	605	CLA	C2C-C1C-NC	5.67	115.93	109.98
24	B	607	CLA	C2D-C1D-ND	5.66	115.73	110.13
24	b	609	CLA	C2D-C1D-ND	5.66	115.73	110.13
24	b	608	CLA	O2D-CGD-CBD	5.66	121.12	111.23
24	A	405	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
24	a	405	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
24	C	511	CLA	C1C-C2C-C3C	-5.65	101.04	106.98
24	c	511	CLA	C1C-C2C-C3C	-5.65	101.04	106.98
24	B	601	CLA	C2D-C1D-ND	5.64	115.71	110.13
24	b	603	CLA	C2D-C1D-ND	5.64	115.71	110.13
24	B	606	CLA	O2D-CGD-CBD	5.64	121.09	111.23
24	B	602	CLA	O2D-CGD-CBD	5.64	121.08	111.23
24	b	604	CLA	O2D-CGD-CBD	5.64	121.08	111.23
24	C	512	CLA	C3B-C4B-NB	5.63	115.55	110.53
24	c	512	CLA	C3B-C4B-NB	5.63	115.55	110.53
24	b	608	CLA	C2D-C1D-ND	5.62	115.69	110.13
24	B	613	CLA	C2D-C1D-ND	5.62	115.69	110.13
24	b	615	CLA	C2D-C1D-ND	5.62	115.69	110.13
24	B	614	CLA	CMD-C2D-C1D	5.61	134.62	124.73
24	B	615	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
24	b	617	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
24	B	606	CLA	C2D-C1D-ND	5.61	115.68	110.13
24	C	507	CLA	C2D-C1D-ND	5.60	115.67	110.13
24	c	507	CLA	C2D-C1D-ND	5.60	115.67	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
24	b	613	CLA	CMD-C2D-C1D	5.57	134.54	124.73
24	B	611	CLA	CMD-C2D-C1D	5.57	134.54	124.73
24	c	502	CLA	CHD-C4C-C3C	-5.57	116.65	124.77
24	b	610	CLA	CHD-C4C-C3C	-5.57	116.65	124.77
24	b	616	CLA	CMD-C2D-C1D	5.57	134.53	124.73
24	c	507	CLA	CHD-C4C-C3C	-5.57	116.66	124.77
24	a	408	CLA	CMD-C2D-C1D	5.55	134.51	124.73
24	B	616	CLA	CMD-C2D-C1D	5.55	134.51	124.73
24	b	618	CLA	CMD-C2D-C1D	5.55	134.51	124.73
24	B	614	CLA	C3B-C2B-C1B	-5.55	100.62	107.17
24	A	408	CLA	CMD-C2D-C1D	5.55	134.50	124.73
24	b	611	CLA	C2C-C1C-NC	5.55	115.81	109.98
24	C	502	CLA	CHD-C4C-C3C	-5.55	116.69	124.77
24	C	507	CLA	CHD-C4C-C3C	-5.54	116.69	124.77
24	C	502	CLA	C2C-C1C-NC	5.54	115.80	109.98
24	c	502	CLA	C2C-C1C-NC	5.54	115.80	109.98
24	b	616	CLA	C3B-C2B-C1B	-5.53	100.65	107.17
24	B	613	CLA	CHD-C4C-C3C	-5.51	116.73	124.77
24	b	615	CLA	CHD-C4C-C3C	-5.51	116.73	124.77
24	C	509	CLA	C2C-C1C-NC	5.50	115.76	109.98
24	c	509	CLA	C2C-C1C-NC	5.50	115.76	109.98
24	B	605	CLA	CHD-C4C-C3C	-5.50	116.75	124.77
24	b	607	CLA	CHD-C4C-C3C	-5.50	116.75	124.77
24	b	616	CLA	C2B-C1B-NB	5.49	116.02	110.33
24	B	614	CLA	C2B-C1B-NB	5.49	116.02	110.33
24	C	511	CLA	CHD-C4C-C3C	-5.48	116.79	124.77
24	c	511	CLA	CHD-C4C-C3C	-5.48	116.79	124.77
24	B	603	CLA	O2D-CGD-CBD	5.48	120.81	111.23
24	b	605	CLA	O2D-CGD-CBD	5.48	120.81	111.23
24	b	612	CLA	CHD-C4C-C3C	-5.48	116.79	124.77
24	D	405	CLA	O2D-CGD-CBD	5.48	120.80	111.23
24	d	405	CLA	O2D-CGD-CBD	5.48	120.80	111.23
24	B	609	CLA	C2C-C1C-NC	5.47	115.72	109.98
24	B	610	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
24	a	405	CLA	C2C-C1C-NC	5.45	115.70	109.98
24	A	405	CLA	C2C-C1C-NC	5.45	115.70	109.98
24	C	505	CLA	C2D-C1D-ND	5.44	115.51	110.13
24	c	505	CLA	C2D-C1D-ND	5.44	115.51	110.13
24	C	503	CLA	C2D-C1D-ND	5.40	115.47	110.13
24	c	503	CLA	C2D-C1D-ND	5.40	115.47	110.13
24	b	614	CLA	C2D-C1D-ND	5.40	115.47	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	O2D-CGD-CBD	5.39	120.66	111.23
24	c	511	CLA	O2D-CGD-CBD	5.39	120.66	111.23
24	D	401	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
24	d	401	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
24	b	613	CLA	C3D-C2D-C1D	-5.38	98.48	105.83
24	B	612	CLA	C2D-C1D-ND	5.38	115.45	110.13
24	B	613	CLA	C2C-C1C-NC	5.37	115.63	109.98
24	B	606	CLA	C3B-C4B-NB	5.36	115.32	110.53
24	b	608	CLA	C3B-C4B-NB	5.36	115.32	110.53
24	b	615	CLA	C2C-C1C-NC	5.36	115.61	109.98
24	B	611	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
24	b	612	CLA	C2C-C1C-NC	5.35	115.60	109.98
24	b	603	CLA	C2C-C1C-NC	5.34	115.59	109.98
24	A	408	CLA	CHD-C4C-C3C	-5.34	116.99	124.77
24	a	408	CLA	CHD-C4C-C3C	-5.34	116.99	124.77
24	B	604	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
24	b	606	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
24	D	401	CLA	C1C-C2C-C3C	-5.33	101.38	106.98
24	d	401	CLA	C1C-C2C-C3C	-5.33	101.38	106.98
24	a	408	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
24	D	405	CLA	C3B-C4B-NB	5.33	115.29	110.53
24	d	405	CLA	C3B-C4B-NB	5.33	115.29	110.53
24	A	408	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
24	C	513	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
24	c	513	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
24	C	502	CLA	C1C-C2C-C3C	-5.31	101.40	106.98
24	D	405	CLA	CHD-C4C-C3C	-5.31	117.04	124.77
24	B	603	CLA	CMD-C2D-C1D	5.31	134.07	124.73
24	b	605	CLA	CMD-C2D-C1D	5.31	134.07	124.73
24	C	509	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
24	c	509	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
24	c	502	CLA	C1C-C2C-C3C	-5.29	101.41	106.98
24	B	604	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
24	b	606	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
24	d	405	CLA	CHD-C4C-C3C	-5.29	117.06	124.77
24	C	507	CLA	C4B-C3B-C2B	-5.28	100.73	107.30
24	c	507	CLA	C4B-C3B-C2B	-5.28	100.73	107.30
24	D	401	CLA	CHD-C1D-ND	-5.27	117.38	124.80
24	d	401	CLA	CHD-C1D-ND	-5.27	117.38	124.80
24	C	506	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
24	c	506	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
24	B	601	CLA	CHD-C4C-C3C	-5.27	117.09	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
24	C	503	CLA	CHD-C4C-C3C	-5.25	117.11	124.77
24	c	503	CLA	CHD-C4C-C3C	-5.25	117.12	124.77
24	B	601	CLA	C2C-C1C-NC	5.25	115.50	109.98
24	C	510	CLA	C2D-C1D-ND	5.24	115.31	110.13
24	c	510	CLA	C2D-C1D-ND	5.24	115.31	110.13
27	A	412	SQD	C4-C3-C2	5.23	120.02	110.83
24	B	610	CLA	C2C-C1C-NC	5.23	115.48	109.98
24	C	510	CLA	O2D-CGD-CBD	5.22	120.36	111.23
24	c	510	CLA	O2D-CGD-CBD	5.22	120.36	111.23
27	a	412	SQD	C4-C3-C2	5.22	119.99	110.83
24	B	610	CLA	CMD-C2D-C1D	5.21	133.91	124.73
24	d	405	CLA	C2D-C1D-ND	5.21	115.28	110.13
24	b	612	CLA	CMD-C2D-C1D	5.21	133.90	124.73
24	D	405	CLA	C2D-C1D-ND	5.20	115.27	110.13
24	c	502	CLA	C3B-C2B-C1B	-5.20	101.05	107.17
24	c	510	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
24	B	613	CLA	C1C-C2C-C3C	-5.17	101.54	106.98
24	C	502	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
24	b	616	CLA	CHD-C4C-C3C	-5.16	117.25	124.77
24	B	613	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
24	b	615	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
24	C	510	CLA	CHD-C4C-C3C	-5.15	117.26	124.77
24	B	614	CLA	CHD-C4C-C3C	-5.15	117.26	124.77
24	A	405	CLA	CAA-C2A-C3A	-5.15	99.08	113.00
24	a	405	CLA	CAA-C2A-C3A	-5.15	99.08	113.00
24	B	607	CLA	CHD-C4C-C3C	-5.13	117.30	124.77
24	b	609	CLA	CHD-C4C-C3C	-5.13	117.30	124.77
24	b	615	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
24	C	507	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
24	c	507	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
24	C	508	CLA	C2C-C1C-NC	5.10	115.34	109.98
24	c	508	CLA	C2C-C1C-NC	5.10	115.34	109.98
24	B	614	CLA	O2D-CGD-CBD	5.10	120.14	111.23
24	C	503	CLA	O2D-CGD-CBD	5.10	120.14	111.23
24	b	616	CLA	O2D-CGD-CBD	5.10	120.14	111.23
24	c	503	CLA	O2D-CGD-CBD	5.09	120.13	111.23
24	b	616	CLA	C3D-C4D-ND	5.07	118.22	109.99
24	B	605	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
24	b	607	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
24	C	512	CLA	C2B-C1B-NB	5.06	115.57	110.33
24	c	512	CLA	C2B-C1B-NB	5.06	115.57	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	CLA	C4A-NA-C1A	-5.05	104.38	106.68
24	c	514	CLA	C4A-NA-C1A	-5.05	104.38	106.68
33	D	403	BCT	O2-C-O1	5.05	132.58	119.68
24	B	614	CLA	C3D-C4D-ND	5.04	118.19	109.99
33	d	403	BCT	O2-C-O1	5.04	132.56	119.68
24	b	603	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
24	B	602	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
24	b	604	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
24	B	601	CLA	C3B-C2B-C1B	-5.02	101.26	107.17
24	B	612	CLA	C3C-C4C-NC	5.01	116.85	110.43
24	b	614	CLA	C3C-C4C-NC	5.01	116.85	110.43
24	c	502	CLA	C2B-C1B-NB	5.00	115.52	110.33
24	D	401	CLA	O2D-CGD-CBD	5.00	119.97	111.23
24	B	615	CLA	CMD-C2D-C1D	5.00	133.53	124.73
24	b	617	CLA	CMD-C2D-C1D	5.00	133.53	124.73
24	b	603	CLA	C2B-C1B-NB	4.99	115.50	110.33
24	d	401	CLA	O2D-CGD-CBD	4.99	119.96	111.23
24	B	615	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
24	b	617	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
24	B	601	CLA	C2B-C1B-NB	4.98	115.49	110.33
24	C	506	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
24	c	506	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
24	C	502	CLA	C2B-C1B-NB	4.97	115.48	110.33
24	c	512	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	C	502	CLA	O2D-CGD-CBD	4.94	119.87	111.23
24	c	502	CLA	O2D-CGD-CBD	4.94	119.87	111.23
24	C	508	CLA	O2D-CGD-CBD	4.94	119.87	111.23
24	c	508	CLA	O2D-CGD-CBD	4.94	119.87	111.23
24	D	405	CLA	C3D-C4D-ND	4.93	118.01	109.99
24	d	405	CLA	C3D-C4D-ND	4.93	118.01	109.99
24	C	512	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
24	C	514	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
24	c	514	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
24	B	616	CLA	C2D-C1D-ND	4.91	114.98	110.13
24	b	618	CLA	C2D-C1D-ND	4.91	114.98	110.13
24	B	605	CLA	CMD-C2D-C1D	4.91	133.37	124.73
24	b	607	CLA	CMD-C2D-C1D	4.91	133.37	124.73
38	X	101	RRX	C7-C8-C9	-4.90	118.98	126.23
38	x	101	RRX	C7-C8-C9	-4.90	118.98	126.23
24	B	607	CLA	C3B-C4B-NB	4.89	114.90	110.53
24	B	606	CLA	C4B-C3B-C2B	-4.89	101.22	107.30
24	b	608	CLA	C4B-C3B-C2B	-4.89	101.22	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	C3B-C4B-NB	4.89	114.89	110.53
24	b	607	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
24	B	605	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
24	C	504	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	c	504	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	A	408	CLA	O2D-CGD-CBD	4.87	119.74	111.23
24	a	408	CLA	O2D-CGD-CBD	4.87	119.74	111.23
24	C	514	CLA	CHD-C4C-C3C	-4.87	117.68	124.77
24	c	514	CLA	CHD-C4C-C3C	-4.87	117.68	124.77
24	B	616	CLA	O2D-CGD-CBD	4.87	119.74	111.23
24	b	618	CLA	O2D-CGD-CBD	4.86	119.73	111.23
24	B	604	CLA	C4A-NA-C1A	-4.85	104.47	106.68
24	B	609	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	D	401	CLA	CMD-C2D-C1D	4.83	133.24	124.73
24	d	401	CLA	CMD-C2D-C1D	4.83	133.24	124.73
24	C	510	CLA	C2C-C1C-NC	4.83	115.06	109.98
24	c	510	CLA	C2C-C1C-NC	4.83	115.06	109.98
24	C	505	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
24	c	505	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
24	b	611	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
24	B	603	CLA	CHD-C4C-C3C	-4.82	117.74	124.77
24	b	605	CLA	CHD-C4C-C3C	-4.82	117.75	124.77
24	B	606	CLA	C2C-C1C-NC	4.82	115.04	109.98
24	C	513	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
24	c	513	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
24	b	608	CLA	C2C-C1C-NC	4.81	115.04	109.98
38	X	101	RRX	C16-C17-C18	-4.80	120.55	127.28
38	x	101	RRX	C16-C17-C18	-4.80	120.55	127.28
24	B	607	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	b	609	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	A	408	CLA	C2C-C1C-NC	4.79	115.01	109.98
24	a	408	CLA	C2C-C1C-NC	4.79	115.01	109.98
24	a	408	CLA	CHD-C1D-ND	-4.78	118.07	124.80
27	F	101	SQD	O9-S-O7	-4.77	98.30	113.82
24	C	507	CLA	C3B-C4B-NB	4.77	114.79	110.53
24	c	507	CLA	C3B-C4B-NB	4.77	114.79	110.53
27	f	101	SQD	O9-S-O7	-4.77	98.30	113.82
24	b	606	CLA	C4A-NA-C1A	-4.77	104.50	106.68
24	C	505	CLA	C2C-C1C-NC	4.77	114.99	109.98
24	c	505	CLA	C2C-C1C-NC	4.77	114.99	109.98
24	b	612	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
24	B	616	CLA	C2C-C1C-NC	4.75	114.97	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	C2C-C1C-NC	4.75	114.97	109.98
24	B	610	CLA	C3D-C2D-C1D	-4.75	99.36	105.83
24	B	603	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
24	b	605	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
24	A	408	CLA	CHD-C1D-ND	-4.74	118.14	124.80
27	B	620	SQD	O7-S-C6	4.73	113.82	106.76
24	C	510	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
24	c	510	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
24	D	404	CLA	C2C-C1C-NC	4.73	114.95	109.98
24	d	404	CLA	C2C-C1C-NC	4.73	114.95	109.98
24	B	611	CLA	C3D-C4D-ND	4.72	117.67	109.99
24	b	613	CLA	C3D-C4D-ND	4.72	117.67	109.99
27	L	102	SQD	O7-S-C6	4.72	113.80	106.76
24	d	404	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
24	b	606	CLA	C1-C2-C3	-4.71	118.48	126.20
24	b	604	CLA	C2B-C1B-NB	4.70	115.20	110.33
24	C	504	CLA	C2C-C1C-NC	4.70	114.92	109.98
24	c	504	CLA	C2C-C1C-NC	4.70	114.92	109.98
24	D	404	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
24	B	604	CLA	C1-C2-C3	-4.69	118.51	126.20
24	C	503	CLA	CMD-C2D-C1D	4.69	132.99	124.73
24	c	503	CLA	CMD-C2D-C1D	4.69	132.99	124.73
24	C	508	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	c	508	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
24	B	602	CLA	CHD-C1D-ND	-4.69	118.21	124.80
24	b	604	CLA	CHD-C1D-ND	-4.69	118.21	124.80
24	B	616	CLA	C1D-CHD-C4C	-4.69	116.06	126.02
24	b	618	CLA	C1D-CHD-C4C	-4.69	116.06	126.02
24	C	506	CLA	C2B-C1B-NB	4.68	115.18	110.33
24	c	506	CLA	C2B-C1B-NB	4.68	115.18	110.33
24	C	506	CLA	C2C-C1C-NC	4.68	114.90	109.98
24	c	506	CLA	C2C-C1C-NC	4.68	114.90	109.98
24	B	614	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
24	d	404	CLA	CHD-C4C-C3C	-4.67	117.96	124.77
24	A	408	CLA	C1C-C2C-C3C	-4.67	102.07	106.98
24	a	408	CLA	C1C-C2C-C3C	-4.67	102.07	106.98
24	C	507	CLA	C2C-C1C-NC	4.66	114.88	109.98
24	c	507	CLA	C2C-C1C-NC	4.66	114.88	109.98
24	B	602	CLA	C2B-C1B-NB	4.66	115.16	110.33
24	b	616	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
24	D	404	CLA	CHD-C4C-C3C	-4.65	117.99	124.77
24	C	505	CLA	C3D-C2D-C1D	-4.65	99.48	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	B	615	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	b	617	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	C	502	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	D	404	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	b	608	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	B	616	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	b	618	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	A	408	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
24	a	408	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
24	d	404	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	B	615	CLA	C2B-C1B-NB	4.63	115.13	110.33
24	b	617	CLA	C2B-C1B-NB	4.63	115.13	110.33
24	B	606	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
24	d	404	CLA	C3D-C4D-ND	4.63	117.51	109.99
24	D	404	CLA	C3D-C4D-ND	4.62	117.50	109.99
24	a	405	CLA	C3C-C4C-NC	4.62	116.35	110.43
24	A	405	CLA	C3C-C4C-NC	4.62	116.35	110.43
24	C	505	CLA	C2B-C1B-NB	4.62	115.12	110.33
24	c	505	CLA	C2B-C1B-NB	4.62	115.12	110.33
35	e	103	HEM	CBD-CAD-C3D	-4.62	99.76	112.53
24	b	607	CLA	C2C-C1C-NC	4.61	114.83	109.98
24	D	404	CLA	CAA-C2A-C3A	-4.61	100.54	113.00
24	d	404	CLA	CAA-C2A-C3A	-4.61	100.54	113.00
24	A	406	CLA	C3C-C4C-NC	4.61	116.33	110.43
24	C	512	CLA	C3D-C4D-ND	4.61	117.48	109.99
24	c	512	CLA	C3D-C4D-ND	4.61	117.48	109.99
35	E	103	HEM	CBD-CAD-C3D	-4.60	99.80	112.53
24	c	502	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	B	607	CLA	CAC-C3C-C4C	4.60	130.77	124.79
24	b	609	CLA	CAC-C3C-C4C	4.60	130.77	124.79
24	A	408	CLA	C2B-C1B-NB	4.60	115.09	110.33
24	a	406	CLA	C3C-C4C-NC	4.60	116.32	110.43
24	a	408	CLA	C2B-C1B-NB	4.59	115.09	110.33
24	B	615	CLA	C2C-C1C-NC	4.59	114.80	109.98
24	b	617	CLA	C2C-C1C-NC	4.59	114.80	109.98
24	B	614	CLA	CHD-C1D-ND	-4.58	118.35	124.80
24	b	616	CLA	CHD-C1D-ND	-4.58	118.35	124.80
24	C	505	CLA	CHD-C4C-C3C	-4.58	118.09	124.77
24	c	505	CLA	CHD-C4C-C3C	-4.58	118.09	124.77
24	B	601	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	b	603	CLA	C3D-C2D-C1D	-4.58	99.58	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C2C-C1C-NC	4.58	114.79	109.98
24	C	504	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
24	c	504	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
38	X	101	RRX	C20-C21-C22	-4.57	120.87	127.28
38	x	101	RRX	C20-C21-C22	-4.57	120.87	127.28
24	C	513	CLA	C3C-C4C-NC	4.57	116.29	110.43
24	c	513	CLA	C3C-C4C-NC	4.57	116.29	110.43
24	b	604	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
24	C	512	CLA	C2C-C1C-NC	4.55	114.77	109.98
24	c	512	CLA	C2C-C1C-NC	4.55	114.77	109.98
24	D	401	CLA	C3D-C4D-ND	4.55	117.39	109.99
24	d	401	CLA	C3D-C4D-ND	4.55	117.39	109.99
24	B	603	CLA	C2D-C1D-ND	4.55	114.63	110.13
24	B	602	CLA	C3B-C2B-C1B	-4.54	101.82	107.17
32	J	102	LMT	C3'-C4'-C5'	-4.54	102.01	110.23
24	b	605	CLA	C2D-C1D-ND	4.53	114.61	110.13
24	B	611	CLA	C2C-C1C-NC	4.53	114.74	109.98
24	C	508	CLA	C1C-C2C-C3C	-4.53	102.22	106.98
24	c	508	CLA	C1C-C2C-C3C	-4.53	102.22	106.98
24	b	617	CLA	CHD-C1D-ND	-4.52	118.44	124.80
24	C	510	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
24	c	510	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
24	b	613	CLA	C2C-C1C-NC	4.51	114.72	109.98
32	j	102	LMT	C3'-C4'-C5'	-4.51	102.06	110.23
24	b	607	CLA	C2B-C1B-NB	4.50	115.00	110.33
24	B	615	CLA	CHD-C1D-ND	-4.50	118.47	124.80
24	a	408	CLA	C3D-C4D-ND	4.50	117.30	109.99
24	b	608	CLA	C3C-C4C-NC	4.50	116.19	110.43
24	A	408	CLA	C3D-C4D-ND	4.50	117.30	109.99
24	B	614	CLA	C2C-C1C-NC	4.49	114.70	109.98
24	b	616	CLA	C2C-C1C-NC	4.49	114.70	109.98
24	C	509	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
24	c	509	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
24	B	605	CLA	C2B-C1B-NB	4.49	114.98	110.33
24	C	509	CLA	C3C-C4C-NC	4.48	116.17	110.43
24	c	509	CLA	C3C-C4C-NC	4.48	116.17	110.43
24	C	507	CLA	O2D-CGD-CBD	4.48	119.06	111.23
24	c	507	CLA	O2D-CGD-CBD	4.48	119.06	111.23
25	D	402	PHO	CMB-C2B-C3B	4.48	133.63	124.68
25	d	402	PHO	CMB-C2B-C3B	4.48	133.63	124.68
24	B	606	CLA	C3C-C4C-NC	4.48	116.17	110.43
24	C	507	CLA	C4A-NA-C1A	-4.47	104.64	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C4A-NA-C1A	-4.47	104.64	106.68
24	b	604	CLA	C4A-NA-C1A	-4.47	104.64	106.68
24	C	504	CLA	C3D-C4D-ND	4.47	117.25	109.99
24	c	504	CLA	C3D-C4D-ND	4.47	117.25	109.99
24	b	614	CLA	CMD-C2D-C1D	4.46	132.59	124.73
24	b	605	CLA	CAC-C3C-C4C	4.45	130.59	124.79
24	A	406	CLA	C2C-C1C-NC	4.44	114.65	109.98
24	B	603	CLA	CAC-C3C-C4C	4.44	130.57	124.79
34	D	410	LHG	O4-P-O5	4.44	133.09	112.44
34	d	410	LHG	O4-P-O5	4.44	133.09	112.44
24	B	612	CLA	C2C-C1C-NC	4.44	114.64	109.98
24	b	614	CLA	C2C-C1C-NC	4.44	114.64	109.98
24	C	504	CLA	C3C-C4C-NC	4.43	116.10	110.43
24	c	504	CLA	C3C-C4C-NC	4.43	116.10	110.43
24	B	611	CLA	O2D-CGD-CBD	4.42	118.96	111.23
24	b	613	CLA	O2D-CGD-CBD	4.42	118.96	111.23
24	d	404	CLA	C3C-C4C-NC	4.42	116.09	110.43
24	B	612	CLA	CMD-C2D-C1D	4.42	132.50	124.73
24	a	406	CLA	C2C-C1C-NC	4.41	114.61	109.98
24	B	607	CLA	C3D-C4D-ND	4.41	117.15	109.99
24	b	609	CLA	C3D-C4D-ND	4.41	117.15	109.99
24	B	608	CLA	C1C-C2C-C3C	-4.40	102.35	106.98
24	C	506	CLA	C2D-C1D-ND	4.40	114.48	110.13
24	c	506	CLA	C2D-C1D-ND	4.40	114.48	110.13
24	D	404	CLA	C3C-C4C-NC	4.40	116.06	110.43
34	l	101	LHG	O4-P-O5	4.39	132.88	112.44
34	L	101	LHG	O4-P-O5	4.39	132.88	112.44
24	C	505	CLA	C3B-C4B-NB	4.39	114.45	110.53
24	c	505	CLA	C3B-C4B-NB	4.39	114.45	110.53
24	b	610	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
37	V	201	HEC	CBB-CAB-C3B	-4.39	118.67	127.43
37	v	201	HEC	CBB-CAB-C3B	-4.39	118.67	127.43
24	b	612	CLA	C2B-C1B-NB	4.38	114.87	110.33
24	b	611	CLA	C3C-C4C-NC	4.38	116.04	110.43
24	c	509	CLA	C3D-C4D-ND	4.38	117.10	109.99
24	B	613	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
24	c	502	CLA	CHD-C1D-ND	-4.37	118.66	124.80
24	b	603	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
24	B	609	CLA	CMB-C2B-C1B	4.36	132.06	125.42
24	c	507	CLA	C4A-NA-C1A	-4.36	104.69	106.68
24	C	509	CLA	C3D-C4D-ND	4.36	117.07	109.99
24	b	610	CLA	C1D-CHD-C4C	-4.36	116.76	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
24	b	614	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
24	b	615	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
24	B	609	CLA	C3C-C4C-NC	4.34	116.00	110.43
24	B	608	CLA	C1D-CHD-C4C	-4.34	116.79	126.02
24	A	406	CLA	O2D-CGD-CBD	4.34	118.82	111.23
24	a	406	CLA	O2D-CGD-CBD	4.34	118.82	111.23
27	A	410	SQD	O9-S-O7	-4.34	99.71	113.82
27	a	410	SQD	O9-S-O7	-4.34	99.71	113.82
24	B	614	CLA	C3B-C4B-NB	4.34	114.40	110.53
24	B	608	CLA	C2D-C1D-ND	4.33	114.42	110.13
24	b	610	CLA	C2D-C1D-ND	4.33	114.41	110.13
24	C	508	CLA	C2B-C1B-NB	4.33	114.82	110.33
24	c	508	CLA	C2B-C1B-NB	4.33	114.82	110.33
24	C	512	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
24	c	512	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
24	B	603	CLA	C4-C3-C5	4.33	122.74	115.23
24	b	611	CLA	CMB-C2B-C1B	4.33	132.01	125.42
24	C	502	CLA	CHD-C1D-ND	-4.33	118.72	124.80
24	B	616	CLA	C2B-C1B-NB	4.32	114.81	110.33
24	b	618	CLA	C2B-C1B-NB	4.32	114.81	110.33
24	b	612	CLA	C3B-C2B-C1B	-4.32	102.08	107.17
24	b	605	CLA	C4-C3-C5	4.32	122.72	115.23
24	B	601	CLA	C1C-C2C-C3C	-4.32	102.44	106.98
27	L	102	SQD	O8-S-C6	4.31	114.30	105.97
24	C	512	CLA	C1-C2-C3	-4.31	119.13	126.20
24	c	512	CLA	C1-C2-C3	-4.31	119.13	126.20
24	d	404	CLA	CAC-C3C-C4C	4.31	130.40	124.79
24	c	514	CLA	CAC-C3C-C4C	4.31	130.40	124.79
28	A	411	PL9	C7-C3-C4	4.31	120.46	116.91
24	b	610	CLA	O2D-CGD-CBD	4.30	118.75	111.23
24	b	616	CLA	C1C-C2C-C3C	-4.30	102.45	106.98
27	B	620	SQD	O8-S-C6	4.30	114.28	105.97
24	B	607	CLA	C3C-C4C-NC	4.30	115.94	110.43
24	b	609	CLA	C3C-C4C-NC	4.30	115.94	110.43
32	C	521	LMT	O1B-C4'-C3'	4.30	118.15	107.23
32	c	521	LMT	O1B-C4'-C3'	4.30	118.15	107.23
24	C	512	CLA	C4B-C3B-C2B	-4.30	101.96	107.30
24	c	512	CLA	C4B-C3B-C2B	-4.30	101.96	107.30
24	C	514	CLA	CAC-C3C-C4C	4.30	130.38	124.79
24	B	610	CLA	C3B-C2B-C1B	-4.29	102.11	107.17
24	C	508	CLA	C3C-C4C-NC	4.29	115.93	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	C3C-C4C-NC	4.29	115.93	110.43
24	D	404	CLA	CAC-C3C-C4C	4.29	130.37	124.79
24	C	513	CLA	C2C-C1C-NC	4.29	114.48	109.98
24	c	513	CLA	C2C-C1C-NC	4.29	114.48	109.98
24	b	616	CLA	C3B-C4B-NB	4.29	114.36	110.53
24	B	602	CLA	C3D-C4D-ND	4.28	116.95	109.99
24	b	604	CLA	C3D-C4D-ND	4.28	116.95	109.99
24	B	608	CLA	O2D-CGD-CBD	4.28	118.72	111.23
24	D	401	CLA	CHD-C4C-C3C	-4.28	118.53	124.77
24	d	401	CLA	CHD-C4C-C3C	-4.28	118.53	124.77
28	d	407	PL9	O1-C4-C3	-4.28	116.21	120.73
24	D	405	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
24	C	513	CLA	C4A-NA-C1A	-4.28	104.73	106.68
24	c	513	CLA	C4A-NA-C1A	-4.28	104.73	106.68
27	a	412	SQD	O7-S-C6	4.27	113.14	106.76
24	B	614	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
28	D	407	PL9	O1-C4-C3	-4.27	116.22	120.73
27	F	101	SQD	O47-C7-C8	4.27	120.72	111.48
27	f	101	SQD	O47-C7-C8	4.27	120.72	111.48
24	B	609	CLA	C3D-C4D-ND	4.27	116.93	109.99
24	C	510	CLA	C3B-C4B-NB	4.27	114.34	110.53
34	E	101	LHG	O4-P-O5	4.26	132.28	112.44
34	e	101	LHG	O4-P-O5	4.26	132.28	112.44
24	c	510	CLA	C3B-C4B-NB	4.26	114.33	110.53
24	d	405	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
27	F	101	SQD	O9-S-C6	4.25	113.10	106.76
24	D	405	CLA	C2C-C1C-NC	4.25	114.44	109.98
24	d	405	CLA	C2C-C1C-NC	4.25	114.44	109.98
24	D	401	CLA	C2B-C1B-NB	4.24	114.73	110.33
24	d	401	CLA	C2B-C1B-NB	4.24	114.73	110.33
28	a	411	PL9	C7-C3-C4	4.24	120.41	116.91
24	D	405	CLA	C2B-C1B-NB	4.24	114.73	110.33
24	d	405	CLA	C2B-C1B-NB	4.24	114.73	110.33
24	b	611	CLA	C3D-C4D-ND	4.24	116.87	109.99
27	f	101	SQD	O9-S-C6	4.23	113.08	106.76
24	B	612	CLA	C4C-C3C-C2C	-4.23	100.73	106.89
24	b	614	CLA	C4C-C3C-C2C	-4.23	100.73	106.89
27	A	412	SQD	O7-S-C6	4.23	113.07	106.76
24	C	503	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
24	c	503	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
24	B	603	CLA	C3D-C4D-ND	4.22	116.84	109.99
24	B	606	CLA	C3D-C4D-ND	4.22	116.84	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C1D-CHD-C4C	-4.21	117.06	126.02
24	a	406	CLA	C1D-CHD-C4C	-4.21	117.06	126.02
24	b	605	CLA	C3D-C4D-ND	4.21	116.84	109.99
24	c	511	CLA	C3B-C4B-NB	4.21	114.29	110.53
24	B	610	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	b	608	CLA	C3D-C4D-ND	4.21	116.83	109.99
24	D	401	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
24	d	401	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
24	C	504	CLA	C1D-CHD-C4C	-4.20	117.09	126.02
24	c	504	CLA	C1D-CHD-C4C	-4.20	117.09	126.02
24	C	511	CLA	C3B-C4B-NB	4.20	114.28	110.53
24	B	603	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
24	b	605	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
24	C	503	CLA	C3D-C4D-ND	4.20	116.81	109.99
24	c	503	CLA	C3D-C4D-ND	4.20	116.81	109.99
24	C	511	CLA	C3C-C4C-NC	4.19	115.80	110.43
24	c	511	CLA	C3C-C4C-NC	4.19	115.80	110.43
24	D	405	CLA	C4B-C3B-C2B	-4.19	102.09	107.30
24	d	405	CLA	C4B-C3B-C2B	-4.19	102.09	107.30
24	B	606	CLA	C4A-NA-C1A	-4.18	104.77	106.68
24	b	608	CLA	C4A-NA-C1A	-4.18	104.77	106.68
24	B	602	CLA	C1-O2A-CGA	4.18	126.78	116.65
24	C	513	CLA	C2B-C1B-NB	4.18	114.66	110.33
24	c	513	CLA	C2B-C1B-NB	4.18	114.66	110.33
24	C	509	CLA	O2D-CGD-O1D	-4.17	115.72	123.85
24	c	509	CLA	O2D-CGD-O1D	-4.17	115.72	123.85
24	D	405	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
24	d	405	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
24	c	514	CLA	O2D-CGD-O1D	-4.17	115.73	123.85
24	C	514	CLA	O2D-CGD-O1D	-4.17	115.73	123.85
24	C	511	CLA	C3B-C2B-C1B	-4.17	102.26	107.17
24	b	604	CLA	C1-O2A-CGA	4.16	126.73	116.65
24	B	615	CLA	C3C-C4C-NC	4.16	115.76	110.43
24	b	617	CLA	C3C-C4C-NC	4.16	115.76	110.43
24	C	504	CLA	C2B-C1B-NB	4.15	114.63	110.33
24	c	504	CLA	C2B-C1B-NB	4.15	114.63	110.33
24	B	607	CLA	C4B-C3B-C2B	-4.15	102.14	107.30
24	b	609	CLA	C4B-C3B-C2B	-4.15	102.14	107.30
24	C	508	CLA	C3D-C4D-ND	4.15	116.72	109.99
24	c	508	CLA	C3D-C4D-ND	4.15	116.72	109.99
24	c	511	CLA	C3B-C2B-C1B	-4.14	102.28	107.17
24	c	507	CLA	CBC-CAC-C3C	-4.14	101.20	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	CBC-CAC-C3C	-4.14	101.20	112.42
24	c	514	CLA	CHD-C1D-ND	-4.14	118.98	124.80
24	C	514	CLA	CHD-C1D-ND	-4.13	118.99	124.80
24	B	615	CLA	C4A-NA-C1A	-4.13	104.80	106.68
24	b	617	CLA	C4A-NA-C1A	-4.13	104.80	106.68
24	D	405	CLA	CHD-C1D-ND	-4.13	119.00	124.80
24	d	405	CLA	CHD-C1D-ND	-4.13	119.00	124.80
24	A	406	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
24	a	406	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
24	B	615	CLA	C3B-C4B-NB	4.12	114.21	110.53
24	b	617	CLA	C3B-C4B-NB	4.12	114.21	110.53
24	C	512	CLA	O2D-CGD-CBD	4.12	118.44	111.23
24	c	512	CLA	O2D-CGD-CBD	4.12	118.43	111.23
24	B	613	CLA	CHD-C1D-ND	-4.12	119.00	124.80
24	b	615	CLA	CHD-C1D-ND	-4.12	119.00	124.80
24	C	512	CLA	C3C-C4C-NC	4.12	115.70	110.43
24	c	512	CLA	C3C-C4C-NC	4.11	115.70	110.43
24	C	505	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
24	c	505	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
24	b	605	CLA	O2A-CGA-CBA	4.11	124.37	111.83
24	A	405	CLA	C3B-C2B-C1B	-4.11	102.32	107.17
24	a	405	CLA	C3B-C2B-C1B	-4.11	102.32	107.17
24	b	611	CLA	C4B-C3B-C2B	-4.11	102.19	107.30
24	B	605	CLA	C3D-C4D-ND	4.11	116.66	109.99
24	b	607	CLA	C3D-C4D-ND	4.11	116.66	109.99
24	C	504	CLA	CAC-C3C-C4C	4.10	130.13	124.79
24	c	504	CLA	CAC-C3C-C4C	4.10	130.13	124.79
24	C	510	CLA	C2B-C1B-NB	4.10	114.58	110.33
24	c	510	CLA	C2B-C1B-NB	4.10	114.58	110.33
24	B	603	CLA	O2A-CGA-CBA	4.09	124.32	111.83
24	C	503	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
24	c	503	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
27	B	620	SQD	O47-C7-C8	4.07	120.29	111.48
27	L	102	SQD	O47-C7-C8	4.07	120.29	111.48
24	B	604	CLA	C4B-C3B-C2B	-4.07	102.25	107.30
24	b	606	CLA	C4B-C3B-C2B	-4.07	102.25	107.30
24	B	607	CLA	CHD-C1D-ND	-4.06	119.09	124.80
24	b	609	CLA	CHD-C1D-ND	-4.06	119.09	124.80
24	B	615	CLA	C3D-C4D-ND	4.06	116.58	109.99
24	b	617	CLA	C3D-C4D-ND	4.06	116.58	109.99
24	C	510	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
24	c	510	CLA	C1C-C2C-C3C	-4.04	102.73	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	C4B-C3B-C2B	-4.04	102.27	107.30
24	b	612	CLA	C3D-C4D-ND	4.04	116.56	109.99
24	C	509	CLA	CMD-C2D-C1D	4.04	131.84	124.73
24	c	509	CLA	CMD-C2D-C1D	4.04	131.84	124.73
24	C	513	CLA	C3D-C4D-ND	4.03	116.55	109.99
24	c	513	CLA	C3D-C4D-ND	4.03	116.55	109.99
24	b	607	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
24	B	610	CLA	C3D-C4D-ND	4.03	116.53	109.99
24	b	611	CLA	C3B-C4B-NB	4.03	114.12	110.53
24	c	503	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
24	B	605	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
24	B	611	CLA	C4B-C3B-C2B	-4.02	102.31	107.30
24	C	506	CLA	C3D-C4D-ND	4.02	116.52	109.99
24	c	506	CLA	C3D-C4D-ND	4.02	116.52	109.99
24	b	610	CLA	C3D-C4D-ND	4.02	116.52	109.99
24	D	405	CLA	C3C-C4C-NC	4.01	115.56	110.43
24	B	608	CLA	CAC-C3C-C4C	4.01	130.00	124.79
24	b	610	CLA	CAC-C3C-C4C	4.00	130.00	124.79
24	C	510	CLA	CHD-C1D-ND	-4.00	119.17	124.80
24	c	510	CLA	CHD-C1D-ND	-4.00	119.17	124.80
24	B	609	CLA	C4B-C3B-C2B	-3.99	102.34	107.30
24	C	509	CLA	C2B-C1B-NB	3.99	114.47	110.33
24	c	509	CLA	C2B-C1B-NB	3.99	114.47	110.33
24	B	608	CLA	C3D-C4D-ND	3.99	116.47	109.99
24	d	405	CLA	C3C-C4C-NC	3.99	115.54	110.43
24	A	405	CLA	C3D-C4D-ND	3.99	116.47	109.99
24	a	405	CLA	C3D-C4D-ND	3.99	116.47	109.99
24	C	503	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
24	B	604	CLA	C2D-C1D-ND	3.98	114.06	110.13
24	b	606	CLA	C2D-C1D-ND	3.98	114.06	110.13
24	b	614	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
24	C	502	CLA	C3D-C4D-ND	3.97	116.44	109.99
24	c	502	CLA	C3D-C4D-ND	3.97	116.43	109.99
24	B	612	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
24	d	404	CLA	CHD-C1D-ND	-3.95	119.25	124.80
24	b	611	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
24	a	405	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
24	A	406	CLA	C2D-C1D-ND	3.94	114.03	110.13
24	a	406	CLA	C2D-C1D-ND	3.94	114.03	110.13
24	B	601	CLA	C3D-C4D-ND	3.94	116.39	109.99
24	b	603	CLA	C3D-C4D-ND	3.94	116.39	109.99
24	A	405	CLA	C1C-C2C-C3C	-3.94	102.83	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	CLA	C3D-C4D-ND	3.94	116.39	109.99
24	c	514	CLA	C3D-C4D-ND	3.94	116.39	109.99
24	C	508	CLA	C3B-C4B-NB	3.94	114.05	110.53
24	c	508	CLA	C3B-C4B-NB	3.94	114.05	110.53
24	B	607	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
24	b	609	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
24	B	609	CLA	C3B-C4B-NB	3.94	114.04	110.53
24	B	611	CLA	CAC-C3C-C4C	3.93	129.91	124.79
24	b	613	CLA	CAC-C3C-C4C	3.93	129.91	124.79
24	D	404	CLA	CHD-C1D-ND	-3.93	119.27	124.80
24	C	513	CLA	CHD-C1D-ND	-3.93	119.27	124.80
24	c	513	CLA	CHD-C1D-ND	-3.93	119.27	124.80
24	C	509	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
24	c	509	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
24	C	506	CLA	C3C-C4C-NC	3.93	115.46	110.43
24	c	506	CLA	C3C-C4C-NC	3.93	115.46	110.43
24	b	612	CLA	C3C-C4C-NC	3.92	115.46	110.43
27	a	412	SQD	O9-S-O7	-3.92	101.06	113.82
24	C	505	CLA	C3D-C4D-ND	3.92	116.36	109.99
24	c	505	CLA	C3D-C4D-ND	3.92	116.36	109.99
24	b	608	CLA	CHD-C1D-ND	-3.92	119.29	124.80
27	A	412	SQD	O9-S-O7	-3.91	101.09	113.82
24	B	604	CLA	C1D-CHD-C4C	-3.91	117.72	126.02
24	b	606	CLA	C1D-CHD-C4C	-3.91	117.72	126.02
27	f	101	SQD	C4-C3-C2	3.90	117.68	110.83
24	B	606	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	C	503	CLA	C1-C2-C3	-3.90	119.81	126.20
24	c	503	CLA	C1-C2-C3	-3.90	119.81	126.20
24	c	503	CLA	C3C-C4C-NC	3.90	115.42	110.43
27	F	101	SQD	C4-C3-C2	3.89	117.66	110.83
24	C	503	CLA	C3B-C4B-NB	3.89	114.00	110.53
24	b	614	CLA	C3B-C4B-NB	3.89	114.00	110.53
24	c	503	CLA	C3B-C4B-NB	3.89	114.00	110.53
24	C	504	CLA	O2D-CGD-CBD	3.89	118.02	111.23
24	c	504	CLA	O2D-CGD-CBD	3.89	118.02	111.23
24	C	507	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
24	c	507	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
24	B	605	CLA	C4-C3-C5	3.88	121.96	115.23
24	b	614	CLA	C2B-C1B-NB	3.88	114.35	110.33
24	b	614	CLA	C3D-C4D-ND	3.87	116.28	109.99
24	B	603	CLA	C3C-C4C-NC	3.87	115.39	110.43
24	b	605	CLA	C3C-C4C-NC	3.87	115.39	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	406	BCR	C24-C23-C22	-3.87	120.51	126.23
24	B	609	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
26	d	406	BCR	C24-C23-C22	-3.87	120.52	126.23
24	b	607	CLA	C4-C3-C5	3.87	121.94	115.23
24	C	503	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
24	c	503	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
28	A	411	PL9	C7-C3-C2	-3.86	118.84	123.39
24	B	612	CLA	C2B-C1B-NB	3.86	114.32	110.33
24	A	405	CLA	C2D-C1D-ND	3.85	113.94	110.13
24	a	405	CLA	C2D-C1D-ND	3.85	113.94	110.13
24	B	608	CLA	C3B-C2B-C1B	-3.85	102.63	107.17
24	B	612	CLA	C3B-C4B-NB	3.85	113.97	110.53
24	c	502	CLA	C3B-C4B-NB	3.85	113.97	110.53
24	B	606	CLA	C2B-C1B-NB	3.85	114.32	110.33
24	b	608	CLA	C2B-C1B-NB	3.85	114.32	110.33
24	B	612	CLA	C3D-C4D-ND	3.85	116.24	109.99
24	C	503	CLA	C3C-C4C-NC	3.85	115.36	110.43
24	b	610	CLA	C3B-C2B-C1B	-3.85	102.63	107.17
24	C	508	CLA	CHD-C1D-ND	-3.85	119.39	124.80
24	c	508	CLA	CHD-C1D-ND	-3.85	119.39	124.80
24	B	616	CLA	C4A-NA-C1A	-3.84	104.92	106.68
24	b	618	CLA	C4A-NA-C1A	-3.84	104.92	106.68
24	b	611	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
34	D	409	LHG	O4-P-O5	3.84	130.30	112.44
34	d	409	LHG	O4-P-O5	3.84	130.30	112.44
24	B	609	CLA	C1D-CHD-C4C	-3.83	117.87	126.02
24	B	611	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
24	d	404	CLA	CMC-C2C-C1C	3.83	131.02	125.03
24	B	613	CLA	C3B-C4B-NB	3.82	113.94	110.53
24	b	615	CLA	C3B-C4B-NB	3.82	113.94	110.53
24	D	404	CLA	CMC-C2C-C1C	3.82	131.01	125.03
24	A	406	CLA	C4B-C3B-C2B	-3.82	102.56	107.30
24	A	408	CLA	C4-C3-C5	3.81	121.85	115.23
24	a	408	CLA	C4-C3-C5	3.81	121.85	115.23
28	a	411	PL9	C7-C3-C2	-3.81	118.89	123.39
24	b	613	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
24	C	510	CLA	C3D-C4D-ND	3.81	116.18	109.99
24	c	510	CLA	C3D-C4D-ND	3.81	116.18	109.99
24	B	615	CLA	C4C-C3C-C2C	-3.81	101.34	106.89
24	b	617	CLA	C4C-C3C-C2C	-3.81	101.34	106.89
24	C	502	CLA	C3B-C4B-NB	3.81	113.93	110.53
24	a	406	CLA	C4B-C3B-C2B	-3.81	102.57	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
24	C	510	CLA	C3C-C4C-NC	3.80	115.30	110.43
24	B	603	CLA	CBA-CAA-C2A	3.80	125.11	113.79
24	b	605	CLA	CBA-CAA-C2A	3.80	125.11	113.79
34	D	408	LHG	O4-P-O5	3.80	130.11	112.44
34	d	408	LHG	O4-P-O5	3.80	130.11	112.44
24	C	507	CLA	C1D-CHD-C4C	-3.79	117.95	126.02
24	d	401	CLA	CMA-C3A-C2A	-3.79	99.31	113.98
24	D	401	CLA	CMA-C3A-C2A	-3.79	99.31	113.98
38	x	101	RRX	C38-C26-C25	-3.79	120.34	124.48
24	B	604	CLA	C3C-C4C-NC	3.79	115.29	110.43
24	b	606	CLA	C3C-C4C-NC	3.79	115.29	110.43
24	d	404	CLA	C4C-C3C-C2C	-3.79	101.38	106.89
24	B	610	CLA	C3C-C4C-NC	3.79	115.28	110.43
24	B	610	CLA	CAA-C2A-C3A	-3.79	102.77	113.00
24	c	510	CLA	C3C-C4C-NC	3.79	115.28	110.43
38	X	101	RRX	C38-C26-C25	-3.78	120.36	124.48
24	A	408	CLA	CAA-C2A-C3A	-3.78	102.78	113.00
24	D	404	CLA	C4C-C3C-C2C	-3.78	101.39	106.89
38	X	101	RRX	C11-C10-C9	-3.78	121.98	127.28
38	x	101	RRX	C11-C10-C9	-3.78	121.98	127.28
24	A	405	CLA	C3B-C4B-NB	3.78	113.90	110.53
24	a	405	CLA	C3B-C4B-NB	3.78	113.90	110.53
24	B	616	CLA	C3B-C4B-NB	3.78	113.90	110.53
24	b	618	CLA	C3B-C4B-NB	3.78	113.90	110.53
31	C	517	DGD	O3G-C3G-C2G	-3.77	101.64	110.82
31	c	517	DGD	O3G-C3G-C2G	-3.77	101.65	110.82
24	a	408	CLA	CAA-C2A-C3A	-3.77	102.81	113.00
24	B	607	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
24	b	609	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
24	C	509	CLA	C4C-C3C-C2C	-3.76	101.42	106.89
24	c	509	CLA	C4C-C3C-C2C	-3.76	101.42	106.89
38	X	101	RRX	C33-C5-C6	-3.76	120.38	124.48
38	x	101	RRX	C33-C5-C6	-3.76	120.38	124.48
24	b	612	CLA	CAA-C2A-C3A	-3.74	102.88	113.00
24	B	613	CLA	C2B-C1B-NB	3.74	114.21	110.33
24	B	601	CLA	C3C-C4C-NC	3.73	115.21	110.43
24	b	603	CLA	C3C-C4C-NC	3.73	115.21	110.43
24	B	616	CLA	C3D-C4D-ND	3.73	116.05	109.99
24	b	618	CLA	C3D-C4D-ND	3.73	116.05	109.99
24	b	610	CLA	CMC-C2C-C1C	3.73	130.86	125.03
27	A	410	SQD	O8-S-C6	3.73	113.17	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	CMC-C2C-C1C	3.73	130.86	125.03
24	c	502	CLA	CMC-C2C-C1C	3.73	130.86	125.03
24	A	406	CLA	C4C-C3C-C2C	-3.72	101.47	106.89
24	C	511	CLA	C3D-C4D-ND	3.72	116.04	109.99
24	c	511	CLA	C3D-C4D-ND	3.72	116.04	109.99
24	B	608	CLA	CMC-C2C-C1C	3.72	130.84	125.03
24	B	613	CLA	C3D-C4D-ND	3.72	116.03	109.99
24	b	615	CLA	C3D-C4D-ND	3.72	116.03	109.99
24	B	605	CLA	C3C-C4C-NC	3.71	115.19	110.43
24	b	607	CLA	C3C-C4C-NC	3.71	115.19	110.43
27	a	410	SQD	O8-S-C6	3.71	113.13	105.97
24	b	616	CLA	CAC-C3C-C4C	3.71	129.61	124.79
27	a	412	SQD	O47-C7-C8	3.70	119.49	111.48
24	b	610	CLA	C4A-NA-C1A	-3.70	104.99	106.68
24	C	505	CLA	CHD-C1D-ND	-3.70	119.60	124.80
24	c	505	CLA	CHD-C1D-ND	-3.70	119.60	124.80
24	C	504	CLA	C4C-C3C-C2C	-3.70	101.51	106.89
24	c	504	CLA	C4C-C3C-C2C	-3.70	101.51	106.89
24	b	608	CLA	C4C-C3C-C2C	-3.70	101.51	106.89
27	A	412	SQD	O47-C7-C8	3.69	119.47	111.48
24	B	606	CLA	C3B-C2B-C1B	-3.69	102.82	107.17
24	b	608	CLA	C3B-C2B-C1B	-3.69	102.82	107.17
24	B	603	CLA	CAA-C2A-C3A	-3.69	103.03	113.00
24	b	605	CLA	CAA-C2A-C3A	-3.69	103.03	113.00
24	a	406	CLA	C4C-C3C-C2C	-3.69	101.52	106.89
24	B	608	CLA	C4A-NA-C1A	-3.69	105.00	106.68
24	B	610	CLA	O2D-CGD-CBD	3.69	117.68	111.23
24	b	615	CLA	C2B-C1B-NB	3.69	114.15	110.33
24	B	610	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
26	C	522	BCR	C24-C23-C22	-3.68	120.79	126.23
26	c	522	BCR	C24-C23-C22	-3.68	120.79	126.23
24	b	605	CLA	O2A-CGA-O1A	-3.68	114.42	123.63
24	b	612	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
25	D	402	PHO	C2B-C1B-NB	-3.67	106.78	109.43
25	d	402	PHO	C2B-C1B-NB	-3.67	106.78	109.43
24	B	603	CLA	O2A-CGA-O1A	-3.67	114.44	123.63
24	B	603	CLA	C3D-C2D-C1D	-3.67	100.82	105.83
26	c	515	BCR	C24-C23-C22	-3.67	120.81	126.23
24	B	614	CLA	CAC-C3C-C4C	3.67	129.56	124.79
24	B	611	CLA	C2B-C1B-NB	3.67	114.13	110.33
24	B	603	CLA	C2B-C1B-NB	3.66	114.13	110.33
24	b	605	CLA	C2B-C1B-NB	3.66	114.13	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
24	B	610	CLA	O2A-CGA-CBA	3.66	122.99	111.83
24	b	605	CLA	C3D-C2D-C1D	-3.66	100.84	105.83
24	B	606	CLA	C4C-C3C-C2C	-3.66	101.57	106.89
26	D	406	BCR	C7-C8-C9	-3.66	120.83	126.23
26	d	406	BCR	C7-C8-C9	-3.66	120.83	126.23
24	C	514	CLA	C1D-CHD-C4C	-3.66	118.25	126.02
24	b	612	CLA	O2A-CGA-CBA	3.65	122.98	111.83
24	B	605	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
24	b	607	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
24	c	514	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
24	b	606	CLA	O2D-CGD-O1D	-3.65	116.75	123.85
24	C	509	CLA	CAC-C3C-C4C	3.65	129.53	124.79
24	c	509	CLA	CAC-C3C-C4C	3.65	129.53	124.79
24	B	608	CLA	CMD-C2D-C1D	3.64	131.15	124.73
24	B	612	CLA	C4B-C3B-C2B	-3.64	102.77	107.30
24	b	614	CLA	C4B-C3B-C2B	-3.64	102.77	107.30
24	D	401	CLA	C4B-C3B-C2B	-3.64	102.78	107.30
24	d	401	CLA	C4B-C3B-C2B	-3.64	102.78	107.30
27	B	620	SQD	O9-S-O7	-3.64	101.99	113.82
27	L	102	SQD	O9-S-O7	-3.64	101.99	113.82
32	c	521	LMT	C3'-C4'-C5'	-3.64	102.87	110.93
24	B	607	CLA	C2B-C1B-NB	3.63	114.09	110.33
24	C	503	CLA	C2B-C1B-NB	3.63	114.09	110.33
24	c	503	CLA	C2B-C1B-NB	3.63	114.09	110.33
26	C	515	BCR	C24-C23-C22	-3.63	120.86	126.23
27	B	620	SQD	C4-C3-C2	3.63	117.20	110.83
24	b	609	CLA	C2B-C1B-NB	3.63	114.09	110.33
24	B	608	CLA	C1-C2-C3	-3.63	120.25	126.20
24	b	610	CLA	C1-C2-C3	-3.63	120.25	126.20
24	b	604	CLA	CAA-C2A-C3A	-3.63	103.20	113.00
24	B	602	CLA	CAA-C2A-C3A	-3.62	103.20	113.00
24	A	408	CLA	C3B-C4B-NB	3.62	113.77	110.53
27	L	102	SQD	C4-C3-C2	3.62	117.19	110.83
32	C	521	LMT	C3'-C4'-C5'	-3.62	102.90	110.93
31	C	517	DGD	C6D-O5D-C1E	3.62	121.56	113.80
24	A	405	CLA	C2B-C1B-NB	3.62	114.08	110.33
24	a	405	CLA	C2B-C1B-NB	3.62	114.08	110.33
24	B	614	CLA	CMC-C2C-C1C	3.62	130.69	125.03
24	b	616	CLA	CMC-C2C-C1C	3.62	130.69	125.03
31	c	517	DGD	C6D-O5D-C1E	3.62	121.55	113.80
24	a	408	CLA	C3B-C4B-NB	3.62	113.76	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	V	201	HEC	C2A-C1A-NA	-3.61	106.83	110.32
24	b	611	CLA	CBC-CAC-C3C	-3.61	102.63	112.42
24	b	610	CLA	CMD-C2D-C1D	3.61	131.09	124.73
24	b	606	CLA	C1-O2A-CGA	3.61	125.39	116.65
24	B	604	CLA	C1-O2A-CGA	3.61	125.39	116.65
24	B	609	CLA	CHD-C1D-ND	-3.61	119.73	124.80
27	f	101	SQD	O7-S-C6	3.61	112.14	106.76
24	C	511	CLA	CHD-C1D-ND	-3.60	119.73	124.80
24	c	511	CLA	CHD-C1D-ND	-3.60	119.73	124.80
24	C	507	CLA	CHD-C1D-ND	-3.60	119.73	124.80
24	C	513	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
24	c	513	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
24	c	507	CLA	CHD-C1D-ND	-3.60	119.74	124.80
24	B	604	CLA	C3B-C4B-NB	3.60	113.74	110.53
24	b	606	CLA	C3B-C4B-NB	3.60	113.74	110.53
24	B	609	CLA	CBC-CAC-C3C	-3.60	102.67	112.42
24	B	616	CLA	CHD-C1D-ND	-3.60	119.74	124.80
24	b	618	CLA	CHD-C1D-ND	-3.60	119.74	124.80
37	v	201	HEC	C2A-C1A-NA	-3.60	106.85	110.32
24	C	512	CLA	C4C-C3C-C2C	-3.59	101.66	106.89
24	B	603	CLA	C4A-NA-C1A	-3.59	105.04	106.68
24	b	605	CLA	C4A-NA-C1A	-3.59	105.04	106.68
24	B	615	CLA	O2D-CGD-CBD	3.59	117.50	111.23
24	b	617	CLA	O2D-CGD-CBD	3.59	117.50	111.23
24	B	601	CLA	CHD-C1D-ND	-3.59	119.75	124.80
24	b	603	CLA	CHD-C1D-ND	-3.59	119.75	124.80
24	C	503	CLA	C1D-CHD-C4C	-3.59	118.40	126.02
24	C	512	CLA	CHD-C1D-ND	-3.59	119.76	124.80
24	c	512	CLA	CHD-C1D-ND	-3.59	119.76	124.80
24	c	512	CLA	C4C-C3C-C2C	-3.58	101.67	106.89
24	B	613	CLA	C1-C2-C3	-3.58	120.33	126.20
24	b	614	CLA	C2A-C1A-CHA	-3.58	117.65	123.87
24	A	408	CLA	CBC-CAC-C3C	-3.58	102.72	112.42
24	a	408	CLA	CBC-CAC-C3C	-3.58	102.72	112.42
24	C	507	CLA	CHC-C1C-C2C	-3.58	116.78	126.95
24	c	507	CLA	CHC-C1C-C2C	-3.58	116.78	126.95
24	b	611	CLA	CHD-C1D-ND	-3.58	119.77	124.80
27	F	101	SQD	O7-S-C6	3.57	112.09	106.76
24	c	503	CLA	C1D-CHD-C4C	-3.57	118.43	126.02
24	C	506	CLA	C1D-CHD-C4C	-3.57	118.43	126.02
24	c	506	CLA	C1D-CHD-C4C	-3.57	118.43	126.02
24	b	615	CLA	C1-C2-C3	-3.57	120.35	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	C2B-C1B-NB	3.57	114.03	110.33
24	C	513	CLA	CMB-C2B-C1B	3.57	130.85	125.42
24	c	513	CLA	CMB-C2B-C1B	3.57	130.85	125.42
24	B	607	CLA	C4C-C3C-C2C	-3.56	101.71	106.89
24	b	609	CLA	C4C-C3C-C2C	-3.56	101.71	106.89
24	B	604	CLA	CMC-C2C-C1C	3.55	130.59	125.03
24	b	606	CLA	CMC-C2C-C1C	3.55	130.59	125.03
24	B	612	CLA	C2A-C1A-CHA	-3.55	117.70	123.87
24	b	606	CLA	C3D-C4D-ND	3.55	115.76	109.99
24	b	612	CLA	O2D-CGD-CBD	3.55	117.44	111.23
24	C	506	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
24	c	506	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
24	A	405	CLA	C3D-C2D-C1D	-3.55	100.99	105.83
24	a	405	CLA	C3D-C2D-C1D	-3.55	100.99	105.83
24	A	406	CLA	C3D-C4D-ND	3.54	115.74	109.99
24	a	406	CLA	C3D-C4D-ND	3.54	115.74	109.99
24	B	604	CLA	C3D-C4D-ND	3.54	115.73	109.99
24	C	513	CLA	CMD-C2D-C1D	3.53	130.94	124.73
24	c	513	CLA	CMD-C2D-C1D	3.53	130.94	124.73
24	B	611	CLA	CHD-C1D-ND	-3.52	119.84	124.80
24	b	613	CLA	CHD-C1D-ND	-3.52	119.84	124.80
24	A	405	CLA	C4C-C3C-C2C	-3.52	101.77	106.89
24	a	405	CLA	C4C-C3C-C2C	-3.52	101.77	106.89
24	C	511	CLA	C3D-C2D-C1D	-3.52	101.03	105.83
24	c	511	CLA	C3D-C2D-C1D	-3.52	101.03	105.83
27	A	410	SQD	O9-S-C6	3.51	112.00	106.76
27	a	410	SQD	O9-S-C6	3.51	112.00	106.76
24	b	608	CLA	C1D-CHD-C4C	-3.51	118.56	126.02
24	b	610	CLA	CMA-C3A-C2A	-3.50	100.43	113.98
24	B	608	CLA	CMA-C3A-C2A	-3.50	100.43	113.98
24	B	616	CLA	CHD-C4C-NC	3.50	129.66	124.23
24	b	618	CLA	CHD-C4C-NC	3.50	129.66	124.23
24	C	511	CLA	C2D-C1D-ND	3.50	113.59	110.13
24	c	511	CLA	C2D-C1D-ND	3.50	113.59	110.13
24	B	613	CLA	C3C-C4C-NC	3.50	114.91	110.43
24	b	615	CLA	C3C-C4C-NC	3.50	114.91	110.43
24	b	612	CLA	CHC-C1C-C2C	-3.49	117.02	126.95
24	B	606	CLA	C1D-CHD-C4C	-3.49	118.60	126.02
24	C	503	CLA	C4B-C3B-C2B	-3.49	102.96	107.30
24	b	612	CLA	C4B-C3B-C2B	-3.49	102.96	107.30
24	c	503	CLA	C4B-C3B-C2B	-3.49	102.96	107.30
24	c	503	CLA	CHC-C1C-C2C	-3.49	117.03	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	C3B-C4B-NB	3.49	113.64	110.53
24	C	507	CLA	CAA-C2A-C3A	-3.48	103.58	113.00
24	c	510	CLA	CAC-C3C-C4C	3.48	129.32	124.79
24	c	514	CLA	C2C-C1C-NC	3.48	113.64	109.98
24	B	616	CLA	CAC-C3C-C4C	3.48	129.32	124.79
24	b	618	CLA	CAC-C3C-C4C	3.48	129.32	124.79
38	X	101	RRX	C10-C11-C12	-3.48	113.11	123.20
38	x	101	RRX	C10-C11-C12	-3.48	113.11	123.20
24	D	401	CLA	C3B-C4B-NB	3.48	113.64	110.53
24	d	401	CLA	C3B-C4B-NB	3.48	113.64	110.53
24	C	510	CLA	CAC-C3C-C4C	3.48	129.32	124.79
24	c	507	CLA	CAA-C2A-C3A	-3.48	103.60	113.00
24	b	608	CLA	CAA-C2A-C3A	-3.48	103.60	113.00
24	B	608	CLA	C2B-C1B-NB	3.48	113.93	110.33
24	B	608	CLA	C4B-C3B-C2B	-3.48	102.98	107.30
24	C	503	CLA	CHC-C1C-C2C	-3.47	117.08	126.95
24	B	602	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
24	b	604	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
24	B	602	CLA	C2C-C1C-NC	3.47	113.63	109.98
24	b	604	CLA	C2C-C1C-NC	3.47	113.63	109.98
24	B	605	CLA	CHD-C1D-ND	-3.47	119.92	124.80
24	b	607	CLA	CHD-C1D-ND	-3.47	119.92	124.80
24	B	611	CLA	C3B-C2B-C1B	-3.47	103.08	107.17
24	B	602	CLA	C3C-C4C-NC	3.47	114.87	110.43
24	b	604	CLA	C3C-C4C-NC	3.47	114.87	110.43
24	B	606	CLA	CAA-C2A-C3A	-3.47	103.63	113.00
24	C	506	CLA	C4A-NA-C1A	-3.47	105.10	106.68
24	c	506	CLA	C4A-NA-C1A	-3.47	105.10	106.68
24	D	405	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
31	C	518	DGD	O6D-C1D-O3G	-3.47	101.85	110.04
24	D	401	CLA	CED-O2D-CGD	3.47	123.78	115.92
24	d	401	CLA	CED-O2D-CGD	3.47	123.78	115.92
24	b	612	CLA	C4C-C3C-C2C	-3.46	101.85	106.89
24	c	511	CLA	C4B-C3B-C2B	-3.46	103.00	107.30
31	c	518	DGD	O6D-C1D-O3G	-3.46	101.87	110.04
24	B	611	CLA	C3B-C4B-NB	3.46	113.62	110.53
24	B	610	CLA	CHC-C1C-C2C	-3.46	117.12	126.95
24	C	505	CLA	C3C-C4C-NC	3.46	114.86	110.43
24	c	505	CLA	C3C-C4C-NC	3.46	114.86	110.43
24	D	404	CLA	C2B-C1B-NB	3.46	113.91	110.33
24	d	404	CLA	C2B-C1B-NB	3.46	113.91	110.33
24	b	610	CLA	C4B-C3B-C2B	-3.45	103.01	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	CLA	C2C-C1C-NC	3.45	113.61	109.98
24	d	405	CLA	C1C-C2C-C3C	-3.45	103.36	106.98
24	b	603	CLA	CMB-C2B-C1B	3.45	130.67	125.42
24	b	608	CLA	CAC-C3C-C4C	3.44	129.27	124.79
24	B	602	CLA	C3B-C4B-NB	3.44	113.60	110.53
24	B	601	CLA	CMB-C2B-C1B	3.43	130.65	125.42
24	c	510	CLA	C4B-C3B-C2B	-3.43	103.03	107.30
24	b	610	CLA	C2B-C1B-NB	3.43	113.88	110.33
24	A	405	CLA	C4B-C3B-C2B	-3.43	103.04	107.30
24	a	405	CLA	C4B-C3B-C2B	-3.43	103.04	107.30
24	C	511	CLA	C4B-C3B-C2B	-3.43	103.04	107.30
24	B	604	CLA	C3D-C2D-C1D	-3.43	101.15	105.83
24	B	610	CLA	C4B-C3B-C2B	-3.43	103.04	107.30
24	b	613	CLA	C3B-C2B-C1B	-3.42	103.13	107.17
24	d	404	CLA	C3B-C4B-NB	3.42	113.58	110.53
24	C	510	CLA	C4B-C3B-C2B	-3.42	103.05	107.30
24	B	603	CLA	C3B-C4B-NB	3.42	113.58	110.53
24	b	605	CLA	C3B-C4B-NB	3.42	113.58	110.53
24	B	606	CLA	CAC-C3C-C4C	3.42	129.24	124.79
24	b	603	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
24	B	610	CLA	C4C-C3C-C2C	-3.41	101.93	106.89
24	b	617	CLA	C1-O2A-CGA	3.41	124.89	116.65
24	b	606	CLA	C3D-C2D-C1D	-3.41	101.18	105.83
24	B	601	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
24	C	507	CLA	C3D-C4D-ND	3.40	115.52	109.99
24	c	507	CLA	C3D-C4D-ND	3.40	115.52	109.99
24	B	616	CLA	C1-O2A-CGA	3.40	124.87	116.65
24	D	404	CLA	C3B-C4B-NB	3.39	113.56	110.53
24	C	511	CLA	CHC-C1C-C2C	-3.39	117.32	126.95
24	c	511	CLA	CHC-C1C-C2C	-3.39	117.32	126.95
24	B	615	CLA	CED-O2D-CGD	3.39	123.59	115.92
24	b	617	CLA	CED-O2D-CGD	3.39	123.59	115.92
24	B	615	CLA	C1-O2A-CGA	3.38	124.84	116.65
24	b	618	CLA	C1-O2A-CGA	3.38	124.83	116.65
38	x	101	RRX	C23-C24-C25	-3.38	117.98	127.00
24	b	615	CLA	CMC-C2C-C1C	3.37	130.31	125.03
24	b	616	CLA	CAA-C2A-C3A	-3.37	103.88	113.00
24	B	613	CLA	CMC-C2C-C1C	3.37	130.30	125.03
24	C	507	CLA	C2B-C1B-NB	3.37	113.82	110.33
24	c	507	CLA	C2B-C1B-NB	3.37	113.82	110.33
24	B	614	CLA	CAA-C2A-C3A	-3.37	103.90	113.00
24	b	616	CLA	C3C-C4C-NC	3.37	114.74	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C1D-CHD-C4C	-3.37	118.87	126.02
24	b	613	CLA	C1D-CHD-C4C	-3.37	118.87	126.02
24	C	505	CLA	C4B-C3B-C2B	-3.36	103.12	107.30
24	c	505	CLA	C4B-C3B-C2B	-3.36	103.12	107.30
24	C	505	CLA	CHC-C1C-C2C	-3.36	117.40	126.95
24	c	505	CLA	CHC-C1C-C2C	-3.36	117.40	126.95
38	x	101	RRX	C24-C23-C22	-3.36	121.27	126.23
24	b	604	CLA	C3B-C4B-NB	3.36	113.53	110.53
24	B	614	CLA	C3C-C4C-NC	3.35	114.73	110.43
38	X	101	RRX	C23-C24-C25	-3.35	118.04	127.00
24	D	405	CLA	C4C-C3C-C2C	-3.35	102.02	106.89
25	D	402	PHO	C3B-C4B-NB	-3.35	105.28	107.46
25	d	402	PHO	C3B-C4B-NB	-3.35	105.28	107.46
24	d	405	CLA	C4C-C3C-C2C	-3.35	102.02	106.89
24	B	611	CLA	CHC-C1C-C2C	-3.34	117.44	126.95
24	C	510	CLA	CMC-C2C-C1C	3.34	130.26	125.03
24	c	510	CLA	CMC-C2C-C1C	3.34	130.26	125.03
24	b	611	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
24	B	608	CLA	C11-C12-C13	-3.34	104.87	115.97
24	b	610	CLA	C11-C12-C13	-3.34	104.87	115.97
24	B	609	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
28	d	407	PL9	O2-C1-C6	3.34	125.79	120.48
24	C	513	CLA	C4C-C3C-C2C	-3.33	102.04	106.89
24	c	513	CLA	C4C-C3C-C2C	-3.33	102.04	106.89
24	C	509	CLA	CHC-C1C-C2C	-3.33	117.48	126.95
24	c	509	CLA	CHC-C1C-C2C	-3.33	117.48	126.95
24	b	613	CLA	CHC-C1C-C2C	-3.33	117.49	126.95
24	C	510	CLA	C1-O2A-CGA	3.33	124.71	116.65
24	B	605	CLA	CMC-C2C-C1C	3.33	130.24	125.03
24	B	608	CLA	C3D-C2D-C1D	-3.33	101.29	105.83
38	X	101	RRX	C24-C23-C22	-3.33	121.31	126.23
24	B	616	CLA	C3C-C4C-NC	3.33	114.69	110.43
24	b	618	CLA	C3C-C4C-NC	3.33	114.69	110.43
24	C	512	CLA	C1D-CHD-C4C	-3.32	118.95	126.02
24	b	609	CLA	C1-C2-C3	-3.32	120.76	126.20
26	A	409	BCR	C15-C14-C13	-3.32	122.62	127.28
24	c	510	CLA	C1-O2A-CGA	3.32	124.68	116.65
24	C	513	CLA	CMC-C2C-C1C	3.32	130.22	125.03
31	C	518	DGD	O3G-C3G-C2G	-3.32	102.75	110.82
31	c	518	DGD	O3G-C3G-C2G	-3.32	102.75	110.82
24	B	615	CLA	CHC-C1C-C2C	-3.32	117.52	126.95
24	b	617	CLA	CHC-C1C-C2C	-3.32	117.52	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	CED-O2D-CGD	3.32	123.44	115.92
24	c	512	CLA	C1D-CHD-C4C	-3.31	118.97	126.02
24	C	504	CLA	C4A-NA-C1A	-3.31	105.17	106.68
24	c	504	CLA	C4A-NA-C1A	-3.31	105.17	106.68
24	c	513	CLA	CMC-C2C-C1C	3.31	130.21	125.03
24	C	514	CLA	CAA-C2A-C3A	-3.31	104.05	113.00
24	c	514	CLA	CAA-C2A-C3A	-3.31	104.05	113.00
24	A	405	CLA	C1D-CHD-C4C	-3.31	118.98	126.02
24	a	405	CLA	C1D-CHD-C4C	-3.31	118.98	126.02
24	C	512	CLA	CAC-C3C-C4C	3.31	129.10	124.79
26	a	409	BCR	C15-C14-C13	-3.31	122.64	127.28
24	b	607	CLA	CMC-C2C-C1C	3.31	130.20	125.03
24	C	511	CLA	CAA-C2A-C3A	-3.31	104.07	113.00
24	B	616	CLA	CHC-C1C-C2C	-3.31	117.56	126.95
24	b	618	CLA	CHC-C1C-C2C	-3.31	117.56	126.95
24	c	512	CLA	CAC-C3C-C4C	3.30	129.09	124.79
24	B	610	CLA	C1D-CHD-C4C	-3.30	119.00	126.02
24	B	613	CLA	O2D-CGD-CBD	3.30	117.00	111.23
24	b	615	CLA	O2D-CGD-CBD	3.30	117.00	111.23
24	C	512	CLA	CED-O2D-CGD	3.30	123.40	115.92
24	C	504	CLA	CHD-C1D-ND	-3.29	120.17	124.80
24	c	504	CLA	CHD-C1D-ND	-3.29	120.17	124.80
24	c	511	CLA	CAA-C2A-C3A	-3.29	104.10	113.00
24	c	502	CLA	C3C-C4C-NC	3.29	114.65	110.43
24	b	612	CLA	C1D-CHD-C4C	-3.29	119.02	126.02
24	B	603	CLA	C4C-C3C-C2C	-3.29	102.10	106.89
24	b	605	CLA	C4C-C3C-C2C	-3.29	102.10	106.89
24	C	506	CLA	CAC-C3C-C4C	3.29	129.07	124.79
24	c	506	CLA	CAC-C3C-C4C	3.29	129.07	124.79
24	B	607	CLA	C1-C2-C3	-3.29	120.81	126.20
28	D	407	PL9	O2-C1-C6	3.29	125.71	120.48
24	A	406	CLA	C3B-C4B-NB	3.29	113.46	110.53
24	a	406	CLA	C3B-C4B-NB	3.29	113.46	110.53
24	b	610	CLA	C3D-C2D-C1D	-3.29	101.35	105.83
24	B	616	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
24	b	618	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
27	A	412	SQD	O5-C5-C4	3.27	115.60	109.70
24	a	406	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
24	b	610	CLA	C3C-C4C-NC	3.27	114.62	110.43
25	D	402	PHO	O1D-CGD-CBD	3.27	129.68	124.72
25	d	402	PHO	O1D-CGD-CBD	3.27	129.68	124.72
24	B	612	CLA	O2D-CGD-O1D	-3.27	117.49	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
24	C	502	CLA	C3C-C4C-NC	3.26	114.61	110.43
24	B	603	CLA	C1D-CHD-C4C	-3.26	119.08	126.02
24	C	502	CLA	C1D-CHD-C4C	-3.26	119.08	126.02
24	B	608	CLA	C3C-C4C-NC	3.26	114.61	110.43
24	C	506	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
24	c	506	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
24	B	616	CLA	CMB-C2B-C1B	3.26	130.38	125.42
24	b	618	CLA	CMB-C2B-C1B	3.26	130.38	125.42
24	B	615	CLA	CAC-C3C-C4C	3.26	129.03	124.79
24	b	617	CLA	CAC-C3C-C4C	3.26	129.03	124.79
24	A	408	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
24	a	408	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
25	D	402	PHO	O2D-CGD-O1D	-3.26	117.51	123.85
25	d	402	PHO	O2D-CGD-O1D	-3.26	117.51	123.85
27	a	412	SQD	O5-C5-C4	3.25	115.56	109.70
24	A	406	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
24	b	605	CLA	C1D-CHD-C4C	-3.25	119.11	126.02
24	b	612	CLA	C3B-C4B-NB	3.25	113.43	110.53
24	c	502	CLA	C1D-CHD-C4C	-3.24	119.12	126.02
24	D	401	CLA	CBC-CAC-C3C	-3.24	103.62	112.42
24	B	601	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
24	b	603	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
24	B	616	CLA	C4-C3-C5	3.24	120.86	115.23
24	b	618	CLA	C4-C3-C5	3.24	120.86	115.23
24	A	408	CLA	CHB-C4A-NA	3.24	129.08	124.40
24	a	408	CLA	CHB-C4A-NA	3.24	129.07	124.40
24	d	401	CLA	CBC-CAC-C3C	-3.24	103.64	112.42
24	B	606	CLA	C1C-C2C-C3C	-3.24	103.58	106.98
24	C	508	CLA	C1D-CHD-C4C	-3.23	119.14	126.02
24	c	508	CLA	C1D-CHD-C4C	-3.23	119.14	126.02
24	C	509	CLA	C4B-C3B-C2B	-3.23	103.29	107.30
24	c	509	CLA	C4B-C3B-C2B	-3.23	103.29	107.30
24	C	505	CLA	CAC-C3C-C4C	3.23	128.99	124.79
24	c	505	CLA	CAC-C3C-C4C	3.23	128.99	124.79
24	C	506	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
24	c	506	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
24	A	408	CLA	C3C-C4C-NC	3.22	114.56	110.43
24	a	408	CLA	C3C-C4C-NC	3.22	114.56	110.43
24	b	612	CLA	CHD-C1D-ND	-3.22	120.27	124.80
26	B	618	BCR	C29-C30-C25	3.22	115.11	110.44
26	b	620	BCR	C29-C30-C25	3.22	115.11	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	621	LMG	O7-C10-O9	-3.22	116.18	123.70
30	b	622	LMG	O7-C10-O9	-3.22	116.18	123.70
31	C	519	DGD	O3G-C3G-C2G	-3.22	103.00	110.82
31	c	519	DGD	O3G-C3G-C2G	-3.22	103.00	110.82
24	A	406	CLA	CAC-C3C-C4C	3.21	128.97	124.79
24	b	608	CLA	C1C-C2C-C3C	-3.21	103.61	106.98
24	C	513	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
24	a	406	CLA	CAC-C3C-C4C	3.21	128.96	124.79
27	B	620	SQD	O47-C7-O49	-3.21	116.21	123.70
27	L	102	SQD	O47-C7-O49	-3.21	116.21	123.70
24	C	505	CLA	CAA-CBA-CGA	3.20	122.31	113.21
24	c	505	CLA	CAA-CBA-CGA	3.20	122.31	113.21
24	B	615	CLA	C1D-CHD-C4C	-3.20	119.21	126.02
24	B	602	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
24	b	604	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
24	C	502	CLA	CHC-C1C-C2C	-3.20	117.85	126.95
24	c	502	CLA	CHC-C1C-C2C	-3.20	117.85	126.95
24	B	616	CLA	CBC-CAC-C3C	-3.19	103.76	112.42
24	b	618	CLA	CBC-CAC-C3C	-3.19	103.76	112.42
24	c	503	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
24	B	611	CLA	CHD-C4C-NC	3.19	129.18	124.23
24	b	617	CLA	C1D-CHD-C4C	-3.19	119.24	126.02
24	b	613	CLA	CHD-C4C-NC	3.19	129.17	124.23
30	C	501	LMG	O6-C1-O1	-3.19	102.51	110.04
30	c	501	LMG	O6-C1-O1	-3.19	102.51	110.04
26	B	617	BCR	C29-C30-C25	3.18	115.06	110.44
26	b	619	BCR	C29-C30-C25	3.18	115.06	110.44
24	C	504	CLA	CMC-C2C-C1C	3.18	130.01	125.03
24	c	504	CLA	CMC-C2C-C1C	3.18	130.01	125.03
24	B	604	CLA	O2A-CGA-CBA	3.18	121.53	111.83
24	C	503	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
24	b	614	CLA	CHD-C1D-ND	-3.18	120.33	124.80
24	B	613	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
24	b	615	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
24	c	513	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
24	b	606	CLA	O2A-CGA-CBA	3.17	121.51	111.83
24	C	504	CLA	C1C-C2C-C3C	-3.17	103.64	106.98
24	c	504	CLA	C1C-C2C-C3C	-3.17	103.64	106.98
24	b	613	CLA	C1-C2-C3	-3.17	121.00	126.20
24	C	512	CLA	C1C-C2C-C3C	-3.16	103.66	106.98
24	c	512	CLA	C1C-C2C-C3C	-3.16	103.66	106.98
26	C	515	BCR	C7-C8-C9	-3.15	121.57	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
24	b	605	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
24	b	614	CLA	C4-C3-C5	3.15	120.69	115.23
24	A	408	CLA	CMC-C2C-C1C	3.15	129.95	125.03
24	a	408	CLA	CMC-C2C-C1C	3.15	129.95	125.03
24	C	508	CLA	CAC-C3C-C2C	3.15	133.34	127.56
24	B	611	CLA	C1-C2-C3	-3.15	121.04	126.20
24	B	602	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
24	B	612	CLA	CHD-C1D-ND	-3.14	120.38	124.80
24	c	508	CLA	CAC-C3C-C2C	3.14	133.33	127.56
26	C	515	BCR	C27-C26-C25	3.14	126.95	122.70
26	c	515	BCR	C27-C26-C25	3.14	126.95	122.70
24	C	507	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
24	c	507	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
32	Z	101	LMT	C3'-C4'-C5'	-3.14	103.97	110.93
24	D	401	CLA	C1-O2A-CGA	3.14	124.25	116.65
24	d	401	CLA	C1-O2A-CGA	3.14	124.25	116.65
24	B	612	CLA	C4-C3-C5	3.14	120.67	115.23
24	D	401	CLA	C1-C2-C3	-3.14	121.06	126.20
24	d	401	CLA	C1-C2-C3	-3.14	121.06	126.20
32	z	101	LMT	C3'-C4'-C5'	-3.13	103.98	110.93
24	C	502	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
24	B	614	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
24	b	616	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
24	D	405	CLA	CMC-C2C-C1C	3.13	129.92	125.03
24	d	405	CLA	CMC-C2C-C1C	3.13	129.92	125.03
24	b	604	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
24	c	507	CLA	CHD-C4C-NC	3.11	129.06	124.23
26	c	515	BCR	C7-C8-C9	-3.11	121.63	126.23
24	c	502	CLA	C4B-C3B-C2B	-3.11	103.44	107.30
31	C	519	DGD	O6D-C1D-O3G	-3.10	102.71	110.04
24	c	510	CLA	C1-C2-C3	-3.10	121.11	126.20
24	c	514	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
24	C	514	CLA	C1C-C2C-C3C	-3.10	103.72	106.98
24	B	610	CLA	CHD-C1D-ND	-3.10	120.44	124.80
24	C	507	CLA	CHD-C4C-NC	3.09	129.03	124.23
31	c	519	DGD	O6D-C1D-O3G	-3.09	102.73	110.04
24	B	615	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
24	b	617	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
24	C	506	CLA	CMB-C2B-C1B	3.09	130.13	125.42
24	c	506	CLA	CMB-C2B-C1B	3.09	130.13	125.42
24	C	510	CLA	C1-C2-C3	-3.09	121.13	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C1-C2-C3	-3.09	121.13	126.20
25	A	407	PHO	CMB-C2B-C3B	3.09	130.85	124.68
25	a	407	PHO	CMB-C2B-C3B	3.09	130.85	124.68
24	b	613	CLA	C3C-C4C-NC	3.08	114.38	110.43
24	c	503	CLA	CAC-C3C-C4C	3.08	128.80	124.79
24	B	611	CLA	C3C-C4C-NC	3.08	114.38	110.43
24	b	603	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
24	b	611	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
24	c	514	CLA	C1C-C2C-C3C	-3.07	103.75	106.98
24	b	611	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
24	B	605	CLA	C1-C2-C3	-3.07	121.17	126.20
24	C	509	CLA	CMB-C2B-C3B	3.07	133.77	126.55
24	c	509	CLA	CMB-C2B-C3B	3.07	133.77	126.55
24	B	601	CLA	CHC-C1C-C2C	-3.07	118.24	126.95
24	c	508	CLA	CBC-CAC-C3C	-3.06	104.11	112.42
24	B	609	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
24	C	503	CLA	CAC-C3C-C4C	3.06	128.77	124.79
24	C	514	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
27	F	101	SQD	O48-C23-C24	3.05	121.14	111.83
27	f	101	SQD	O48-C23-C24	3.05	121.14	111.83
24	B	604	CLA	CHC-C1C-C2C	-3.05	118.28	126.95
24	b	606	CLA	CHC-C1C-C2C	-3.05	118.28	126.95
24	B	601	CLA	C1D-CHD-C4C	-3.05	119.54	126.02
24	b	603	CLA	C1D-CHD-C4C	-3.05	119.54	126.02
24	B	606	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
24	C	508	CLA	CBC-CAC-C3C	-3.04	104.17	112.42
24	C	504	CLA	C3B-C4B-NB	3.04	113.25	110.53
24	c	504	CLA	C3B-C4B-NB	3.04	113.25	110.53
31	c	519	DGD	CDB-CCB-CBB	-3.04	99.00	114.37
24	B	612	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
24	b	614	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
24	a	405	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
24	A	405	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
24	A	408	CLA	CED-O2D-CGD	3.04	122.81	115.92
24	a	408	CLA	CED-O2D-CGD	3.04	122.81	115.92
31	C	519	DGD	CDB-CCB-CBB	-3.03	99.03	114.37
24	a	406	CLA	C2B-C1B-NB	3.03	113.47	110.33
24	d	404	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
24	b	608	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
27	B	620	SQD	C1-O5-C5	-3.03	107.80	113.72
26	B	618	BCR	C30-C25-C26	-3.03	118.50	122.64
26	b	620	BCR	C30-C25-C26	-3.03	118.50	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	C1-C2-C3	-3.02	121.25	126.20
24	c	513	CLA	C1-C2-C3	-3.02	121.25	126.20
24	D	404	CLA	C4B-C3B-C2B	-3.02	103.55	107.30
24	B	610	CLA	C3B-C4B-NB	3.02	113.22	110.53
27	L	102	SQD	C1-O5-C5	-3.02	107.83	113.72
24	a	406	CLA	C3B-C2B-C1B	-3.02	103.61	107.17
24	B	612	CLA	O1D-CGD-CBD	-3.02	118.57	124.52
24	A	406	CLA	C2B-C1B-NB	3.02	113.45	110.33
24	C	503	CLA	CHD-C1D-ND	-3.01	120.56	124.80
24	c	503	CLA	CHD-C1D-ND	-3.01	120.56	124.80
24	C	509	CLA	C1D-CHD-C4C	-3.01	119.61	126.02
24	c	509	CLA	C1D-CHD-C4C	-3.01	119.61	126.02
24	B	609	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
24	b	614	CLA	O1D-CGD-CBD	-3.01	118.58	124.52
31	c	518	DGD	CBB-CAB-C9B	-3.01	99.17	114.37
24	b	604	CLA	CMB-C2B-C1B	3.00	129.99	125.42
28	D	407	PL9	C8-C7-C3	3.00	119.79	112.03
28	d	407	PL9	C8-C7-C3	3.00	119.79	112.03
27	F	101	SQD	O5-C1-C2	-3.00	104.21	110.37
24	C	507	CLA	C3C-C4C-NC	3.00	114.27	110.43
24	c	507	CLA	C3C-C4C-NC	3.00	114.27	110.43
31	C	518	DGD	CBB-CAB-C9B	-3.00	99.21	114.37
24	B	616	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
24	b	618	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
24	A	406	CLA	C3B-C2B-C1B	-3.00	103.64	107.17
24	c	514	CLA	C3B-C4B-NB	3.00	113.20	110.53
24	B	606	CLA	CMB-C2B-C3B	2.99	133.59	126.55
24	b	608	CLA	CMB-C2B-C3B	2.99	133.59	126.55
27	f	101	SQD	O5-C1-C2	-2.99	104.22	110.37
24	A	406	CLA	C1-C2-C3	-2.99	121.30	126.20
24	a	406	CLA	C1-C2-C3	-2.99	121.30	126.20
24	C	514	CLA	C3C-C4C-NC	2.99	114.26	110.43
24	D	405	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	d	405	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	B	607	CLA	CHC-C1C-C2C	-2.99	118.46	126.95
24	b	609	CLA	CHC-C1C-C2C	-2.99	118.46	126.95
35	E	103	HEM	C3B-C2B-C1B	2.99	108.65	106.41
35	e	103	HEM	C3B-C2B-C1B	2.99	108.65	106.41
24	c	514	CLA	C3C-C4C-NC	2.99	114.25	110.43
24	B	609	CLA	CHD-C4C-NC	2.98	128.86	124.23
24	D	404	CLA	O2A-CGA-CBA	2.98	120.94	111.83
24	d	404	CLA	O2A-CGA-CBA	2.98	120.94	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	401	CLA	CHC-C1C-C2C	-2.98	118.47	126.95
24	d	401	CLA	CHC-C1C-C2C	-2.98	118.47	126.95
24	C	513	CLA	C3B-C4B-NB	2.98	113.19	110.53
24	c	513	CLA	C3B-C4B-NB	2.98	113.19	110.53
24	B	602	CLA	CMB-C2B-C1B	2.98	129.96	125.42
24	d	404	CLA	C1C-C2C-C3C	-2.97	103.85	106.98
24	A	405	CLA	CHD-C1D-ND	-2.97	120.63	124.80
24	a	405	CLA	CHD-C1D-ND	-2.97	120.63	124.80
24	b	611	CLA	CHD-C4C-NC	2.96	128.83	124.23
30	C	523	LMG	O8-C28-O10	-2.96	116.22	123.63
30	c	523	LMG	O8-C28-O10	-2.96	116.22	123.63
24	B	605	CLA	C1D-CHD-C4C	-2.96	119.73	126.02
24	b	607	CLA	C1D-CHD-C4C	-2.96	119.73	126.02
24	B	601	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
24	b	603	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
24	B	602	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
24	b	604	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
24	D	404	CLA	C1C-C2C-C3C	-2.96	103.87	106.98
28	a	411	PL9	O1-C4-C3	-2.95	117.62	120.73
24	B	604	CLA	C6-C7-C8	-2.95	106.16	115.97
24	b	606	CLA	C6-C7-C8	-2.95	106.16	115.97
24	C	513	CLA	C1D-CHD-C4C	-2.95	119.75	126.02
24	c	513	CLA	C1D-CHD-C4C	-2.95	119.75	126.02
24	C	514	CLA	C3B-C4B-NB	2.95	113.16	110.53
34	d	408	LHG	O8-C23-C24	2.95	120.82	111.83
24	B	613	CLA	C4A-NA-C1A	-2.94	105.34	106.68
24	b	615	CLA	C4A-NA-C1A	-2.94	105.34	106.68
24	B	605	CLA	C3B-C4B-NB	2.94	113.15	110.53
24	b	607	CLA	C3B-C4B-NB	2.94	113.15	110.53
34	D	408	LHG	O8-C23-C24	2.94	120.79	111.83
28	A	411	PL9	O1-C4-C3	-2.93	117.64	120.73
24	B	608	CLA	CHD-C4C-NC	2.93	128.78	124.23
24	c	510	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
24	C	504	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
24	c	504	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
24	C	505	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
24	c	505	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
24	C	511	CLA	C2B-C1B-NB	2.93	113.36	110.33
24	c	511	CLA	C2B-C1B-NB	2.93	113.36	110.33
24	b	605	CLA	C5-C3-C2	-2.93	114.60	121.17
24	C	510	CLA	C4C-C3C-C2C	-2.92	102.63	106.89
24	c	507	CLA	C1-C2-C3	-2.92	121.41	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C5-C3-C2	-2.92	114.60	121.17
27	A	412	SQD	O6-C1-C2	2.92	112.71	108.27
27	a	412	SQD	O6-C1-C2	2.92	112.71	108.27
24	C	508	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
24	c	508	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
24	B	605	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
24	b	607	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
25	A	407	PHO	C2B-C1B-NB	-2.90	107.33	109.43
25	a	407	PHO	C2B-C1B-NB	-2.90	107.33	109.43
24	C	513	CLA	O2A-CGA-CBA	2.90	120.69	111.83
24	c	513	CLA	O2A-CGA-CBA	2.90	120.69	111.83
24	B	602	CLA	CED-O2D-CGD	2.90	122.50	115.92
24	b	604	CLA	CED-O2D-CGD	2.90	122.50	115.92
24	b	610	CLA	CHD-C4C-NC	2.90	128.73	124.23
24	b	611	CLA	CAC-C3C-C4C	2.90	128.56	124.79
24	B	603	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
24	b	605	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
24	B	602	CLA	CHD-C4C-NC	2.90	128.72	124.23
24	b	604	CLA	CHD-C4C-NC	2.90	128.72	124.23
24	C	507	CLA	C1-C2-C3	-2.90	121.45	126.20
30	B	621	LMG	O6-C1-O1	-2.89	103.21	110.04
30	b	622	LMG	O6-C1-O1	-2.89	103.21	110.04
24	B	611	CLA	CBC-CAC-C3C	-2.89	104.59	112.42
24	b	613	CLA	CBC-CAC-C3C	-2.89	104.59	112.42
24	B	612	CLA	CAC-C3C-C4C	2.88	128.54	124.79
24	b	614	CLA	CAC-C3C-C4C	2.88	128.54	124.79
24	c	508	CLA	C4-C3-C5	2.88	120.22	115.23
27	A	410	SQD	C1-C2-C3	-2.88	103.96	110.01
27	a	410	SQD	C1-C2-C3	-2.88	103.96	110.01
24	A	406	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
24	C	502	CLA	CHD-C4C-NC	2.87	128.68	124.23
24	c	502	CLA	CHD-C4C-NC	2.87	128.68	124.23
24	C	506	CLA	CMC-C2C-C1C	2.87	129.52	125.03
24	c	506	CLA	CMC-C2C-C1C	2.87	129.52	125.03
24	a	406	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
24	B	615	CLA	C6-C7-C8	-2.87	106.43	115.97
28	a	411	PL9	O2-C1-C6	2.87	125.04	120.48
24	b	617	CLA	C6-C7-C8	-2.87	106.44	115.97
24	B	607	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
24	b	609	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
24	b	610	CLA	C3B-C4B-NB	2.87	113.09	110.53
24	b	614	CLA	C4D-CHA-C1A	-2.86	117.83	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	CLA	CMA-C3A-C4A	-2.86	104.08	111.77
24	c	513	CLA	CMA-C3A-C4A	-2.86	104.08	111.77
30	B	621	LMG	C40-C39-C38	-2.86	99.90	114.37
30	b	622	LMG	C40-C39-C38	-2.86	99.90	114.37
28	d	407	PL9	C40-C39-C41	2.86	120.19	115.23
28	A	411	PL9	O2-C1-C6	2.86	125.03	120.48
24	c	510	CLA	C1D-CHD-C4C	-2.86	119.95	126.02
24	C	513	CLA	CHB-C4A-NA	2.86	128.52	124.40
24	c	513	CLA	CHB-C4A-NA	2.86	128.52	124.40
24	B	601	CLA	C4A-NA-C1A	-2.86	105.38	106.68
24	b	603	CLA	C4A-NA-C1A	-2.86	105.38	106.68
24	B	614	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
30	d	411	LMG	O6-C1-O1	-2.86	103.30	110.04
24	c	505	CLA	CED-O2D-CGD	2.86	122.39	115.92
24	B	612	CLA	O2A-CGA-CBA	2.85	120.54	111.83
28	D	407	PL9	C40-C39-C41	2.85	120.18	115.23
24	b	614	CLA	O2A-CGA-CBA	2.85	120.53	111.83
24	C	507	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
24	c	507	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
24	b	616	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
24	C	508	CLA	C4-C3-C5	2.85	120.17	115.23
24	B	609	CLA	CAC-C3C-C4C	2.85	128.50	124.79
24	B	612	CLA	C4D-CHA-C1A	-2.85	117.85	121.24
35	E	103	HEM	CHD-C4C-NC	2.85	127.55	124.45
35	e	103	HEM	CHD-C4C-NC	2.85	127.55	124.45
30	D	411	LMG	O6-C1-O1	-2.85	103.32	110.04
24	B	606	CLA	C4-C3-C5	2.84	120.17	115.23
24	b	608	CLA	C4-C3-C5	2.84	120.17	115.23
24	A	408	CLA	CHC-C1C-C2C	-2.84	118.86	126.95
24	a	408	CLA	CHC-C1C-C2C	-2.84	118.86	126.95
31	H	101	DGD	C6D-C5D-C4D	2.84	118.03	112.07
31	h	101	DGD	C6D-C5D-C4D	2.84	118.03	112.07
27	A	410	SQD	C4-C3-C2	2.84	115.82	110.83
27	a	410	SQD	C4-C3-C2	2.84	115.82	110.83
24	C	505	CLA	CED-O2D-CGD	2.84	122.36	115.92
24	C	510	CLA	C1D-CHD-C4C	-2.84	119.98	126.02
24	B	608	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
24	B	606	CLA	CHC-C1C-C2C	-2.84	118.89	126.95
24	B	608	CLA	C3B-C4B-NB	2.84	113.06	110.53
24	b	610	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
24	B	615	CLA	CHA-C1A-NA	-2.83	119.98	126.39
24	b	617	CLA	CHA-C1A-NA	-2.83	119.98	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
24	d	401	CLA	CAA-C2A-C3A	-2.83	105.35	113.00
24	C	512	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
24	c	509	CLA	CHD-C1D-ND	-2.83	120.82	124.80
24	D	405	CLA	C4A-NA-C1A	-2.83	105.39	106.68
24	d	405	CLA	C4A-NA-C1A	-2.83	105.39	106.68
24	B	613	CLA	C1-O2A-CGA	2.82	123.49	116.65
24	B	612	CLA	C1D-CHD-C4C	-2.82	120.02	126.02
24	D	401	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
24	C	506	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
24	c	506	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
24	b	615	CLA	C1-O2A-CGA	2.82	123.47	116.65
38	X	101	RRX	C16-C15-C14	-2.82	117.75	123.52
24	c	512	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
27	f	101	SQD	O8-S-C6	2.82	111.41	105.97
24	C	509	CLA	CHD-C1D-ND	-2.81	120.84	124.80
24	b	614	CLA	C1D-CHD-C4C	-2.81	120.05	126.02
31	C	518	DGD	CDB-CCB-CBB	-2.81	100.18	114.37
31	c	518	DGD	CDB-CCB-CBB	-2.81	100.18	114.37
24	C	508	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
24	c	508	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
24	C	511	CLA	C1D-CHD-C4C	-2.80	120.06	126.02
24	c	511	CLA	C1D-CHD-C4C	-2.80	120.06	126.02
24	B	605	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
24	B	604	CLA	C11-C12-C13	-2.80	106.65	115.97
24	b	606	CLA	C11-C12-C13	-2.80	106.65	115.97
38	x	101	RRX	C16-C15-C14	-2.80	117.79	123.52
24	C	514	CLA	C4-C3-C5	2.80	120.09	115.23
24	c	514	CLA	C4-C3-C5	2.80	120.09	115.23
26	B	619	BCR	C24-C23-C22	-2.80	122.09	126.23
24	C	505	CLA	CMA-C3A-C4A	-2.80	104.25	111.77
24	c	505	CLA	CMA-C3A-C4A	-2.80	104.25	111.77
31	H	101	DGD	C3D-C4D-C5D	-2.80	105.16	110.23
31	h	101	DGD	C3D-C4D-C5D	-2.80	105.16	110.23
24	b	607	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
24	B	602	CLA	C1D-CHD-C4C	-2.80	120.07	126.02
24	b	604	CLA	C1D-CHD-C4C	-2.80	120.07	126.02
27	F	101	SQD	O8-S-C6	2.80	111.37	105.97
28	D	407	PL9	C7-C8-C9	-2.79	122.02	126.83
28	d	407	PL9	C7-C8-C9	-2.79	122.02	126.83
32	z	101	LMT	C3B-C4B-C5B	-2.79	105.17	110.23
25	D	402	PHO	C4A-C3A-C2A	-2.79	100.19	102.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402	PHO	C4A-C3A-C2A	-2.79	100.19	102.84
34	D	408	LHG	C11-C10-C9	-2.78	100.29	114.37
34	d	408	LHG	C11-C10-C9	-2.78	100.29	114.37
24	B	609	CLA	C2B-C1B-NB	2.78	113.21	110.33
24	B	605	CLA	CAC-C3C-C4C	2.78	128.41	124.79
24	b	607	CLA	CAC-C3C-C4C	2.78	128.41	124.79
24	b	612	CLA	C1-C2-C3	-2.78	121.64	126.20
26	b	621	BCR	C24-C23-C22	-2.78	122.12	126.23
26	B	618	BCR	C15-C16-C17	-2.78	117.83	123.52
26	b	620	BCR	C15-C16-C17	-2.78	117.83	123.52
24	B	610	CLA	C1-C2-C3	-2.78	121.65	126.20
32	Z	101	LMT	C3B-C4B-C5B	-2.78	105.20	110.23
24	D	405	CLA	C2A-C1A-CHA	-2.78	119.05	123.87
24	d	405	CLA	C2A-C1A-CHA	-2.78	119.05	123.87
24	b	609	CLA	CAA-C2A-C3A	-2.77	105.51	113.00
34	D	409	LHG	O8-C23-C24	2.77	120.28	111.83
24	a	405	CLA	C7-C6-C5	-2.77	105.88	113.26
24	C	510	CLA	CAA-C2A-C3A	-2.77	105.53	113.00
24	c	510	CLA	CAA-C2A-C3A	-2.77	105.53	113.00
24	B	605	CLA	O1D-CGD-CBD	-2.77	119.06	124.52
24	b	607	CLA	O1D-CGD-CBD	-2.77	119.06	124.52
26	t	102	BCR	C33-C5-C6	-2.76	121.47	124.48
24	B	607	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
34	e	101	LHG	C11-C10-C9	-2.76	100.42	114.37
24	A	405	CLA	C7-C6-C5	-2.76	105.92	113.26
34	d	409	LHG	O8-C23-C24	2.75	120.23	111.83
34	E	101	LHG	C11-C10-C9	-2.75	100.46	114.37
24	D	405	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
24	d	405	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
24	B	607	CLA	C1D-CHD-C4C	-2.75	120.17	126.02
24	b	609	CLA	C1D-CHD-C4C	-2.75	120.17	126.02
24	B	603	CLA	CHD-C1D-ND	-2.75	120.93	124.80
24	d	404	CLA	C1-C2-C3	-2.75	121.70	126.20
24	c	514	CLA	CHB-C1B-C2B	-2.74	119.46	127.43
24	C	505	CLA	C1D-CHD-C4C	-2.74	120.19	126.02
24	c	505	CLA	C1D-CHD-C4C	-2.74	120.19	126.02
26	T	101	BCR	C33-C5-C6	-2.74	121.49	124.48
26	C	516	BCR	C7-C8-C9	-2.74	122.18	126.23
26	c	516	BCR	C7-C8-C9	-2.74	122.18	126.23
28	D	407	PL9	C7-C3-C2	-2.74	120.16	123.39
28	d	407	PL9	C7-C3-C2	-2.74	120.16	123.39
24	C	511	CLA	CMD-C2D-C3D	-2.74	121.41	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	CMD-C2D-C3D	-2.74	121.41	127.69
24	b	605	CLA	CHD-C1D-ND	-2.74	120.95	124.80
24	C	511	CLA	C4-C3-C5	2.74	119.98	115.23
24	D	405	CLA	C4-C3-C5	2.74	119.98	115.23
24	d	405	CLA	C4-C3-C5	2.74	119.98	115.23
24	C	514	CLA	CHB-C1B-C2B	-2.74	119.49	127.43
31	C	517	DGD	O2G-C1B-O1B	-2.73	117.31	123.70
31	c	517	DGD	O2G-C1B-O1B	-2.73	117.31	123.70
24	B	616	CLA	C7-C6-C5	-2.73	105.97	113.26
24	b	618	CLA	C7-C6-C5	-2.73	105.97	113.26
35	E	103	HEM	CMC-C2C-C1C	-2.73	119.91	124.73
35	e	103	HEM	CMC-C2C-C1C	-2.73	119.91	124.73
24	D	405	CLA	C1-C2-C3	-2.73	121.72	126.20
24	d	405	CLA	C1-C2-C3	-2.73	121.72	126.20
24	B	614	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
24	D	404	CLA	C1-C2-C3	-2.73	121.72	126.20
24	D	401	CLA	O2A-CGA-CBA	2.73	120.16	111.83
24	d	401	CLA	O2A-CGA-CBA	2.73	120.16	111.83
24	A	405	CLA	CHB-C4A-NA	2.73	128.34	124.40
24	a	405	CLA	CHB-C4A-NA	2.73	128.34	124.40
26	C	515	BCR	C15-C16-C17	-2.72	117.94	123.52
24	B	602	CLA	C1-C2-C3	-2.72	121.73	126.20
24	b	604	CLA	C1-C2-C3	-2.72	121.73	126.20
24	C	510	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	c	510	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	A	408	CLA	CHD-C4C-NC	2.72	128.45	124.23
24	a	408	CLA	CHD-C4C-NC	2.72	128.45	124.23
24	c	506	CLA	C1-C2-C3	-2.72	121.74	126.20
24	a	406	CLA	CMB-C2B-C1B	2.72	129.56	125.42
24	b	616	CLA	C4C-C3C-C2C	-2.72	102.93	106.89
31	H	101	DGD	C3E-C4E-C5E	-2.72	105.30	110.23
31	h	101	DGD	C3E-C4E-C5E	-2.72	105.30	110.23
24	B	613	CLA	CHC-C1C-C2C	-2.72	119.23	126.95
24	b	611	CLA	C4A-NA-C1A	-2.71	105.44	106.68
24	C	506	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
24	c	506	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
31	C	518	DGD	O6D-C5D-C6D	-2.71	101.32	106.69
31	c	518	DGD	O3G-C1D-C2D	-2.71	104.16	108.27
26	c	515	BCR	C15-C16-C17	-2.71	117.98	123.52
31	C	518	DGD	O3G-C1D-C2D	-2.71	104.16	108.27
30	B	621	LMG	O8-C28-O10	-2.70	116.86	123.63
34	e	101	LHG	C20-C19-C18	-2.70	100.70	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	CMB-C2B-C1B	2.70	129.54	125.42
24	b	617	CLA	CMB-C2B-C1B	2.70	129.54	125.42
34	E	101	LHG	C20-C19-C18	-2.70	100.71	114.37
38	X	101	RRX	C15-C14-C13	-2.70	123.49	127.28
28	D	407	PL9	C22-C23-C24	-2.70	121.44	127.62
28	d	407	PL9	C22-C23-C24	-2.70	121.44	127.62
24	b	615	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
24	b	611	CLA	C2B-C1B-NB	2.70	113.12	110.33
24	A	406	CLA	CMB-C2B-C1B	2.70	129.53	125.42
24	c	511	CLA	C4-C3-C5	2.70	119.91	115.23
38	x	101	RRX	C15-C14-C13	-2.70	123.50	127.28
30	b	622	LMG	O8-C28-O10	-2.70	116.89	123.63
24	B	616	CLA	CMA-C3A-C4A	-2.70	104.53	111.77
24	b	618	CLA	CMA-C3A-C4A	-2.70	104.53	111.77
24	C	510	CLA	C4A-NA-C1A	-2.69	105.45	106.68
24	C	510	CLA	O2A-CGA-CBA	2.69	120.04	111.83
24	c	510	CLA	O2A-CGA-CBA	2.69	120.04	111.83
24	C	506	CLA	C1-C2-C3	-2.69	121.79	126.20
31	c	518	DGD	O6D-C5D-C6D	-2.69	101.36	106.69
24	B	609	CLA	C3B-C2B-C1B	-2.69	104.00	107.17
24	c	502	CLA	C1-C2-C3	-2.69	121.80	126.20
24	C	502	CLA	C1-C2-C3	-2.68	121.80	126.20
24	B	604	CLA	C3B-C2B-C1B	-2.68	104.01	107.17
24	b	606	CLA	C3B-C2B-C1B	-2.68	104.01	107.17
24	B	602	CLA	CBC-CAC-C3C	-2.68	105.15	112.42
24	b	604	CLA	CBC-CAC-C3C	-2.68	105.15	112.42
24	D	404	CLA	CMA-C3A-C2A	-2.68	103.62	113.98
24	d	404	CLA	CMA-C3A-C2A	-2.68	103.62	113.98
24	c	510	CLA	C4A-NA-C1A	-2.68	105.46	106.68
31	C	517	DGD	CDB-CCB-CBB	-2.68	100.85	114.37
24	b	607	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
24	B	605	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
24	C	504	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
24	c	504	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
24	C	507	CLA	CHC-C1C-NC	2.67	128.34	124.31
24	c	507	CLA	CHC-C1C-NC	2.67	128.34	124.31
24	B	609	CLA	C4A-NA-C1A	-2.67	105.46	106.68
31	c	517	DGD	CDB-CCB-CBB	-2.67	100.87	114.37
30	D	411	LMG	C6-C5-C4	-2.67	106.46	113.02
30	d	411	LMG	C6-C5-C4	-2.67	106.46	113.02
24	B	601	CLA	CAC-C3C-C4C	2.67	128.26	124.79
24	b	603	CLA	CAC-C3C-C4C	2.67	128.26	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C27-C26-C25	2.67	126.31	122.70
26	b	621	BCR	C27-C26-C25	2.67	126.31	122.70
24	b	611	CLA	CHA-C1A-NA	-2.67	120.35	126.39
24	B	615	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
24	b	617	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
26	D	406	BCR	C1-C6-C5	-2.67	118.99	122.64
26	d	406	BCR	C1-C6-C5	-2.67	118.99	122.64
28	d	407	PL9	O2-C1-C2	-2.66	115.77	121.83
30	c	523	LMG	O1-C1-C2	-2.66	104.23	108.27
24	C	505	CLA	C1-C2-C3	-2.66	121.83	126.20
24	c	505	CLA	C1-C2-C3	-2.66	121.83	126.20
24	C	508	CLA	CMB-C2B-C1B	2.66	129.47	125.42
24	B	609	CLA	CMC-C2C-C1C	2.66	129.19	125.03
28	D	407	PL9	O2-C1-C2	-2.66	115.78	121.83
24	B	609	CLA	CHA-C1A-NA	-2.66	120.38	126.39
24	A	408	CLA	O2A-CGA-CBA	2.66	119.93	111.83
24	a	408	CLA	O2A-CGA-CBA	2.66	119.93	111.83
24	c	508	CLA	CMB-C2B-C1B	2.65	129.46	125.42
24	A	406	CLA	C4A-NA-C1A	-2.65	105.47	106.68
24	a	406	CLA	C4A-NA-C1A	-2.65	105.47	106.68
24	c	511	CLA	C1-O2A-CGA	2.65	123.08	116.65
24	b	609	CLA	CAA-CBA-CGA	2.65	120.73	113.21
30	C	523	LMG	O1-C1-C2	-2.65	104.25	108.27
24	C	511	CLA	C1-O2A-CGA	2.65	123.06	116.65
24	B	607	CLA	CAA-CBA-CGA	2.64	120.72	113.21
24	C	502	CLA	CAA-C2A-C3A	-2.64	105.85	113.00
24	c	502	CLA	CAA-C2A-C3A	-2.64	105.85	113.00
30	C	501	LMG	C40-C39-C38	-2.64	101.01	114.37
30	c	501	LMG	C40-C39-C38	-2.64	101.01	114.37
31	H	101	DGD	CDB-CCB-CBB	-2.64	101.02	114.37
31	h	101	DGD	CDB-CCB-CBB	-2.64	101.02	114.37
38	X	101	RRX	C30-C29-C28	-2.64	107.80	113.59
38	x	101	RRX	C30-C29-C28	-2.64	107.80	113.59
24	D	401	CLA	C3C-C4C-NC	2.64	113.81	110.43
24	d	401	CLA	C3C-C4C-NC	2.64	113.81	110.43
28	D	407	PL9	C12-C13-C14	-2.63	121.59	127.62
28	d	407	PL9	C12-C13-C14	-2.63	121.59	127.62
24	B	613	CLA	CHD-C4C-NC	2.63	128.32	124.23
24	b	615	CLA	CHD-C4C-NC	2.63	128.32	124.23
24	A	408	CLA	CAC-C3C-C4C	2.63	128.22	124.79
24	a	408	CLA	CAC-C3C-C4C	2.63	128.22	124.79
24	C	503	CLA	CAA-C2A-C3A	-2.63	105.89	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	503	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
24	c	514	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
24	B	616	CLA	CAA-C2A-C3A	-2.63	105.90	113.00
24	b	618	CLA	CAA-C2A-C3A	-2.63	105.90	113.00
24	C	510	CLA	CMB-C2B-C3B	2.63	132.73	126.55
24	c	510	CLA	CMB-C2B-C3B	2.63	132.73	126.55
24	C	511	CLA	C4C-C3C-C2C	-2.63	103.07	106.89
24	c	511	CLA	C4C-C3C-C2C	-2.63	103.07	106.89
30	C	523	LMG	C1-C2-C3	-2.62	104.49	110.01
30	c	523	LMG	C1-C2-C3	-2.62	104.49	110.01
24	D	401	CLA	CMC-C2C-C3C	2.62	133.25	126.15
24	d	401	CLA	CMC-C2C-C3C	2.62	133.25	126.15
24	C	514	CLA	CHB-C4A-NA	2.62	128.18	124.40
24	c	514	CLA	CHB-C4A-NA	2.62	128.18	124.40
38	X	101	RRX	C8-C7-C6	-2.62	120.00	127.00
38	x	101	RRX	C8-C7-C6	-2.62	120.00	127.00
24	C	514	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
24	C	502	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
24	b	611	CLA	CMC-C2C-C1C	2.61	129.12	125.03
24	C	513	CLA	C1-O2A-CGA	2.61	122.97	116.65
24	c	513	CLA	C1-O2A-CGA	2.61	122.97	116.65
24	B	601	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
24	b	603	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
24	c	502	CLA	CBC-CAC-C3C	-2.61	105.34	112.42
24	C	514	CLA	O2A-CGA-CBA	2.61	119.79	111.83
24	c	514	CLA	O2A-CGA-CBA	2.61	119.79	111.83
24	C	502	CLA	CBC-CAC-C3C	-2.61	105.35	112.42
27	a	412	SQD	C3-C4-C5	2.61	114.96	110.23
24	A	405	CLA	CAA-C2A-C1A	-2.61	103.43	111.97
24	a	405	CLA	CAA-C2A-C1A	-2.61	103.43	111.97
26	T	101	BCR	C31-C1-C6	2.60	114.32	110.24
26	t	102	BCR	C31-C1-C6	2.60	114.32	110.24
24	c	502	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
24	b	616	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
24	C	510	CLA	C11-C12-C13	-2.60	107.33	115.97
24	c	510	CLA	C11-C12-C13	-2.60	107.33	115.97
24	c	503	CLA	C16-C17-C18	-2.60	104.35	115.94
24	C	508	CLA	C1-C2-C3	-2.60	121.94	126.20
32	J	102	LMT	C1-O1'-C1'	2.60	118.11	113.68
32	j	102	LMT	C1-O1'-C1'	2.60	118.11	113.68
24	C	503	CLA	C16-C17-C18	-2.60	104.35	115.94
24	C	505	CLA	CHB-C4A-NA	2.60	128.15	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	CHB-C4A-NA	2.60	128.15	124.40
24	B	601	CLA	CBC-CAC-C3C	-2.59	105.39	112.42
24	b	603	CLA	CBC-CAC-C3C	-2.59	105.39	112.42
24	C	510	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
24	c	510	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
24	c	502	CLA	CMB-C2B-C3B	2.59	132.65	126.55
24	B	615	CLA	CMA-C3A-C4A	-2.59	104.81	111.77
24	b	617	CLA	CMA-C3A-C4A	-2.59	104.81	111.77
24	b	607	CLA	CHB-C4A-NA	2.59	128.14	124.40
24	C	510	CLA	CED-O2D-CGD	2.59	121.79	115.92
24	c	510	CLA	CED-O2D-CGD	2.59	121.79	115.92
26	D	406	BCR	C4-C5-C6	2.59	126.20	122.70
26	d	406	BCR	C4-C5-C6	2.59	126.20	122.70
24	D	405	CLA	CHB-C4A-NA	2.59	128.13	124.40
24	d	405	CLA	CHB-C4A-NA	2.59	128.13	124.40
24	C	504	CLA	C1-O2A-CGA	2.58	122.91	116.65
24	c	504	CLA	C1-O2A-CGA	2.58	122.91	116.65
24	B	614	CLA	O2A-CGA-O1A	-2.58	117.16	123.63
30	C	520	LMG	O1-C1-C2	-2.58	104.35	108.27
30	c	520	LMG	O1-C1-C2	-2.58	104.35	108.27
24	c	508	CLA	C1-C2-C3	-2.58	121.97	126.20
24	c	514	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
27	A	412	SQD	C3-C4-C5	2.58	114.91	110.23
24	B	605	CLA	CHB-C4A-NA	2.58	128.12	124.40
24	C	506	CLA	CHD-C1D-ND	-2.57	121.18	124.80
24	c	506	CLA	CHD-C1D-ND	-2.57	121.18	124.80
24	B	611	CLA	CMC-C2C-C1C	2.57	129.05	125.03
31	C	518	DGD	O3D-C3D-C4D	-2.57	104.32	110.38
31	c	518	DGD	O3D-C3D-C4D	-2.57	104.32	110.38
24	b	610	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
24	B	608	CLA	CHD-C1D-ND	-2.57	121.19	124.80
24	B	608	CLA	C4C-C3C-C2C	-2.57	103.16	106.89
24	C	514	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
24	C	502	CLA	CMB-C2B-C3B	2.56	132.58	126.55
24	D	405	CLA	O2A-CGA-CBA	2.56	119.65	111.83
24	d	405	CLA	O2A-CGA-CBA	2.56	119.65	111.83
26	A	409	BCR	C27-C26-C25	2.56	126.17	122.70
26	a	409	BCR	C27-C26-C25	2.56	126.17	122.70
30	c	501	LMG	O7-C10-O9	-2.56	117.72	123.70
24	c	502	CLA	CAC-C3C-C4C	2.56	128.12	124.79
32	C	521	LMT	O5B-C5B-C4B	2.56	114.31	109.70
32	c	521	LMT	O5B-C5B-C4B	2.56	114.31	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	412	SQD	O9-S-C6	2.56	110.58	106.76
30	C	520	LMG	C40-C39-C38	-2.56	101.44	114.37
24	B	614	CLA	CMA-C3A-C2A	-2.56	104.09	113.98
24	C	506	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
24	c	506	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
30	C	501	LMG	O7-C10-O9	-2.56	117.73	123.70
26	C	515	BCR	C38-C26-C27	-2.56	108.15	113.60
26	c	515	BCR	C38-C26-C27	-2.56	108.15	113.60
24	B	603	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
24	b	605	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
24	B	601	CLA	C3B-C4B-NB	2.55	112.81	110.53
24	b	603	CLA	C3B-C4B-NB	2.55	112.81	110.53
24	C	507	CLA	C3B-C2B-C1B	-2.55	104.16	107.17
24	c	507	CLA	C3B-C2B-C1B	-2.55	104.16	107.17
24	C	506	CLA	C1-O2A-CGA	2.55	122.83	116.65
30	c	520	LMG	C40-C39-C38	-2.55	101.46	114.37
24	A	408	CLA	C1D-CHD-C4C	-2.55	120.59	126.02
24	b	616	CLA	CMA-C3A-C2A	-2.55	104.11	113.98
24	b	616	CLA	C4-C3-C5	2.55	119.65	115.23
24	D	404	CLA	CHC-C1C-C2C	-2.55	119.71	126.95
24	d	404	CLA	CHC-C1C-C2C	-2.55	119.71	126.95
27	A	412	SQD	O9-S-C6	2.55	110.56	106.76
32	z	101	LMT	O5B-C5B-C4B	2.54	114.28	109.70
24	C	510	CLA	CBC-CAC-C3C	-2.54	105.52	112.42
24	c	510	CLA	CBC-CAC-C3C	-2.54	105.52	112.42
24	B	614	CLA	C4-C3-C5	2.54	119.64	115.23
24	B	602	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
24	b	604	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
24	a	405	CLA	O2A-CGA-CBA	2.54	119.59	111.83
24	b	610	CLA	CHD-C1D-ND	-2.54	121.22	124.80
24	b	611	CLA	C3B-C2B-C1B	-2.54	104.17	107.17
28	D	407	PL9	C20-C19-C21	2.54	119.64	115.23
32	m	102	LMT	O1'-C1-C2	-2.54	100.74	109.37
24	C	514	CLA	CMB-C2B-C3B	2.54	132.53	126.55
24	c	506	CLA	C1-O2A-CGA	2.54	122.80	116.65
24	A	405	CLA	O2A-CGA-CBA	2.54	119.58	111.83
24	a	408	CLA	C1D-CHD-C4C	-2.54	120.62	126.02
24	A	406	CLA	CHD-C4C-NC	2.54	128.17	124.23
24	a	406	CLA	CHD-C4C-NC	2.54	128.17	124.23
24	b	610	CLA	O2A-CGA-CBA	2.54	119.58	111.83
28	d	407	PL9	C20-C19-C21	2.54	119.63	115.23
31	C	518	DGD	O2E-C2E-C1E	-2.54	104.03	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	518	DGD	O2E-C2E-C1E	-2.54	104.03	110.08
24	B	602	CLA	C4-C3-C5	2.54	119.63	115.23
24	b	604	CLA	C4-C3-C5	2.54	119.63	115.23
24	B	608	CLA	O2A-CGA-CBA	2.53	119.56	111.83
32	M	101	LMT	O1'-C1-C2	-2.53	100.77	109.37
24	b	614	CLA	CAA-C2A-C3A	-2.53	106.16	113.00
26	B	619	BCR	C2-C1-C6	2.53	114.11	110.44
24	b	616	CLA	O2A-CGA-CBA	2.53	119.54	111.83
24	b	607	CLA	CED-O2D-CGD	2.53	121.65	115.92
31	c	517	DGD	O3E-C3E-C2E	-2.53	104.42	110.38
24	B	616	CLA	C4-C3-C2	-2.53	117.14	123.63
24	b	618	CLA	C4-C3-C2	-2.53	117.14	123.63
31	C	517	DGD	O3E-C3E-C2E	-2.52	104.42	110.38
24	C	506	CLA	C3B-C4B-NB	2.52	112.78	110.53
24	c	506	CLA	C3B-C4B-NB	2.52	112.78	110.53
24	c	514	CLA	CMB-C2B-C3B	2.52	132.48	126.55
24	B	612	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
24	B	610	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
24	B	605	CLA	CED-O2D-CGD	2.52	121.62	115.92
24	B	614	CLA	O2A-CGA-CBA	2.52	119.50	111.83
28	A	411	PL9	C37-C38-C39	-2.52	121.87	127.62
28	a	411	PL9	C37-C38-C39	-2.52	121.87	127.62
26	b	621	BCR	C2-C1-C6	2.51	114.09	110.44
24	b	612	CLA	O2A-CGA-O1A	-2.51	117.34	123.63
24	b	613	CLA	CMC-C2C-C1C	2.51	128.96	125.03
26	C	515	BCR	C16-C15-C14	-2.51	118.38	123.52
30	C	501	LMG	O3-C3-C2	-2.51	104.46	110.38
30	c	501	LMG	O3-C3-C2	-2.51	104.46	110.38
26	C	516	BCR	C27-C26-C25	2.51	126.10	122.70
32	Z	101	LMT	O5B-C5B-C4B	2.51	114.22	109.70
24	B	604	CLA	CHD-C1D-ND	-2.51	121.27	124.80
24	b	606	CLA	CHD-C1D-ND	-2.51	121.27	124.80
31	C	517	DGD	O2D-C2D-C3D	-2.51	104.46	110.38
31	c	517	DGD	O2D-C2D-C3D	-2.51	104.46	110.38
24	C	502	CLA	C7-C6-C5	-2.51	106.58	113.26
24	c	502	CLA	C7-C6-C5	-2.51	106.58	113.26
26	B	619	BCR	C1-C6-C5	-2.51	119.21	122.64
24	B	612	CLA	CMA-C3A-C2A	-2.50	104.30	113.98
24	b	614	CLA	CMA-C3A-C2A	-2.50	104.30	113.98
24	B	609	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	c	505	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
24	C	505	CLA	O2D-CGD-O1D	-2.49	118.99	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	CBC-CAC-C3C	-2.49	105.66	112.42
24	C	505	CLA	CBC-CAC-C3C	-2.49	105.66	112.42
24	c	505	CLA	CBC-CAC-C3C	-2.49	105.66	112.42
30	C	523	LMG	O7-C10-O9	-2.49	117.88	123.70
30	c	523	LMG	O7-C10-O9	-2.49	117.88	123.70
24	C	502	CLA	CAC-C3C-C4C	2.49	128.03	124.79
28	d	407	PL9	C36-C34-C33	-2.49	115.58	121.17
34	d	410	LHG	O8-C23-C24	2.49	119.42	111.83
26	T	101	BCR	C15-C14-C13	-2.49	123.79	127.28
26	t	102	BCR	C15-C14-C13	-2.49	123.79	127.28
26	c	516	BCR	C27-C26-C25	2.49	126.06	122.70
28	D	407	PL9	C36-C34-C33	-2.49	115.59	121.17
24	B	606	CLA	C11-C10-C8	-2.48	107.71	115.97
24	b	608	CLA	C11-C10-C8	-2.48	107.71	115.97
30	C	520	LMG	C38-C37-C36	-2.48	101.81	114.37
24	B	605	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
25	D	402	PHO	C4B-NB-C1B	2.48	112.44	108.82
25	d	402	PHO	C4B-NB-C1B	2.48	112.44	108.82
24	B	609	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
28	A	411	PL9	C22-C23-C24	-2.48	121.94	127.62
28	a	411	PL9	C22-C23-C24	-2.48	121.94	127.62
24	C	508	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
24	c	508	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
24	C	510	CLA	CMA-C3A-C2A	-2.48	104.39	113.98
24	C	504	CLA	CMB-C2B-C1B	2.48	129.20	125.42
24	c	504	CLA	CMB-C2B-C1B	2.48	129.20	125.42
24	C	505	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
24	c	505	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
24	C	511	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
24	c	505	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
30	d	411	LMG	C40-C39-C38	-2.48	101.84	114.37
24	B	605	CLA	CAA-C2A-C3A	-2.48	106.30	113.00
24	b	607	CLA	CAA-C2A-C3A	-2.48	106.30	113.00
24	c	510	CLA	CMA-C3A-C2A	-2.48	104.40	113.98
30	c	520	LMG	C38-C37-C36	-2.48	101.84	114.37
24	B	603	CLA	CMB-C2B-C3B	2.48	132.38	126.55
24	b	611	CLA	CHB-C4A-NA	2.48	127.97	124.40
24	B	611	CLA	C4C-C3C-C2C	-2.48	103.29	106.89
26	b	621	BCR	C1-C6-C5	-2.48	119.25	122.64
24	C	513	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
24	c	513	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
26	c	515	BCR	C16-C15-C14	-2.48	118.45	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	CMB-C2B-C3B	2.47	132.37	126.55
24	c	514	CLA	CHD-C4C-NC	2.47	128.07	124.23
30	D	411	LMG	C40-C39-C38	-2.47	101.87	114.37
34	D	410	LHG	O8-C23-C24	2.47	119.37	111.83
24	C	505	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
24	C	514	CLA	CHD-C4C-NC	2.47	128.06	124.23
24	B	612	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
24	A	406	CLA	CMA-C3A-C2A	-2.47	104.44	113.98
24	a	406	CLA	CMA-C3A-C2A	-2.47	104.44	113.98
26	B	617	BCR	C30-C25-C26	-2.47	119.26	122.64
26	b	619	BCR	C30-C25-C26	-2.47	119.26	122.64
28	D	407	PL9	C7-C3-C4	2.47	118.94	116.91
28	d	407	PL9	C7-C3-C4	2.47	118.94	116.91
24	b	614	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
24	B	606	CLA	C11-C12-C13	-2.46	107.77	115.97
24	c	509	CLA	C1-C2-C3	-2.46	122.16	126.20
24	b	613	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
24	c	511	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
33	D	403	BCT	O3-C-O1	-2.46	113.39	119.68
24	b	608	CLA	C11-C12-C13	-2.46	107.80	115.97
24	B	611	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
24	b	611	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
24	C	505	CLA	C4-C3-C5	2.45	119.49	115.23
24	c	505	CLA	C4-C3-C5	2.45	119.49	115.23
24	C	507	CLA	OBD-CAD-C3D	-2.45	122.68	128.42
24	c	507	CLA	OBD-CAD-C3D	-2.45	122.68	128.42
24	D	405	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
24	d	405	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
24	b	613	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
24	C	504	CLA	CHD-C4C-NC	2.45	128.03	124.23
24	c	504	CLA	CHD-C4C-NC	2.45	128.03	124.23
24	A	406	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
24	a	406	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
24	C	508	CLA	CHD-C4C-NC	2.45	128.03	124.23
24	c	508	CLA	CHD-C4C-NC	2.45	128.03	124.23
24	D	405	CLA	C1D-CHD-C4C	-2.45	120.82	126.02
24	d	405	CLA	C1D-CHD-C4C	-2.45	120.82	126.02
24	C	503	CLA	C6-C5-C3	-2.44	107.51	113.47
24	c	503	CLA	C6-C5-C3	-2.44	107.51	113.47
24	C	514	CLA	C2A-C1A-CHA	-2.44	119.63	123.87
24	c	514	CLA	C2A-C1A-CHA	-2.44	119.63	123.87
24	B	614	CLA	CED-O2D-CGD	2.44	121.45	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	CED-O2D-CGD	2.44	121.45	115.92
24	B	610	CLA	CAC-C3C-C4C	2.44	127.97	124.79
24	C	513	CLA	CHA-C1A-NA	-2.44	120.87	126.39
24	c	513	CLA	CHA-C1A-NA	-2.44	120.87	126.39
24	C	507	CLA	C2A-C1A-CHA	-2.44	119.64	123.87
24	c	507	CLA	C2A-C1A-CHA	-2.44	119.64	123.87
33	d	403	BCT	O3-C-O1	-2.44	113.44	119.68
24	B	605	CLA	CHD-C4C-NC	2.44	128.01	124.23
24	b	607	CLA	CHD-C4C-NC	2.44	128.01	124.23
24	B	602	CLA	CMC-C2C-C1C	2.44	128.84	125.03
24	b	604	CLA	CMC-C2C-C1C	2.44	128.84	125.03
26	C	522	BCR	C11-C10-C9	-2.43	123.87	127.28
26	c	522	BCR	C11-C10-C9	-2.43	123.87	127.28
24	C	509	CLA	C1-C2-C3	-2.43	122.22	126.20
30	C	520	LMG	O2-C2-C1	-2.43	104.29	110.08
30	c	520	LMG	O2-C2-C1	-2.43	104.29	110.08
26	A	409	BCR	C20-C21-C22	-2.43	123.87	127.28
26	a	409	BCR	C20-C21-C22	-2.43	123.87	127.28
31	C	518	DGD	C6D-O5D-C1E	2.43	119.00	113.80
31	c	518	DGD	C6D-O5D-C1E	2.43	119.00	113.80
24	C	512	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
24	c	512	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
24	C	508	CLA	O2A-CGA-CBA	2.42	119.23	111.83
24	c	508	CLA	O2A-CGA-CBA	2.42	119.23	111.83
24	B	614	CLA	CHD-C4C-NC	2.42	127.99	124.23
24	b	616	CLA	CHD-C4C-NC	2.42	127.99	124.23
24	b	608	CLA	CMC-C2C-C1C	2.42	128.82	125.03
35	E	103	HEM	CAC-C3C-C4C	-2.42	119.04	124.82
35	e	103	HEM	CAC-C3C-C4C	-2.42	119.04	124.82
24	C	505	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
24	c	505	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
26	B	618	BCR	C27-C26-C25	2.42	125.97	122.70
26	b	620	BCR	C27-C26-C25	2.42	125.97	122.70
24	C	508	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	c	508	CLA	CHB-C4A-NA	2.42	127.89	124.40
31	H	101	DGD	O6D-C1D-O3G	-2.42	104.33	110.04
31	h	101	DGD	O6D-C1D-O3G	-2.42	104.33	110.04
24	C	512	CLA	C1-O2A-CGA	2.42	122.51	116.65
24	c	512	CLA	C1-O2A-CGA	2.42	122.51	116.65
24	B	613	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
24	b	615	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
24	C	509	CLA	O2A-CGA-O1A	-2.42	117.59	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	O2A-CGA-O1A	-2.42	117.59	123.63
24	b	611	CLA	C1-C2-C3	-2.41	122.24	126.20
24	B	604	CLA	C4C-C3C-C2C	-2.41	103.38	106.89
24	b	606	CLA	C4C-C3C-C2C	-2.41	103.38	106.89
24	B	601	CLA	CHB-C4A-NA	2.41	127.88	124.40
24	b	603	CLA	CHB-C4A-NA	2.41	127.88	124.40
24	A	408	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
24	a	408	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
24	B	609	CLA	C1-C2-C3	-2.41	122.25	126.20
35	e	103	HEM	CBA-CAA-C2A	-2.41	105.87	112.53
28	A	411	PL9	C21-C19-C18	-2.41	115.76	121.17
28	a	411	PL9	C21-C19-C18	-2.41	115.76	121.17
35	E	103	HEM	CBA-CAA-C2A	-2.41	105.88	112.53
24	D	401	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
24	d	401	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
24	C	510	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
24	c	510	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
24	C	511	CLA	C4A-NA-C1A	-2.40	105.58	106.68
24	c	511	CLA	C4A-NA-C1A	-2.40	105.58	106.68
24	B	613	CLA	C1D-CHD-C4C	-2.40	120.91	126.02
24	b	615	CLA	C1D-CHD-C4C	-2.40	120.91	126.02
24	C	509	CLA	C3B-C4B-NB	2.40	112.68	110.53
24	c	509	CLA	C3B-C4B-NB	2.40	112.68	110.53
31	h	101	DGD	C1D-C2D-C3D	-2.40	104.95	110.01
26	B	617	BCR	C38-C26-C27	-2.40	108.47	113.60
26	b	619	BCR	C38-C26-C27	-2.40	108.47	113.60
24	C	514	CLA	CBC-CAC-C3C	-2.40	105.91	112.42
24	a	406	CLA	CBC-CAC-C3C	-2.40	105.91	112.42
24	B	606	CLA	CMC-C2C-C1C	2.40	128.78	125.03
24	C	512	CLA	O2A-CGA-CBA	2.40	119.15	111.83
24	B	604	CLA	CAC-C3C-C4C	2.40	127.91	124.79
24	b	606	CLA	CAC-C3C-C4C	2.40	127.91	124.79
24	C	513	CLA	CHD-C4C-NC	2.40	127.95	124.23
24	c	513	CLA	CHD-C4C-NC	2.40	127.95	124.23
24	A	406	CLA	CBC-CAC-C3C	-2.40	105.92	112.42
24	c	514	CLA	CBC-CAC-C3C	-2.40	105.92	112.42
31	C	519	DGD	C1E-O6E-C5E	2.39	118.39	113.72
31	c	519	DGD	C1E-O6E-C5E	2.39	118.39	113.72
24	B	613	CLA	CHB-C4A-NA	2.39	127.85	124.40
24	b	615	CLA	CHB-C4A-NA	2.39	127.85	124.40
24	A	406	CLA	CED-O2D-CGD	2.39	121.34	115.92
24	a	406	CLA	CED-O2D-CGD	2.39	121.34	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
24	A	405	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
24	a	405	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
24	c	502	CLA	O2A-CGA-CBA	2.39	119.11	111.83
24	c	512	CLA	O2A-CGA-CBA	2.39	119.11	111.83
26	C	516	BCR	C30-C25-C26	-2.38	119.38	122.64
26	c	516	BCR	C30-C25-C26	-2.38	119.38	122.64
24	c	514	CLA	CMC-C2C-C1C	2.38	128.75	125.03
24	D	401	CLA	C4A-NA-C1A	-2.38	105.59	106.68
24	d	401	CLA	C4A-NA-C1A	-2.38	105.59	106.68
24	A	406	CLA	CAA-CBA-CGA	2.38	119.96	113.21
31	H	101	DGD	C1D-C2D-C3D	-2.38	105.01	110.01
24	b	606	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
30	C	520	LMG	O1-C7-C8	-2.38	105.04	110.82
30	c	520	LMG	O1-C7-C8	-2.38	105.04	110.82
24	C	502	CLA	O2A-CGA-CBA	2.37	119.08	111.83
24	b	613	CLA	C6-C5-C3	2.37	119.25	113.47
37	V	201	HEC	CBC-CAC-C3C	-2.37	122.69	127.43
37	v	201	HEC	CBC-CAC-C3C	-2.37	122.69	127.43
26	D	406	BCR	C27-C26-C25	2.37	125.91	122.70
26	d	406	BCR	C27-C26-C25	2.37	125.91	122.70
24	C	508	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
24	c	508	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
24	B	610	CLA	CHD-C4C-NC	2.37	127.91	124.23
27	B	620	SQD	O48-C23-C24	2.37	119.06	111.83
27	L	102	SQD	O48-C23-C24	2.37	119.06	111.83
24	c	508	CLA	C11-C12-C13	-2.37	108.09	115.97
24	a	406	CLA	CAA-CBA-CGA	2.36	119.91	113.21
24	C	513	CLA	CAC-C3C-C4C	2.36	127.86	124.79
24	c	513	CLA	CAC-C3C-C4C	2.36	127.86	124.79
24	B	611	CLA	C7-C6-C5	-2.36	106.97	113.26
24	B	611	CLA	C6-C5-C3	2.36	119.21	113.47
26	C	515	BCR	C11-C10-C9	-2.36	123.97	127.28
26	c	515	BCR	C11-C10-C9	-2.36	123.97	127.28
24	C	508	CLA	C11-C12-C13	-2.36	108.13	115.97
38	X	101	RRX	C4-C5-C6	-2.36	119.52	122.70
38	x	101	RRX	C4-C5-C6	-2.36	119.52	122.70
30	D	411	LMG	C38-C37-C36	-2.36	102.46	114.37
24	b	612	CLA	CAC-C3C-C4C	2.35	127.85	124.79
24	B	607	CLA	CED-O2D-CGD	2.35	121.25	115.92
24	b	609	CLA	CED-O2D-CGD	2.35	121.25	115.92
30	d	411	LMG	C38-C37-C36	-2.35	102.48	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
24	C	514	CLA	CMC-C2C-C1C	2.35	128.71	125.03
24	D	401	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
24	d	401	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
24	C	513	CLA	CHC-C1C-C2C	-2.35	120.28	126.95
24	c	513	CLA	CHC-C1C-C2C	-2.35	120.28	126.95
24	C	505	CLA	C1-O2A-CGA	2.35	122.33	116.65
24	c	505	CLA	C1-O2A-CGA	2.35	122.33	116.65
24	C	512	CLA	CHD-C4C-NC	2.35	127.87	124.23
28	d	407	PL9	C41-C39-C38	-2.35	115.90	121.17
24	B	615	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	b	617	CLA	CHB-C4A-NA	2.34	127.78	124.40
24	b	606	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
24	c	509	CLA	C11-C10-C8	-2.34	108.18	115.97
24	C	508	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
24	c	508	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
24	B	614	CLA	CHB-C4A-NA	2.34	127.77	124.40
24	b	616	CLA	CHB-C4A-NA	2.34	127.77	124.40
24	B	604	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
24	C	513	CLA	CBC-CAC-C3C	-2.34	106.08	112.42
24	c	513	CLA	CBC-CAC-C3C	-2.34	106.08	112.42
30	C	523	LMG	O6-C1-O1	-2.34	104.52	110.04
24	C	509	CLA	C11-C10-C8	-2.33	108.20	115.97
24	b	613	CLA	C7-C6-C5	-2.33	107.04	113.26
24	b	610	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
24	c	512	CLA	CHD-C4C-NC	2.33	127.85	124.23
30	C	523	LMG	C38-C37-C36	-2.33	102.58	114.37
30	c	523	LMG	C38-C37-C36	-2.33	102.58	114.37
24	C	509	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
28	a	411	PL9	O2-C1-C2	-2.33	116.53	121.83
26	T	101	BCR	C39-C30-C25	2.33	113.89	110.24
26	t	102	BCR	C39-C30-C25	2.33	113.89	110.24
30	c	523	LMG	O6-C1-O1	-2.33	104.54	110.04
28	A	411	PL9	O2-C1-C2	-2.33	116.54	121.83
24	B	614	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
24	b	616	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
31	c	518	DGD	O2D-C2D-C1D	-2.32	104.53	110.08
24	B	613	CLA	C7-C6-C5	-2.32	107.07	113.26
24	b	615	CLA	C7-C6-C5	-2.32	107.07	113.26
24	C	511	CLA	CHC-C4B-NB	2.32	127.53	124.05
24	c	511	CLA	CHC-C4B-NB	2.32	127.53	124.05
24	D	401	CLA	CHB-C4A-NA	2.32	127.75	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	C	507	CLA	CGD-CBD-CAD	-2.32	103.34	110.85
24	c	507	CLA	CGD-CBD-CAD	-2.32	103.34	110.85
24	b	603	CLA	O2A-CGA-CBA	2.32	118.90	111.83
24	b	612	CLA	C4-C3-C5	2.32	119.25	115.23
24	b	616	CLA	CBA-CAA-C2A	2.32	120.69	113.79
24	B	608	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
24	B	601	CLA	O2A-CGA-CBA	2.32	118.90	111.83
26	C	522	BCR	C27-C26-C25	2.32	125.83	122.70
26	c	522	BCR	C27-C26-C25	2.32	125.83	122.70
24	D	405	CLA	CMA-C3A-C4A	-2.31	105.55	111.77
24	d	405	CLA	CMA-C3A-C4A	-2.31	105.55	111.77
31	C	518	DGD	O2D-C2D-C1D	-2.31	104.56	110.08
24	c	511	CLA	O2A-CGA-CBA	2.31	118.88	111.83
24	B	610	CLA	C4-C3-C5	2.31	119.24	115.23
27	F	101	SQD	O5-C5-C4	2.31	113.86	109.70
28	D	407	PL9	C41-C39-C38	-2.31	115.98	121.17
24	C	509	CLA	CBC-CAC-C3C	-2.31	106.16	112.42
24	c	509	CLA	CBC-CAC-C3C	-2.31	106.16	112.42
27	f	101	SQD	O5-C5-C4	2.31	113.86	109.70
35	E	103	HEM	C4C-NC-C1C	2.31	109.58	105.82
35	e	103	HEM	C4C-NC-C1C	2.31	109.58	105.82
24	b	611	CLA	CMA-C3A-C2A	-2.31	105.07	113.98
24	B	614	CLA	CBA-CAA-C2A	2.30	120.65	113.79
24	B	611	CLA	CED-O2D-CGD	2.30	121.13	115.92
24	b	613	CLA	CED-O2D-CGD	2.30	121.13	115.92
24	B	609	CLA	CMA-C3A-C2A	-2.30	105.09	113.98
24	B	614	CLA	C1D-CHD-C4C	-2.30	121.14	126.02
24	b	616	CLA	C1D-CHD-C4C	-2.30	121.14	126.02
24	B	607	CLA	CBC-CAC-C3C	-2.30	106.19	112.42
24	b	609	CLA	CBC-CAC-C3C	-2.30	106.19	112.42
24	C	511	CLA	O2A-CGA-CBA	2.30	118.84	111.83
26	a	409	BCR	C16-C17-C18	-2.29	124.06	127.28
24	B	610	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
24	B	603	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
24	b	605	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
24	D	405	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
24	d	405	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
26	C	515	BCR	C31-C1-C6	2.29	113.84	110.24
26	J	104	BCR	C1-C6-C5	-2.29	119.51	122.64
24	B	609	CLA	O2A-CGA-CBA	2.29	118.82	111.83
24	B	614	CLA	CMB-C2B-C1B	2.28	128.90	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C2A-C1A-CHA	-2.28	119.90	123.87
24	c	506	CLA	C2A-C1A-CHA	-2.28	119.90	123.87
24	B	611	CLA	CHC-C1C-NC	2.28	127.75	124.31
24	b	611	CLA	O2A-CGA-CBA	2.28	118.78	111.83
34	L	101	LHG	C11-C10-C9	-2.28	102.86	114.37
34	l	101	LHG	C11-C10-C9	-2.28	102.86	114.37
24	b	615	CLA	C4C-C3C-C2C	-2.28	103.58	106.89
24	B	607	CLA	C4-C3-C5	2.27	119.17	115.23
24	b	609	CLA	C4-C3-C5	2.27	119.17	115.23
32	Z	101	LMT	O5B-C5B-C6B	2.27	112.07	106.44
34	d	408	LHG	C27-C26-C25	-2.27	102.88	114.37
30	B	621	LMG	O3-C3-C2	-2.27	105.02	110.38
30	b	622	LMG	O3-C3-C2	-2.27	105.02	110.38
24	b	612	CLA	CHD-C4C-NC	2.27	127.75	124.23
26	D	406	BCR	C35-C13-C12	2.27	121.56	118.09
34	D	408	LHG	C27-C26-C25	-2.27	102.89	114.37
26	c	515	BCR	C31-C1-C6	2.27	113.80	110.24
24	b	616	CLA	CMB-C2B-C1B	2.27	128.87	125.42
24	b	608	CLA	CHD-C4C-NC	2.27	127.75	124.23
26	B	618	BCR	C24-C23-C22	-2.27	122.88	126.23
26	b	620	BCR	C24-C23-C22	-2.27	122.88	126.23
24	C	507	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
24	b	613	CLA	CHC-C1C-NC	2.27	127.72	124.31
31	C	519	DGD	C3G-C2G-C1G	-2.27	106.50	111.78
31	c	519	DGD	C3G-C2G-C1G	-2.27	106.50	111.78
24	c	507	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
34	e	101	LHG	C18-C17-C16	-2.26	102.93	114.37
28	d	407	PL9	C32-C33-C34	-2.26	122.45	127.62
26	J	104	BCR	C27-C26-C25	2.26	125.76	122.70
26	j	104	BCR	C27-C26-C25	2.26	125.76	122.70
32	z	101	LMT	O5B-C5B-C6B	2.26	112.04	106.44
24	D	404	CLA	CED-O2D-CGD	2.26	121.05	115.92
24	d	404	CLA	CED-O2D-CGD	2.26	121.05	115.92
24	C	503	CLA	CHB-C4A-NA	2.26	127.66	124.40
24	c	503	CLA	CHB-C4A-NA	2.26	127.66	124.40
26	A	409	BCR	C16-C17-C18	-2.26	124.11	127.28
24	a	406	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
24	C	509	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
34	E	101	LHG	C18-C17-C16	-2.26	102.96	114.37
24	A	406	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
24	b	610	CLA	C4-C3-C5	2.26	119.14	115.23
26	j	104	BCR	C1-C6-C5	-2.26	119.55	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C28-C27-C26	-2.25	110.04	114.06
28	D	407	PL9	C32-C33-C34	-2.25	122.47	127.62
24	B	613	CLA	C4C-C3C-C2C	-2.25	103.61	106.89
24	c	509	CLA	CAA-C2A-C3A	-2.25	106.92	113.00
24	b	613	CLA	CMA-C3A-C4A	-2.25	105.72	111.77
24	B	616	CLA	CMC-C2C-C1C	2.25	128.55	125.03
24	b	618	CLA	CMC-C2C-C1C	2.25	128.55	125.03
26	d	406	BCR	C35-C13-C12	2.25	121.52	118.09
34	D	410	LHG	O8-C23-O10	-2.25	118.01	123.63
28	a	411	PL9	C15-C14-C16	-2.25	111.33	115.23
31	H	101	DGD	CAB-C9B-C8B	-2.24	103.02	114.37
31	h	101	DGD	CAB-C9B-C8B	-2.24	103.02	114.37
26	b	620	BCR	C28-C27-C26	-2.24	110.05	114.06
24	B	604	CLA	CHD-C4C-NC	2.24	127.71	124.23
24	b	606	CLA	CHD-C4C-NC	2.24	127.71	124.23
24	B	606	CLA	CHD-C4C-NC	2.24	127.71	124.23
24	B	611	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
24	B	608	CLA	C4-C3-C5	2.24	119.12	115.23
28	A	411	PL9	C15-C14-C16	-2.24	111.34	115.23
24	C	508	CLA	CMC-C2C-C1C	2.24	128.53	125.03
24	c	508	CLA	CMC-C2C-C1C	2.24	128.53	125.03
34	d	410	LHG	O8-C23-O10	-2.24	118.04	123.63
24	B	603	CLA	CMC-C2C-C1C	2.24	128.53	125.03
24	b	605	CLA	CMC-C2C-C1C	2.24	128.53	125.03
24	B	605	CLA	CMB-C2B-C3B	2.23	131.81	126.55
24	b	607	CLA	CMB-C2B-C3B	2.23	131.81	126.55
24	B	610	CLA	CMC-C2C-C1C	2.23	128.53	125.03
24	C	502	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
24	c	502	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
24	B	612	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
24	B	601	CLA	CHD-C4C-NC	2.23	127.69	124.23
24	b	603	CLA	CHD-C4C-NC	2.23	127.69	124.23
24	b	609	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
24	b	614	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
26	C	516	BCR	C2-C1-C6	2.23	113.68	110.44
26	c	516	BCR	C2-C1-C6	2.23	113.68	110.44
24	B	607	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
24	b	609	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
24	C	502	CLA	CHB-C4A-NA	2.22	127.61	124.40
24	B	615	CLA	CHC-C1C-NC	2.22	127.66	124.31
24	b	617	CLA	CHC-C1C-NC	2.22	127.66	124.31
24	C	512	CLA	CBC-CAC-C3C	-2.22	106.39	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
25	D	402	PHO	CED-O2D-CGD	2.22	120.95	115.92
25	d	402	PHO	CED-O2D-CGD	2.22	120.95	115.92
34	e	101	LHG	C5-O7-C7	-2.22	112.48	117.80
24	B	616	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
24	b	618	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
24	c	502	CLA	CHB-C4A-NA	2.22	127.60	124.40
24	B	607	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
24	b	612	CLA	CAA-CBA-CGA	-2.22	106.91	113.21
24	A	408	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
24	a	408	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
31	H	101	DGD	C4E-C3E-C2E	-2.22	106.93	110.83
31	h	101	DGD	C4E-C3E-C2E	-2.22	106.93	110.83
24	C	511	CLA	CMC-C2C-C1C	2.22	128.50	125.03
24	c	511	CLA	CMC-C2C-C1C	2.22	128.50	125.03
24	b	603	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
24	C	512	CLA	C7-C6-C5	-2.21	107.36	113.26
24	c	512	CLA	C7-C6-C5	-2.21	107.36	113.26
24	D	401	CLA	CAA-CBA-CGA	2.21	119.48	113.21
24	d	401	CLA	CAA-CBA-CGA	2.21	119.48	113.21
24	B	610	CLA	CAA-CBA-CGA	-2.21	106.94	113.21
24	C	509	CLA	CMA-C3A-C2A	-2.21	105.44	113.98
34	E	101	LHG	C5-O7-C7	-2.21	112.52	117.80
30	D	411	LMG	C1-C2-C3	-2.21	105.37	110.01
30	d	411	LMG	C1-C2-C3	-2.21	105.37	110.01
24	B	615	CLA	CHD-C4C-NC	2.21	127.65	124.23
24	b	617	CLA	CHD-C4C-NC	2.21	127.65	124.23
28	A	411	PL9	C12-C13-C14	-2.20	122.58	127.62
28	a	411	PL9	C12-C13-C14	-2.20	122.58	127.62
24	c	509	CLA	CMA-C3A-C2A	-2.20	105.46	113.98
24	B	613	CLA	CHC-C4B-NB	2.20	127.35	124.05
24	C	511	CLA	C1-C2-C3	-2.20	122.59	126.20
24	c	511	CLA	C1-C2-C3	-2.20	122.59	126.20
24	B	616	CLA	CHA-C1A-NA	-2.20	121.41	126.39
24	b	618	CLA	CHA-C1A-NA	-2.20	121.41	126.39
24	b	612	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
26	t	102	BCR	C7-C8-C9	-2.20	122.98	126.23
24	b	612	CLA	CMC-C2C-C1C	2.20	128.47	125.03
26	T	101	BCR	C7-C8-C9	-2.20	122.98	126.23
24	B	606	CLA	CHA-C1A-NA	-2.20	121.42	126.39
24	b	608	CLA	CHA-C1A-NA	-2.20	121.42	126.39
24	B	604	CLA	CHA-C1A-NA	-2.20	121.42	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	CHA-C1A-NA	-2.20	121.42	126.39
24	B	601	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
24	B	609	CLA	CED-O2D-CGD	2.19	120.89	115.92
26	C	522	BCR	C2-C1-C6	2.19	113.63	110.44
26	c	522	BCR	C2-C1-C6	2.19	113.63	110.44
24	b	615	CLA	CHC-C4B-NB	2.19	127.34	124.05
27	f	101	SQD	C1-C2-C3	-2.19	105.39	110.01
24	C	509	CLA	O2A-CGA-CBA	2.19	118.52	111.83
24	c	509	CLA	O2A-CGA-CBA	2.19	118.52	111.83
24	b	611	CLA	CED-O2D-CGD	2.19	120.89	115.92
24	C	507	CLA	CMC-C2C-C3C	2.19	132.08	126.15
24	c	507	CLA	CMC-C2C-C3C	2.19	132.08	126.15
27	B	620	SQD	O5-C1-C2	-2.19	105.87	110.37
27	L	102	SQD	O5-C1-C2	-2.19	105.87	110.37
24	C	505	CLA	CHC-C1C-NC	2.19	127.61	124.31
24	c	505	CLA	CHC-C1C-NC	2.19	127.61	124.31
27	A	412	SQD	C45-O47-C7	2.19	123.04	117.80
27	a	412	SQD	C45-O47-C7	2.19	123.04	117.80
28	A	411	PL9	C20-C19-C18	-2.19	118.00	123.63
28	a	411	PL9	C20-C19-C18	-2.19	118.00	123.63
30	D	411	LMG	C22-C21-C20	-2.19	103.30	114.37
30	d	411	LMG	C22-C21-C20	-2.19	103.30	114.37
24	B	613	CLA	CMB-C2B-C3B	2.19	131.70	126.55
24	b	615	CLA	CMB-C2B-C3B	2.19	131.70	126.55
26	a	409	BCR	C24-C23-C22	-2.19	123.00	126.23
26	D	406	BCR	C38-C26-C27	-2.18	108.94	113.60
26	d	406	BCR	C38-C26-C27	-2.18	108.94	113.60
24	b	611	CLA	C4-C3-C5	2.18	119.02	115.23
34	L	101	LHG	C27-C26-C25	-2.18	103.33	114.37
24	D	401	CLA	CHD-C4C-NC	2.18	127.62	124.23
24	d	401	CLA	CHD-C4C-NC	2.18	127.62	124.23
31	c	517	DGD	O5D-C6D-C5D	-2.18	104.50	109.42
24	B	612	CLA	CHD-C4C-NC	2.18	127.61	124.23
24	b	614	CLA	CHD-C4C-NC	2.18	127.61	124.23
24	D	404	CLA	O2D-CGD-CBD	2.18	115.04	111.23
24	d	404	CLA	O2D-CGD-CBD	2.18	115.04	111.23
31	C	517	DGD	O5D-C6D-C5D	-2.18	104.51	109.42
24	B	603	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
24	b	605	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
24	B	606	CLA	CMA-C3A-C2A	-2.18	105.56	113.98
34	l	101	LHG	C27-C26-C25	-2.18	103.37	114.37
24	B	615	CLA	CBC-CAC-C3C	-2.17	106.53	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
24	b	608	CLA	CMA-C3A-C2A	-2.17	105.59	113.98
31	C	517	DGD	O6E-C1E-O5D	-2.17	104.92	110.04
24	d	401	CLA	C2A-C1A-CHA	-2.17	120.10	123.87
31	C	517	DGD	O5E-C6E-C5E	-2.17	103.95	111.33
30	c	501	LMG	C38-C37-C36	-2.17	103.42	114.37
27	F	101	SQD	C1-C2-C3	-2.17	105.45	110.01
24	B	616	CLA	C6-C5-C3	2.17	118.74	113.47
24	b	618	CLA	C6-C5-C3	2.17	118.74	113.47
24	B	609	CLA	C4-C3-C5	2.16	118.98	115.23
25	D	402	PHO	C3D-C4D-ND	2.16	110.48	107.71
25	d	402	PHO	C3D-C4D-ND	2.16	110.48	107.71
30	C	501	LMG	C38-C37-C36	-2.16	103.43	114.37
26	C	522	BCR	C40-C30-C25	2.16	113.64	110.24
26	c	522	BCR	C40-C30-C25	2.16	113.64	110.24
27	A	412	SQD	O48-C23-C24	2.16	118.42	111.83
27	a	412	SQD	O48-C23-C24	2.16	118.42	111.83
24	C	512	CLA	CAA-C2A-C1A	2.16	119.06	111.97
24	c	512	CLA	CAA-C2A-C1A	2.16	119.06	111.97
24	b	603	CLA	C4-C3-C5	2.16	118.98	115.23
31	C	519	DGD	CBB-CAB-C9B	-2.16	103.45	114.37
31	c	519	DGD	CBB-CAB-C9B	-2.16	103.45	114.37
31	c	517	DGD	O5E-C6E-C5E	-2.16	103.98	111.33
24	B	603	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
34	d	410	LHG	C18-C17-C16	-2.16	103.46	114.37
24	C	507	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
31	c	517	DGD	O6E-C1E-O5D	-2.16	104.94	110.04
24	A	408	CLA	OBD-CAD-C3D	-2.15	123.38	128.42
24	a	408	CLA	OBD-CAD-C3D	-2.15	123.38	128.42
34	D	410	LHG	C18-C17-C16	-2.15	103.48	114.37
34	D	408	LHG	O8-C6-C5	-2.15	102.19	108.40
31	c	517	DGD	C3G-C2G-C1G	-2.15	106.77	111.78
30	C	523	LMG	O2-C2-C1	-2.15	104.95	110.08
30	c	523	LMG	O2-C2-C1	-2.15	104.95	110.08
24	C	514	CLA	CMA-C3A-C2A	-2.15	105.67	113.98
24	c	514	CLA	CMA-C3A-C2A	-2.15	105.67	113.98
24	C	505	CLA	CMC-C2C-C1C	2.15	128.39	125.03
24	c	505	CLA	CMC-C2C-C1C	2.15	128.39	125.03
24	b	605	CLA	CBC-CAC-C3C	-2.15	106.59	112.42
26	A	409	BCR	C24-C23-C22	-2.15	123.06	126.23
24	D	401	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
34	d	408	LHG	O8-C6-C5	-2.15	102.21	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	511	CLA	O1D-CGD-CBD	-2.15	120.29	124.52
24	C	506	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
24	c	506	CLA	CMD-C2D-C3D	-2.14	122.77	127.69
24	c	507	CLA	CMA-C3A-C4A	-2.14	106.01	111.77
31	H	101	DGD	O3G-C3G-C2G	-2.14	105.61	110.82
31	h	101	DGD	O3G-C3G-C2G	-2.14	105.61	110.82
27	A	410	SQD	O48-C23-C24	2.14	118.36	111.83
27	a	410	SQD	O48-C23-C24	2.14	118.36	111.83
24	B	604	CLA	C11-C10-C8	-2.14	108.85	115.97
24	b	606	CLA	C11-C10-C8	-2.14	108.85	115.97
24	B	613	CLA	CHA-C1A-NA	-2.14	121.55	126.39
24	b	615	CLA	CHA-C1A-NA	-2.14	121.55	126.39
31	C	517	DGD	C3G-C2G-C1G	-2.14	106.80	111.78
24	B	604	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
24	B	601	CLA	C4-C3-C5	2.14	118.94	115.23
24	C	513	CLA	CMA-C3A-C2A	-2.13	105.73	113.98
24	c	513	CLA	CMA-C3A-C2A	-2.13	105.73	113.98
24	A	408	CLA	C5-C3-C2	-2.13	116.38	121.17
24	a	408	CLA	C5-C3-C2	-2.13	116.38	121.17
24	B	616	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
24	b	618	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
24	C	511	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
38	x	101	RRX	C37-C22-C23	2.13	121.34	118.09
24	c	509	CLA	CED-O2D-CGD	2.13	120.74	115.92
24	b	606	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
24	c	511	CLA	CHC-C4B-C3B	-2.12	118.15	127.37
38	X	101	RRX	C21-C20-C19	-2.12	117.05	123.20
38	x	101	RRX	C21-C20-C19	-2.12	117.05	123.20
26	A	409	BCR	C2-C1-C6	2.12	113.52	110.44
26	a	409	BCR	C2-C1-C6	2.12	113.52	110.44
24	C	511	CLA	CHC-C4B-C3B	-2.12	118.16	127.37
24	a	408	CLA	C7-C6-C5	-2.12	107.61	113.26
24	C	503	CLA	CHD-C4C-NC	2.12	127.52	124.23
24	B	609	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
24	b	611	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
30	B	621	LMG	C38-C37-C36	-2.12	103.66	114.37
30	b	622	LMG	C38-C37-C36	-2.12	103.66	114.37
24	C	509	CLA	CED-O2D-CGD	2.12	120.72	115.92
38	X	101	RRX	C37-C22-C23	2.12	121.32	118.09
38	x	101	RRX	C34-C9-C8	2.12	121.32	118.09
37	V	201	HEC	CHA-C1A-C2A	2.12	128.20	124.86
24	c	511	CLA	OBD-CAD-C3D	-2.11	123.47	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Z	101	LMT	C1B-O5B-C5B	2.11	117.85	113.72
24	C	511	CLA	OBD-CAD-C3D	-2.11	123.48	128.42
34	D	409	LHG	C20-C19-C18	-2.11	103.69	114.37
34	d	409	LHG	C20-C19-C18	-2.11	103.69	114.37
24	C	507	CLA	CAC-C3C-C4C	2.11	127.54	124.79
24	c	507	CLA	CAC-C3C-C4C	2.11	127.54	124.79
24	C	513	CLA	C16-C15-C13	-2.11	108.95	115.97
24	c	513	CLA	C16-C15-C13	-2.11	108.95	115.97
24	A	408	CLA	C7-C6-C5	-2.11	107.64	113.26
24	c	510	CLA	CHD-C4C-NC	2.11	127.50	124.23
24	B	613	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
24	b	615	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
24	B	606	CLA	O2A-CGA-CBA	2.11	118.25	111.83
24	b	608	CLA	O2A-CGA-CBA	2.11	118.25	111.83
24	B	603	CLA	CHB-C4A-NA	2.10	127.44	124.40
24	b	605	CLA	CHB-C4A-NA	2.10	127.44	124.40
32	z	101	LMT	C1B-O5B-C5B	2.10	117.83	113.72
37	V	201	HEC	CAA-CBA-CGA	-2.10	108.09	113.67
38	X	101	RRX	C34-C9-C8	2.10	121.30	118.09
24	D	404	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
24	d	404	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
30	C	523	LMG	C40-C39-C38	-2.09	103.78	114.37
30	c	523	LMG	C40-C39-C38	-2.09	103.78	114.37
24	C	513	CLA	CAA-C2A-C1A	2.09	118.83	111.97
24	c	513	CLA	CAA-C2A-C1A	2.09	118.83	111.97
37	v	201	HEC	CAA-CBA-CGA	-2.09	108.11	113.67
26	T	101	BCR	C2-C1-C6	2.09	113.48	110.44
26	t	102	BCR	C2-C1-C6	2.09	113.48	110.44
24	B	616	CLA	CHC-C1C-NC	2.09	127.46	124.31
24	b	618	CLA	CHC-C1C-NC	2.09	127.46	124.31
30	C	520	LMG	O8-C28-O10	-2.09	118.40	123.63
30	c	520	LMG	O8-C28-O10	-2.09	118.40	123.63
30	c	501	LMG	O2-C2-C1	-2.09	105.10	110.08
26	a	409	BCR	C20-C19-C18	-2.09	120.64	126.36
24	B	605	CLA	C4A-NA-C1A	-2.09	105.73	106.68
30	C	501	LMG	C7-O1-C1	-2.09	109.32	113.80
30	c	501	LMG	C7-O1-C1	-2.09	109.32	113.80
24	C	512	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
34	d	408	LHG	O8-C23-O10	-2.08	118.42	123.63
24	B	606	CLA	CED-O2D-CGD	2.08	120.64	115.92
24	c	503	CLA	CHD-C4C-NC	2.08	127.46	124.23
26	A	409	BCR	C20-C19-C18	-2.08	120.66	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	620	SQD	C1-C2-C3	-2.08	105.63	110.01
27	L	102	SQD	C1-C2-C3	-2.08	105.63	110.01
25	A	407	PHO	CBA-CAA-C2A	-2.08	107.65	113.78
30	C	501	LMG	O2-C2-C1	-2.08	105.12	110.08
35	E	103	HEM	C1B-NB-C4B	2.08	107.67	105.21
35	e	103	HEM	C1B-NB-C4B	2.08	107.67	105.21
24	B	612	CLA	CHB-C4A-NA	2.08	127.39	124.40
24	b	614	CLA	CHB-C4A-NA	2.08	127.39	124.40
26	C	515	BCR	C15-C14-C13	-2.07	124.37	127.28
31	C	517	DGD	C1E-O6E-C5E	2.07	117.77	113.72
26	J	104	BCR	C38-C26-C27	-2.07	109.17	113.60
26	j	104	BCR	C38-C26-C27	-2.07	109.17	113.60
24	C	506	CLA	CHD-C4C-NC	2.07	127.45	124.23
24	c	506	CLA	CHD-C4C-NC	2.07	127.45	124.23
24	D	404	CLA	C1D-CHD-C4C	-2.07	121.61	126.02
34	D	408	LHG	O8-C23-O10	-2.07	118.45	123.63
26	D	406	BCR	C30-C25-C26	-2.07	119.81	122.64
26	d	406	BCR	C30-C25-C26	-2.07	119.81	122.64
24	d	404	CLA	C1D-CHD-C4C	-2.07	121.62	126.02
26	B	618	BCR	C15-C14-C13	-2.07	124.38	127.28
26	b	620	BCR	C15-C14-C13	-2.07	124.38	127.28
24	b	608	CLA	CED-O2D-CGD	2.07	120.60	115.92
24	C	510	CLA	CHD-C4C-NC	2.06	127.43	124.23
37	v	201	HEC	CHA-C1A-C2A	2.06	128.12	124.86
25	a	407	PHO	CBA-CAA-C2A	-2.06	107.70	113.78
31	c	517	DGD	C1E-O6E-C5E	2.06	117.75	113.72
34	L	101	LHG	C20-C19-C18	-2.06	103.95	114.37
30	C	520	LMG	O6-C1-O1	-2.06	105.17	110.04
30	c	520	LMG	O6-C1-O1	-2.06	105.17	110.04
24	B	602	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
24	b	604	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
26	a	409	BCR	C38-C26-C27	-2.06	109.20	113.60
34	l	101	LHG	C20-C19-C18	-2.06	103.95	114.37
35	e	103	HEM	O2A-CGA-CBA	2.06	120.50	114.00
24	b	607	CLA	C4A-NA-C1A	-2.06	105.74	106.68
24	A	405	CLA	CMB-C2B-C3B	2.06	131.39	126.55
24	a	405	CLA	CMB-C2B-C3B	2.06	131.39	126.55
27	A	410	SQD	O48-C23-O10	-2.06	118.48	123.63
27	a	410	SQD	O48-C23-O10	-2.06	118.48	123.63
24	C	511	CLA	CHD-C4C-NC	2.06	127.42	124.23
24	c	511	CLA	CHD-C4C-NC	2.06	127.42	124.23
24	a	406	CLA	C6-C5-C3	-2.06	108.46	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	BCR	C35-C13-C14	-2.06	119.49	122.82
26	t	102	BCR	C35-C13-C14	-2.06	119.49	122.82
24	b	611	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
24	b	613	CLA	CMB-C2B-C3B	2.05	131.38	126.55
26	c	515	BCR	C15-C14-C13	-2.05	124.40	127.28
32	J	102	LMT	C1'-C2'-C3'	2.05	114.33	110.01
24	C	504	CLA	CHA-C1A-NA	-2.05	121.74	126.39
24	c	504	CLA	CHA-C1A-NA	-2.05	121.74	126.39
26	A	409	BCR	C38-C26-C27	-2.05	109.22	113.60
24	b	610	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
24	B	614	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
24	b	616	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
24	B	611	CLA	CMB-C2B-C3B	2.05	131.37	126.55
35	E	103	HEM	O2A-CGA-CBA	2.05	120.47	114.00
26	C	522	BCR	C38-C26-C27	-2.05	109.23	113.60
26	c	522	BCR	C38-C26-C27	-2.05	109.23	113.60
24	B	605	CLA	CMA-C3A-C2A	-2.05	106.07	113.98
24	b	607	CLA	CMA-C3A-C2A	-2.05	106.07	113.98
24	C	514	CLA	C1-O2A-CGA	2.05	121.60	116.65
24	c	514	CLA	C1-O2A-CGA	2.05	121.60	116.65
32	j	102	LMT	C1'-C2'-C3'	2.04	114.31	110.01
24	A	406	CLA	C6-C5-C3	-2.04	108.49	113.47
24	B	605	CLA	C6-C7-C8	-2.04	109.18	115.97
24	A	406	CLA	CHA-C1A-NA	-2.04	121.77	126.39
24	a	406	CLA	CHA-C1A-NA	-2.04	121.77	126.39
24	D	405	CLA	CHD-C4C-NC	2.04	127.40	124.23
24	d	405	CLA	CHD-C4C-NC	2.04	127.40	124.23
24	B	601	CLA	C1-O2A-CGA	2.04	121.59	116.65
31	C	519	DGD	O2G-C1B-C2B	2.04	115.89	111.48
31	c	519	DGD	O2G-C1B-C2B	2.04	115.89	111.48
34	E	101	LHG	C27-C26-C25	-2.04	104.07	114.37
24	b	603	CLA	C1-O2A-CGA	2.04	121.58	116.65
24	B	608	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
34	e	101	LHG	C27-C26-C25	-2.04	104.08	114.37
24	C	509	CLA	CHD-C4C-NC	2.04	127.39	124.23
24	c	509	CLA	CHD-C4C-NC	2.04	127.39	124.23
24	D	405	CLA	CAC-C3C-C4C	2.03	127.44	124.79
24	B	611	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
24	b	613	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
24	A	405	CLA	CAC-C3C-C4C	2.03	127.44	124.79
24	a	405	CLA	CAC-C3C-C4C	2.03	127.44	124.79
24	c	512	CLA	O1D-CGD-CBD	-2.03	120.51	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C6-C7-C8	-2.03	109.22	115.97
24	B	609	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
34	E	101	LHG	O8-C6-C5	-2.03	102.55	108.40
34	D	408	LHG	C18-C17-C16	-2.03	104.12	114.37
34	d	408	LHG	C18-C17-C16	-2.03	104.12	114.37
24	B	610	CLA	CHC-C1C-NC	2.03	127.36	124.31
26	J	104	BCR	C29-C30-C25	2.03	113.38	110.44
26	j	104	BCR	C29-C30-C25	2.03	113.38	110.44
27	F	101	SQD	O48-C23-O10	-2.03	118.56	123.63
24	b	612	CLA	CHC-C1C-NC	2.03	127.36	124.31
30	d	411	LMG	C17-C16-C15	-2.02	104.13	114.37
24	C	514	CLA	OBD-CAD-C3D	-2.02	123.68	128.42
24	c	514	CLA	OBD-CAD-C3D	-2.02	123.68	128.42
25	d	402	PHO	CMD-C2D-C3D	2.02	128.73	124.68
31	C	519	DGD	CAB-C9B-C8B	-2.02	104.14	114.37
31	c	519	DGD	CAB-C9B-C8B	-2.02	104.14	114.37
34	e	101	LHG	O8-C6-C5	-2.02	102.56	108.40
24	c	502	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
27	F	101	SQD	C45-O47-C7	2.02	122.64	117.80
27	f	101	SQD	C45-O47-C7	2.02	122.64	117.80
27	f	101	SQD	O48-C23-O10	-2.02	118.57	123.63
34	D	408	LHG	C20-C19-C18	-2.02	104.15	114.37
34	d	408	LHG	C20-C19-C18	-2.02	104.15	114.37
26	D	406	BCR	C2-C1-C6	2.02	113.38	110.44
26	d	406	BCR	C2-C1-C6	2.02	113.38	110.44
24	B	606	CLA	C1-O2A-CGA	2.02	121.54	116.65
24	b	608	CLA	C1-O2A-CGA	2.02	121.54	116.65
24	C	512	CLA	CMB-C2B-C1B	2.02	128.49	125.42
24	c	512	CLA	CMB-C2B-C1B	2.02	128.49	125.42
27	F	101	SQD	O47-C7-O49	-2.02	118.99	123.70
30	D	411	LMG	C17-C16-C15	-2.01	104.19	114.37
24	B	616	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
24	B	605	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
24	b	607	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
24	b	618	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
27	f	101	SQD	O47-C7-O49	-2.01	119.00	123.70
24	c	513	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
25	D	402	PHO	CMD-C2D-C3D	2.01	128.70	124.68
26	C	515	BCR	C16-C17-C18	-2.01	124.46	127.28
26	c	515	BCR	C16-C17-C18	-2.01	124.46	127.28
24	B	613	CLA	CED-O2D-CGD	2.01	120.47	115.92
24	b	615	CLA	CED-O2D-CGD	2.01	120.47	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	521	LMT	O5'-C1'-O1'	-2.01	105.30	110.04
32	c	521	LMT	O5'-C1'-O1'	-2.01	105.30	110.04
24	c	502	CLA	C4A-NA-C1A	-2.00	105.77	106.68
24	b	604	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
27	a	410	SQD	C46-C45-C44	2.00	116.45	111.78

All (60) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	601	CLA	ND
24	B	602	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	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	C	514	CLA	ND
24	D	401	CLA	ND
24	D	404	CLA	ND
24	a	405	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	608	CLA	ND
24	b	609	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	b	617	CLA	ND
24	b	618	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	c	514	CLA	ND
24	d	401	CLA	ND
24	d	404	CLA	ND

All (1472) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C14-C13-C15-C16
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2B-C3B-CAB-CBB
24	B	615	CLA	C4B-C3B-CAB-CBB
24	B	616	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	506	CLA	C4B-C3B-CAB-CBB
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	C2-C1-O2A-CGA
24	b	603	CLA	C14-C13-C15-C16
24	b	616	CLA	CAD-CBD-CGD-O1D
24	b	616	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	C2B-C3B-CAB-CBB
24	b	617	CLA	C4B-C3B-CAB-CBB
24	b	618	CLA	CHA-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O1D
24	c	503	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	C4B-C3B-CAB-CBB
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	C2-C1-O2A-CGA
26	A	409	BCR	C36-C18-C19-C20
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	C	516	BCR	C11-C12-C13-C14
26	C	516	BCR	C11-C12-C13-C35
26	C	522	BCR	C11-C10-C9-C8
26	C	522	BCR	C11-C10-C9-C34
26	D	406	BCR	C7-C8-C9-C10
26	D	406	BCR	C21-C22-C23-C24
26	D	406	BCR	C22-C23-C24-C25
26	J	104	BCR	C5-C6-C7-C8
26	J	104	BCR	C7-C8-C9-C34
26	J	104	BCR	C21-C22-C23-C24
26	J	104	BCR	C37-C22-C23-C24
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C7-C8-C9-C10
26	T	101	BCR	C21-C22-C23-C24
26	a	409	BCR	C36-C18-C19-C20
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	516	BCR	C11-C12-C13-C14
26	c	516	BCR	C11-C12-C13-C35
26	c	522	BCR	C11-C10-C9-C8
26	c	522	BCR	C11-C10-C9-C34
26	d	406	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	d	406	BCR	C21-C22-C23-C24
26	d	406	BCR	C22-C23-C24-C25
26	j	104	BCR	C5-C6-C7-C8
26	j	104	BCR	C7-C8-C9-C34
26	j	104	BCR	C21-C22-C23-C24
26	j	104	BCR	C37-C22-C23-C24
26	t	102	BCR	C1-C6-C7-C8
26	t	102	BCR	C7-C8-C9-C10
26	t	102	BCR	C21-C22-C23-C24
27	A	412	SQD	C5-C6-S-O7
27	A	412	SQD	C5-C6-S-O8
27	A	412	SQD	C5-C6-S-O9
27	B	620	SQD	O10-C23-O48-C46
27	B	620	SQD	C24-C23-O48-C46
27	L	102	SQD	O10-C23-O48-C46
27	L	102	SQD	C24-C23-O48-C46
27	a	412	SQD	C5-C6-S-O7
27	a	412	SQD	C5-C6-S-O8
27	a	412	SQD	C5-C6-S-O9
28	A	411	PL9	C12-C13-C14-C16
28	A	411	PL9	C27-C28-C29-C30
28	A	411	PL9	C27-C28-C29-C31
28	A	411	PL9	C37-C38-C39-C40
28	D	407	PL9	C42-C43-C44-C45
28	D	407	PL9	C44-C46-C47-C48
28	a	411	PL9	C12-C13-C14-C16
28	a	411	PL9	C27-C28-C29-C30
28	a	411	PL9	C27-C28-C29-C31
28	a	411	PL9	C37-C38-C39-C40
28	d	407	PL9	C42-C43-C44-C45
28	d	407	PL9	C44-C46-C47-C48
34	D	408	LHG	C3-O3-P-O4
34	D	409	LHG	O1-C1-C2-C3
34	D	409	LHG	O2-C2-C3-O3
34	D	409	LHG	C3-O3-P-O5
34	D	409	LHG	C3-O3-P-O6
34	D	409	LHG	C4-O6-P-O3
34	D	409	LHG	C4-O6-P-O4
34	D	409	LHG	C4-O6-P-O5
34	E	101	LHG	C3-O3-P-O5
34	E	101	LHG	C3-O3-P-O6
34	L	101	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
34	d	408	LHG	C3-O3-P-O4
34	d	409	LHG	O1-C1-C2-C3
34	d	409	LHG	O2-C2-C3-O3
34	d	409	LHG	C3-O3-P-O5
34	d	409	LHG	C3-O3-P-O6
34	d	409	LHG	C4-O6-P-O3
34	d	409	LHG	C4-O6-P-O4
34	d	409	LHG	C4-O6-P-O5
34	e	101	LHG	C3-O3-P-O5
34	e	101	LHG	C3-O3-P-O6
34	l	101	LHG	C4-O6-P-O3
37	V	201	HEC	C2B-C3B-CAB-CBB
37	V	201	HEC	C4B-C3B-CAB-CBB
37	V	201	HEC	C2C-C3C-CAC-CBC
37	V	201	HEC	C4C-C3C-CAC-CBC
37	v	201	HEC	C2B-C3B-CAB-CBB
37	v	201	HEC	C4B-C3B-CAB-CBB
37	v	201	HEC	C2C-C3C-CAC-CBC
37	v	201	HEC	C4C-C3C-CAC-CBC
28	D	407	PL9	C47-C48-C49-C51
28	d	407	PL9	C47-C48-C49-C51
27	F	101	SQD	O10-C23-O48-C46
27	f	101	SQD	O10-C23-O48-C46
32	C	521	LMT	C3'-C4'-O1B-C1B
32	c	521	LMT	C3'-C4'-O1B-C1B
24	B	614	CLA	C3-C5-C6-C7
24	B	615	CLA	C3-C5-C6-C7
24	b	616	CLA	C3-C5-C6-C7
24	b	617	CLA	C3-C5-C6-C7
27	F	101	SQD	C24-C23-O48-C46
27	f	101	SQD	C24-C23-O48-C46
32	Z	101	LMT	O5'-C5'-C6'-O6'
32	z	101	LMT	O5'-C5'-C6'-O6'
24	B	601	CLA	C4-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6
24	B	605	CLA	C4-C3-C5-C6
24	D	405	CLA	C4-C3-C5-C6
24	b	603	CLA	C4-C3-C5-C6
24	b	605	CLA	C4-C3-C5-C6
24	b	607	CLA	C4-C3-C5-C6
24	d	405	CLA	C4-C3-C5-C6
24	B	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C2-C3-C5-C6
24	D	405	CLA	C2-C3-C5-C6
24	b	605	CLA	C2-C3-C5-C6
24	b	607	CLA	C2-C3-C5-C6
24	d	405	CLA	C2-C3-C5-C6
28	A	411	PL9	C18-C19-C21-C22
28	A	411	PL9	C28-C29-C31-C32
28	a	411	PL9	C18-C19-C21-C22
28	a	411	PL9	C28-C29-C31-C32
28	D	407	PL9	C47-C48-C49-C50
28	d	407	PL9	C47-C48-C49-C50
24	B	601	CLA	C3-C5-C6-C7
24	b	603	CLA	C3-C5-C6-C7
24	C	510	CLA	CBA-CGA-O2A-C1
24	c	510	CLA	CBA-CGA-O2A-C1
28	A	411	PL9	C22-C23-C24-C25
28	a	411	PL9	C22-C23-C24-C25
28	A	411	PL9	C17-C18-C19-C21
28	A	411	PL9	C22-C23-C24-C26
28	a	411	PL9	C17-C18-C19-C21
28	a	411	PL9	C22-C23-C24-C26
30	C	523	LMG	C4-C5-C6-O5
30	c	523	LMG	C4-C5-C6-O5
30	C	523	LMG	C29-C28-O8-C9
30	c	523	LMG	C29-C28-O8-C9
32	J	102	LMT	O5'-C5'-C6'-O6'
32	j	102	LMT	O5'-C5'-C6'-O6'
32	Z	101	LMT	C4'-C5'-C6'-O6'
32	z	101	LMT	C4'-C5'-C6'-O6'
24	A	408	CLA	C4-C3-C5-C6
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
24	C	510	CLA	O1A-CGA-O2A-C1
24	c	510	CLA	O1A-CGA-O2A-C1
28	A	411	PL9	C24-C26-C27-C28
28	A	411	PL9	C44-C46-C47-C48
28	D	407	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
28	a	411	PL9	C24-C26-C27-C28
28	a	411	PL9	C44-C46-C47-C48
28	d	407	PL9	C39-C41-C42-C43
28	A	411	PL9	C47-C48-C49-C50
28	a	411	PL9	C47-C48-C49-C50
27	A	410	SQD	C12-C13-C14-C15
24	B	604	CLA	CBD-CGD-O2D-CED
24	C	514	CLA	CBD-CGD-O2D-CED
24	b	606	CLA	CBD-CGD-O2D-CED
24	c	514	CLA	CBD-CGD-O2D-CED
27	a	410	SQD	C12-C13-C14-C15
30	C	523	LMG	O6-C5-C6-O5
30	c	523	LMG	O6-C5-C6-O5
25	D	402	PHO	CBD-CGD-O2D-CED
25	d	402	PHO	CBD-CGD-O2D-CED
24	C	508	CLA	C4-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
28	A	411	PL9	C20-C19-C21-C22
28	a	411	PL9	C20-C19-C21-C22
24	B	601	CLA	C2-C3-C5-C6
24	C	508	CLA	C2-C3-C5-C6
24	b	603	CLA	C2-C3-C5-C6
24	c	508	CLA	C2-C3-C5-C6
24	B	607	CLA	C6-C7-C8-C9
24	C	503	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	b	609	CLA	C6-C7-C8-C9
24	c	503	CLA	C14-C13-C15-C16
24	c	505	CLA	C11-C12-C13-C14
25	A	407	PHO	C14-C13-C15-C16
25	a	407	PHO	C14-C13-C15-C16
26	B	618	BCR	C7-C8-C9-C34
26	C	515	BCR	C7-C8-C9-C34
26	C	515	BCR	C11-C12-C13-C35
26	C	515	BCR	C37-C22-C23-C24
26	C	516	BCR	C7-C8-C9-C34
26	C	522	BCR	C11-C12-C13-C35
26	D	406	BCR	C37-C22-C23-C24
26	T	101	BCR	C7-C8-C9-C34
26	T	101	BCR	C37-C22-C23-C24
26	b	620	BCR	C7-C8-C9-C34
26	c	515	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
26	c	515	BCR	C11-C12-C13-C35
26	c	515	BCR	C37-C22-C23-C24
26	c	516	BCR	C7-C8-C9-C34
26	c	522	BCR	C11-C12-C13-C35
26	d	406	BCR	C37-C22-C23-C24
26	t	102	BCR	C7-C8-C9-C34
26	t	102	BCR	C37-C22-C23-C24
34	D	408	LHG	C23-C24-C25-C26
34	d	408	LHG	C23-C24-C25-C26
32	M	101	LMT	O5'-C5'-C6'-O6'
32	m	102	LMT	O5'-C5'-C6'-O6'
34	D	409	LHG	O1-C1-C2-O2
34	d	409	LHG	O1-C1-C2-O2
24	B	613	CLA	C11-C10-C8-C7
24	b	615	CLA	C11-C10-C8-C7
30	B	621	LMG	C28-C29-C30-C31
30	b	622	LMG	C28-C29-C30-C31
28	A	411	PL9	C9-C11-C12-C13
28	a	411	PL9	C9-C11-C12-C13
24	B	604	CLA	C3-C5-C6-C7
24	C	514	CLA	C3-C5-C6-C7
24	b	606	CLA	C3-C5-C6-C7
24	c	514	CLA	C3-C5-C6-C7
24	A	406	CLA	C15-C16-C17-C18
24	a	406	CLA	C15-C16-C17-C18
27	F	101	SQD	C7-C8-C9-C10
27	f	101	SQD	C7-C8-C9-C10
30	C	501	LMG	C28-C29-C30-C31
30	C	520	LMG	C28-C29-C30-C31
30	c	501	LMG	C28-C29-C30-C31
30	c	520	LMG	C28-C29-C30-C31
24	A	408	CLA	C8-C10-C11-C12
24	a	408	CLA	C8-C10-C11-C12
24	B	606	CLA	C2A-CAA-CBA-CGA
24	b	608	CLA	C2A-CAA-CBA-CGA
24	B	614	CLA	C10-C11-C12-C13
24	D	405	CLA	C5-C6-C7-C8
24	b	616	CLA	C10-C11-C12-C13
24	c	509	CLA	C8-C10-C11-C12
24	d	405	CLA	C5-C6-C7-C8
31	C	518	DGD	C1A-C2A-C3A-C4A
31	c	518	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	C23-C24-C25-C26
34	e	101	LHG	C23-C24-C25-C26
24	C	512	CLA	C3-C5-C6-C7
24	c	512	CLA	C3-C5-C6-C7
32	Z	101	LMT	O5'-C1'-O1'-C1
32	z	101	LMT	O5'-C1'-O1'-C1
32	J	102	LMT	C4'-C5'-C6'-O6'
32	j	102	LMT	C4'-C5'-C6'-O6'
24	C	504	CLA	C15-C16-C17-C18
24	C	509	CLA	C8-C10-C11-C12
24	C	509	CLA	C10-C11-C12-C13
24	C	513	CLA	C15-C16-C17-C18
24	C	514	CLA	C5-C6-C7-C8
24	c	504	CLA	C15-C16-C17-C18
24	c	509	CLA	C10-C11-C12-C13
24	c	513	CLA	C15-C16-C17-C18
24	c	514	CLA	C5-C6-C7-C8
24	B	613	CLA	C8-C10-C11-C12
24	b	615	CLA	C8-C10-C11-C12
30	C	523	LMG	O9-C10-O7-C8
30	c	523	LMG	O9-C10-O7-C8
24	B	601	CLA	C15-C16-C17-C18
24	b	603	CLA	C15-C16-C17-C18
27	B	620	SQD	C23-C24-C25-C26
27	L	102	SQD	C23-C24-C25-C26
32	C	521	LMT	O5B-C5B-C6B-O6B
32	c	521	LMT	O5B-C5B-C6B-O6B
24	C	513	CLA	CBA-CGA-O2A-C1
24	c	513	CLA	CBA-CGA-O2A-C1
34	D	409	LHG	C1-C2-C3-O3
34	d	409	LHG	C1-C2-C3-O3
24	B	610	CLA	C15-C16-C17-C18
24	b	612	CLA	C15-C16-C17-C18
32	Z	101	LMT	C2B-C1B-O1B-C4'
32	z	101	LMT	C2B-C1B-O1B-C4'
32	Z	101	LMT	O1'-C1-C2-C3
32	z	101	LMT	O1'-C1-C2-C3
24	B	608	CLA	C13-C15-C16-C17
24	b	610	CLA	C13-C15-C16-C17
24	C	512	CLA	CBA-CGA-O2A-C1
24	c	512	CLA	CBA-CGA-O2A-C1
32	z	101	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
27	A	410	SQD	C7-C8-C9-C10
27	a	410	SQD	C7-C8-C9-C10
27	F	101	SQD	C8-C7-O47-C45
27	f	101	SQD	C8-C7-O47-C45
30	C	501	LMG	C11-C10-O7-C8
30	c	501	LMG	C11-C10-O7-C8
32	Z	101	LMT	O5B-C5B-C6B-O6B
28	D	407	PL9	C32-C33-C34-C35
28	d	407	PL9	C32-C33-C34-C35
31	C	518	DGD	C2E-C1E-O5D-C6D
31	c	518	DGD	C2E-C1E-O5D-C6D
32	Z	101	LMT	C2'-C1'-O1'-C1
32	z	101	LMT	C2'-C1'-O1'-C1
26	A	409	BCR	C11-C10-C9-C34
26	A	409	BCR	C20-C21-C22-C37
26	B	617	BCR	C11-C10-C9-C34
26	B	619	BCR	C16-C17-C18-C36
26	C	515	BCR	C20-C21-C22-C37
26	T	101	BCR	C20-C21-C22-C37
26	a	409	BCR	C11-C10-C9-C34
26	a	409	BCR	C20-C21-C22-C37
26	b	619	BCR	C11-C10-C9-C34
26	b	621	BCR	C16-C17-C18-C36
26	c	515	BCR	C20-C21-C22-C37
26	t	102	BCR	C20-C21-C22-C37
26	B	618	BCR	C11-C12-C13-C35
26	B	618	BCR	C37-C22-C23-C24
26	C	515	BCR	C36-C18-C19-C20
26	J	104	BCR	C36-C18-C19-C20
26	b	620	BCR	C11-C12-C13-C35
26	b	620	BCR	C37-C22-C23-C24
26	c	515	BCR	C36-C18-C19-C20
26	j	104	BCR	C36-C18-C19-C20
32	Z	101	LMT	O5B-C1B-O1B-C4'
32	z	101	LMT	O5B-C1B-O1B-C4'
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	513	CLA	O1A-CGA-O2A-C1
24	C	508	CLA	C2A-CAA-CBA-CGA
24	c	508	CLA	C2A-CAA-CBA-CGA
24	C	512	CLA	C8-C10-C11-C12
24	D	404	CLA	C15-C16-C17-C18
24	c	512	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	d	404	CLA	C15-C16-C17-C18
34	D	410	LHG	O1-C1-C2-C3
34	E	101	LHG	O1-C1-C2-C3
34	d	410	LHG	O1-C1-C2-C3
34	e	101	LHG	O1-C1-C2-C3
24	C	502	CLA	C16-C17-C18-C19
24	C	511	CLA	C16-C17-C18-C19
24	C	513	CLA	C16-C17-C18-C19
24	c	502	CLA	C16-C17-C18-C19
24	c	511	CLA	C16-C17-C18-C19
24	c	513	CLA	C16-C17-C18-C19
26	A	409	BCR	C20-C21-C22-C23
26	B	619	BCR	C11-C10-C9-C8
26	C	515	BCR	C20-C21-C22-C23
26	T	101	BCR	C11-C10-C9-C8
26	T	101	BCR	C20-C21-C22-C23
26	a	409	BCR	C20-C21-C22-C23
26	b	621	BCR	C11-C10-C9-C8
26	c	515	BCR	C20-C21-C22-C23
26	t	102	BCR	C11-C10-C9-C8
26	t	102	BCR	C20-C21-C22-C23
31	C	518	DGD	O6D-C1D-O3G-C3G
31	C	518	DGD	O6E-C1E-O5D-C6D
31	c	518	DGD	O6D-C1D-O3G-C3G
31	c	518	DGD	O6E-C1E-O5D-C6D
24	B	603	CLA	CBD-CGD-O2D-CED
24	C	503	CLA	CBD-CGD-O2D-CED
24	b	605	CLA	CBD-CGD-O2D-CED
24	c	503	CLA	CBD-CGD-O2D-CED
24	C	507	CLA	C16-C17-C18-C19
24	C	511	CLA	C16-C17-C18-C20
24	c	507	CLA	C16-C17-C18-C19
24	c	511	CLA	C16-C17-C18-C20
27	L	102	SQD	C11-C10-C9-C8
30	b	622	LMG	C33-C34-C35-C36
27	B	620	SQD	C11-C10-C9-C8
27	F	101	SQD	C34-C35-C36-C37
27	f	101	SQD	C34-C35-C36-C37
30	B	621	LMG	C35-C36-C37-C38
30	b	622	LMG	C35-C36-C37-C38
31	C	517	DGD	C2A-C3A-C4A-C5A
30	B	621	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	C	518	DGD	C6B-C7B-C8B-C9B
31	H	101	DGD	CAA-CBA-CCA-CDA
31	c	517	DGD	C2A-C3A-C4A-C5A
31	c	518	DGD	C6B-C7B-C8B-C9B
31	h	101	DGD	CAA-CBA-CCA-CDA
24	C	512	CLA	O1A-CGA-O2A-C1
24	c	512	CLA	O1A-CGA-O2A-C1
27	A	410	SQD	C10-C11-C12-C13
27	a	410	SQD	C10-C11-C12-C13
30	B	621	LMG	C36-C37-C38-C39
30	C	501	LMG	C35-C36-C37-C38
30	C	520	LMG	C12-C13-C14-C15
30	b	622	LMG	C36-C37-C38-C39
30	c	501	LMG	C35-C36-C37-C38
30	c	520	LMG	C12-C13-C14-C15
34	D	408	LHG	C27-C28-C29-C30
34	d	408	LHG	C27-C28-C29-C30
32	Z	101	LMT	C2-C1-O1'-C1'
32	z	101	LMT	C2-C1-O1'-C1'
24	B	602	CLA	C4B-C3B-CAB-CBB
24	b	604	CLA	C4B-C3B-CAB-CBB
34	D	410	LHG	C12-C13-C14-C15
34	D	410	LHG	C13-C14-C15-C16
34	d	410	LHG	C12-C13-C14-C15
34	d	410	LHG	C13-C14-C15-C16
34	D	408	LHG	C29-C30-C31-C32
34	E	101	LHG	C27-C28-C29-C30
30	B	621	LMG	C15-C16-C17-C18
31	c	517	DGD	C3A-C4A-C5A-C6A
34	d	408	LHG	C29-C30-C31-C32
34	e	101	LHG	C27-C28-C29-C30
24	A	408	CLA	C11-C12-C13-C15
24	a	408	CLA	C11-C12-C13-C15
27	F	101	SQD	C9-C10-C11-C12
27	f	101	SQD	C9-C10-C11-C12
30	C	501	LMG	C39-C40-C41-C42
30	b	622	LMG	C15-C16-C17-C18
30	c	501	LMG	C39-C40-C41-C42
31	C	517	DGD	C3A-C4A-C5A-C6A
30	C	520	LMG	C10-C11-C12-C13
30	c	520	LMG	C10-C11-C12-C13
34	E	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	e	101	LHG	C7-C8-C9-C10
32	C	521	LMT	C1-C2-C3-C4
32	c	521	LMT	C1-C2-C3-C4
30	D	411	LMG	C30-C31-C32-C33
30	d	411	LMG	C30-C31-C32-C33
31	C	518	DGD	C4B-C5B-C6B-C7B
24	b	606	CLA	O1A-CGA-O2A-C1
30	b	622	LMG	C18-C19-C20-C21
31	c	518	DGD	C4B-C5B-C6B-C7B
30	B	621	LMG	C18-C19-C20-C21
24	D	401	CLA	C2C-C3C-CAC-CBC
38	X	101	RRX	C9-C10-C11-C12
38	x	101	RRX	C9-C10-C11-C12
24	B	615	CLA	C16-C17-C18-C19
24	C	502	CLA	C16-C17-C18-C20
24	b	617	CLA	C16-C17-C18-C19
24	c	502	CLA	C16-C17-C18-C20
24	B	604	CLA	O1A-CGA-O2A-C1
27	A	412	SQD	C27-C28-C29-C30
27	a	412	SQD	C27-C28-C29-C30
30	C	523	LMG	C12-C13-C14-C15
30	c	523	LMG	C12-C13-C14-C15
24	d	401	CLA	C2C-C3C-CAC-CBC
30	B	621	LMG	C34-C35-C36-C37
30	C	501	LMG	C37-C38-C39-C40
30	b	622	LMG	C34-C35-C36-C37
30	c	501	LMG	C37-C38-C39-C40
24	B	604	CLA	CBA-CGA-O2A-C1
24	b	606	CLA	CBA-CGA-O2A-C1
30	C	523	LMG	O1-C7-C8-C9
30	c	523	LMG	O1-C7-C8-C9
30	C	520	LMG	C31-C32-C33-C34
30	c	520	LMG	C31-C32-C33-C34
31	C	518	DGD	C6A-C7A-C8A-C9A
31	c	518	DGD	C6A-C7A-C8A-C9A
34	E	101	LHG	C17-C18-C19-C20
34	e	101	LHG	C17-C18-C19-C20
34	D	408	LHG	C7-C8-C9-C10
34	d	408	LHG	C7-C8-C9-C10
27	B	620	SQD	C28-C29-C30-C31
27	L	102	SQD	C28-C29-C30-C31
30	B	621	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
30	b	622	LMG	C38-C39-C40-C41
34	d	410	LHG	C28-C29-C30-C31
34	D	410	LHG	C28-C29-C30-C31
34	E	101	LHG	C16-C17-C18-C19
34	e	101	LHG	C16-C17-C18-C19
27	B	620	SQD	C13-C14-C15-C16
27	L	102	SQD	C13-C14-C15-C16
27	L	102	SQD	C16-C17-C18-C19
27	B	620	SQD	C16-C17-C18-C19
24	A	408	CLA	C16-C17-C18-C19
24	C	510	CLA	C16-C17-C18-C20
24	a	408	CLA	C16-C17-C18-C19
24	c	510	CLA	C16-C17-C18-C20
24	C	506	CLA	C2B-C3B-CAB-CBB
24	c	506	CLA	C2B-C3B-CAB-CBB
26	C	515	BCR	C5-C6-C7-C8
26	J	104	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	c	515	BCR	C5-C6-C7-C8
26	j	104	BCR	C1-C6-C7-C8
26	t	102	BCR	C5-C6-C7-C8
38	X	101	RRX	C23-C24-C25-C30
38	x	101	RRX	C23-C24-C25-C30
24	C	504	CLA	CBD-CGD-O2D-CED
24	c	504	CLA	CBD-CGD-O2D-CED
24	B	606	CLA	C15-C16-C17-C18
24	b	608	CLA	C15-C16-C17-C18
25	D	402	PHO	O1D-CGD-O2D-CED
25	d	402	PHO	O1D-CGD-O2D-CED
30	C	523	LMG	C31-C32-C33-C34
30	c	523	LMG	C31-C32-C33-C34
24	D	401	CLA	C15-C16-C17-C18
24	d	401	CLA	C15-C16-C17-C18
27	B	620	SQD	C24-C25-C26-C27
27	L	102	SQD	C24-C25-C26-C27
31	H	101	DGD	C5B-C6B-C7B-C8B
31	h	101	DGD	C5B-C6B-C7B-C8B
27	A	412	SQD	C25-C26-C27-C28
27	a	412	SQD	C25-C26-C27-C28
30	D	411	LMG	C37-C38-C39-C40
30	b	622	LMG	C30-C31-C32-C33
34	D	408	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
34	d	408	LHG	C30-C31-C32-C33
30	B	621	LMG	C30-C31-C32-C33
30	C	501	LMG	C18-C19-C20-C21
30	c	501	LMG	C18-C19-C20-C21
30	d	411	LMG	C37-C38-C39-C40
24	A	408	CLA	C5-C6-C7-C8
24	D	405	CLA	C13-C15-C16-C17
24	a	408	CLA	C5-C6-C7-C8
27	B	620	SQD	C30-C31-C32-C33
27	L	102	SQD	C30-C31-C32-C33
30	C	523	LMG	C18-C19-C20-C21
30	c	523	LMG	C18-C19-C20-C21
30	d	411	LMG	C35-C36-C37-C38
30	D	411	LMG	C35-C36-C37-C38
30	C	523	LMG	C17-C18-C19-C20
30	c	501	LMG	C30-C31-C32-C33
30	c	523	LMG	C17-C18-C19-C20
31	C	518	DGD	C3B-C4B-C5B-C6B
31	C	519	DGD	CAB-CBB-CCB-CDB
31	c	518	DGD	C3B-C4B-C5B-C6B
31	c	519	DGD	CAB-CBB-CCB-CDB
30	C	501	LMG	C30-C31-C32-C33
30	C	523	LMG	C11-C10-O7-C8
30	c	523	LMG	C11-C10-O7-C8
24	B	612	CLA	C10-C11-C12-C13
24	b	614	CLA	C10-C11-C12-C13
24	d	405	CLA	C13-C15-C16-C17
26	A	409	BCR	C7-C8-C9-C34
26	a	409	BCR	C7-C8-C9-C34
31	C	518	DGD	C4A-C5A-C6A-C7A
31	C	518	DGD	C8A-C9A-CAA-CBA
31	c	518	DGD	C4A-C5A-C6A-C7A
31	c	518	DGD	C8A-C9A-CAA-CBA
30	C	523	LMG	C8-C7-O1-C1
30	c	523	LMG	C8-C7-O1-C1
32	C	521	LMT	C4'-C5'-C6'-O6'
32	c	521	LMT	C4'-C5'-C6'-O6'
32	C	521	LMT	C6-C7-C8-C9
32	c	521	LMT	C6-C7-C8-C9
24	A	408	CLA	C16-C17-C18-C20
24	C	507	CLA	C16-C17-C18-C20
24	C	513	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	a	408	CLA	C16-C17-C18-C20
24	c	507	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C20
30	C	520	LMG	C11-C12-C13-C14
30	c	520	LMG	C11-C12-C13-C14
25	A	407	PHO	C4-C3-C5-C6
25	a	407	PHO	C4-C3-C5-C6
28	D	407	PL9	C45-C44-C46-C47
28	d	407	PL9	C45-C44-C46-C47
27	B	620	SQD	C14-C15-C16-C17
27	L	102	SQD	C14-C15-C16-C17
30	B	621	LMG	C17-C18-C19-C20
30	C	501	LMG	C16-C17-C18-C19
30	b	622	LMG	C17-C18-C19-C20
30	C	520	LMG	C34-C35-C36-C37
30	c	501	LMG	C16-C17-C18-C19
30	c	520	LMG	C34-C35-C36-C37
31	C	518	DGD	C3A-C4A-C5A-C6A
31	c	518	DGD	C3A-C4A-C5A-C6A
30	C	523	LMG	O10-C28-O8-C9
30	c	523	LMG	O10-C28-O8-C9
27	A	412	SQD	C11-C12-C13-C14
27	a	412	SQD	C11-C12-C13-C14
31	C	518	DGD	C5B-C6B-C7B-C8B
31	c	518	DGD	C5B-C6B-C7B-C8B
34	E	101	LHG	C34-C35-C36-C37
30	C	501	LMG	C12-C13-C14-C15
34	e	101	LHG	C34-C35-C36-C37
24	B	604	CLA	C5-C6-C7-C8
24	b	606	CLA	C5-C6-C7-C8
24	B	615	CLA	C16-C17-C18-C20
24	b	617	CLA	C16-C17-C18-C20
31	C	518	DGD	C9A-CAA-CBA-CCA
31	c	518	DGD	C9A-CAA-CBA-CCA
30	D	411	LMG	C14-C15-C16-C17
30	c	501	LMG	C12-C13-C14-C15
30	d	411	LMG	C14-C15-C16-C17
31	C	517	DGD	CBA-CCA-CDA-CEA
31	C	519	DGD	CBA-CCA-CDA-CEA
31	c	517	DGD	CBA-CCA-CDA-CEA
31	c	519	DGD	CBA-CCA-CDA-CEA
24	B	606	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	b	608	CLA	C13-C15-C16-C17
31	H	101	DGD	CBA-CCA-CDA-CEA
31	h	101	DGD	CBA-CCA-CDA-CEA
34	E	101	LHG	C15-C16-C17-C18
34	e	101	LHG	C15-C16-C17-C18
30	D	411	LMG	O6-C5-C6-O5
30	d	411	LMG	O6-C5-C6-O5
27	A	412	SQD	O6-C44-C45-O47
27	a	412	SQD	O6-C44-C45-O47
30	D	411	LMG	C17-C18-C19-C20
30	d	411	LMG	C17-C18-C19-C20
31	C	519	DGD	C7B-C8B-C9B-CAB
31	c	519	DGD	C7B-C8B-C9B-CAB
34	E	101	LHG	C18-C19-C20-C21
27	B	620	SQD	C11-C12-C13-C14
27	L	102	SQD	C11-C12-C13-C14
34	e	101	LHG	C18-C19-C20-C21
25	A	407	PHO	C2-C3-C5-C6
25	a	407	PHO	C2-C3-C5-C6
30	d	411	LMG	C36-C37-C38-C39
31	C	518	DGD	CCA-CDA-CEA-CFA
31	c	518	DGD	CCA-CDA-CEA-CFA
32	Z	101	LMT	C6-C7-C8-C9
32	z	101	LMT	C6-C7-C8-C9
24	C	502	CLA	C2A-CAA-CBA-CGA
24	c	502	CLA	C2A-CAA-CBA-CGA
30	D	411	LMG	C36-C37-C38-C39
24	B	604	CLA	O1D-CGD-O2D-CED
24	b	606	CLA	O1D-CGD-O2D-CED
27	A	412	SQD	C10-C11-C12-C13
27	a	412	SQD	C10-C11-C12-C13
24	B	615	CLA	C8-C10-C11-C12
24	b	617	CLA	C8-C10-C11-C12
27	A	412	SQD	C23-C24-C25-C26
27	a	412	SQD	C23-C24-C25-C26
34	D	409	LHG	C23-C24-C25-C26
34	d	409	LHG	C23-C24-C25-C26
27	A	410	SQD	C34-C35-C36-C37
27	a	410	SQD	C34-C35-C36-C37
31	C	519	DGD	C9B-CAB-CBB-CCB
31	c	519	DGD	C9B-CAB-CBB-CCB
34	E	101	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
34	e	101	LHG	O1-C1-C2-O2
30	C	520	LMG	C16-C17-C18-C19
30	c	520	LMG	C16-C17-C18-C19
24	A	406	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C1A-C2A-CAA-CBA
24	C	503	CLA	C1A-C2A-CAA-CBA
24	C	507	CLA	C1A-C2A-CAA-CBA
24	C	512	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	503	CLA	C1A-C2A-CAA-CBA
24	c	507	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
24	d	401	CLA	C1A-C2A-CAA-CBA
30	C	523	LMG	C16-C17-C18-C19
30	c	523	LMG	C16-C17-C18-C19
31	C	519	DGD	C6B-C7B-C8B-C9B
31	c	519	DGD	C6B-C7B-C8B-C9B
31	C	517	DGD	O6E-C5E-C6E-O5E
31	c	517	DGD	O6E-C5E-C6E-O5E
27	F	101	SQD	O49-C7-O47-C45
27	f	101	SQD	O49-C7-O47-C45
24	B	614	CLA	C6-C7-C8-C10
24	C	505	CLA	C11-C12-C13-C15
24	C	507	CLA	C11-C12-C13-C15
24	C	509	CLA	C12-C13-C15-C16
24	b	616	CLA	C6-C7-C8-C10
24	c	505	CLA	C11-C12-C13-C15
24	c	507	CLA	C11-C12-C13-C15
24	c	509	CLA	C12-C13-C15-C16
27	A	410	SQD	C11-C12-C13-C14
27	a	410	SQD	C11-C12-C13-C14
24	C	504	CLA	C8-C10-C11-C12
34	D	409	LHG	C26-C27-C28-C29
34	d	409	LHG	C26-C27-C28-C29
24	B	609	CLA	C2-C3-C5-C6
24	b	611	CLA	C2-C3-C5-C6
28	A	411	PL9	C13-C14-C16-C17
28	a	411	PL9	C13-C14-C16-C17
31	C	518	DGD	CBA-CCA-CDA-CEA
31	c	518	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
24	c	504	CLA	C8-C10-C11-C12
24	C	507	CLA	C11-C12-C13-C14
24	c	507	CLA	C11-C12-C13-C14
27	A	412	SQD	C24-C25-C26-C27
27	a	412	SQD	C24-C25-C26-C27
31	C	518	DGD	CCB-CDB-CEB-CFB
31	c	518	DGD	CCB-CDB-CEB-CFB
30	C	523	LMG	C7-C8-C9-O8
30	c	523	LMG	C7-C8-C9-O8
31	C	518	DGD	C7A-C8A-C9A-CAA
31	c	518	DGD	C7A-C8A-C9A-CAA
30	C	520	LMG	C15-C16-C17-C18
30	c	520	LMG	C15-C16-C17-C18
30	d	411	LMG	C32-C33-C34-C35
30	D	411	LMG	C32-C33-C34-C35
30	C	523	LMG	C38-C39-C40-C41
30	c	523	LMG	C38-C39-C40-C41
24	C	510	CLA	C10-C11-C12-C13
24	c	510	CLA	C10-C11-C12-C13
26	C	516	BCR	C35-C13-C14-C15
26	C	522	BCR	C20-C21-C22-C37
26	c	516	BCR	C35-C13-C14-C15
26	c	522	BCR	C20-C21-C22-C37
27	A	410	SQD	C30-C31-C32-C33
27	a	410	SQD	C30-C31-C32-C33
24	B	609	CLA	C4-C3-C5-C6
30	c	523	LMG	C32-C33-C34-C35
32	Z	101	LMT	C7-C8-C9-C10
32	z	101	LMT	C7-C8-C9-C10
30	C	501	LMG	C13-C14-C15-C16
30	C	523	LMG	C32-C33-C34-C35
30	c	501	LMG	C13-C14-C15-C16
24	C	514	CLA	O1D-CGD-O2D-CED
31	C	518	DGD	C2B-C3B-C4B-C5B
31	c	518	DGD	C2B-C3B-C4B-C5B
24	A	408	CLA	C15-C16-C17-C18
24	a	408	CLA	C15-C16-C17-C18
30	C	520	LMG	C32-C33-C34-C35
30	c	520	LMG	C32-C33-C34-C35
34	L	101	LHG	C29-C30-C31-C32
34	l	101	LHG	C29-C30-C31-C32
24	c	514	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	C	521	LMT	C4-C5-C6-C7
32	c	521	LMT	C4-C5-C6-C7
26	B	617	BCR	C11-C10-C9-C8
26	C	515	BCR	C16-C17-C18-C19
26	J	104	BCR	C11-C10-C9-C8
26	b	619	BCR	C11-C10-C9-C8
26	c	515	BCR	C16-C17-C18-C19
26	j	104	BCR	C11-C10-C9-C8
27	A	412	SQD	C17-C18-C19-C20
27	a	412	SQD	C17-C18-C19-C20
27	a	412	SQD	C26-C27-C28-C29
27	A	412	SQD	C26-C27-C28-C29
27	B	620	SQD	C27-C28-C29-C30
27	L	102	SQD	C27-C28-C29-C30
30	C	501	LMG	C31-C32-C33-C34
30	c	501	LMG	C31-C32-C33-C34
31	C	517	DGD	C5B-C6B-C7B-C8B
31	c	517	DGD	C5B-C6B-C7B-C8B
24	b	611	CLA	C4-C3-C5-C6
28	A	411	PL9	C30-C29-C31-C32
28	a	411	PL9	C30-C29-C31-C32
30	C	520	LMG	C38-C39-C40-C41
30	c	520	LMG	C38-C39-C40-C41
30	c	501	LMG	C29-C30-C31-C32
34	L	101	LHG	C14-C15-C16-C17
34	l	101	LHG	C14-C15-C16-C17
31	H	101	DGD	CDB-CEB-CFB-CGB
31	h	101	DGD	CDB-CEB-CFB-CGB
30	C	501	LMG	C29-C30-C31-C32
34	D	408	LHG	C33-C34-C35-C36
34	d	408	LHG	C33-C34-C35-C36
31	c	517	DGD	CDA-CEA-CFA-CGA
30	C	501	LMG	C33-C34-C35-C36
30	C	523	LMG	C20-C21-C22-C23
30	c	501	LMG	C33-C34-C35-C36
30	c	523	LMG	C20-C21-C22-C23
32	J	102	LMT	C4-C5-C6-C7
31	C	517	DGD	CDA-CEA-CFA-CGA
30	C	523	LMG	C33-C34-C35-C36
30	c	523	LMG	C33-C34-C35-C36
32	j	102	LMT	C4-C5-C6-C7
27	B	620	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	L	102	SQD	C29-C30-C31-C32
30	c	523	LMG	C34-C35-C36-C37
30	C	523	LMG	C34-C35-C36-C37
28	A	411	PL9	C39-C41-C42-C43
28	a	411	PL9	C39-C41-C42-C43
34	D	410	LHG	C32-C33-C34-C35
24	C	514	CLA	CBA-CGA-O2A-C1
24	c	514	CLA	CBA-CGA-O2A-C1
34	d	410	LHG	C32-C33-C34-C35
27	B	620	SQD	C31-C32-C33-C34
27	L	102	SQD	C31-C32-C33-C34
32	Z	101	LMT	C1-C2-C3-C4
32	z	101	LMT	C1-C2-C3-C4
30	D	411	LMG	C22-C23-C24-C25
30	d	411	LMG	C22-C23-C24-C25
24	C	514	CLA	C4-C3-C5-C6
24	c	514	CLA	C4-C3-C5-C6
30	D	411	LMG	C13-C14-C15-C16
30	d	411	LMG	C13-C14-C15-C16
34	L	101	LHG	C16-C17-C18-C19
34	l	101	LHG	C16-C17-C18-C19
24	B	613	CLA	C11-C10-C8-C9
24	B	614	CLA	C6-C7-C8-C9
24	B	614	CLA	C14-C13-C15-C16
24	B	615	CLA	C14-C13-C15-C16
24	C	509	CLA	C14-C13-C15-C16
24	b	615	CLA	C11-C10-C8-C9
24	b	616	CLA	C6-C7-C8-C9
24	b	616	CLA	C14-C13-C15-C16
24	b	617	CLA	C14-C13-C15-C16
24	c	509	CLA	C14-C13-C15-C16
24	B	601	CLA	C5-C6-C7-C8
24	B	615	CLA	C13-C15-C16-C17
24	b	603	CLA	C5-C6-C7-C8
24	b	617	CLA	C13-C15-C16-C17
24	C	504	CLA	C4B-C3B-CAB-CBB
24	C	513	CLA	C4B-C3B-CAB-CBB
24	c	504	CLA	C4B-C3B-CAB-CBB
24	c	513	CLA	C4B-C3B-CAB-CBB
30	D	411	LMG	C19-C20-C21-C22
30	d	411	LMG	C19-C20-C21-C22
24	C	512	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	D	405	CLA	CBA-CGA-O2A-C1
24	d	405	CLA	CBA-CGA-O2A-C1
30	c	501	LMG	C32-C33-C34-C35
31	C	518	DGD	C2D-C1D-O3G-C3G
31	c	518	DGD	C2D-C1D-O3G-C3G
24	c	512	CLA	C15-C16-C17-C18
30	C	501	LMG	C32-C33-C34-C35
32	Z	101	LMT	C2-C3-C4-C5
32	z	101	LMT	C2-C3-C4-C5
34	D	409	LHG	O6-C4-C5-C6
34	d	409	LHG	O6-C4-C5-C6
24	B	601	CLA	C12-C13-C15-C16
24	B	614	CLA	C12-C13-C15-C16
24	C	512	CLA	C6-C7-C8-C10
24	b	603	CLA	C12-C13-C15-C16
24	b	616	CLA	C12-C13-C15-C16
24	c	512	CLA	C6-C7-C8-C10
24	B	603	CLA	C5-C6-C7-C8
24	b	605	CLA	C5-C6-C7-C8
32	C	521	LMT	O5'-C5'-C6'-O6'
32	c	521	LMT	O5'-C5'-C6'-O6'
30	C	520	LMG	C14-C15-C16-C17
30	c	520	LMG	C14-C15-C16-C17
32	C	521	LMT	C5-C6-C7-C8
32	c	521	LMT	C5-C6-C7-C8
27	a	412	SQD	C19-C20-C21-C22
27	A	412	SQD	C19-C20-C21-C22
26	C	522	BCR	C19-C20-C21-C22
26	c	522	BCR	C19-C20-C21-C22
30	c	523	LMG	C19-C20-C21-C22
30	C	523	LMG	C19-C20-C21-C22
30	B	621	LMG	O9-C10-O7-C8
30	b	622	LMG	O9-C10-O7-C8
34	L	101	LHG	C30-C31-C32-C33
34	l	101	LHG	C30-C31-C32-C33
34	D	408	LHG	C1-C2-C3-O3
34	d	408	LHG	C1-C2-C3-O3
27	A	412	SQD	O6-C44-C45-C46
27	a	412	SQD	O6-C44-C45-C46
30	C	520	LMG	O1-C7-C8-C9
30	c	520	LMG	O1-C7-C8-C9
24	B	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	C8-C10-C11-C12
34	D	408	LHG	C12-C13-C14-C15
34	d	408	LHG	C12-C13-C14-C15
27	A	410	SQD	C32-C33-C34-C35
27	a	410	SQD	C32-C33-C34-C35
30	C	501	LMG	C38-C39-C40-C41
30	c	501	LMG	C38-C39-C40-C41
31	C	517	DGD	C4B-C5B-C6B-C7B
31	C	519	DGD	CCA-CDA-CEA-CFA
31	c	517	DGD	C4B-C5B-C6B-C7B
31	c	519	DGD	CCA-CDA-CEA-CFA
24	C	514	CLA	C2-C3-C5-C6
24	c	514	CLA	C2-C3-C5-C6
24	B	607	CLA	C3-C5-C6-C7
24	b	609	CLA	C3-C5-C6-C7
24	A	405	CLA	C2C-C3C-CAC-CBC
24	a	405	CLA	C2C-C3C-CAC-CBC
31	c	519	DGD	CCB-CDB-CEB-CFB
34	D	409	LHG	C16-C17-C18-C19
34	d	409	LHG	C16-C17-C18-C19
34	L	101	LHG	O6-C4-C5-O7
34	l	101	LHG	O6-C4-C5-O7
31	C	519	DGD	CCB-CDB-CEB-CFB
26	B	617	BCR	C1-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	C	516	BCR	C23-C24-C25-C30
26	C	522	BCR	C1-C6-C7-C8
26	b	619	BCR	C1-C6-C7-C8
26	c	515	BCR	C1-C6-C7-C8
26	c	516	BCR	C23-C24-C25-C30
26	c	522	BCR	C1-C6-C7-C8
27	B	620	SQD	C12-C13-C14-C15
24	B	615	CLA	C10-C11-C12-C13
24	b	617	CLA	C10-C11-C12-C13
30	C	520	LMG	C22-C23-C24-C25
30	c	520	LMG	C22-C23-C24-C25
24	C	503	CLA	O1D-CGD-O2D-CED
24	c	503	CLA	O1D-CGD-O2D-CED
27	L	102	SQD	C12-C13-C14-C15
24	C	510	CLA	C16-C17-C18-C19
24	c	510	CLA	C16-C17-C18-C19
30	C	520	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
30	c	520	LMG	O1-C7-C8-O7
24	B	615	CLA	C2-C3-C5-C6
24	C	508	CLA	C16-C17-C18-C19
24	c	508	CLA	C16-C17-C18-C19
27	B	620	SQD	C32-C33-C34-C35
27	L	102	SQD	C32-C33-C34-C35
27	B	620	SQD	C25-C26-C27-C28
27	L	102	SQD	C25-C26-C27-C28
24	A	408	CLA	C3-C5-C6-C7
24	a	408	CLA	C3-C5-C6-C7
24	C	510	CLA	C6-C7-C8-C9
24	c	510	CLA	C6-C7-C8-C9
30	C	520	LMG	C33-C34-C35-C36
30	c	520	LMG	C33-C34-C35-C36
31	c	519	DGD	CBB-CCB-CDB-CEB
34	d	410	LHG	C11-C12-C13-C14
31	C	519	DGD	CBB-CCB-CDB-CEB
34	D	410	LHG	C11-C12-C13-C14
32	M	101	LMT	C4'-C5'-C6'-O6'
32	m	102	LMT	C4'-C5'-C6'-O6'
24	B	615	CLA	C4-C3-C5-C6
24	b	617	CLA	C2-C3-C5-C6
30	C	520	LMG	C35-C36-C37-C38
30	c	520	LMG	C35-C36-C37-C38
26	B	619	BCR	C20-C21-C22-C37
26	J	104	BCR	C35-C13-C14-C15
26	J	104	BCR	C16-C17-C18-C36
26	J	104	BCR	C20-C21-C22-C37
26	b	621	BCR	C20-C21-C22-C37
26	j	104	BCR	C35-C13-C14-C15
26	j	104	BCR	C16-C17-C18-C36
26	j	104	BCR	C20-C21-C22-C37
24	C	514	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	O1A-CGA-O2A-C1
34	L	101	LHG	O6-C4-C5-C6
34	l	101	LHG	O6-C4-C5-C6
24	C	504	CLA	C16-C17-C18-C20
24	c	504	CLA	C16-C17-C18-C20
34	D	410	LHG	C15-C16-C17-C18
34	d	410	LHG	C15-C16-C17-C18
30	B	621	LMG	C21-C22-C23-C24
24	B	615	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	D	405	CLA	C11-C10-C8-C7
24	b	617	CLA	C12-C13-C15-C16
24	d	405	CLA	C11-C10-C8-C7
30	b	622	LMG	C21-C22-C23-C24
28	d	407	PL9	C37-C38-C39-C40
26	J	104	BCR	C7-C8-C9-C10
26	j	104	BCR	C7-C8-C9-C10
31	H	101	DGD	CCA-CDA-CEA-CFA
31	h	101	DGD	CCA-CDA-CEA-CFA
31	C	518	DGD	C5D-C6D-O5D-C1E
31	c	518	DGD	C5D-C6D-O5D-C1E
24	C	510	CLA	C8-C10-C11-C12
24	c	510	CLA	C8-C10-C11-C12
24	B	601	CLA	C2A-CAA-CBA-CGA
24	b	603	CLA	C2A-CAA-CBA-CGA
27	B	620	SQD	O49-C7-O47-C45
27	L	102	SQD	O49-C7-O47-C45
30	B	621	LMG	C13-C14-C15-C16
30	b	622	LMG	C13-C14-C15-C16
24	b	617	CLA	C4-C3-C5-C6
31	H	101	DGD	O2G-C1B-C2B-C3B
31	h	101	DGD	O2G-C1B-C2B-C3B
24	B	607	CLA	C5-C6-C7-C8
24	C	513	CLA	C10-C11-C12-C13
24	b	609	CLA	C5-C6-C7-C8
24	c	513	CLA	C10-C11-C12-C13
24	B	616	CLA	C13-C15-C16-C17
24	b	618	CLA	C13-C15-C16-C17
34	E	101	LHG	C9-C10-C11-C12
34	e	101	LHG	C9-C10-C11-C12
24	C	503	CLA	C16-C17-C18-C20
24	D	405	CLA	C16-C17-C18-C19
24	c	503	CLA	C16-C17-C18-C20
24	d	405	CLA	C16-C17-C18-C19
24	D	405	CLA	O1A-CGA-O2A-C1
24	d	405	CLA	O1A-CGA-O2A-C1
34	D	409	LHG	O6-C4-C5-O7
34	d	409	LHG	O6-C4-C5-O7
28	D	407	PL9	C37-C38-C39-C40
34	d	410	LHG	C31-C32-C33-C34
24	C	508	CLA	C5-C6-C7-C8
24	c	508	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	C	520	LMG	C40-C41-C42-C43
30	c	520	LMG	C40-C41-C42-C43
34	D	410	LHG	C31-C32-C33-C34
27	A	410	SQD	O6-C44-C45-O47
27	a	410	SQD	O6-C44-C45-O47
30	C	523	LMG	O7-C8-C9-O8
30	c	523	LMG	O7-C8-C9-O8
27	F	101	SQD	C25-C26-C27-C28
27	f	101	SQD	C25-C26-C27-C28
34	d	409	LHG	C30-C31-C32-C33
34	D	409	LHG	C30-C31-C32-C33
30	C	501	LMG	C17-C18-C19-C20
34	e	101	LHG	C10-C11-C12-C13
30	C	523	LMG	C14-C15-C16-C17
30	c	501	LMG	C17-C18-C19-C20
30	c	523	LMG	C14-C15-C16-C17
31	C	517	DGD	C6A-C7A-C8A-C9A
31	c	517	DGD	C6A-C7A-C8A-C9A
34	E	101	LHG	C10-C11-C12-C13
32	M	101	LMT	C4B-C5B-C6B-O6B
32	m	102	LMT	C4B-C5B-C6B-O6B
24	B	612	CLA	CBA-CGA-O2A-C1
24	b	614	CLA	CBA-CGA-O2A-C1
34	l	101	LHG	C31-C32-C33-C34
34	L	101	LHG	C31-C32-C33-C34
30	C	520	LMG	C36-C37-C38-C39
32	c	521	LMT	C3-C4-C5-C6
32	C	521	LMT	C3-C4-C5-C6
24	A	406	CLA	C4B-C3B-CAB-CBB
24	C	514	CLA	C1A-C2A-CAA-CBA
24	a	406	CLA	C4B-C3B-CAB-CBB
24	c	514	CLA	C1A-C2A-CAA-CBA
26	T	101	BCR	C22-C23-C24-C25
26	t	102	BCR	C22-C23-C24-C25
30	c	520	LMG	C36-C37-C38-C39
26	C	515	BCR	C21-C22-C23-C24
26	c	515	BCR	C21-C22-C23-C24
24	B	612	CLA	O1A-CGA-O2A-C1
24	b	614	CLA	O1A-CGA-O2A-C1
30	D	411	LMG	C21-C22-C23-C24
30	d	411	LMG	C21-C22-C23-C24
24	A	406	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	C	503	CLA	C12-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C7
24	C	512	CLA	C12-C13-C15-C16
24	a	406	CLA	C11-C10-C8-C7
24	c	503	CLA	C12-C13-C15-C16
24	c	508	CLA	C11-C10-C8-C7
24	c	512	CLA	C12-C13-C15-C16
34	L	101	LHG	C12-C13-C14-C15
34	l	101	LHG	C12-C13-C14-C15
30	C	520	LMG	C30-C31-C32-C33
30	c	520	LMG	C30-C31-C32-C33
34	L	101	LHG	C34-C35-C36-C37
30	c	501	LMG	C15-C16-C17-C18
34	l	101	LHG	C34-C35-C36-C37
30	C	501	LMG	C15-C16-C17-C18
34	E	101	LHG	C13-C14-C15-C16
34	e	101	LHG	C13-C14-C15-C16
34	D	409	LHG	O9-C7-O7-C5
34	d	409	LHG	O9-C7-O7-C5
31	C	519	DGD	CDA-CEA-CFA-CGA
31	c	519	DGD	CDA-CEA-CFA-CGA
34	E	101	LHG	C28-C29-C30-C31
24	C	512	CLA	C6-C7-C8-C9
24	C	512	CLA	C14-C13-C15-C16
24	D	405	CLA	C11-C10-C8-C9
24	c	512	CLA	C6-C7-C8-C9
24	c	512	CLA	C14-C13-C15-C16
24	d	405	CLA	C11-C10-C8-C9
34	e	101	LHG	C28-C29-C30-C31
31	C	517	DGD	O6D-C5D-C6D-O5D
31	c	517	DGD	O6D-C5D-C6D-O5D
30	C	501	LMG	O1-C7-C8-O7
30	C	523	LMG	O1-C7-C8-O7
30	c	501	LMG	O1-C7-C8-O7
30	c	523	LMG	O1-C7-C8-O7
30	C	523	LMG	C37-C38-C39-C40
30	c	523	LMG	C37-C38-C39-C40
24	A	405	CLA	C13-C15-C16-C17
24	a	405	CLA	C13-C15-C16-C17
30	C	501	LMG	O1-C7-C8-C9
30	c	501	LMG	O1-C7-C8-C9
30	C	501	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
30	c	501	LMG	C36-C37-C38-C39
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	C	505	CLA	CAD-CBD-CGD-O2D
24	b	603	CLA	CAD-CBD-CGD-O2D
24	b	607	CLA	CAD-CBD-CGD-O2D
24	c	505	CLA	CAD-CBD-CGD-O2D
27	A	412	SQD	C16-C17-C18-C19
27	a	412	SQD	C16-C17-C18-C19
30	c	501	LMG	C14-C15-C16-C17
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	605	CLA	CAD-CBD-CGD-O1D
24	B	609	CLA	CAD-CBD-CGD-O1D
24	B	616	CLA	CHA-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	b	603	CLA	CAD-CBD-CGD-O1D
24	b	607	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	b	618	CLA	CHA-CBD-CGD-O1D
24	c	505	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
34	D	408	LHG	C3-O3-P-O6
34	D	409	LHG	C3-O3-P-O4
34	L	101	LHG	C4-O6-P-O5
34	d	408	LHG	C3-O3-P-O6
34	d	409	LHG	C3-O3-P-O4
34	l	101	LHG	C4-O6-P-O5
30	C	501	LMG	C14-C15-C16-C17
24	A	406	CLA	C2B-C3B-CAB-CBB
24	B	602	CLA	C2B-C3B-CAB-CBB
24	a	406	CLA	C2B-C3B-CAB-CBB
24	b	604	CLA	C2B-C3B-CAB-CBB
28	D	407	PL9	C43-C44-C46-C47
28	d	407	PL9	C43-C44-C46-C47
26	C	522	BCR	C7-C8-C9-C34
26	c	522	BCR	C7-C8-C9-C34
34	D	410	LHG	C2-C3-O3-P
34	d	410	LHG	C2-C3-O3-P
30	D	411	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
30	d	411	LMG	C20-C21-C22-C23
34	d	408	LHG	C24-C25-C26-C27
28	A	411	PL9	C4-C3-C7-C8
28	a	411	PL9	C4-C3-C7-C8
34	D	408	LHG	C24-C25-C26-C27
34	L	101	LHG	O10-C23-O8-C6
34	l	101	LHG	O10-C23-O8-C6
24	D	405	CLA	C10-C11-C12-C13
24	d	405	CLA	C10-C11-C12-C13
24	C	508	CLA	C16-C17-C18-C20
24	c	508	CLA	C16-C17-C18-C20
24	B	616	CLA	C10-C11-C12-C13
24	b	618	CLA	C10-C11-C12-C13
24	C	513	CLA	C11-C10-C8-C7
24	c	513	CLA	C11-C10-C8-C7
27	F	101	SQD	O5-C1-O6-C44
27	f	101	SQD	O5-C1-O6-C44
34	D	409	LHG	C34-C35-C36-C37
34	d	409	LHG	C34-C35-C36-C37
34	l	101	LHG	C10-C11-C12-C13
34	l	101	LHG	C13-C14-C15-C16
34	L	101	LHG	C10-C11-C12-C13
30	C	501	LMG	C11-C12-C13-C14
30	c	501	LMG	C11-C12-C13-C14
24	C	504	CLA	C16-C17-C18-C19
24	c	504	CLA	C16-C17-C18-C19
34	L	101	LHG	C13-C14-C15-C16
32	C	521	LMT	C5'-C4'-O1B-C1B
32	c	521	LMT	C5'-C4'-O1B-C1B
30	c	501	LMG	O9-C10-O7-C8
31	C	517	DGD	O1B-C1B-O2G-C2G
30	C	501	LMG	O9-C10-O7-C8
31	c	517	DGD	O1B-C1B-O2G-C2G
34	E	101	LHG	O8-C23-C24-C25
34	e	101	LHG	O8-C23-C24-C25
27	A	412	SQD	C45-C44-O6-C1
27	B	620	SQD	C45-C44-O6-C1
27	F	101	SQD	C45-C44-O6-C1
27	L	102	SQD	C45-C44-O6-C1
27	a	412	SQD	C45-C44-O6-C1
27	f	101	SQD	C45-C44-O6-C1
26	D	406	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
26	d	406	BCR	C13-C14-C15-C16
31	C	519	DGD	O6D-C1D-O3G-C3G
24	A	405	CLA	C4C-C3C-CAC-CBC
24	a	405	CLA	C4C-C3C-CAC-CBC
34	d	410	LHG	C29-C30-C31-C32
24	B	614	CLA	C11-C12-C13-C14
24	C	508	CLA	C11-C10-C8-C9
24	b	616	CLA	C11-C12-C13-C14
24	c	508	CLA	C11-C10-C8-C9
34	D	410	LHG	C29-C30-C31-C32
31	C	517	DGD	C4D-C5D-C6D-O5D
31	c	517	DGD	C4D-C5D-C6D-O5D
24	C	510	CLA	C13-C15-C16-C17
24	c	510	CLA	C13-C15-C16-C17
34	E	101	LHG	O6-C4-C5-O7
34	e	101	LHG	O6-C4-C5-O7
27	B	620	SQD	C26-C27-C28-C29
27	L	102	SQD	C9-C10-C11-C12
27	L	102	SQD	C26-C27-C28-C29
24	D	405	CLA	C16-C17-C18-C20
24	d	405	CLA	C16-C17-C18-C20
27	B	620	SQD	C9-C10-C11-C12
24	A	406	CLA	C6-C7-C8-C10
24	B	610	CLA	C12-C13-C15-C16
24	a	406	CLA	C6-C7-C8-C10
24	b	612	CLA	C12-C13-C15-C16
34	E	101	LHG	O9-C7-O7-C5
34	e	101	LHG	O9-C7-O7-C5
31	C	519	DGD	C8A-C9A-CAA-CBA
31	c	519	DGD	C8A-C9A-CAA-CBA
26	B	619	BCR	C35-C13-C14-C15
26	C	516	BCR	C11-C10-C9-C34
26	b	621	BCR	C35-C13-C14-C15
26	c	516	BCR	C11-C10-C9-C34
31	c	519	DGD	O6D-C1D-O3G-C3G
31	H	101	DGD	C7B-C8B-C9B-CAB
31	h	101	DGD	C7B-C8B-C9B-CAB
24	A	405	CLA	C15-C16-C17-C18
24	a	405	CLA	C15-C16-C17-C18
30	C	523	LMG	C15-C16-C17-C18
30	c	523	LMG	C15-C16-C17-C18
38	X	101	RRX	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
38	x	101	RRX	C19-C20-C21-C22
34	D	410	LHG	C10-C11-C12-C13
34	d	410	LHG	C10-C11-C12-C13
24	B	607	CLA	C8-C10-C11-C12
24	b	609	CLA	C8-C10-C11-C12
32	J	102	LMT	C11-C10-C9-C8
32	j	102	LMT	C11-C10-C9-C8
24	A	406	CLA	C6-C7-C8-C9
24	A	406	CLA	C11-C10-C8-C9
24	B	615	CLA	C6-C7-C8-C9
24	a	406	CLA	C6-C7-C8-C9
24	a	406	CLA	C11-C10-C8-C9
24	b	617	CLA	C6-C7-C8-C9
30	C	523	LMG	C29-C30-C31-C32
30	c	523	LMG	C29-C30-C31-C32
27	a	412	SQD	O49-C7-O47-C45
27	B	620	SQD	C10-C11-C12-C13
27	L	102	SQD	C10-C11-C12-C13
24	B	601	CLA	CAA-CBA-CGA-O2A
24	b	603	CLA	CAA-CBA-CGA-O2A
24	b	612	CLA	C2A-CAA-CBA-CGA
24	B	611	CLA	O1D-CGD-O2D-CED
24	b	613	CLA	O1D-CGD-O2D-CED
24	B	601	CLA	C1A-C2A-CAA-CBA
24	C	504	CLA	C1A-C2A-CAA-CBA
24	b	603	CLA	C1A-C2A-CAA-CBA
24	c	504	CLA	C1A-C2A-CAA-CBA
37	V	201	HEC	CAD-CBD-CGD-O1D
37	v	201	HEC	CAD-CBD-CGD-O1D
30	C	520	LMG	C17-C18-C19-C20
26	A	409	BCR	C1-C6-C7-C8
26	B	617	BCR	C5-C6-C7-C8
26	B	619	BCR	C23-C24-C25-C30
26	C	516	BCR	C23-C24-C25-C26
26	C	522	BCR	C5-C6-C7-C8
26	a	409	BCR	C1-C6-C7-C8
26	b	619	BCR	C5-C6-C7-C8
26	b	621	BCR	C23-C24-C25-C30
26	c	516	BCR	C23-C24-C25-C26
26	c	522	BCR	C5-C6-C7-C8
30	c	520	LMG	C17-C18-C19-C20
27	A	412	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
31	C	519	DGD	O6E-C5E-C6E-O5E
31	c	519	DGD	O6E-C5E-C6E-O5E
24	B	614	CLA	C11-C12-C13-C15
24	B	616	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C12-C13-C15
24	b	618	CLA	C12-C13-C15-C16
31	H	101	DGD	C9B-CAB-CBB-CCB
31	h	101	DGD	C9B-CAB-CBB-CCB
24	B	610	CLA	C2A-CAA-CBA-CGA
31	H	101	DGD	C8A-C9A-CAA-CBA
31	h	101	DGD	C8A-C9A-CAA-CBA
28	D	407	PL9	C4-C3-C7-C8
28	d	407	PL9	C4-C3-C7-C8
27	A	410	SQD	C15-C16-C17-C18
27	A	412	SQD	C31-C32-C33-C34
27	a	410	SQD	C15-C16-C17-C18
27	a	412	SQD	C31-C32-C33-C34
37	V	201	HEC	CAD-CBD-CGD-O2D
37	v	201	HEC	CAD-CBD-CGD-O2D
24	B	602	CLA	C15-C16-C17-C18
24	b	604	CLA	C15-C16-C17-C18
31	c	518	DGD	CBB-CCB-CDB-CEB
31	C	518	DGD	CBB-CCB-CDB-CEB
34	D	408	LHG	C32-C33-C34-C35
34	d	408	LHG	C32-C33-C34-C35
24	A	408	CLA	C14-C13-C15-C16
24	B	614	CLA	C5-C6-C7-C8
24	b	616	CLA	C5-C6-C7-C8
27	A	410	SQD	O6-C44-C45-C46
27	a	410	SQD	O6-C44-C45-C46
24	c	507	CLA	C10-C11-C12-C13
34	D	409	LHG	C13-C14-C15-C16
34	d	409	LHG	C13-C14-C15-C16
24	C	503	CLA	C4B-C3B-CAB-CBB
24	c	503	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	C10-C11-C12-C13
27	A	412	SQD	C28-C29-C30-C31
27	a	412	SQD	C28-C29-C30-C31
34	E	101	LHG	C11-C10-C9-C8
34	e	101	LHG	C11-C10-C9-C8
27	F	101	SQD	O47-C7-C8-C9
27	f	101	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	O1A-CGA-O2A-C1
24	b	604	CLA	O1A-CGA-O2A-C1
30	d	411	LMG	C33-C34-C35-C36
25	A	407	PHO	CHA-CBD-CGD-O1D
25	A	407	PHO	CHA-CBD-CGD-O2D
25	D	402	PHO	CHA-CBD-CGD-O2D
25	a	407	PHO	CHA-CBD-CGD-O1D
25	a	407	PHO	CHA-CBD-CGD-O2D
25	d	402	PHO	CHA-CBD-CGD-O2D
34	D	410	LHG	O10-C23-O8-C6
34	d	410	LHG	O10-C23-O8-C6
30	D	411	LMG	C33-C34-C35-C36
34	l	101	LHG	C25-C26-C27-C28
30	d	411	LMG	C28-C29-C30-C31
34	L	101	LHG	C25-C26-C27-C28
34	e	101	LHG	C33-C34-C35-C36
34	E	101	LHG	C33-C34-C35-C36
34	D	408	LHG	O2-C2-C3-O3
34	d	408	LHG	O2-C2-C3-O3
30	D	411	LMG	C28-C29-C30-C31
24	A	408	CLA	C11-C10-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	a	408	CLA	C11-C10-C8-C9
24	a	408	CLA	C14-C13-C15-C16
24	c	506	CLA	C11-C12-C13-C14
31	C	517	DGD	C5D-C6D-O5D-C1E
31	c	517	DGD	C5D-C6D-O5D-C1E
24	B	614	CLA	C2-C1-O2A-CGA
24	b	616	CLA	C2-C1-O2A-CGA
24	B	607	CLA	C3A-C2A-CAA-CBA
24	b	609	CLA	C3A-C2A-CAA-CBA
34	D	408	LHG	C11-C12-C13-C14
34	d	408	LHG	C11-C12-C13-C14
24	B	610	CLA	O1D-CGD-O2D-CED
24	C	505	CLA	C15-C16-C17-C18
24	c	505	CLA	C15-C16-C17-C18
24	C	504	CLA	O1D-CGD-O2D-CED
24	c	504	CLA	O1D-CGD-O2D-CED
31	C	519	DGD	O1A-C1A-O1G-C1G
31	c	519	DGD	O1A-C1A-O1G-C1G
30	D	411	LMG	C10-C11-C12-C13
30	d	411	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	603	CLA	O1D-CGD-O2D-CED
24	b	605	CLA	O1D-CGD-O2D-CED
24	D	401	CLA	C4C-C3C-CAC-CBC
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	609	CLA	C2A-CAA-CBA-CGA
24	d	401	CLA	C4C-C3C-CAC-CBC
34	d	410	LHG	C14-C15-C16-C17
34	D	410	LHG	C14-C15-C16-C17
24	b	605	CLA	C13-C15-C16-C17
24	b	612	CLA	O1D-CGD-O2D-CED
24	A	408	CLA	C11-C10-C8-C7
24	B	615	CLA	C6-C7-C8-C10
24	C	506	CLA	C11-C12-C13-C15
24	a	408	CLA	C11-C10-C8-C7
24	b	617	CLA	C6-C7-C8-C10
24	c	506	CLA	C11-C12-C13-C15
30	C	501	LMG	C19-C20-C21-C22
30	c	501	LMG	C19-C20-C21-C22
24	A	405	CLA	C2B-C3B-CAB-CBB
24	C	504	CLA	C2B-C3B-CAB-CBB
24	C	513	CLA	C2B-C3B-CAB-CBB
24	a	405	CLA	C2B-C3B-CAB-CBB
24	c	504	CLA	C2B-C3B-CAB-CBB
24	c	513	CLA	C2B-C3B-CAB-CBB
26	A	409	BCR	C5-C6-C7-C8
26	B	619	BCR	C23-C24-C25-C26
26	C	522	BCR	C23-C24-C25-C26
26	C	522	BCR	C23-C24-C25-C30
26	a	409	BCR	C5-C6-C7-C8
26	b	621	BCR	C23-C24-C25-C26
26	c	522	BCR	C23-C24-C25-C26
26	c	522	BCR	C23-C24-C25-C30
24	B	613	CLA	C2-C1-O2A-CGA
24	b	615	CLA	C2-C1-O2A-CGA
24	B	603	CLA	C13-C15-C16-C17
24	C	511	CLA	CAA-CBA-CGA-O2A
24	c	511	CLA	CAA-CBA-CGA-O2A
31	H	101	DGD	CBB-CCB-CDB-CEB
31	h	101	DGD	CBB-CCB-CDB-CEB
31	C	518	DGD	C5A-C6A-C7A-C8A
31	c	518	DGD	C5A-C6A-C7A-C8A
30	C	501	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	A	410	SQD	C9-C10-C11-C12
27	F	101	SQD	C28-C29-C30-C31
27	a	410	SQD	C9-C10-C11-C12
27	f	101	SQD	C28-C29-C30-C31
31	C	518	DGD	CAA-CBA-CCA-CDA
31	c	518	DGD	CAA-CBA-CCA-CDA
27	A	410	SQD	O47-C7-C8-C9
27	a	410	SQD	O47-C7-C8-C9
30	c	501	LMG	O8-C28-C29-C30
34	D	410	LHG	C17-C18-C19-C20
34	d	410	LHG	C17-C18-C19-C20
32	M	101	LMT	O5B-C5B-C6B-O6B
34	D	408	LHG	C25-C26-C27-C28
24	B	607	CLA	O1A-CGA-O2A-C1
24	b	609	CLA	O1A-CGA-O2A-C1
34	d	408	LHG	C25-C26-C27-C28
24	B	616	CLA	C14-C13-C15-C16
24	C	513	CLA	C11-C10-C8-C9
24	b	618	CLA	C14-C13-C15-C16
24	c	513	CLA	C11-C10-C8-C9
24	B	613	CLA	CAA-CBA-CGA-O2A
24	b	615	CLA	CAA-CBA-CGA-O2A
34	D	410	LHG	O8-C23-C24-C25
34	d	410	LHG	O8-C23-C24-C25
32	m	102	LMT	O5B-C5B-C6B-O6B
24	B	616	CLA	C4B-C3B-CAB-CBB
24	b	618	CLA	C4B-C3B-CAB-CBB
24	B	616	CLA	CAA-CBA-CGA-O2A
24	C	513	CLA	CAA-CBA-CGA-O2A
24	c	513	CLA	CAA-CBA-CGA-O2A
30	C	523	LMG	O8-C28-C29-C30
30	c	523	LMG	O8-C28-C29-C30
31	c	517	DGD	O2G-C1B-C2B-C3B
26	C	515	BCR	C11-C12-C13-C14
26	c	515	BCR	C11-C12-C13-C14
24	C	506	CLA	CAA-CBA-CGA-O2A
24	c	506	CLA	CAA-CBA-CGA-O2A
27	B	620	SQD	O48-C23-C24-C25
27	L	102	SQD	O48-C23-C24-C25
31	C	517	DGD	O2G-C1B-C2B-C3B
34	E	101	LHG	O6-C4-C5-C6
34	e	101	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
28	A	411	PL9	C17-C18-C19-C20
28	a	411	PL9	C17-C18-C19-C20
24	b	618	CLA	CAA-CBA-CGA-O2A
24	A	408	CLA	C2-C1-O2A-CGA
24	C	512	CLA	C2-C1-O2A-CGA
24	C	514	CLA	C2-C1-O2A-CGA
24	a	408	CLA	C2-C1-O2A-CGA
24	c	512	CLA	C2-C1-O2A-CGA
24	c	514	CLA	C2-C1-O2A-CGA
24	d	404	CLA	C2-C1-O2A-CGA
24	B	607	CLA	C6-C7-C8-C10
24	B	612	CLA	C11-C10-C8-C7
24	b	609	CLA	C6-C7-C8-C10
24	b	614	CLA	C11-C10-C8-C7
24	D	401	CLA	C16-C17-C18-C20
24	d	401	CLA	C16-C17-C18-C20
24	B	602	CLA	C13-C15-C16-C17
24	b	604	CLA	C13-C15-C16-C17
24	c	506	CLA	C16-C17-C18-C19
34	l	101	LHG	C17-C18-C19-C20
30	C	501	LMG	O9-C10-C11-C12
30	c	501	LMG	O9-C10-C11-C12
30	C	520	LMG	C4-C5-C6-O5
34	L	101	LHG	C17-C18-C19-C20
30	c	520	LMG	C4-C5-C6-O5
24	C	506	CLA	C16-C17-C18-C19
30	C	501	LMG	C20-C21-C22-C23
30	c	501	LMG	C20-C21-C22-C23
24	B	605	CLA	C10-C11-C12-C13
24	c	511	CLA	CAA-CBA-CGA-O1A
27	B	620	SQD	O49-C7-C8-C9
27	L	102	SQD	O49-C7-C8-C9
24	C	511	CLA	CAA-CBA-CGA-O1A
24	b	607	CLA	C10-C11-C12-C13
24	B	612	CLA	C11-C10-C8-C9
24	b	614	CLA	C11-C10-C8-C9
31	C	518	DGD	C8B-C9B-CAB-CBB
31	C	518	DGD	O1B-C1B-C2B-C3B
31	c	518	DGD	O1B-C1B-C2B-C3B
31	c	518	DGD	C8B-C9B-CAB-CBB
24	C	506	CLA	C2-C3-C5-C6
24	c	506	CLA	C2-C3-C5-C6

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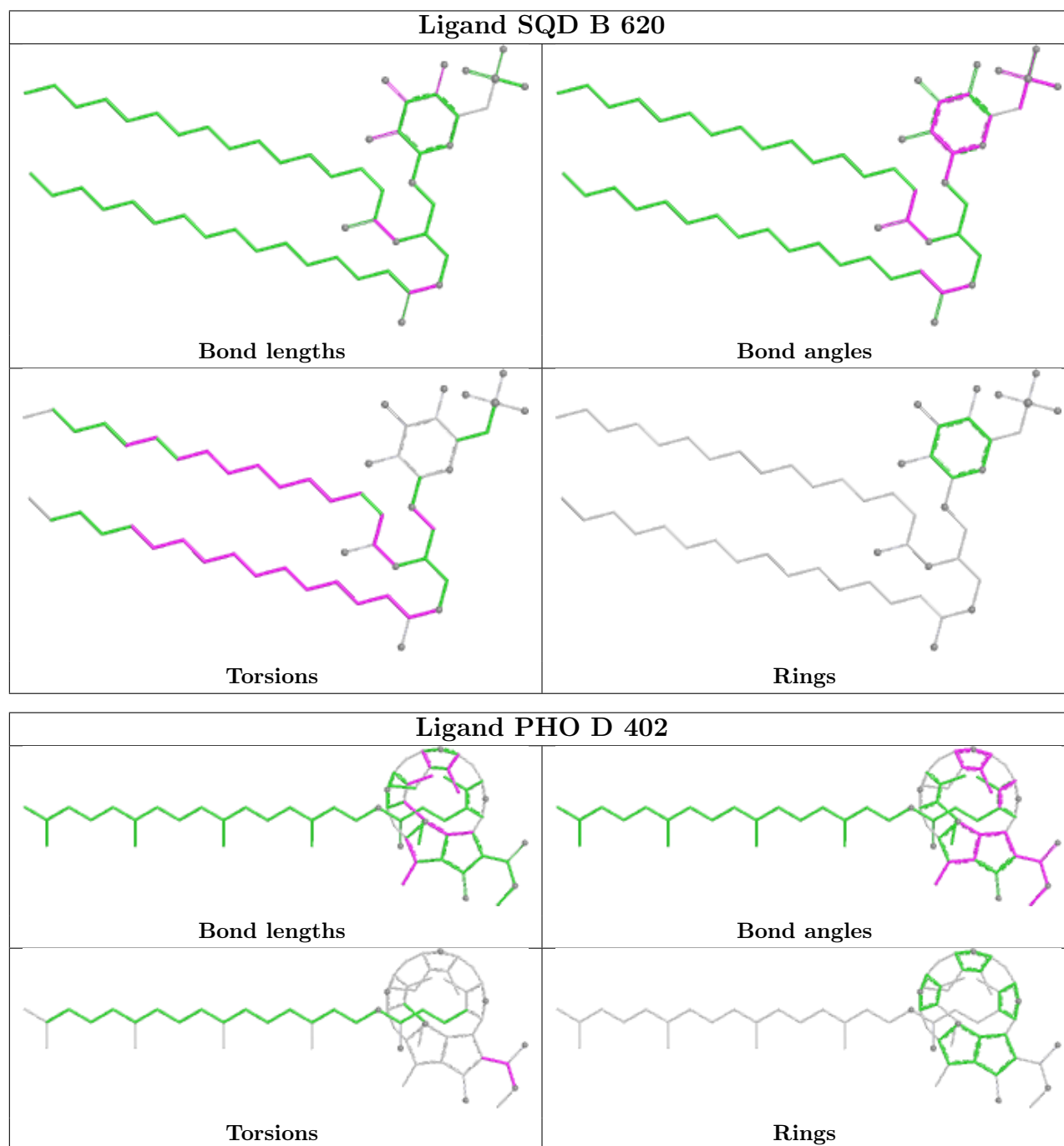
Mol	Chain	Res	Type	Atoms
35	E	103	HEM	CAA-CBA-CGA-O2A
35	e	103	HEM	CAA-CBA-CGA-O2A
24	C	511	CLA	C8-C10-C11-C12
24	c	511	CLA	C8-C10-C11-C12
30	B	621	LMG	C8-C7-O1-C1
30	b	622	LMG	C8-C7-O1-C1
31	H	101	DGD	C2G-C3G-O3G-C1D
31	h	101	DGD	C2G-C3G-O3G-C1D
24	C	506	CLA	CAA-CBA-CGA-O1A
24	c	506	CLA	CAA-CBA-CGA-O1A
34	E	101	LHG	C31-C32-C33-C34
34	e	101	LHG	C31-C32-C33-C34
24	C	513	CLA	C8-C10-C11-C12
24	c	513	CLA	C8-C10-C11-C12
24	B	611	CLA	CBD-CGD-O2D-CED
24	b	613	CLA	CBD-CGD-O2D-CED
24	B	609	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	b	611	CLA	CAD-CBD-CGD-O2D
24	c	510	CLA	CAD-CBD-CGD-O2D
34	e	101	LHG	C30-C31-C32-C33
34	E	101	LHG	C30-C31-C32-C33
24	B	608	CLA	C2-C1-O2A-CGA
24	D	404	CLA	C2-C1-O2A-CGA
24	b	610	CLA	C2-C1-O2A-CGA
24	B	613	CLA	CAA-CBA-CGA-O1A
24	B	616	CLA	CAA-CBA-CGA-O1A
24	b	615	CLA	CAA-CBA-CGA-O1A
24	b	618	CLA	CAA-CBA-CGA-O1A
27	B	620	SQD	O10-C23-C24-C25
27	L	102	SQD	O10-C23-C24-C25
30	B	621	LMG	O8-C28-C29-C30
30	b	622	LMG	O8-C28-C29-C30

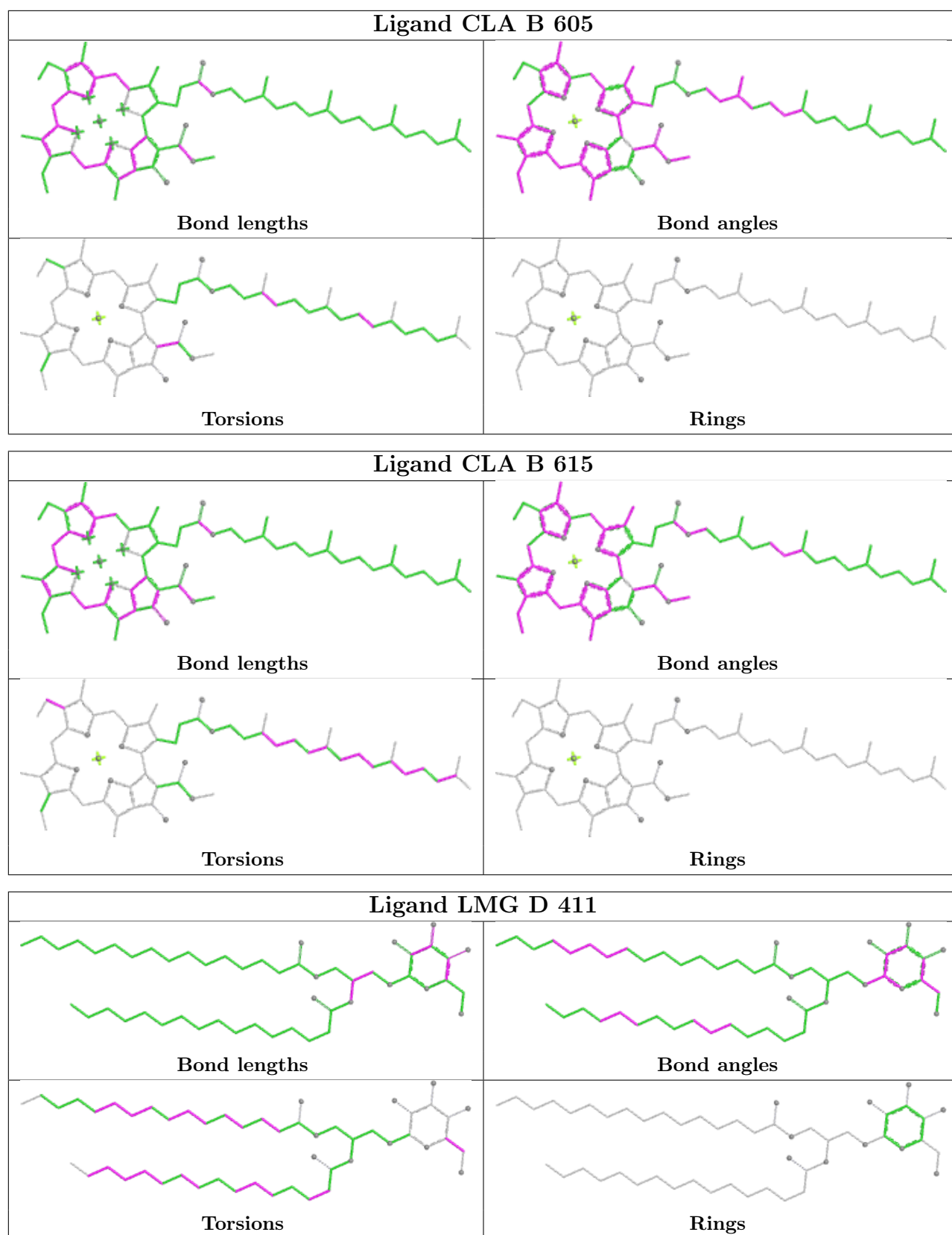
There are no ring outliers.

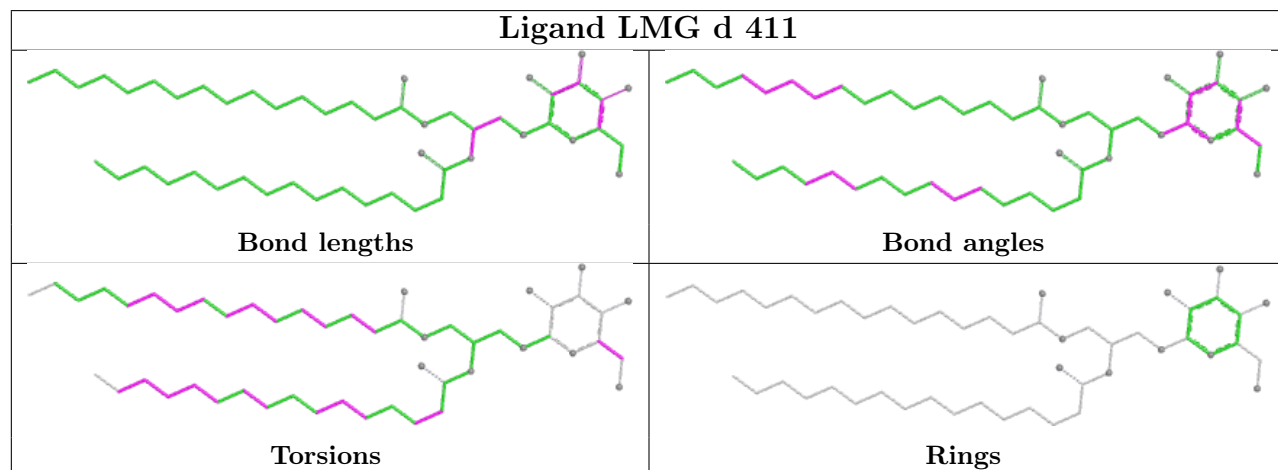
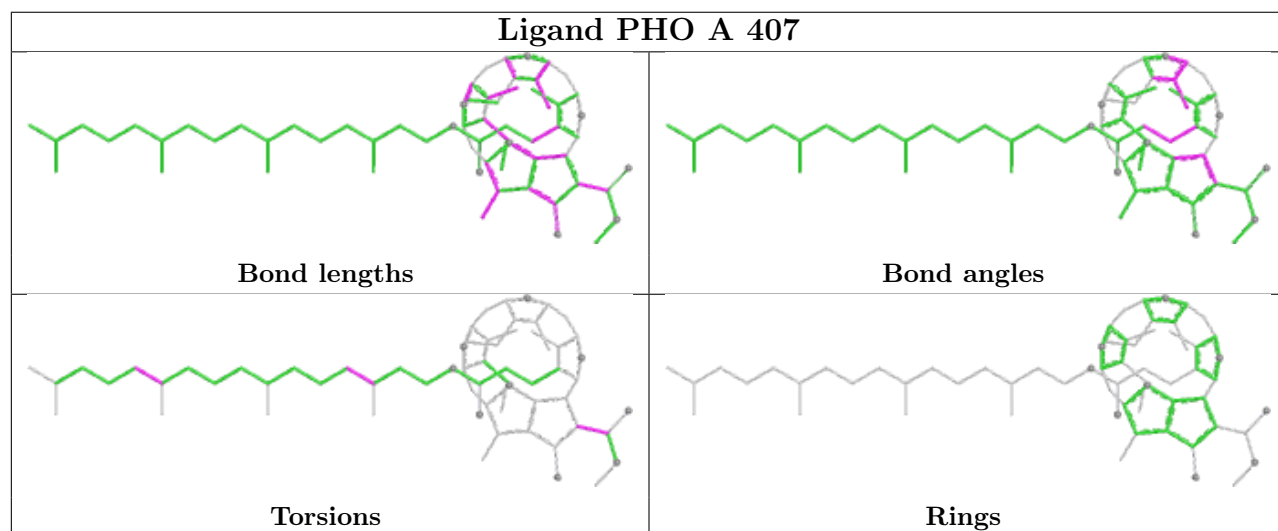
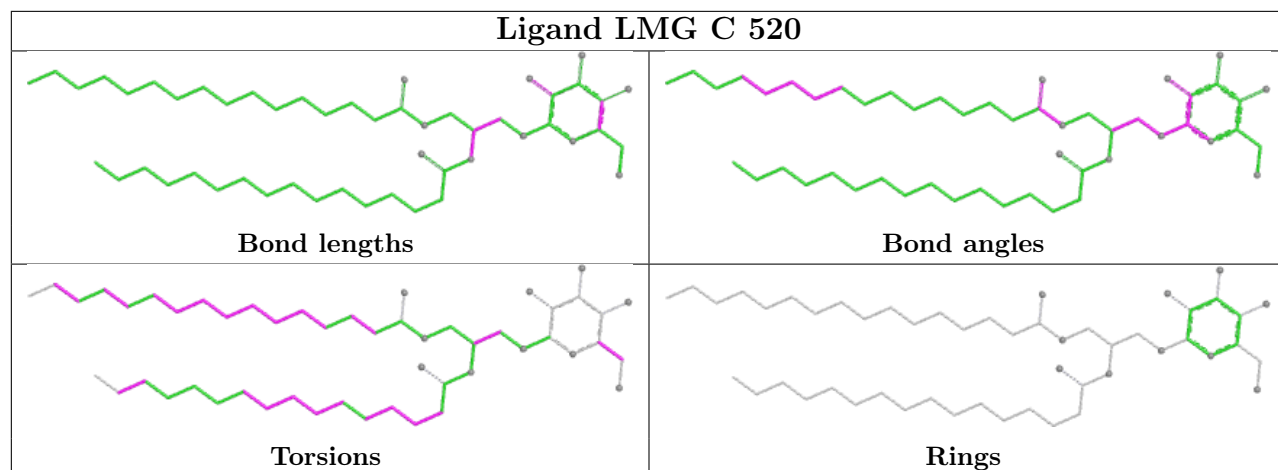
No monomer is involved in short contacts.

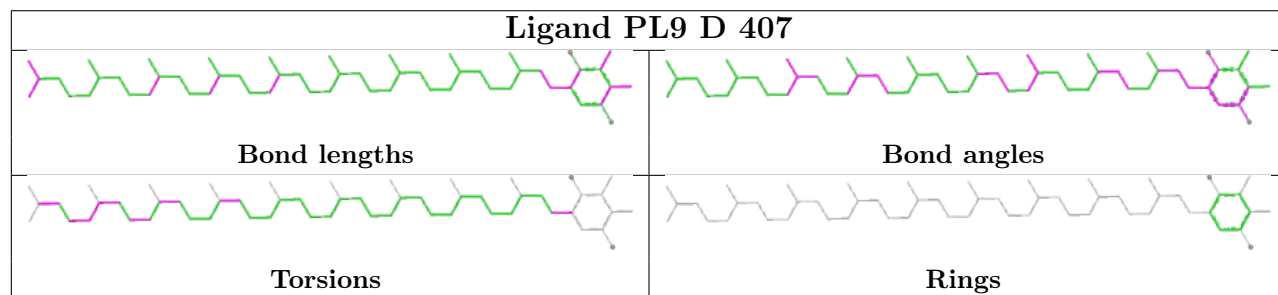
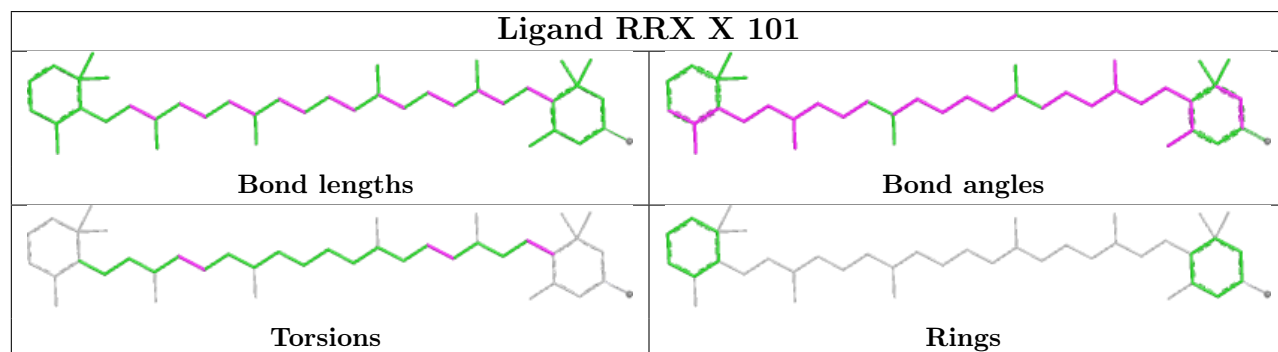
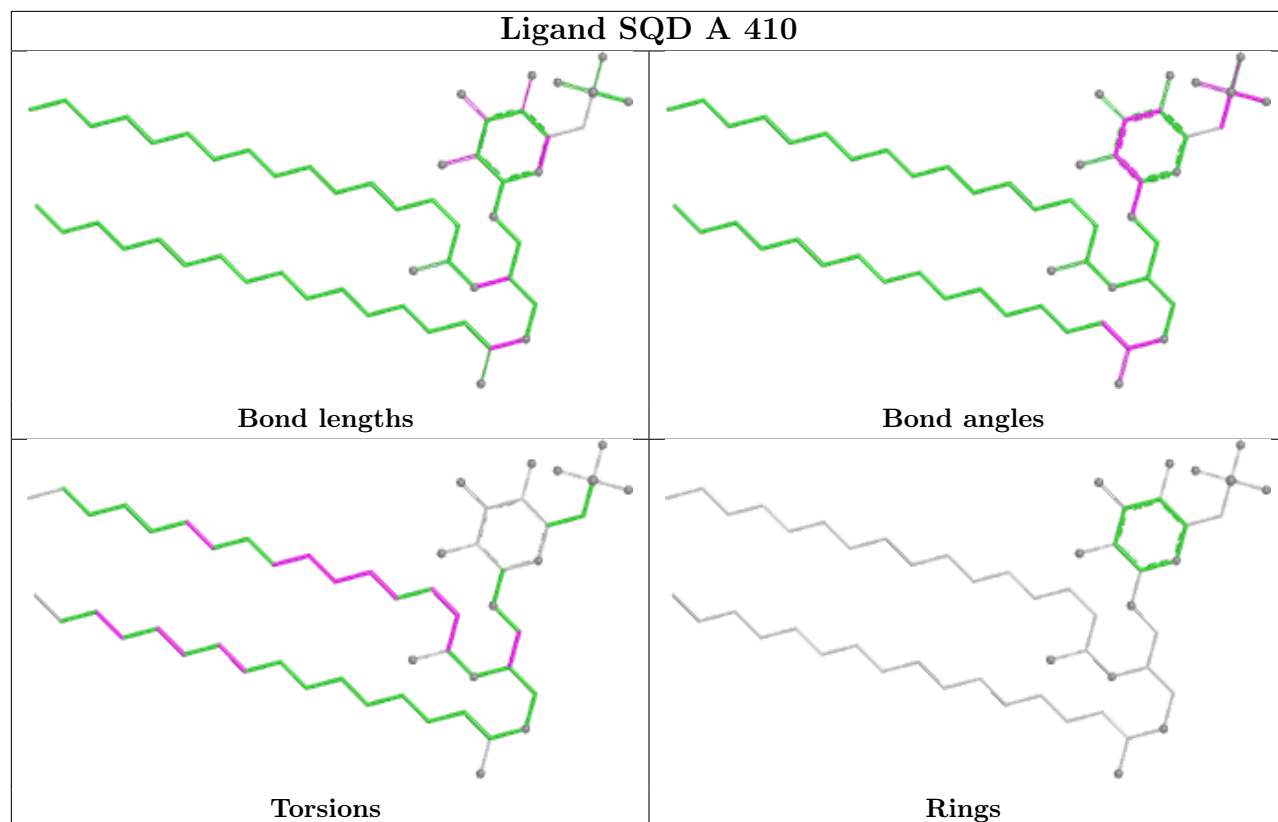
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

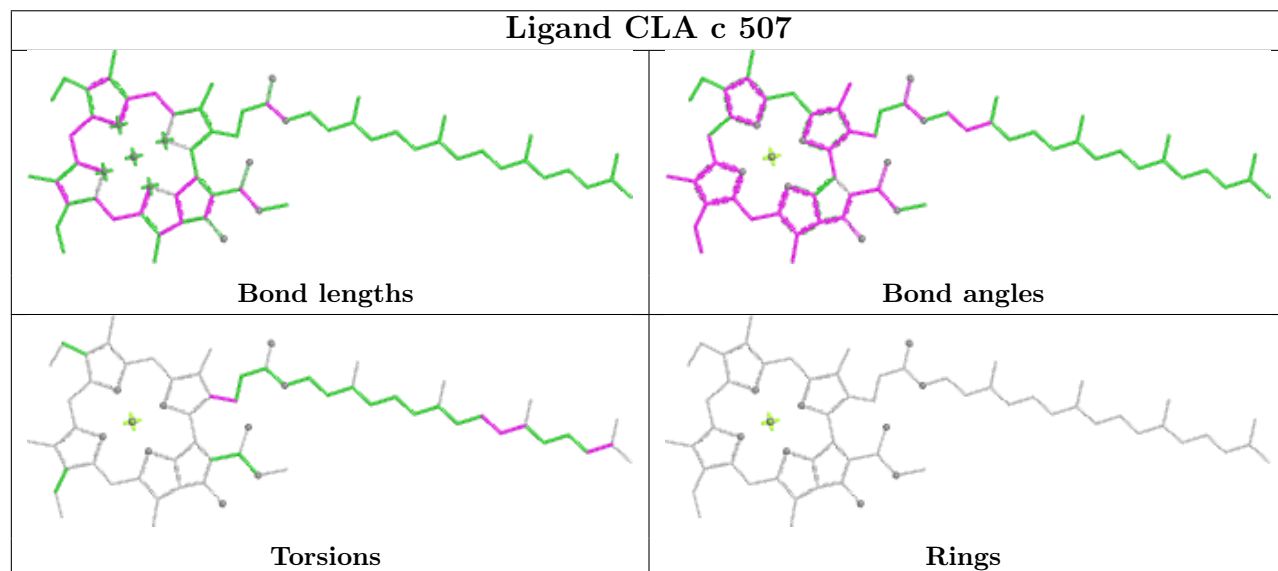
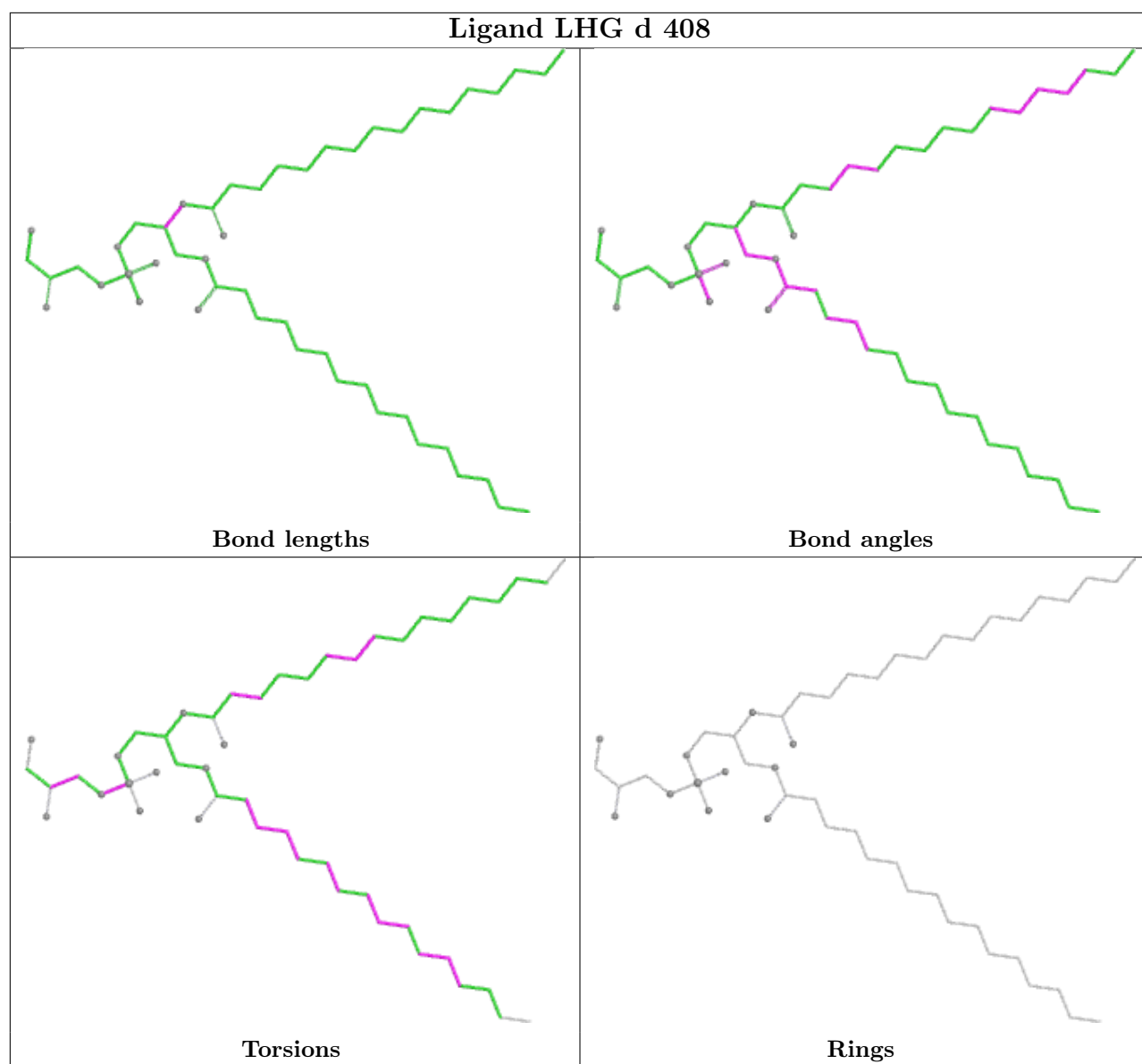
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

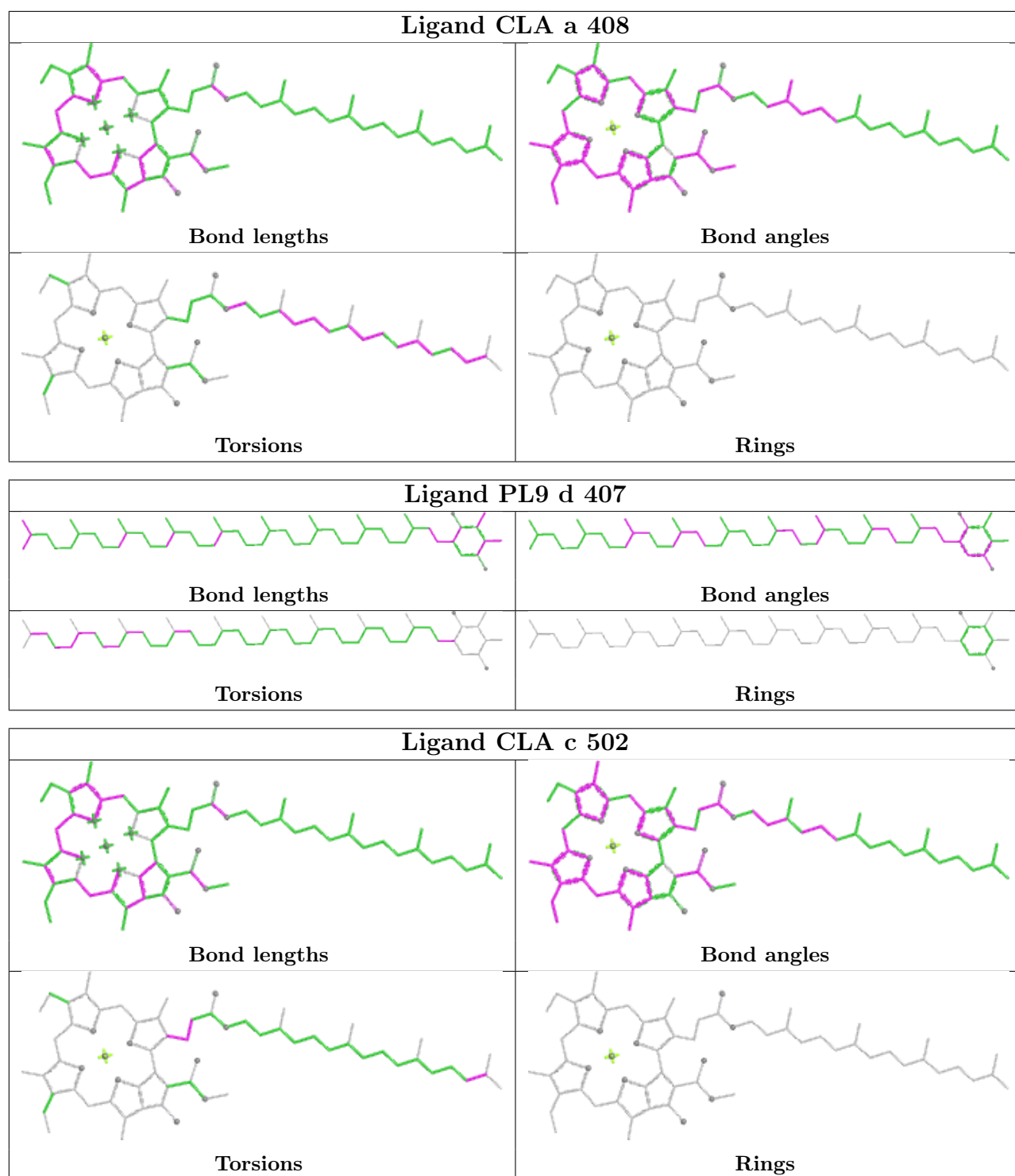


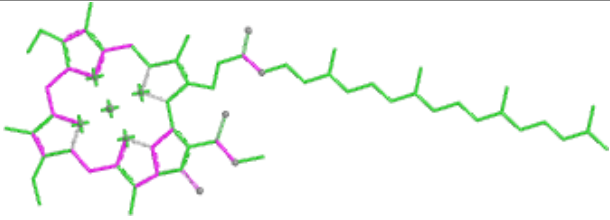
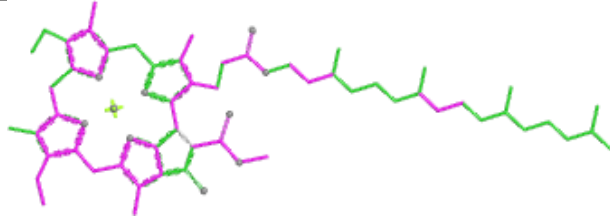
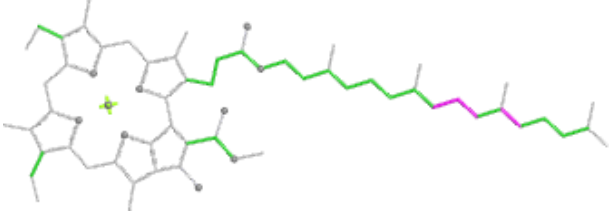
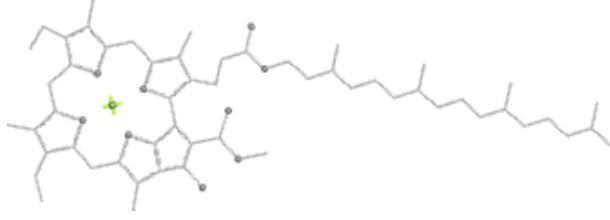
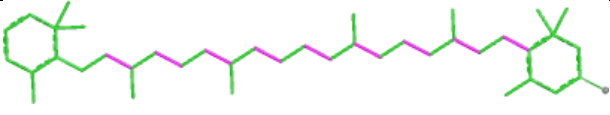
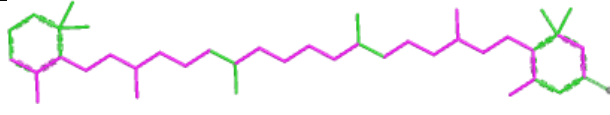
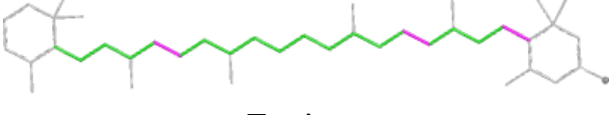
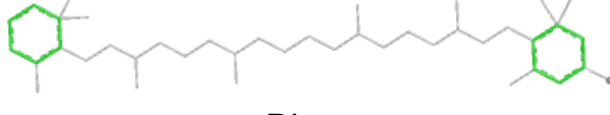
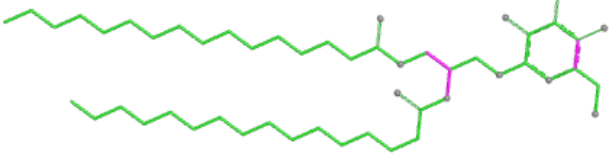
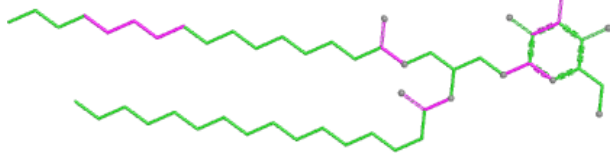
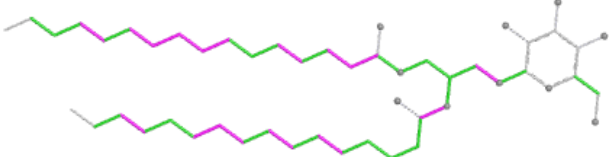
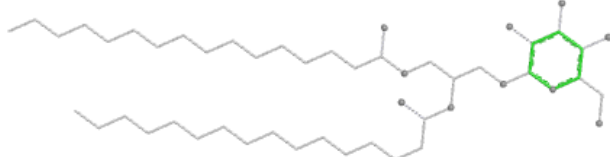


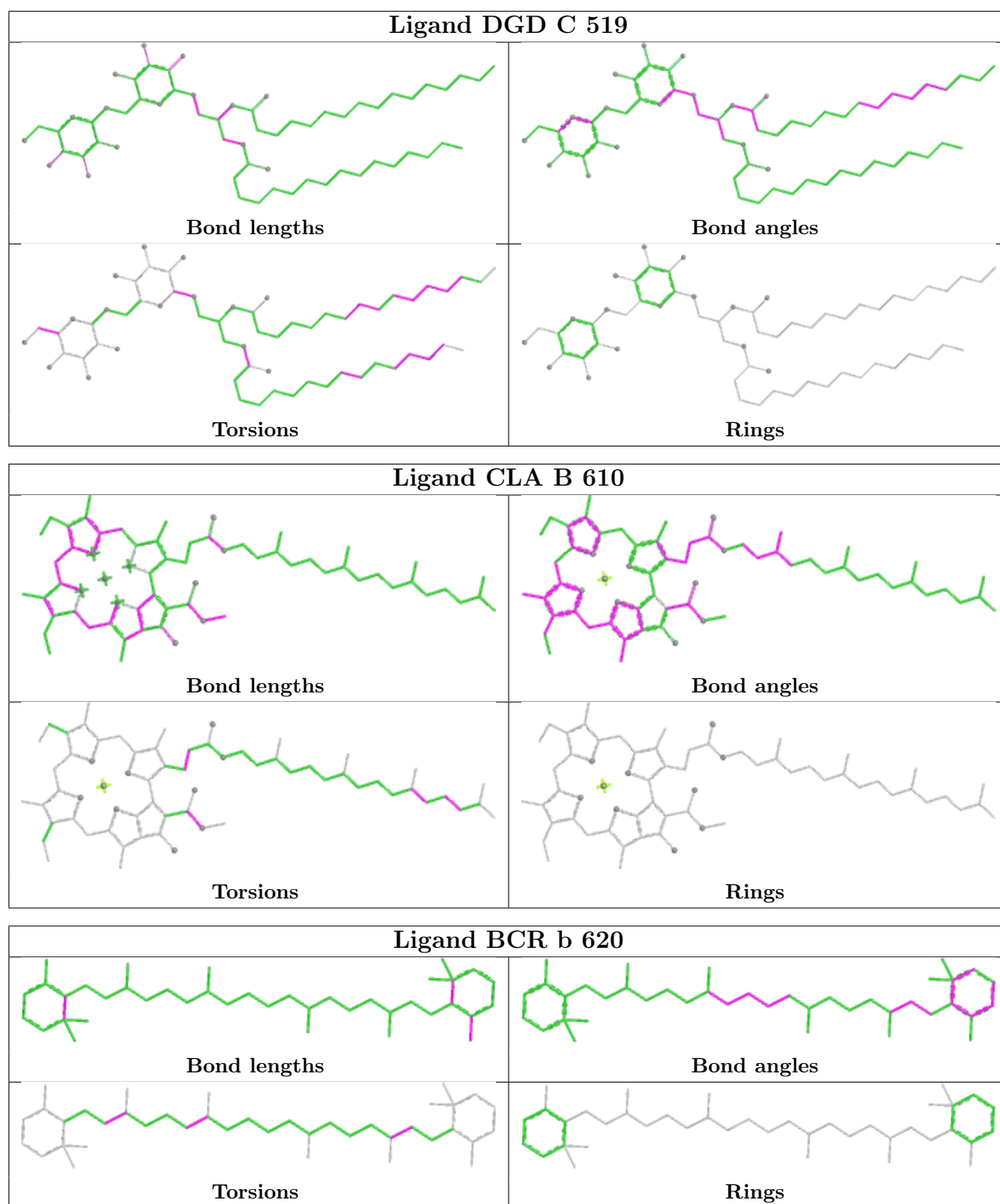


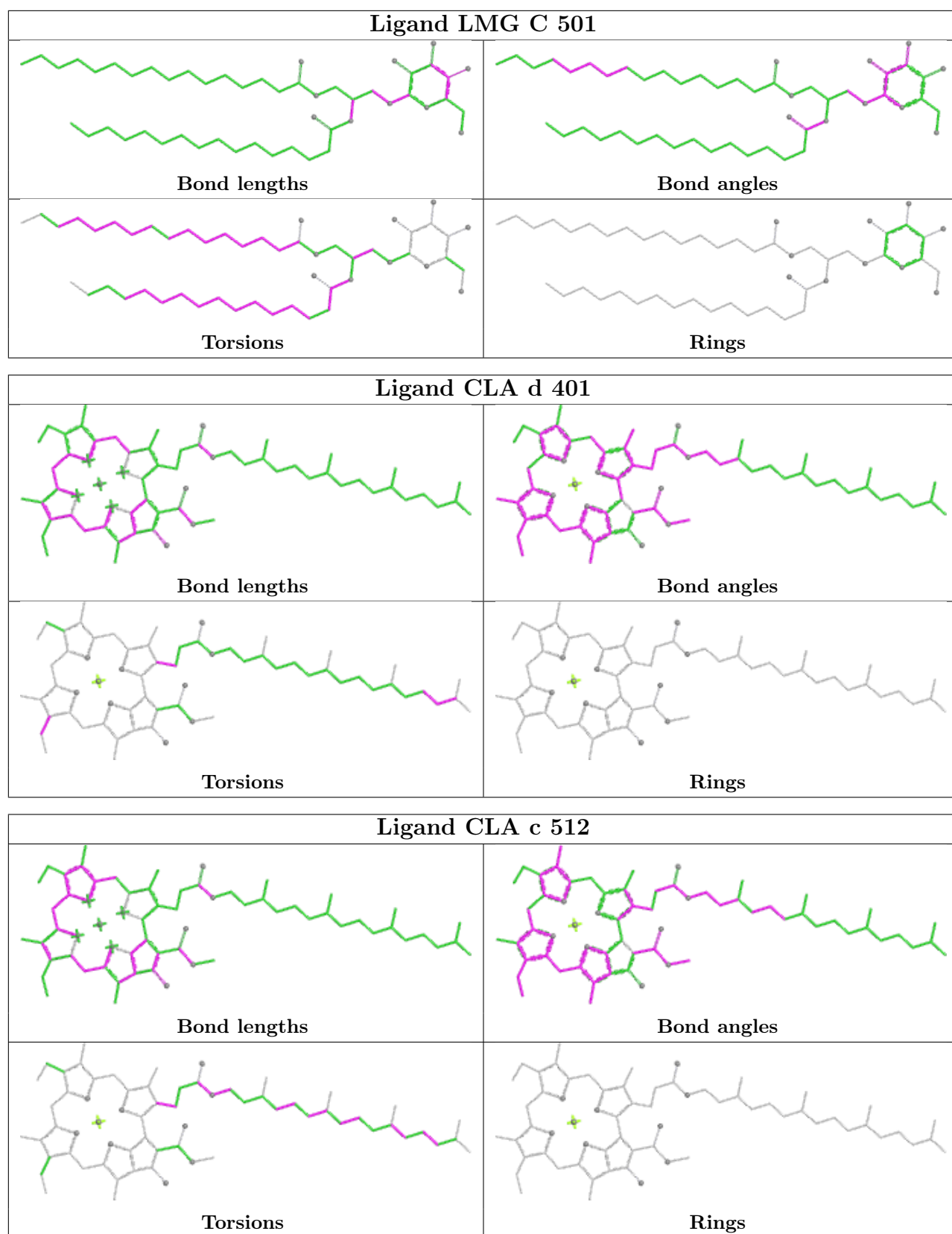


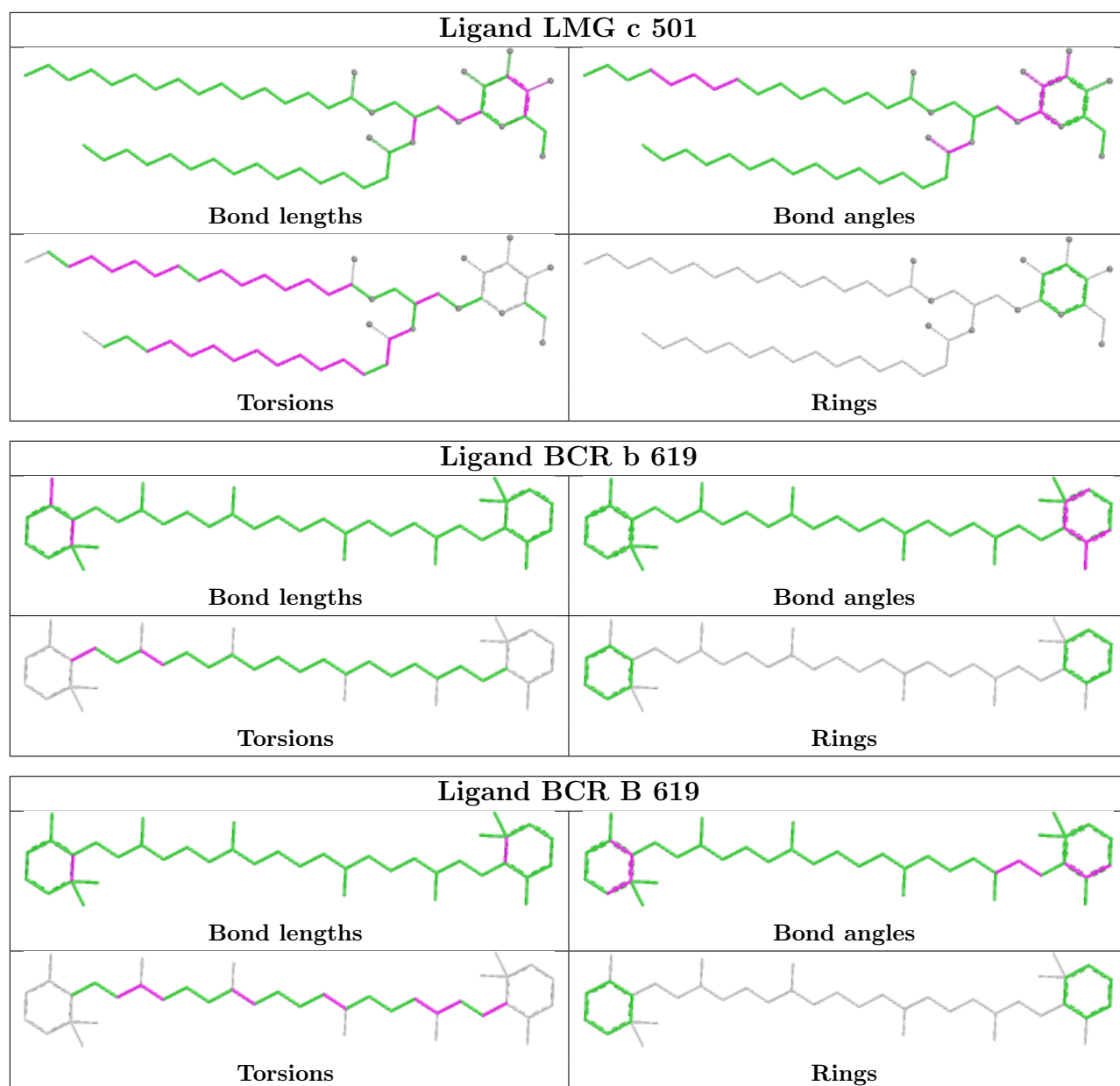


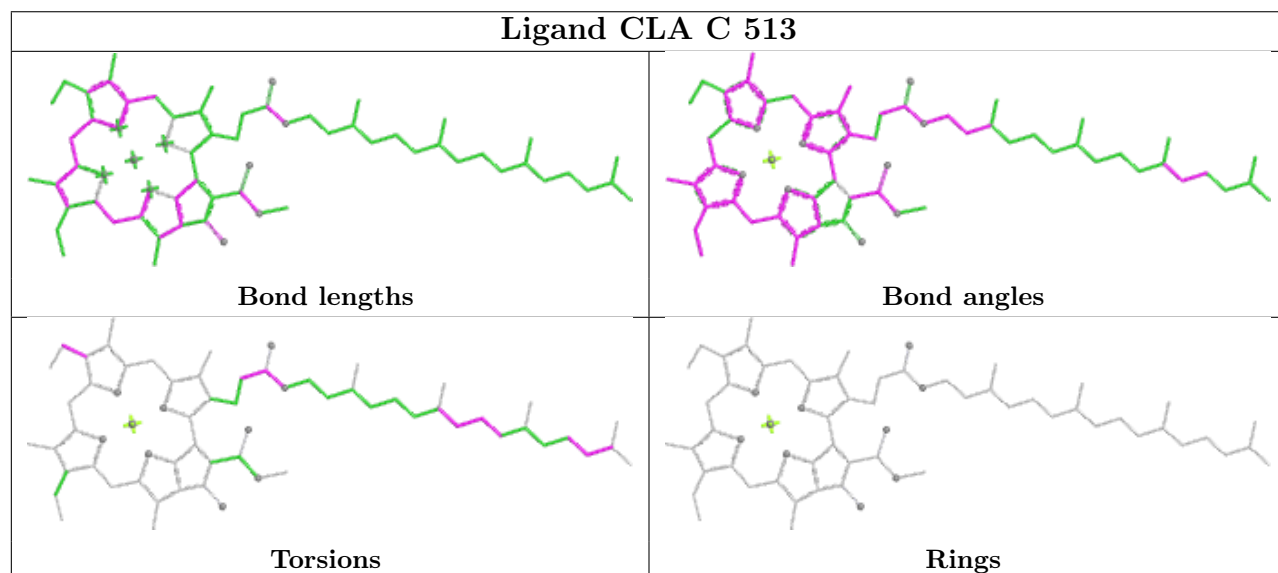
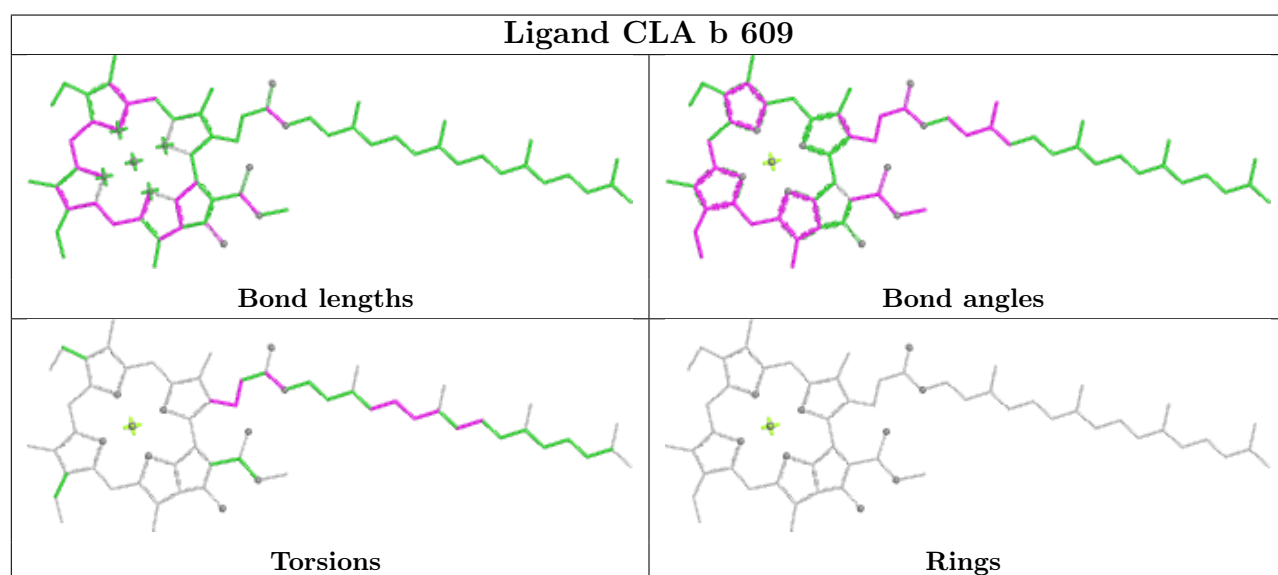
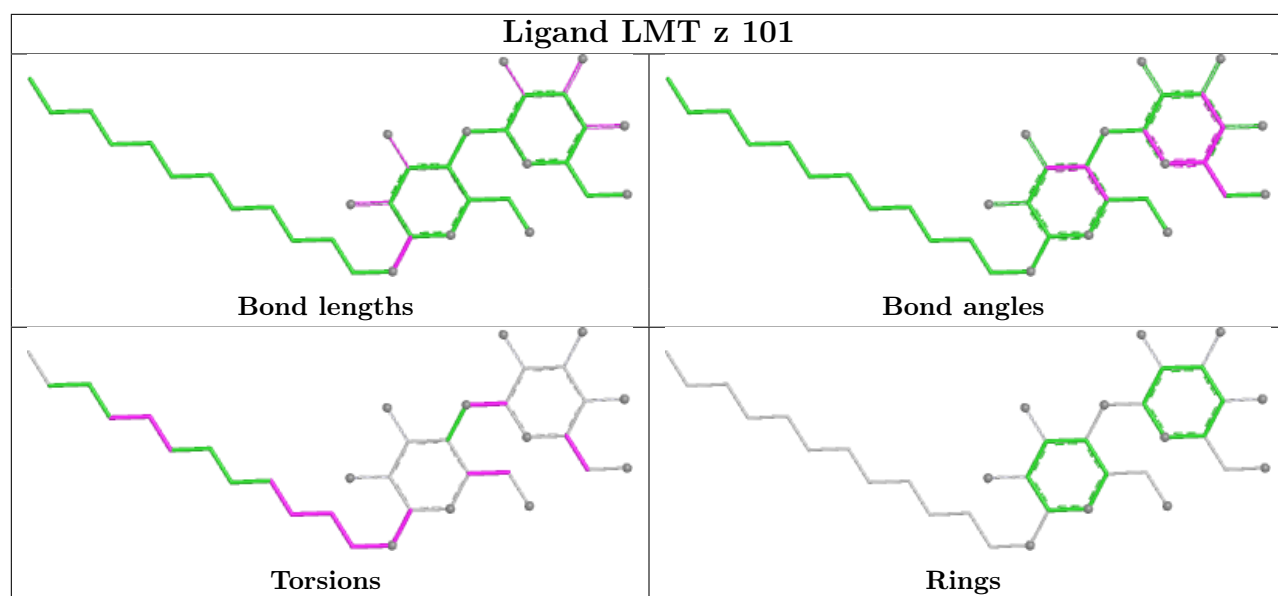


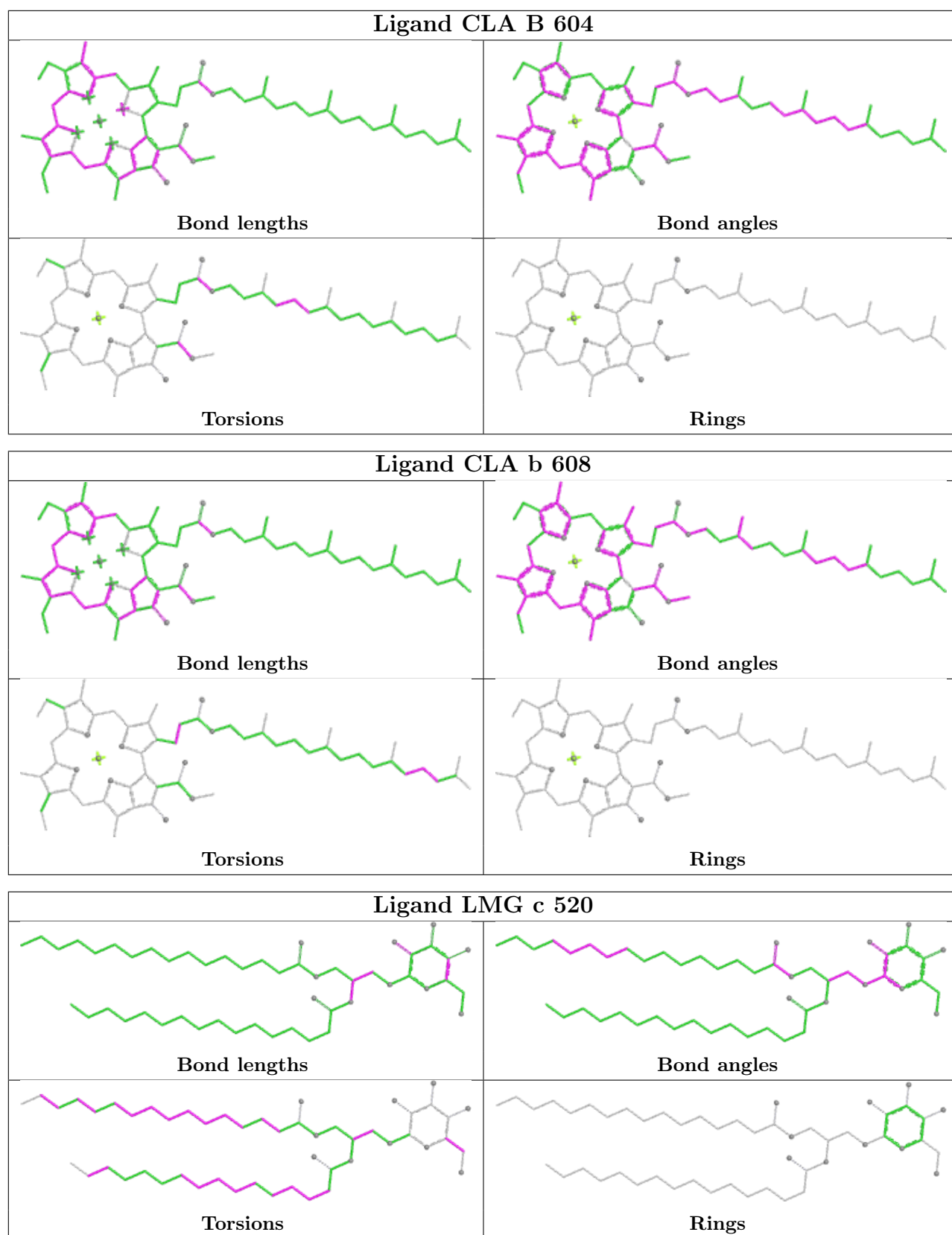
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand RRX x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

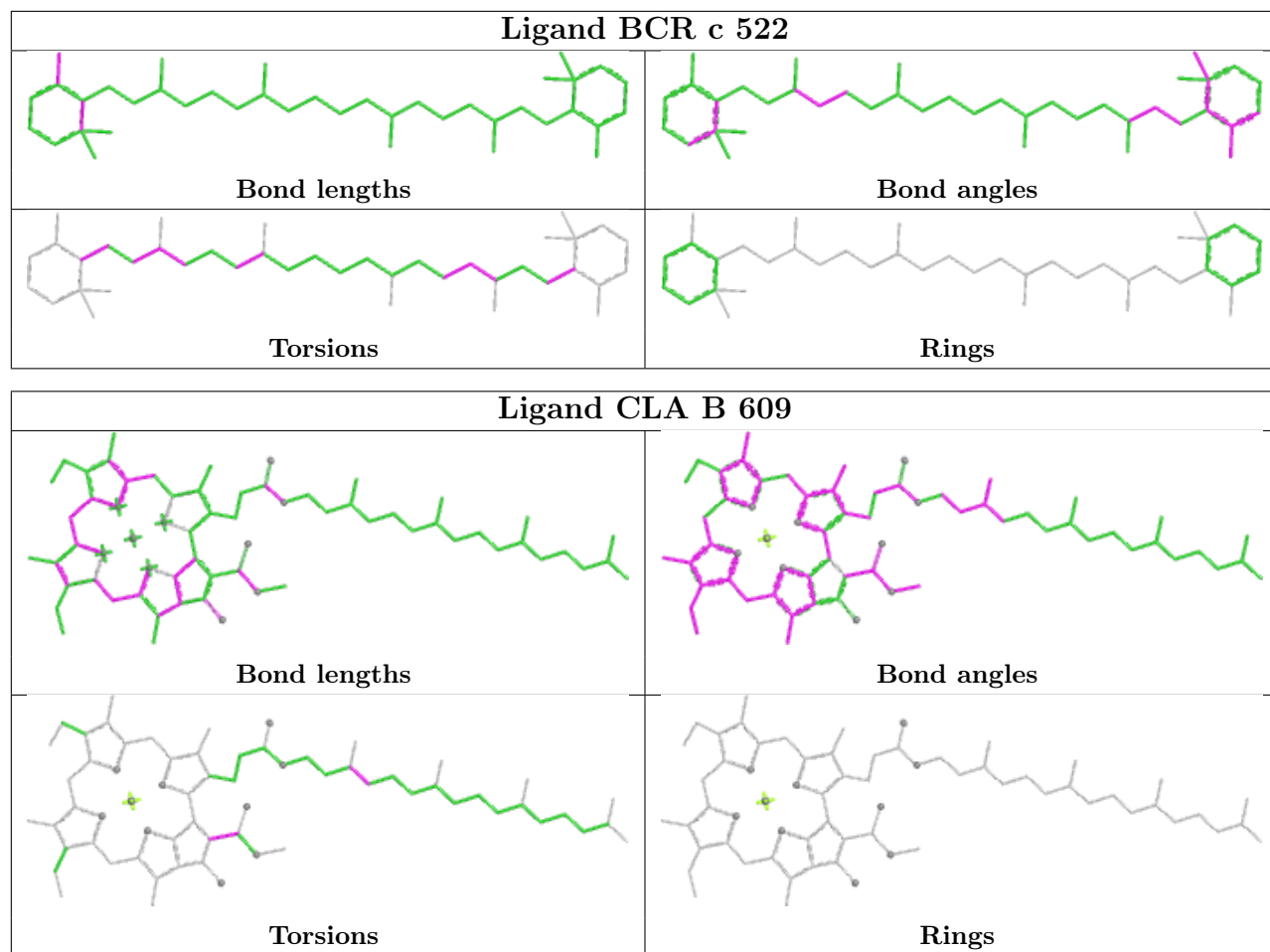


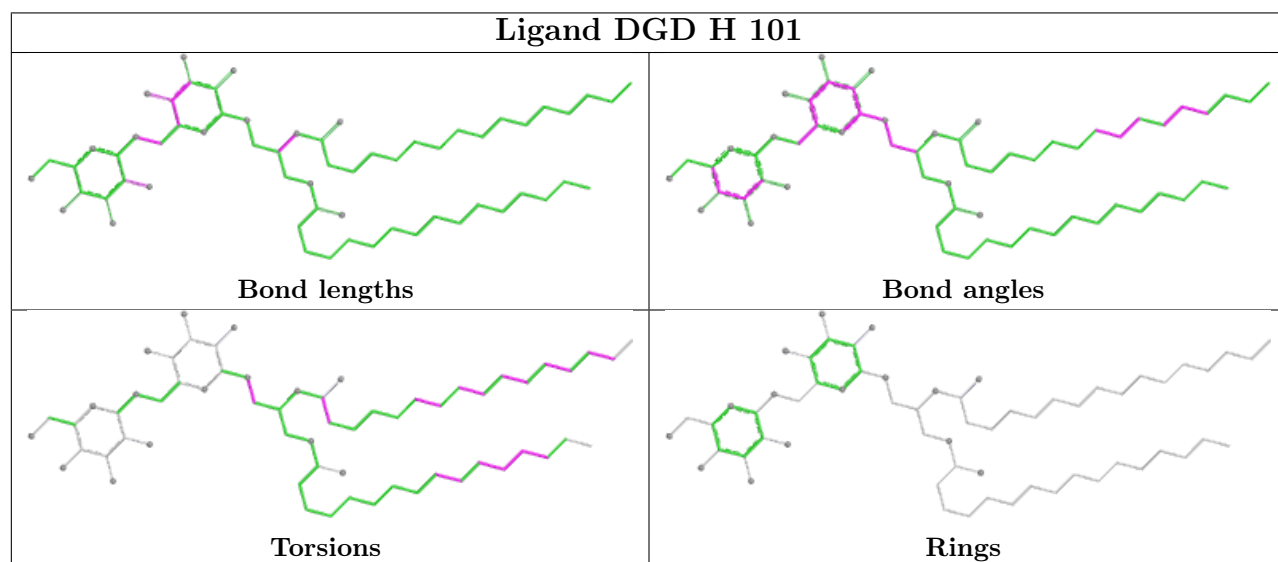
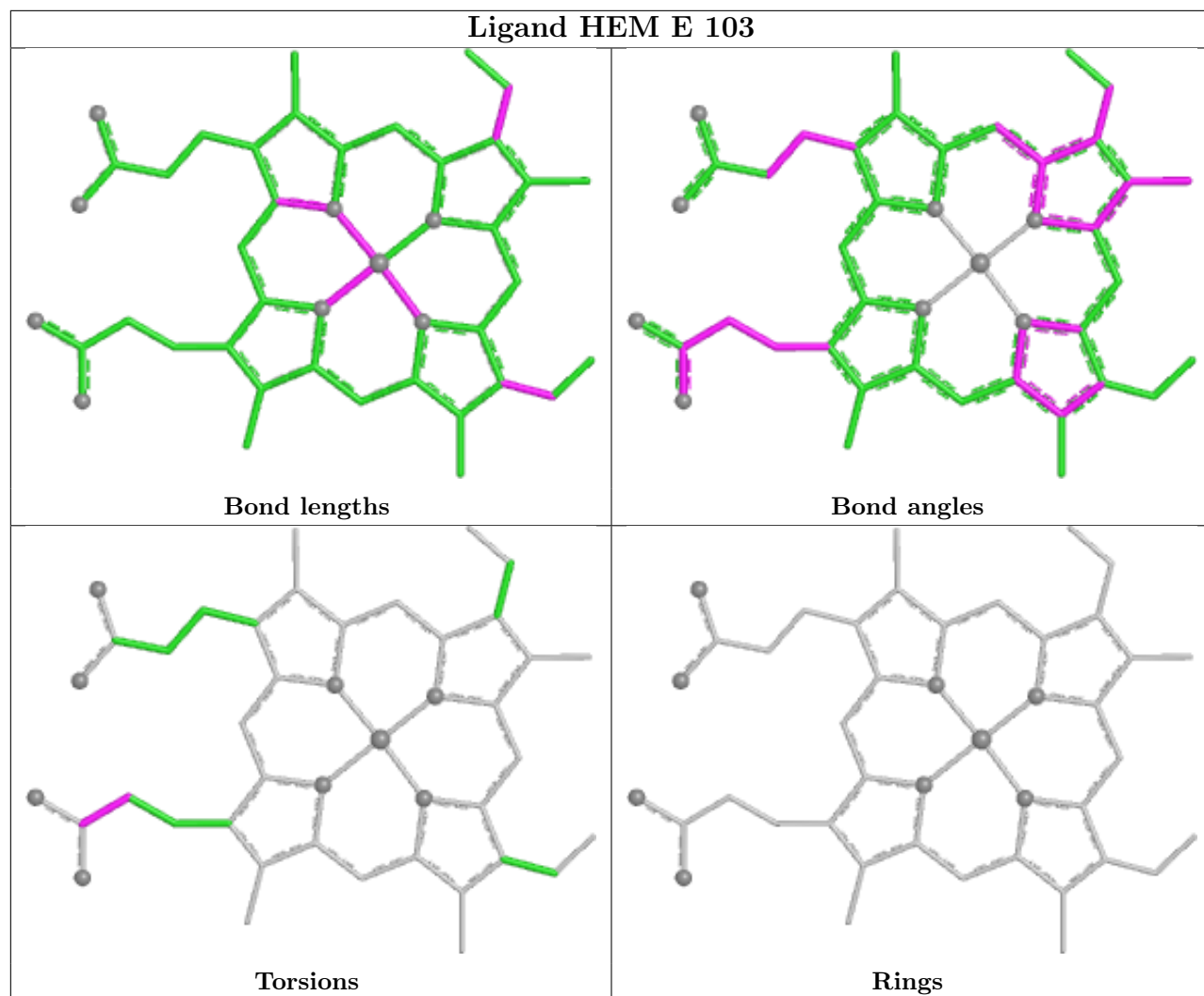


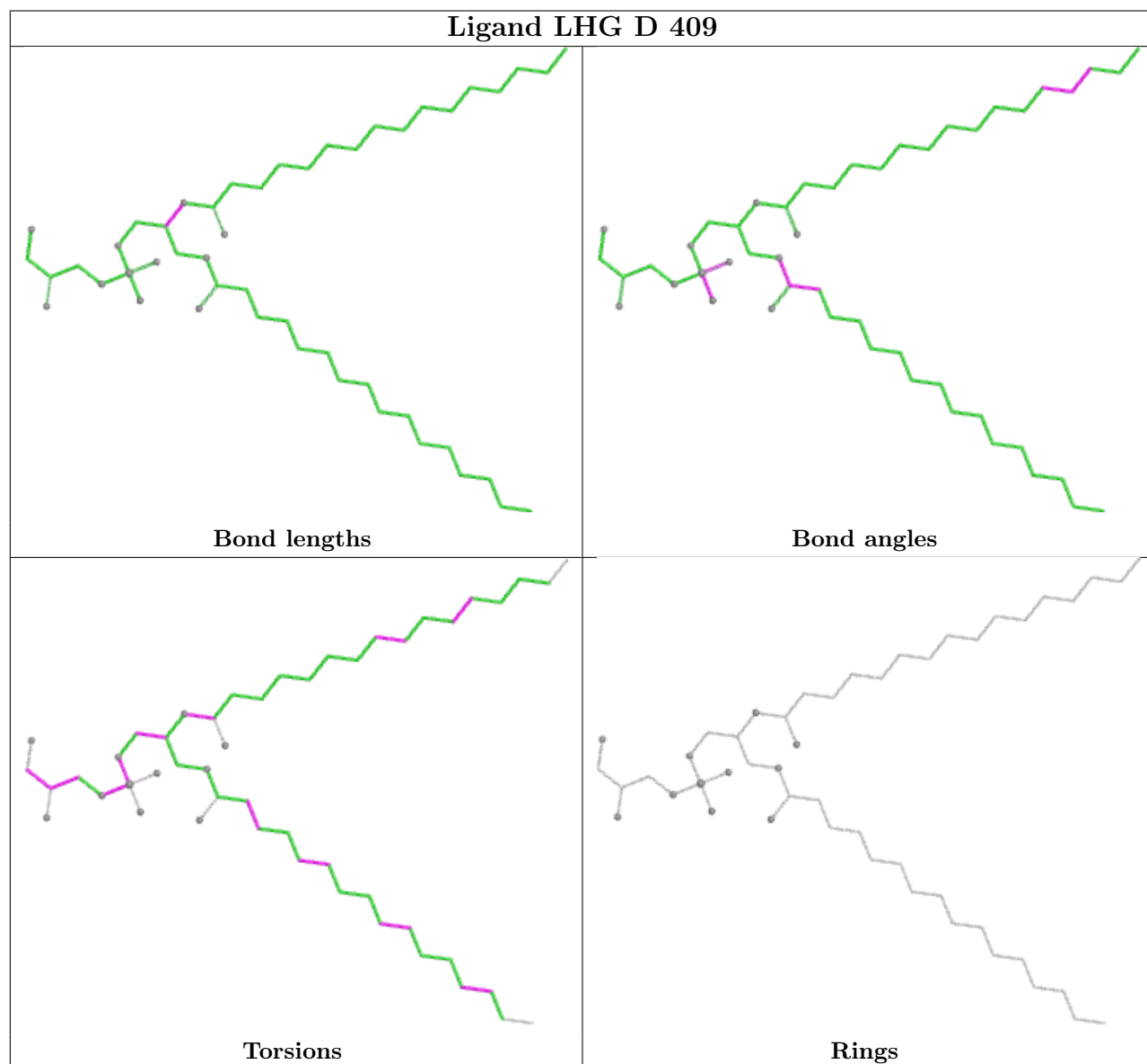
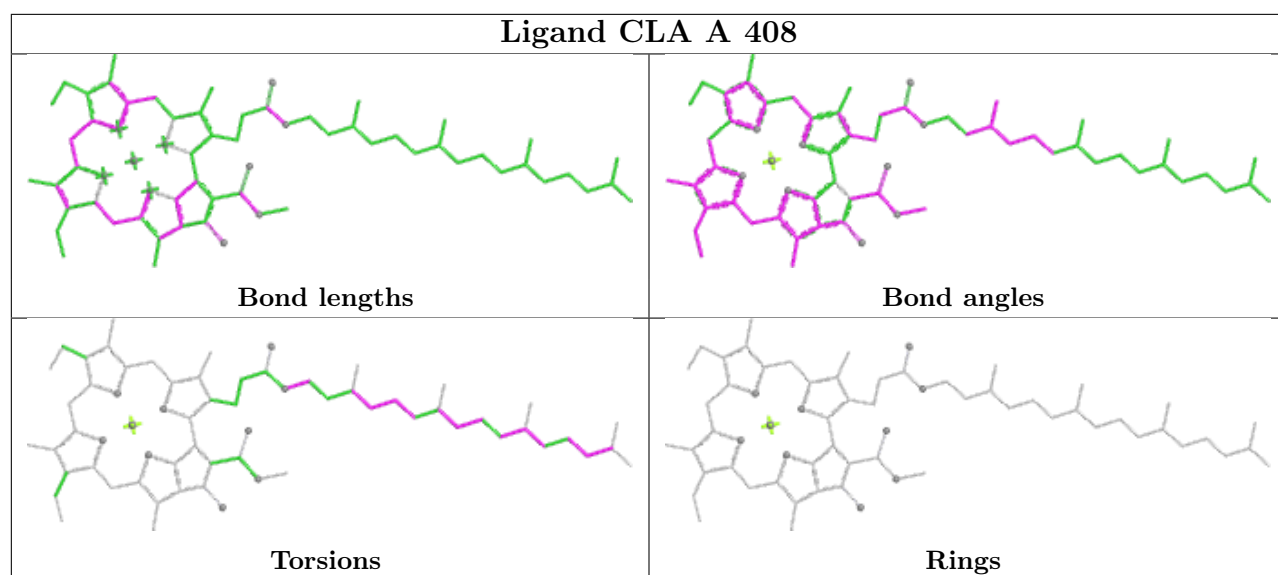


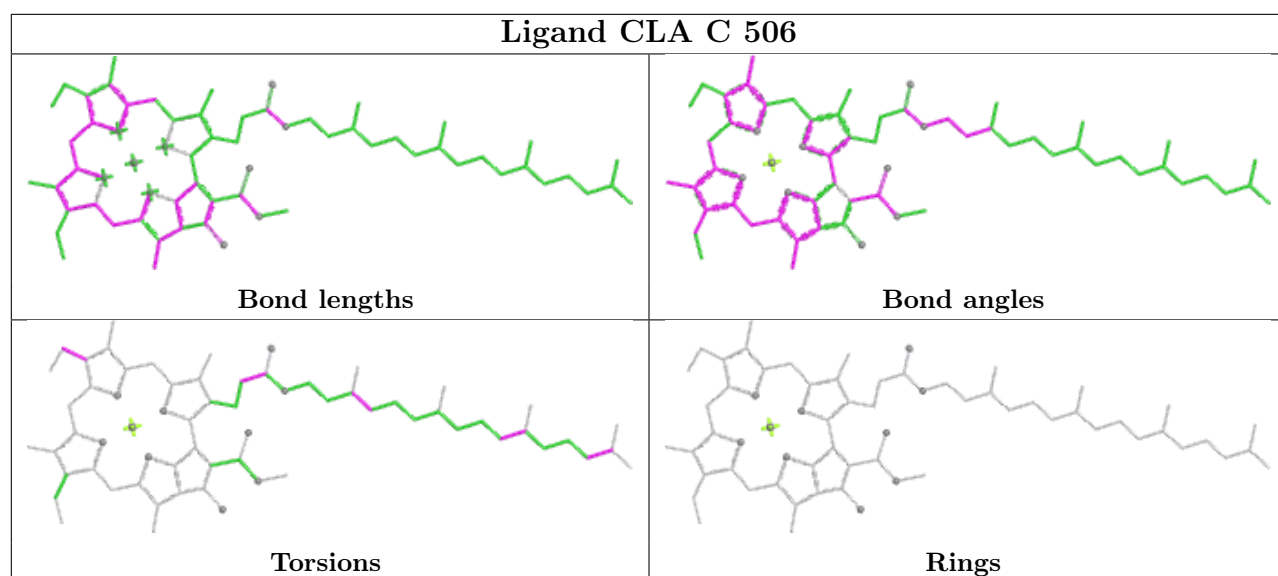
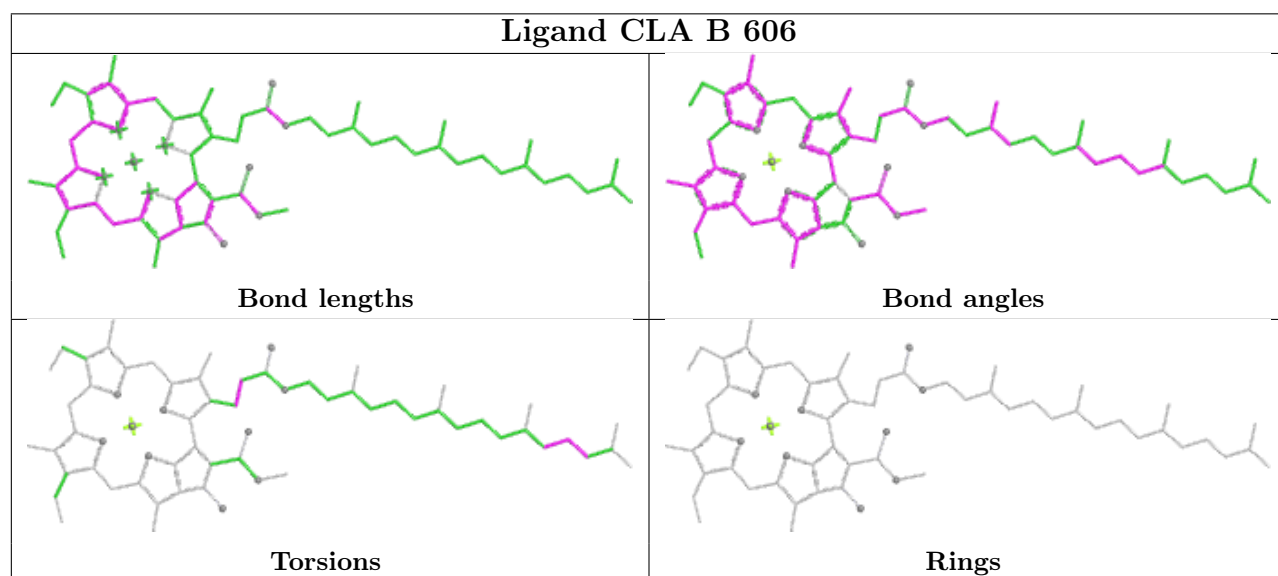
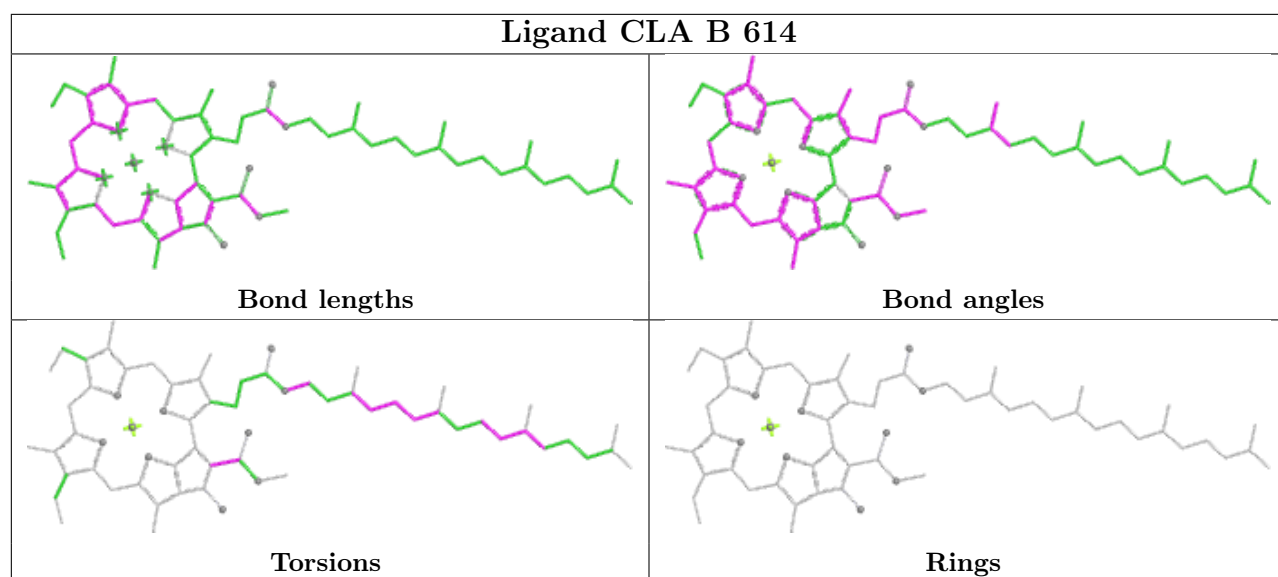


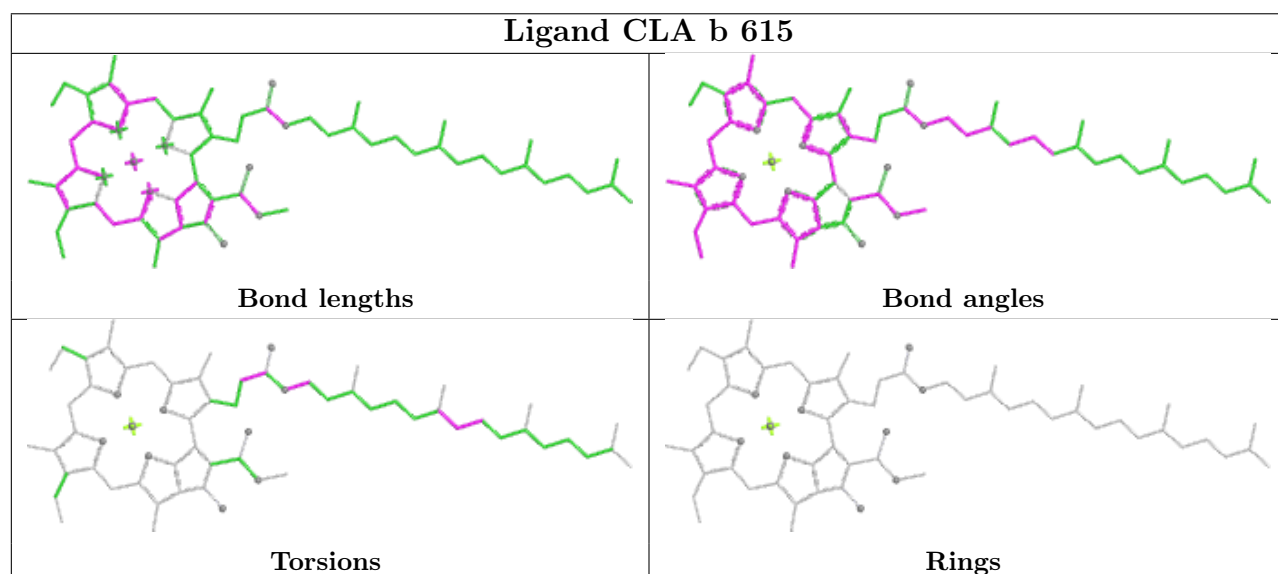
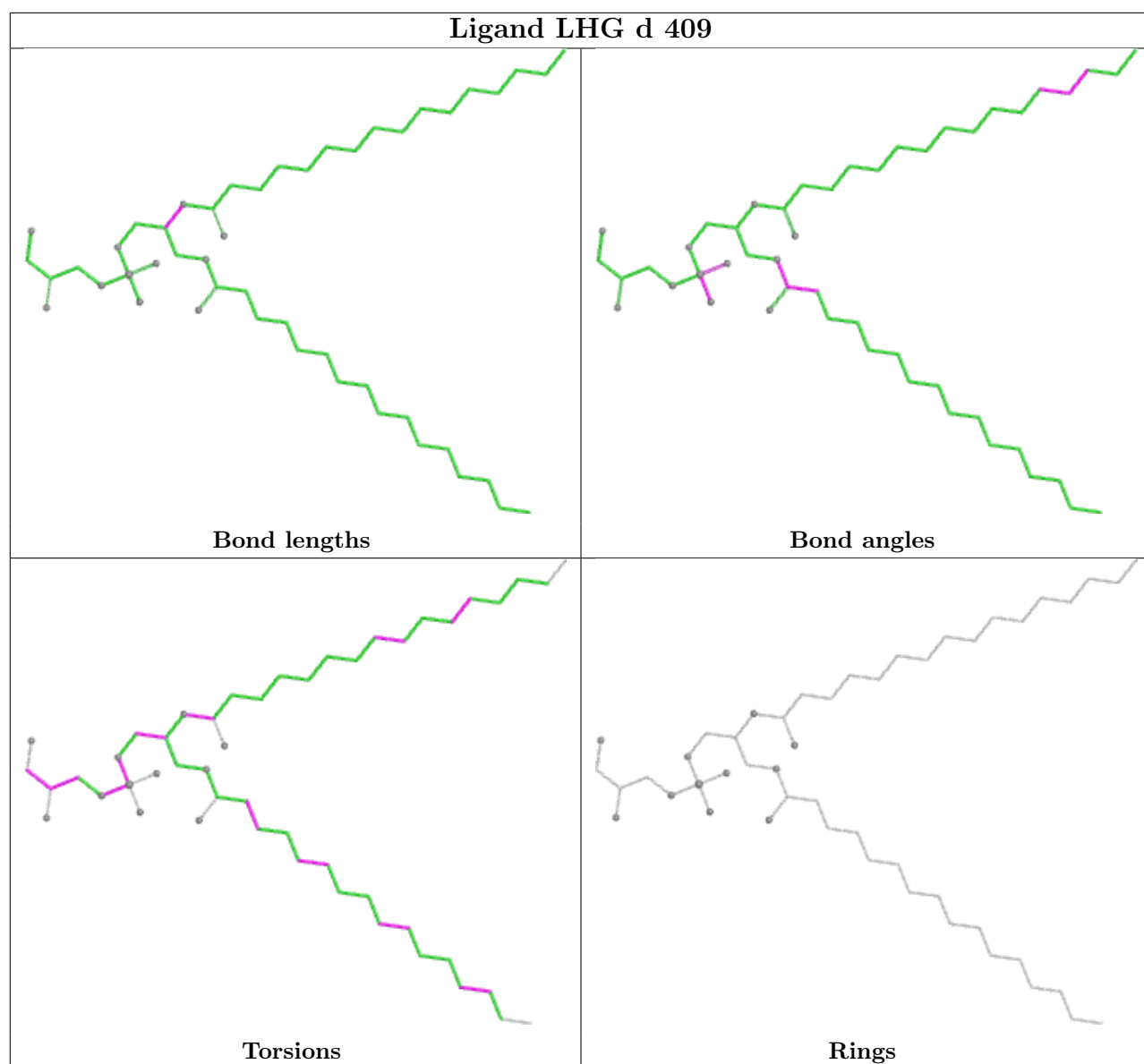


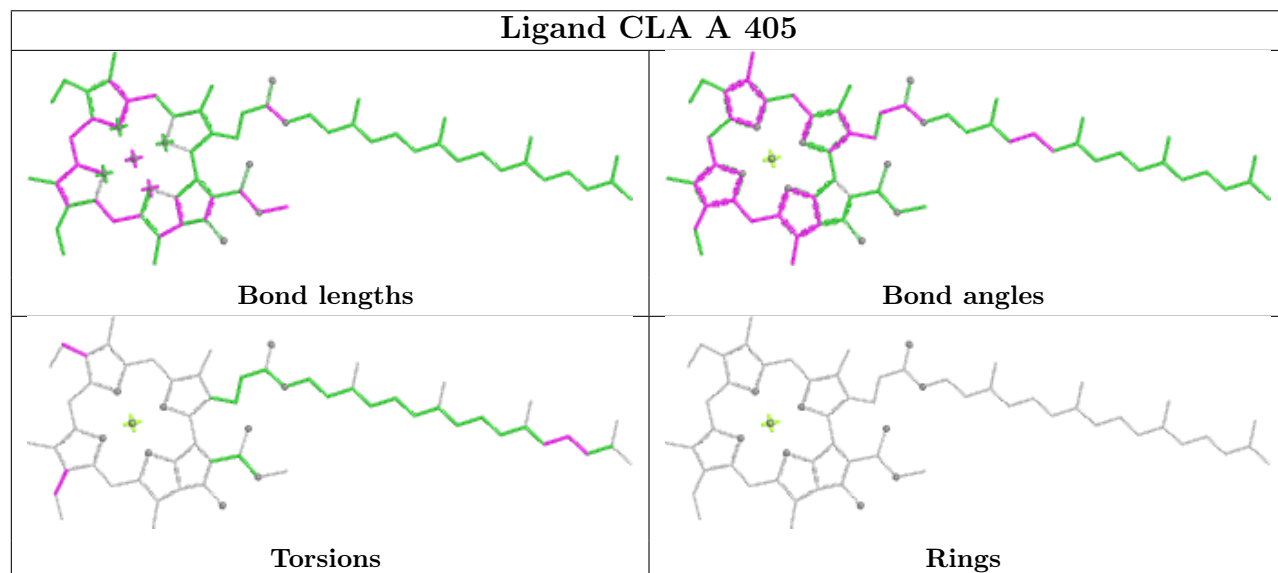
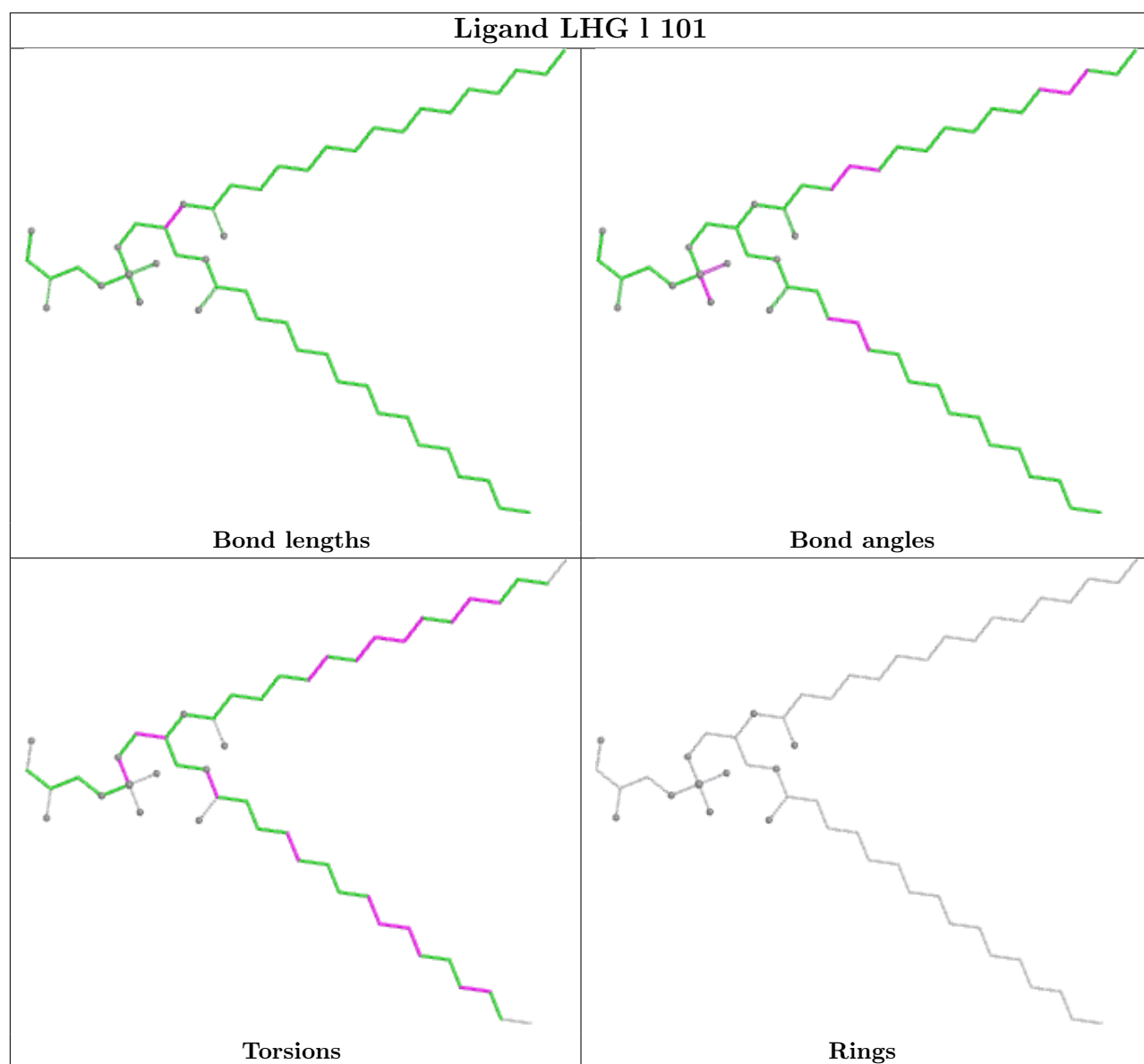


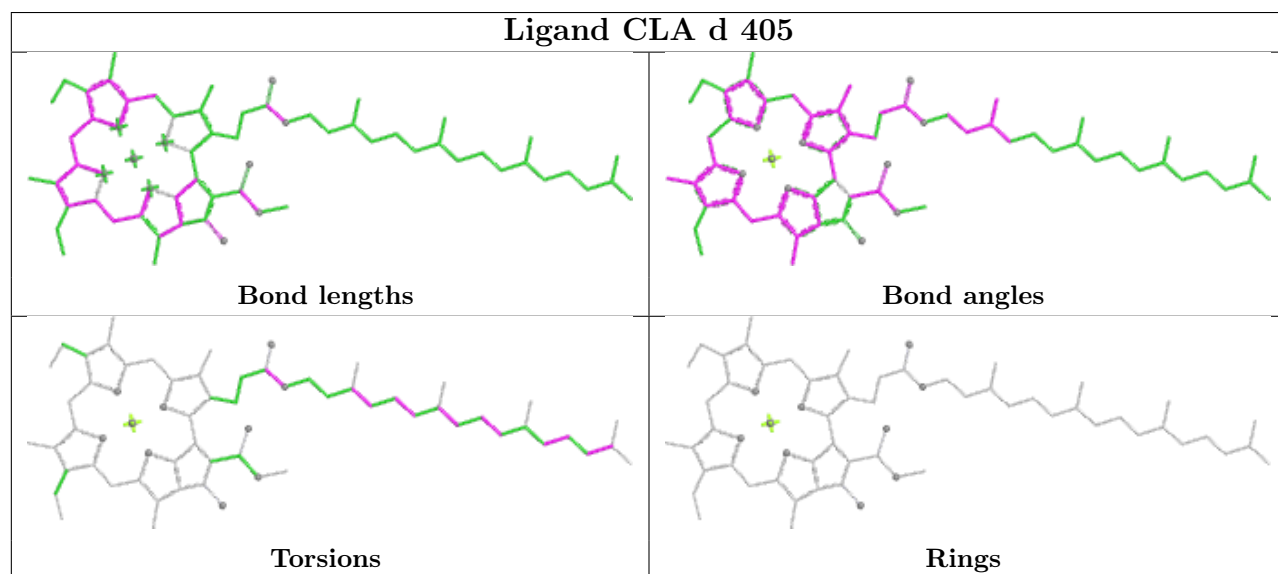
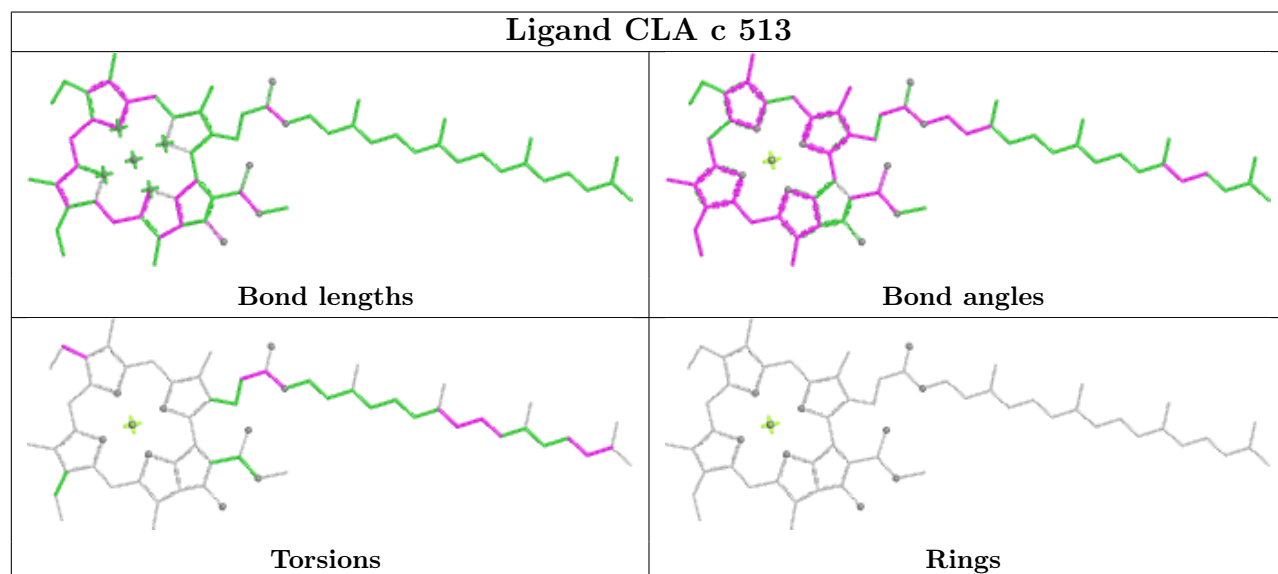
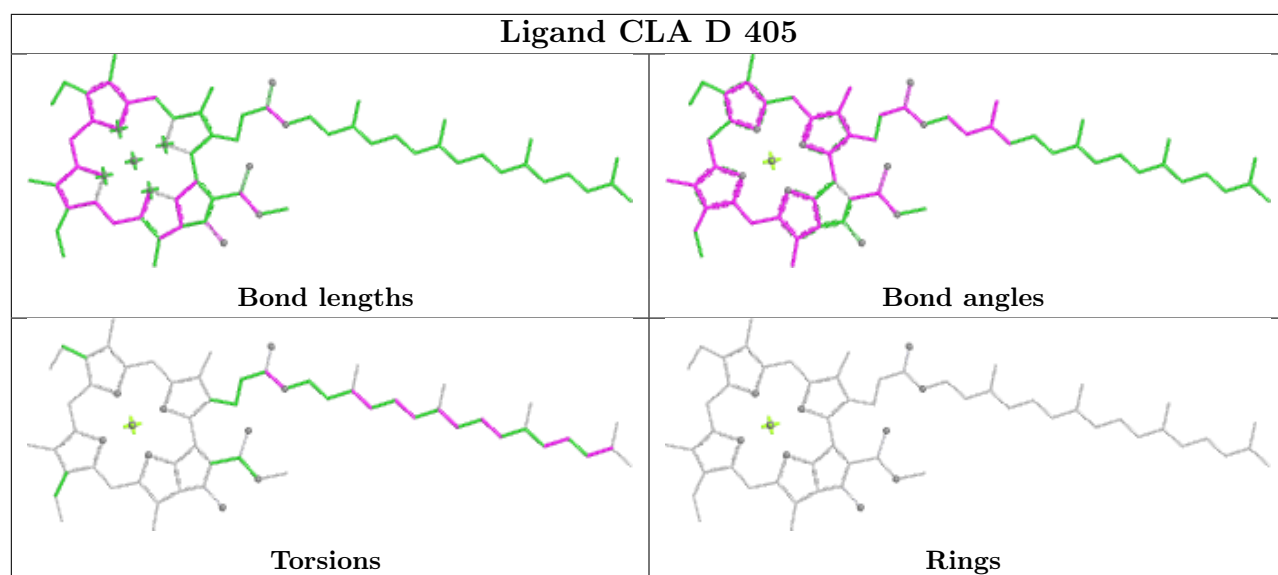


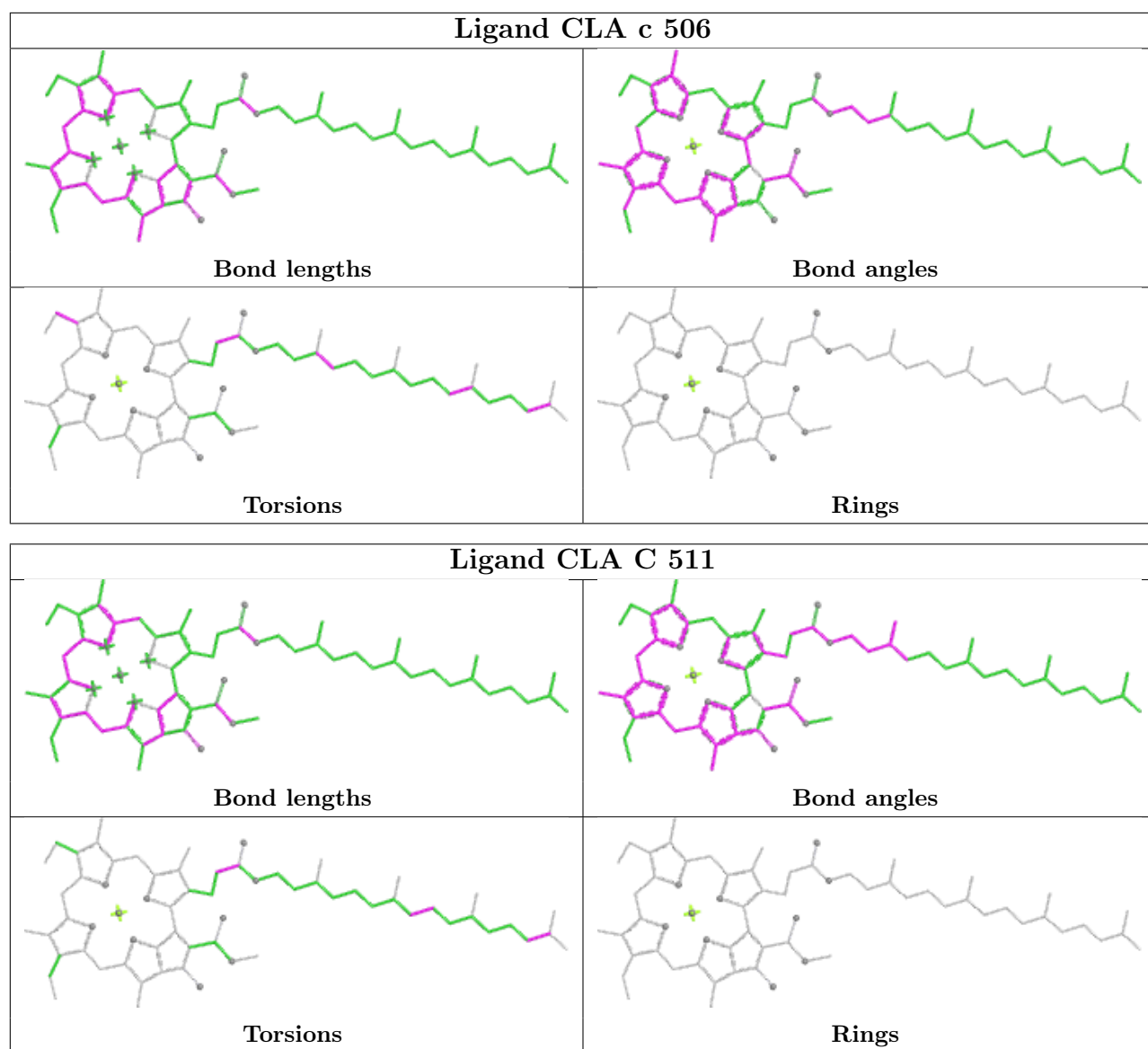


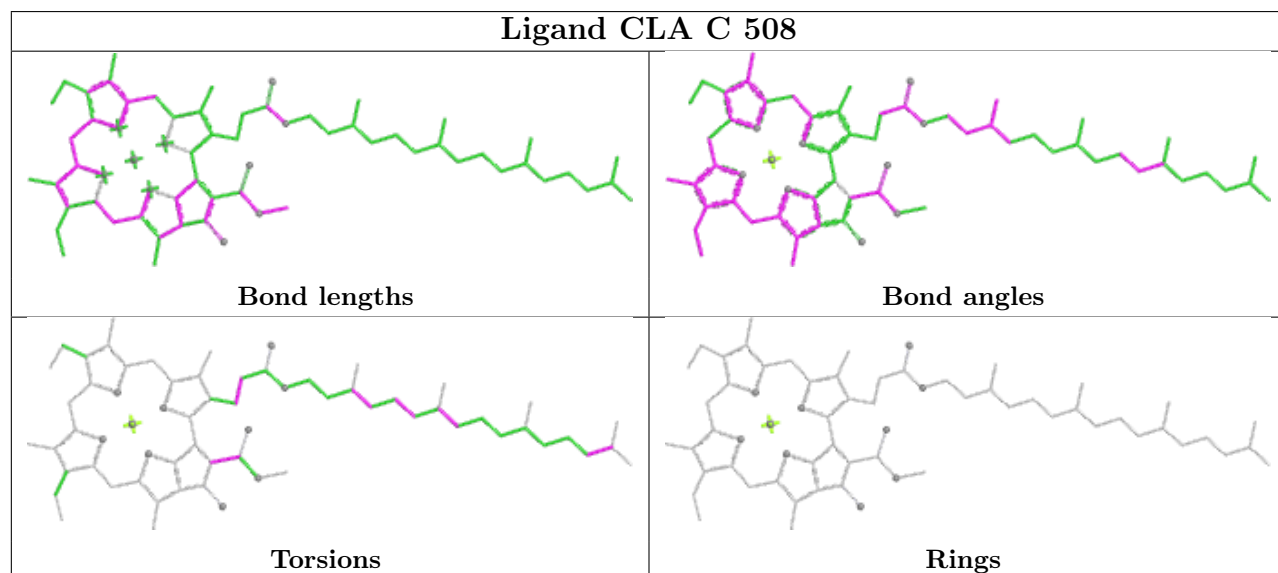
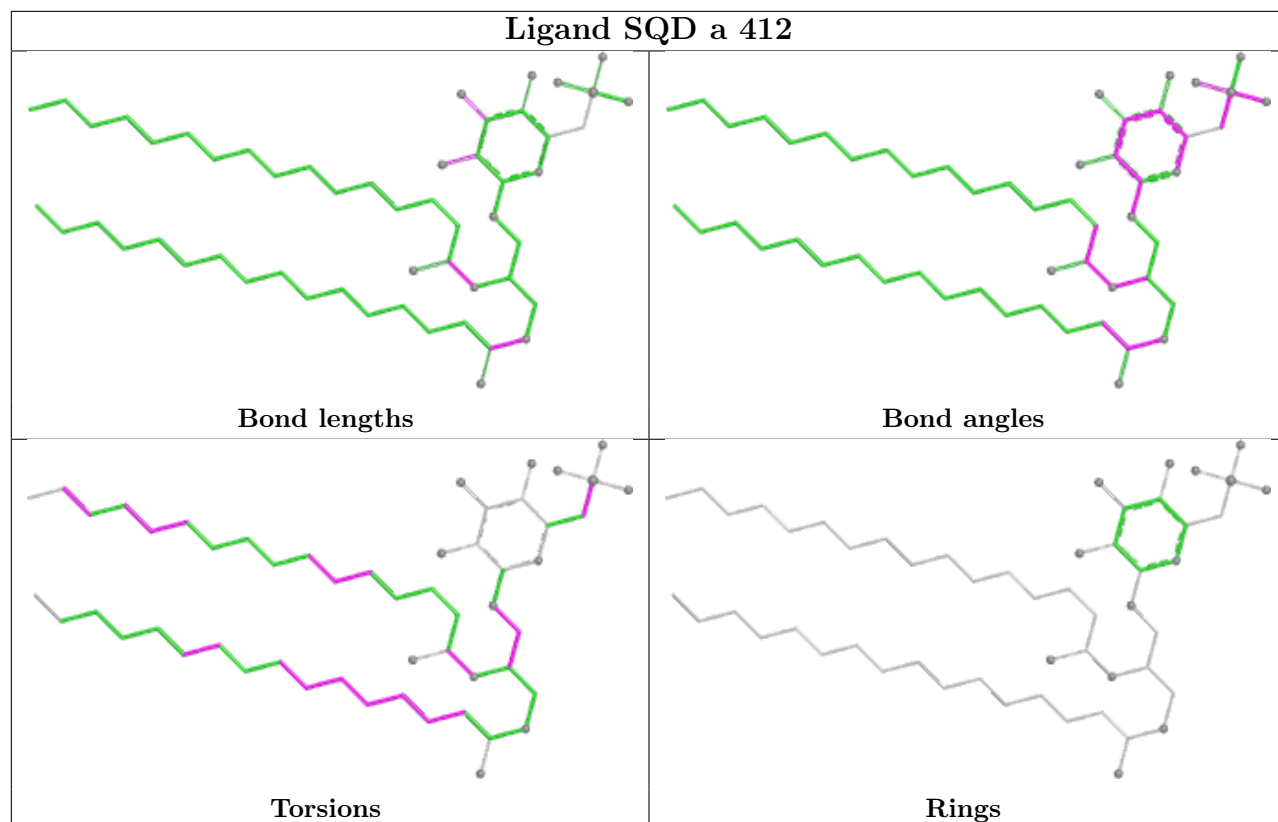


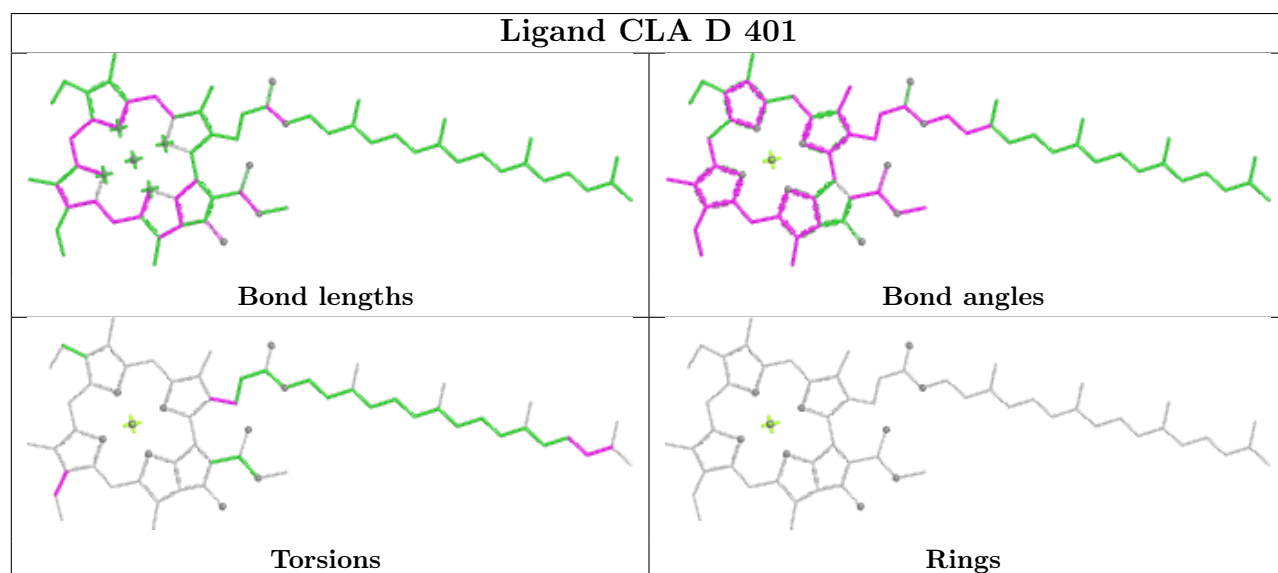
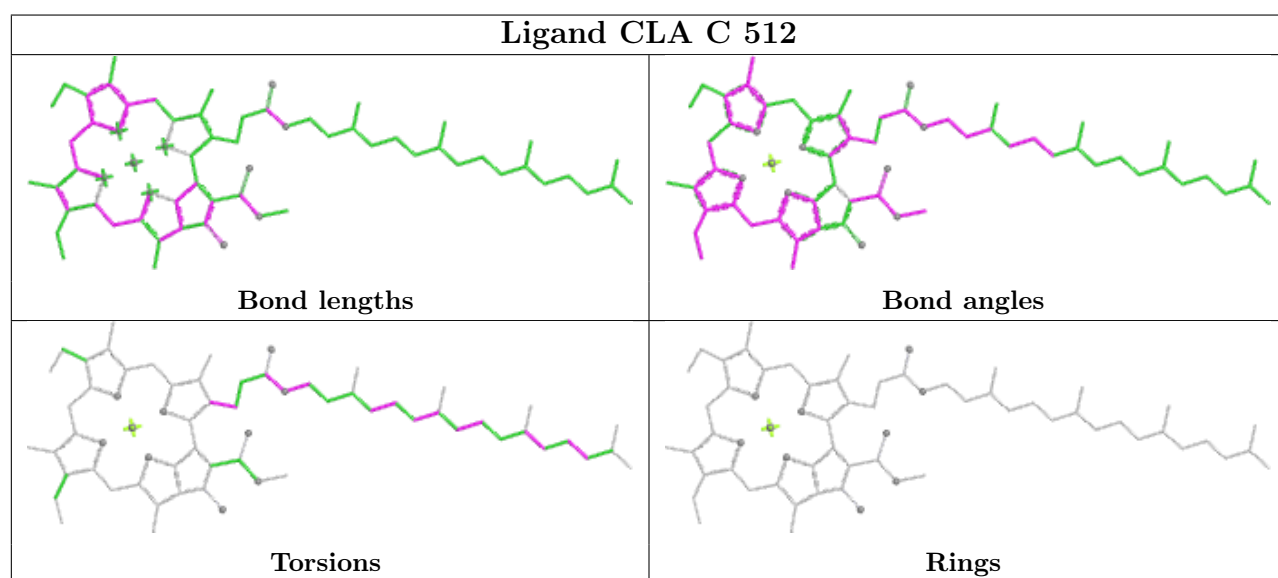
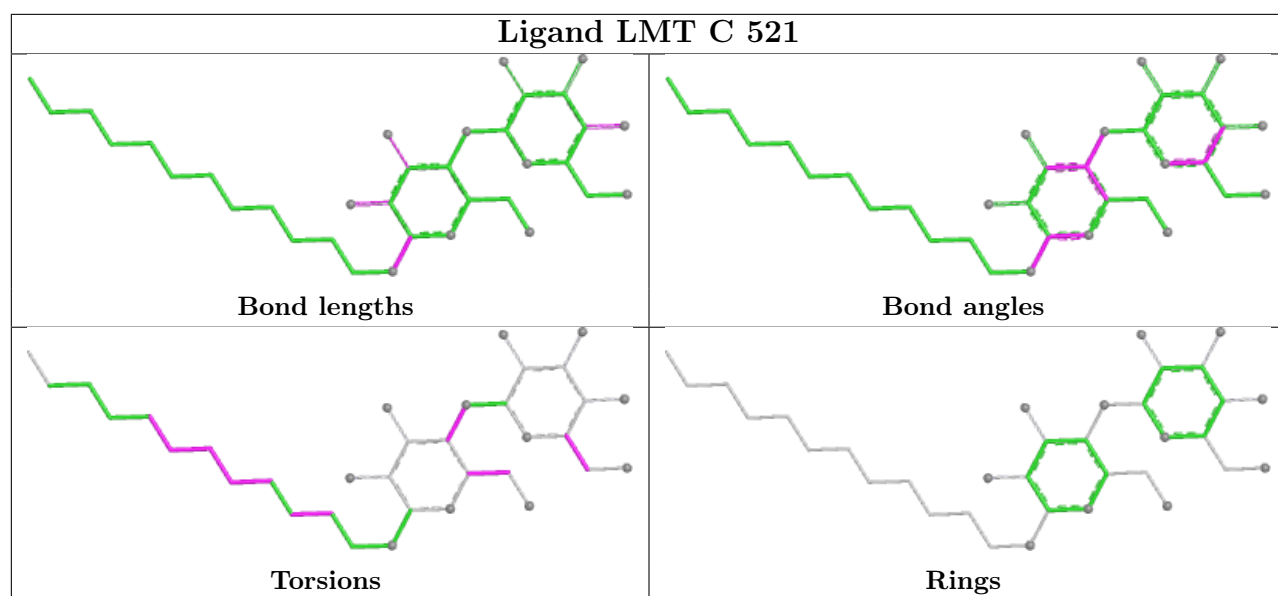


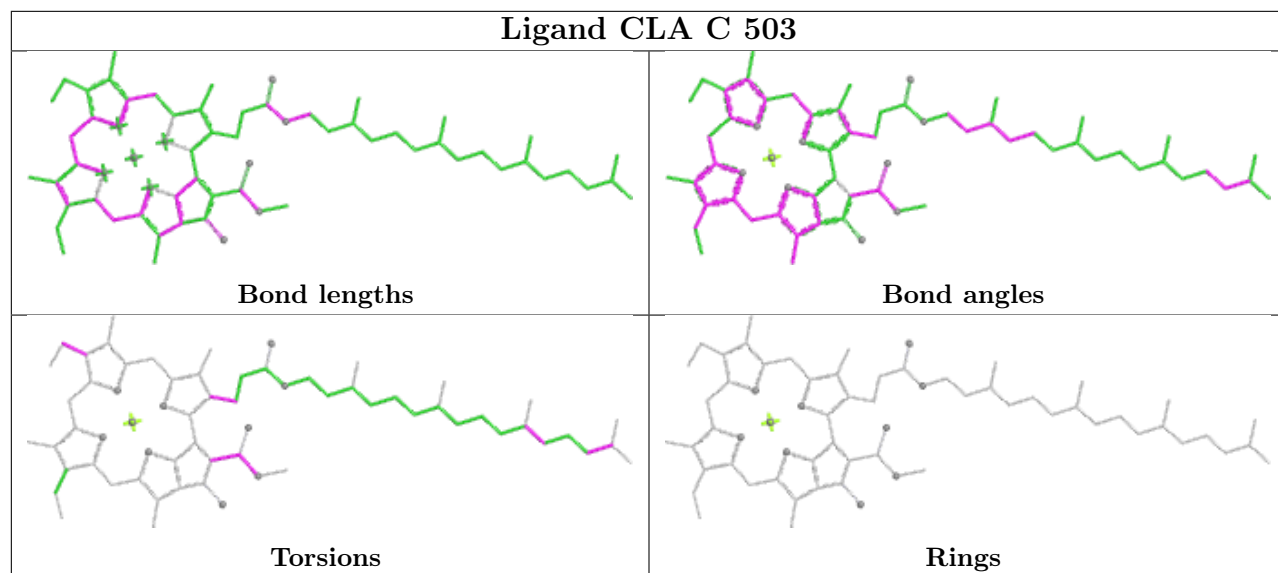
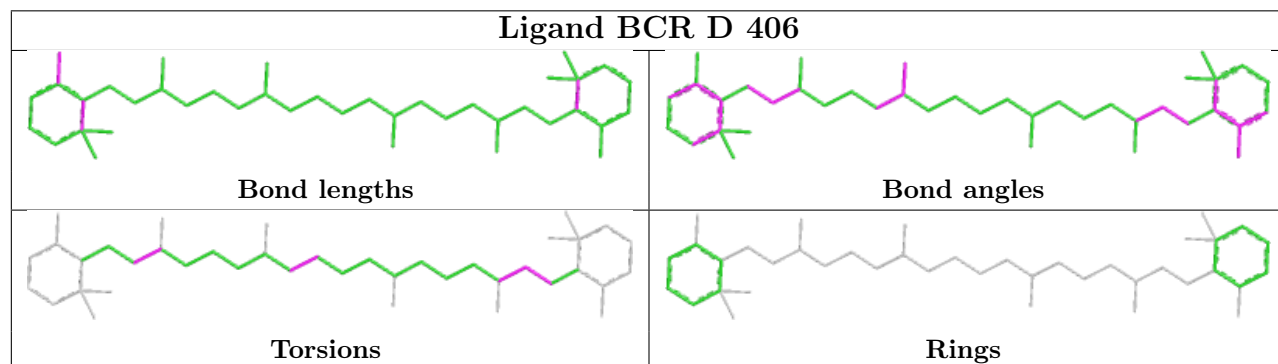
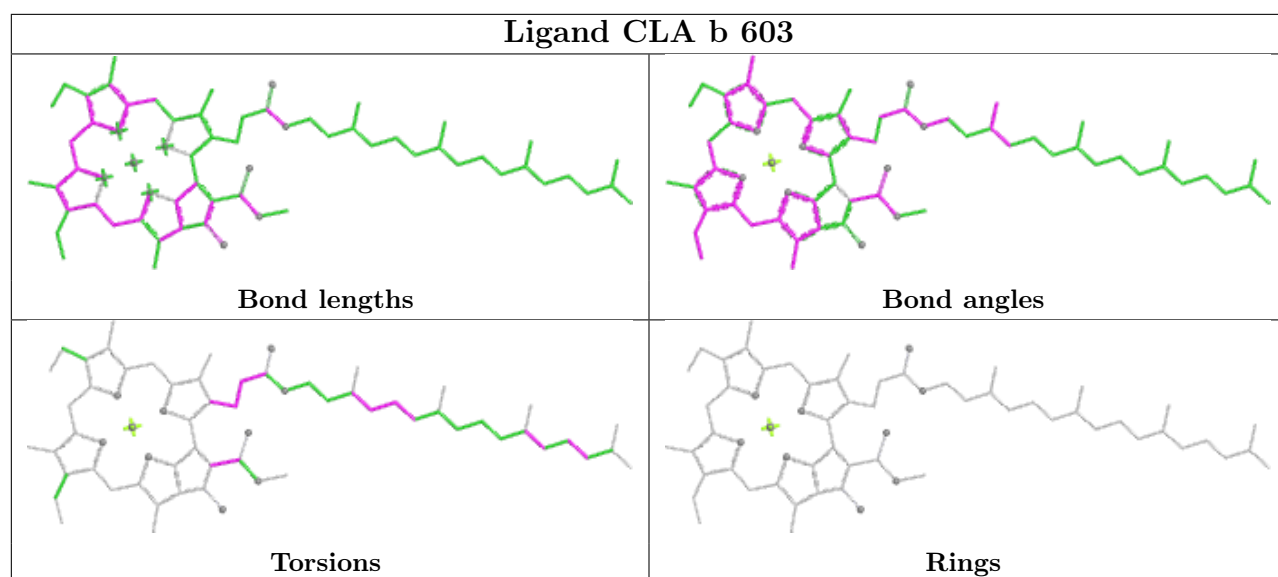


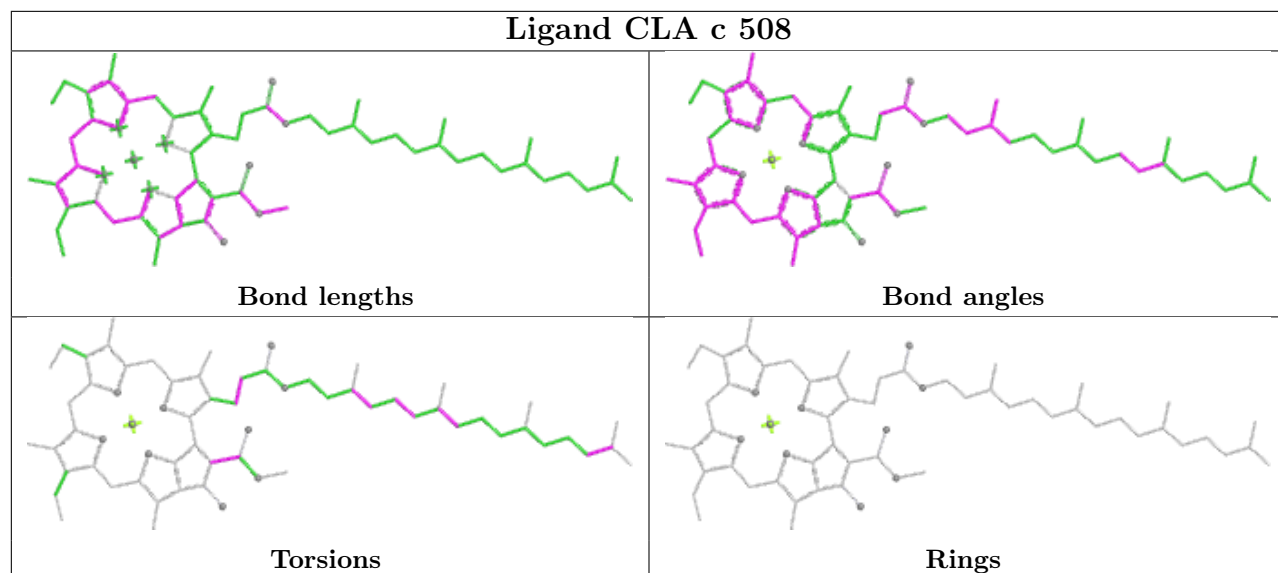
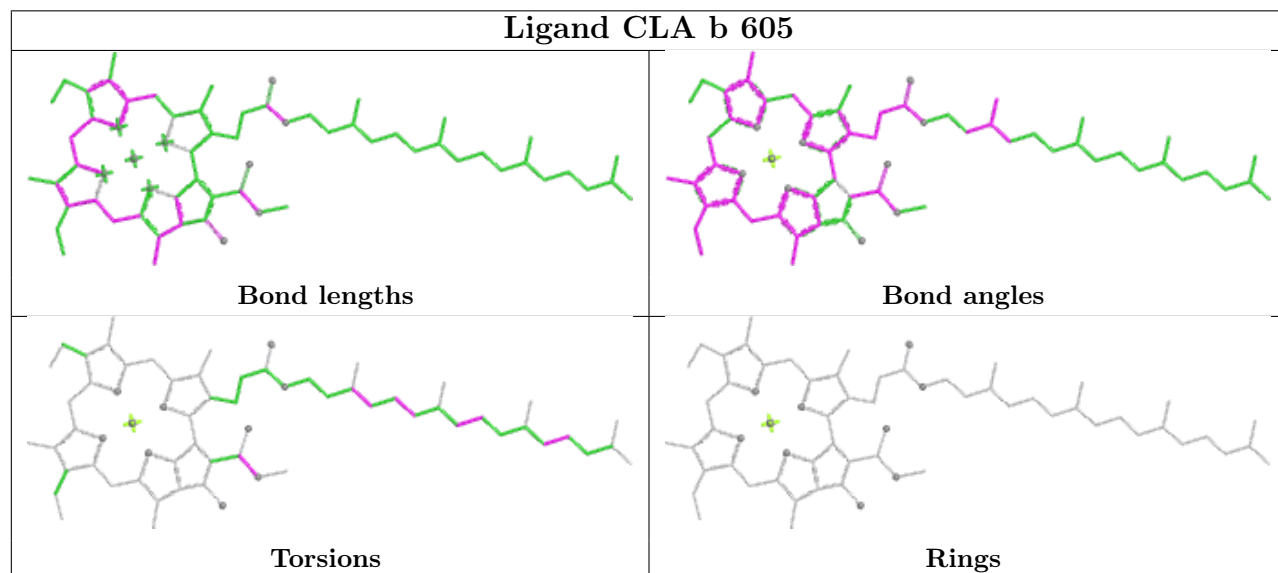
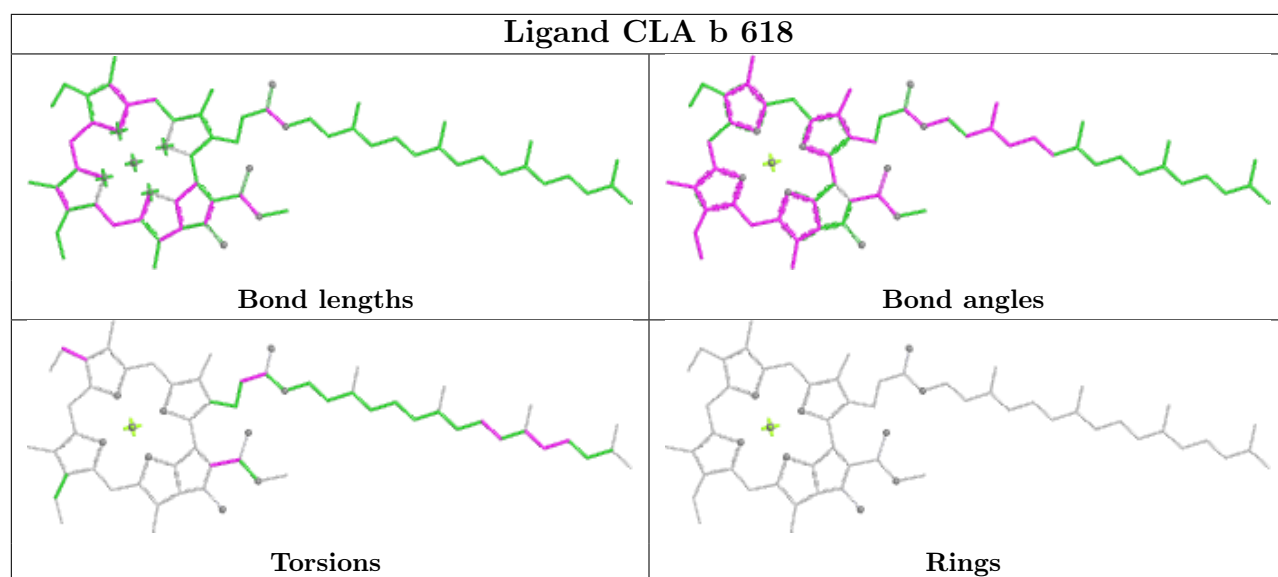


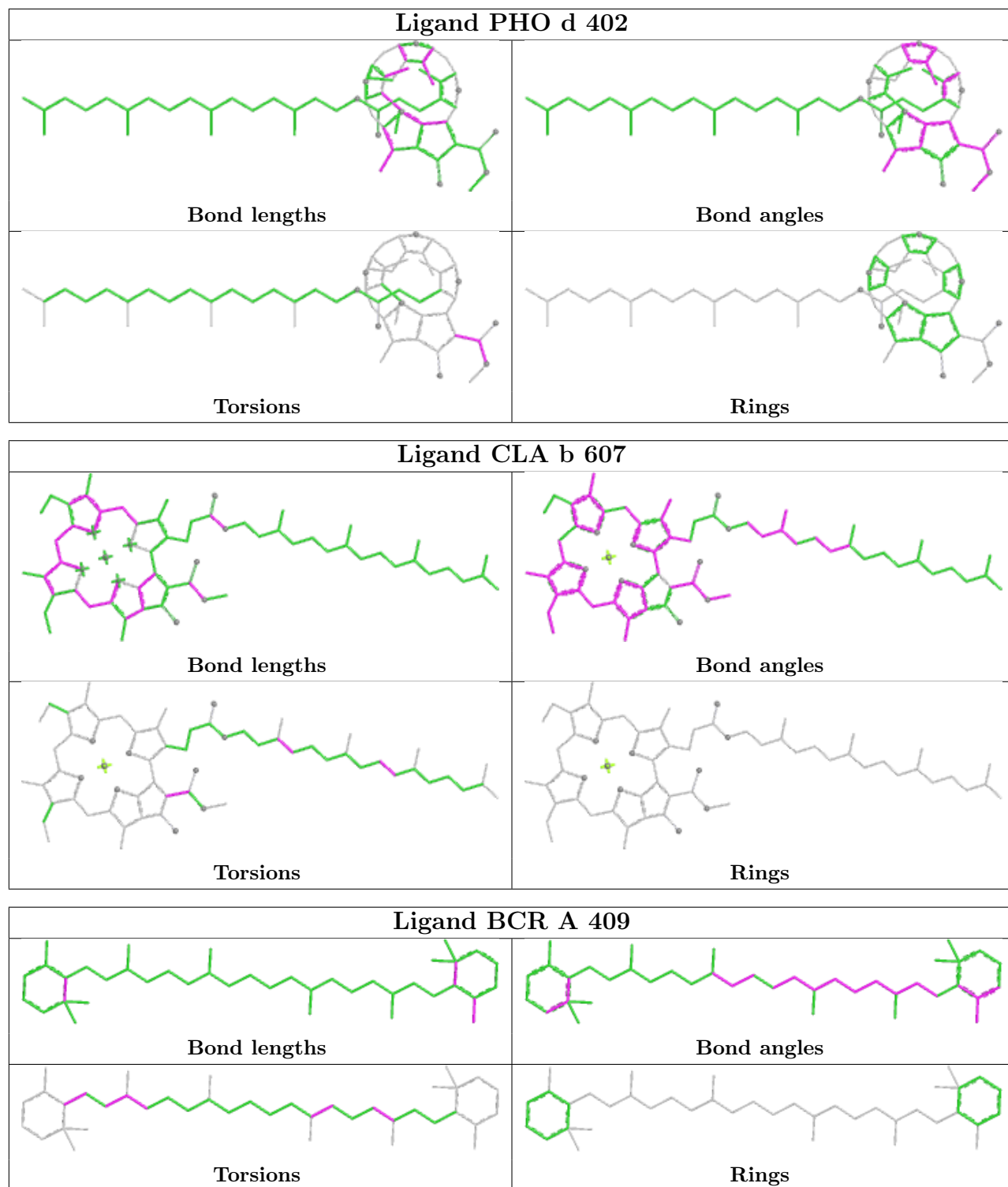


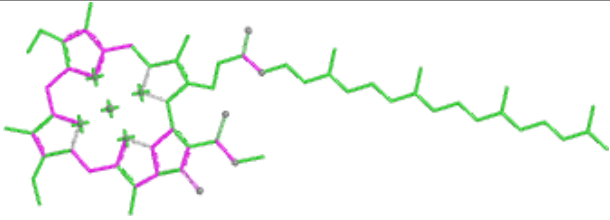
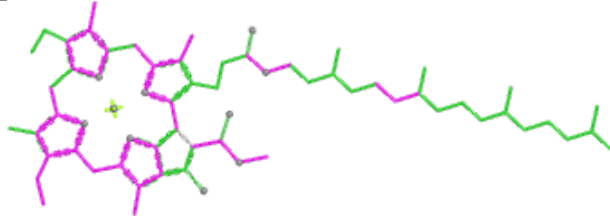
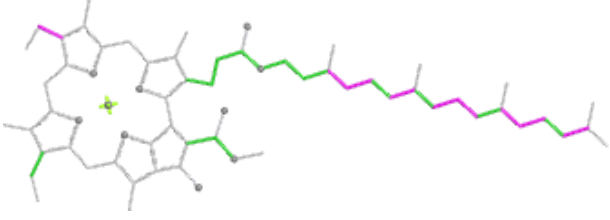
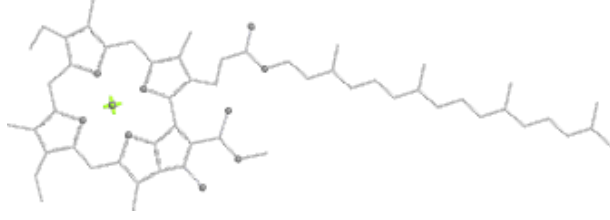
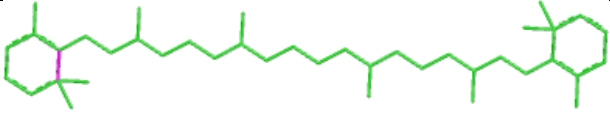
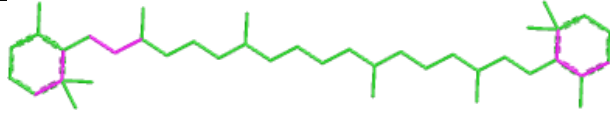
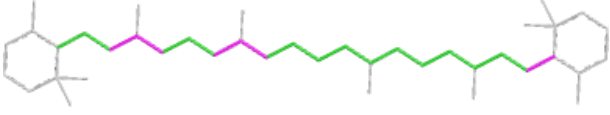
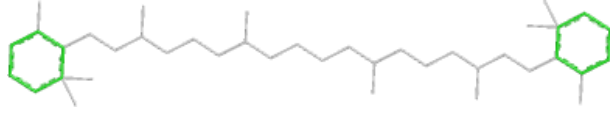
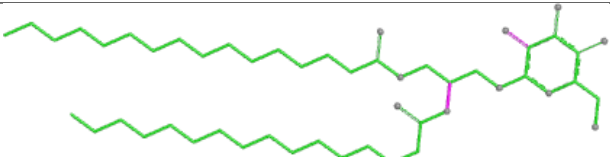
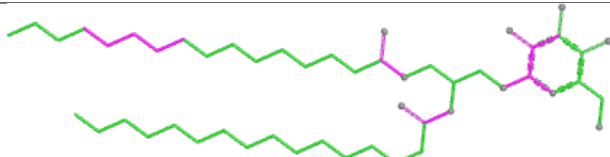
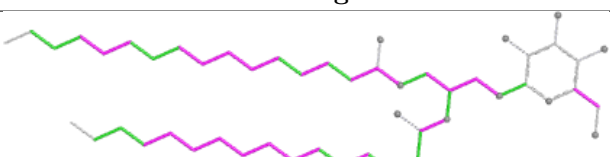
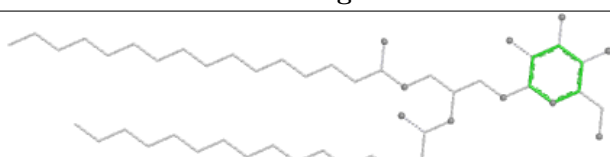


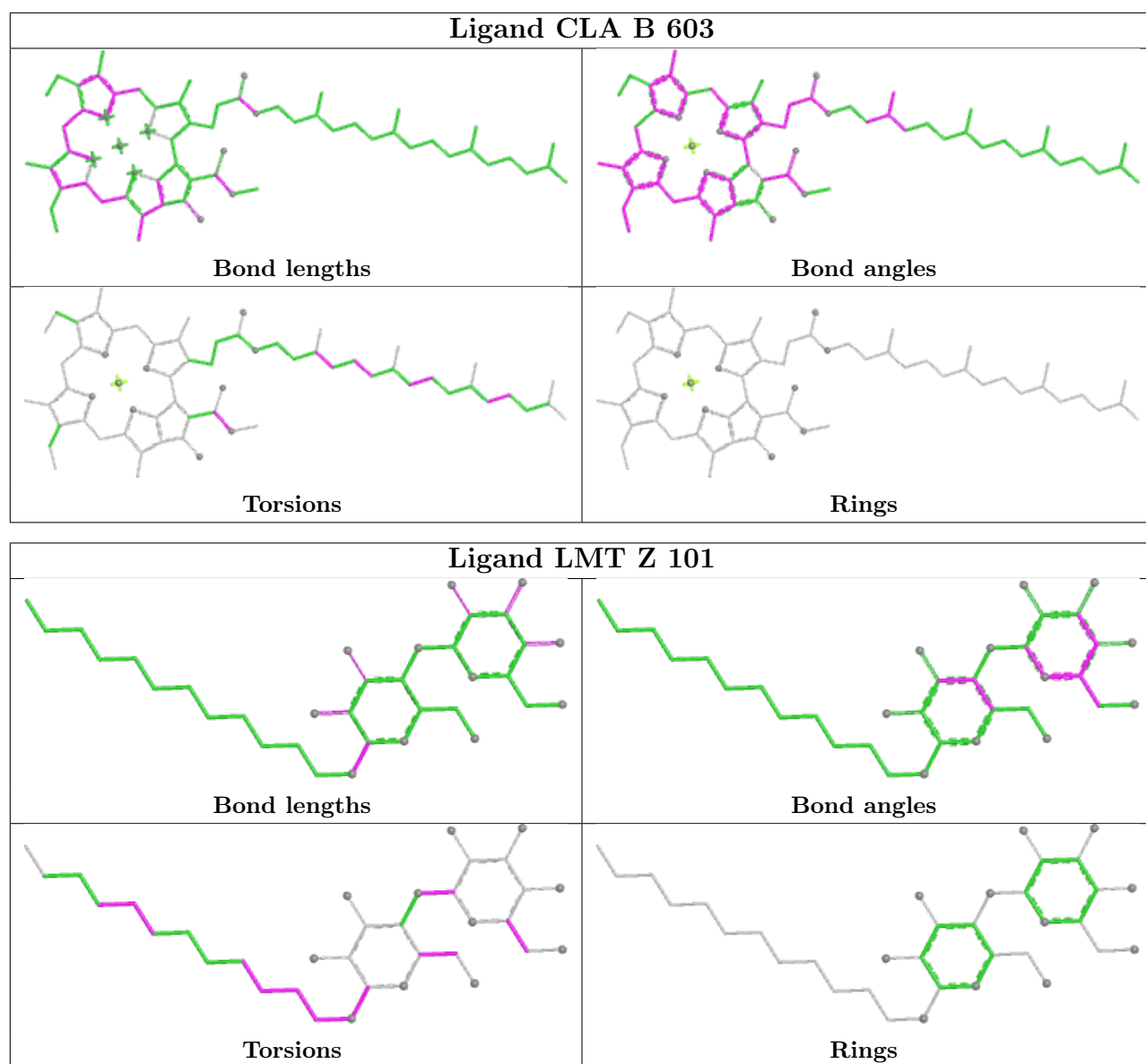


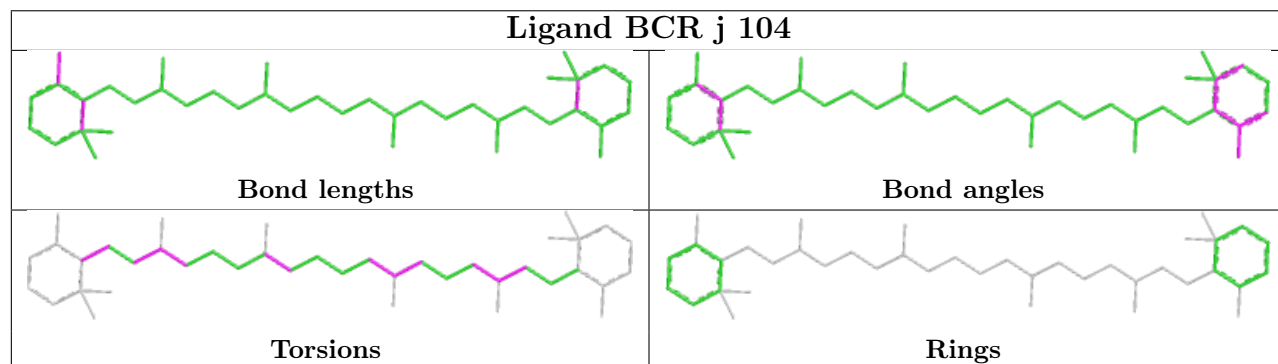
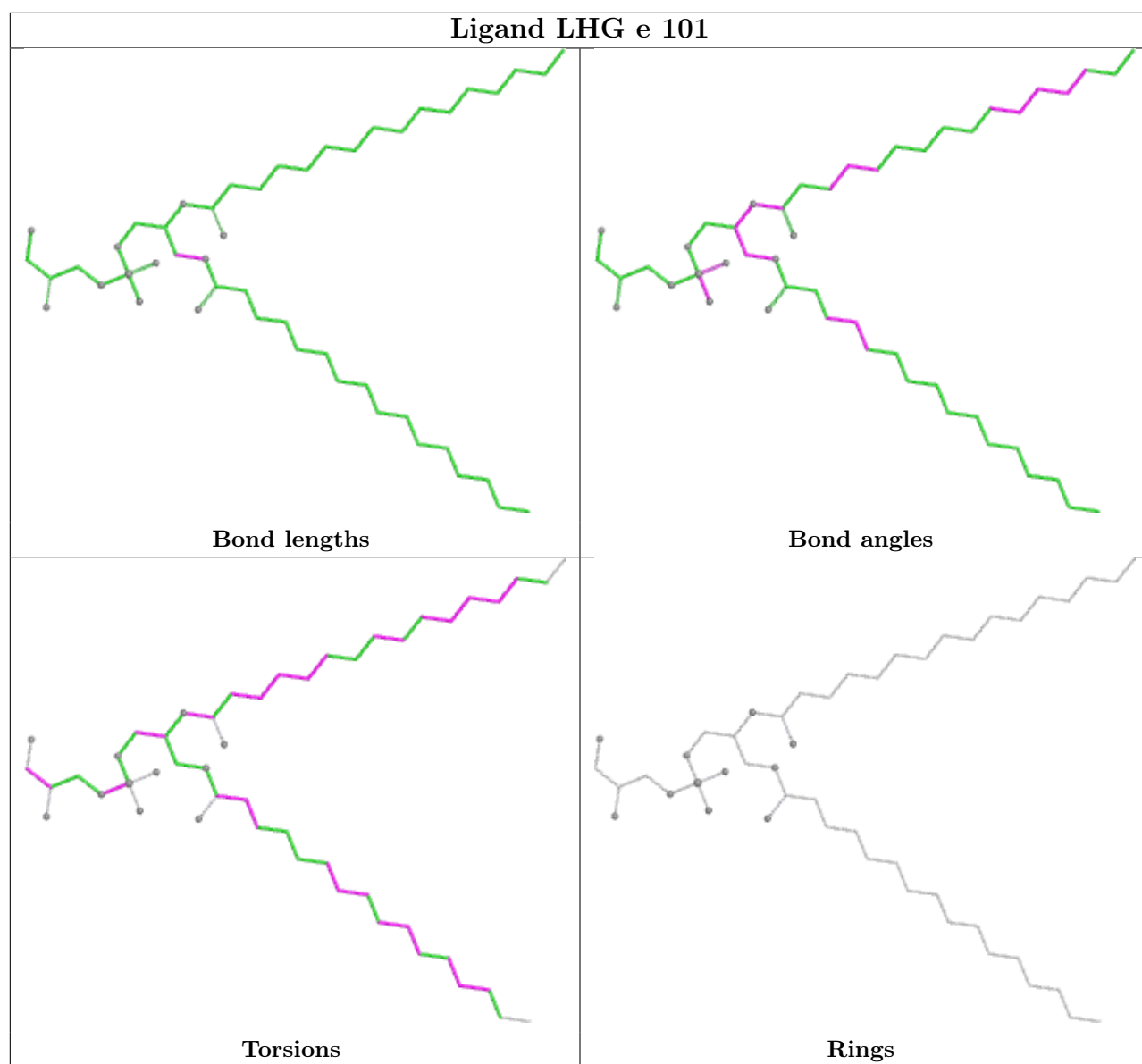


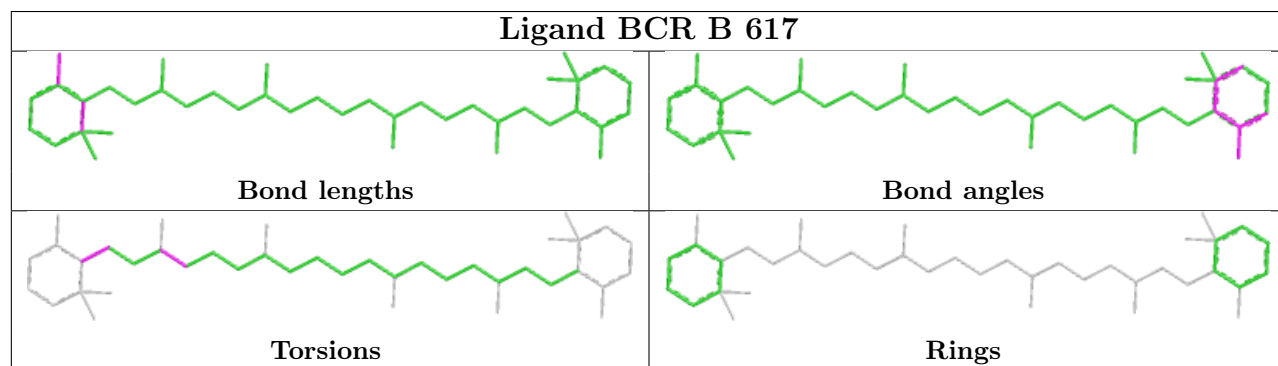
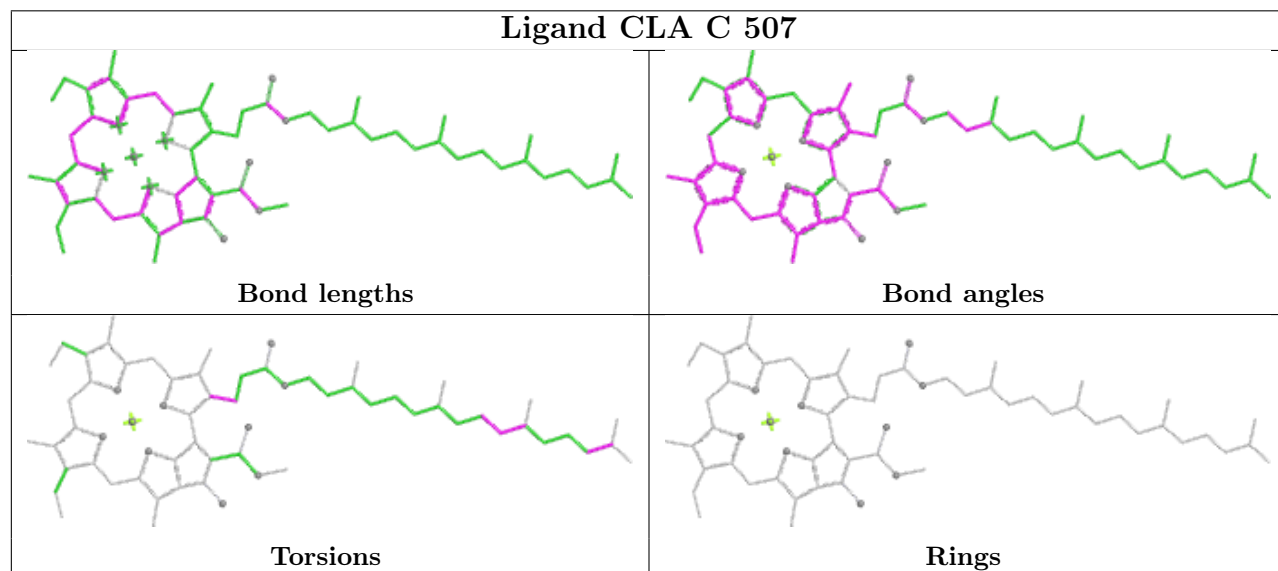
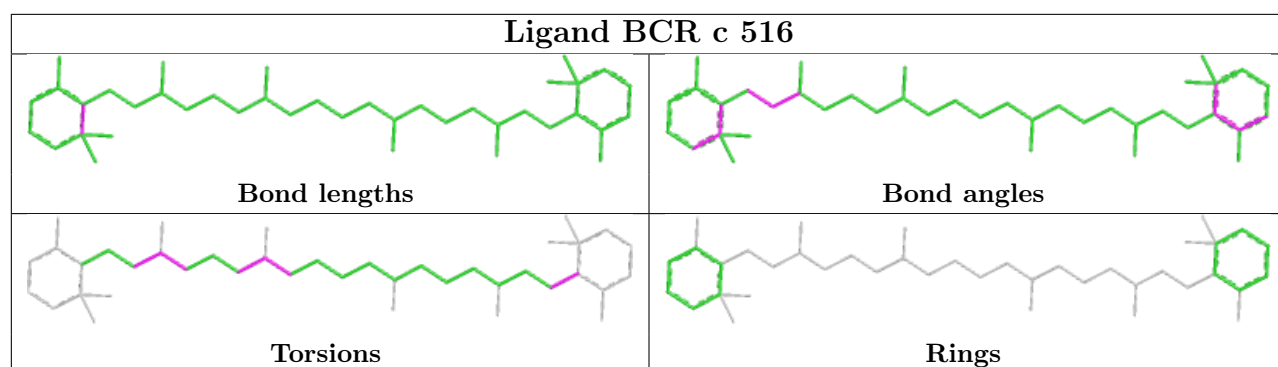


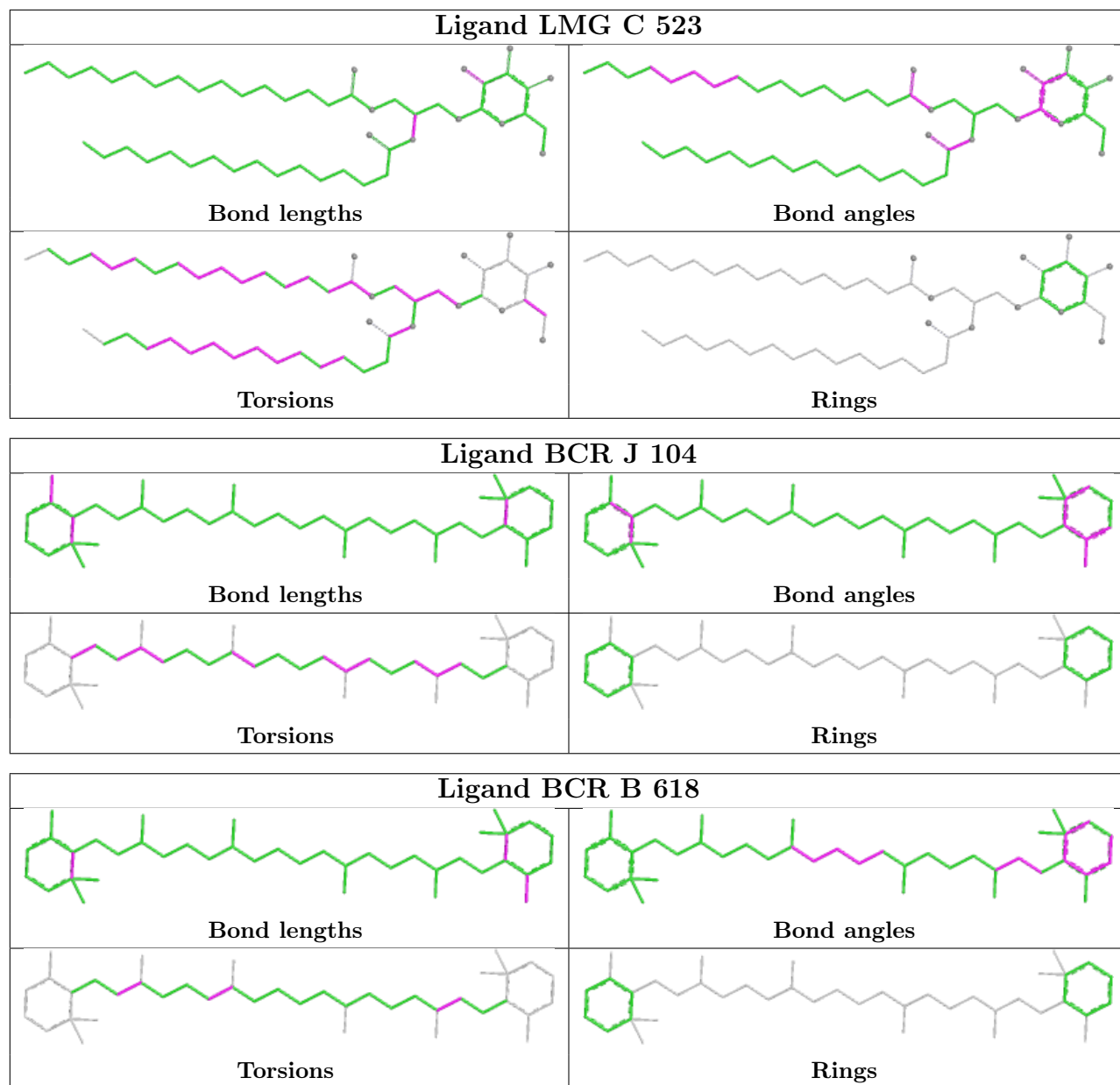


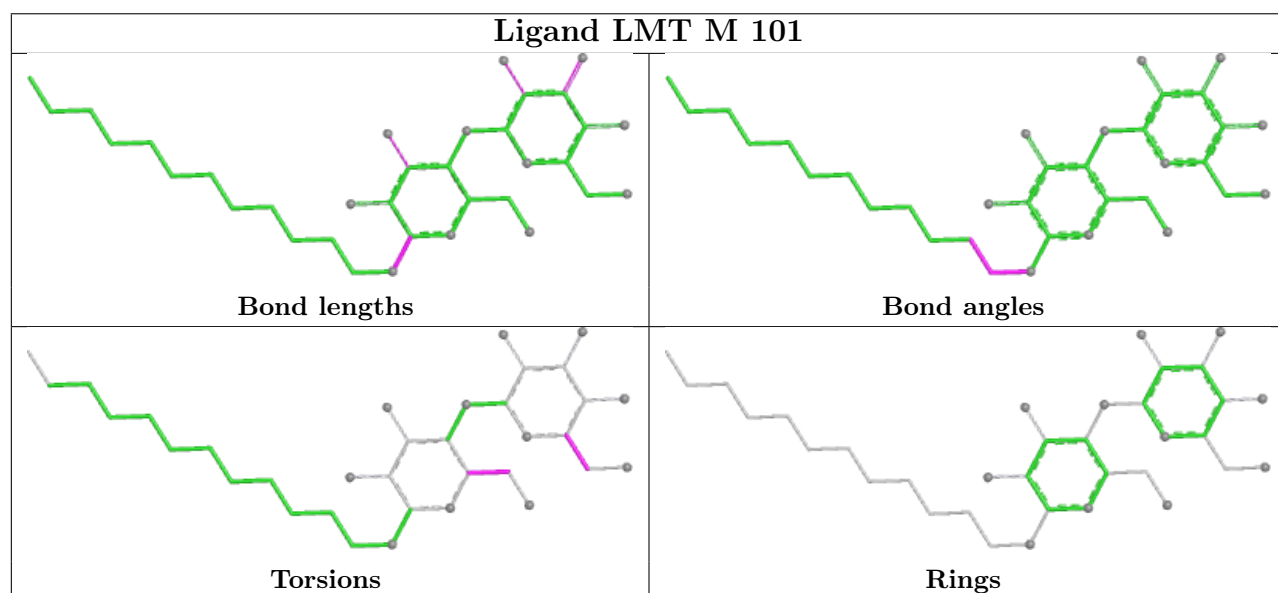
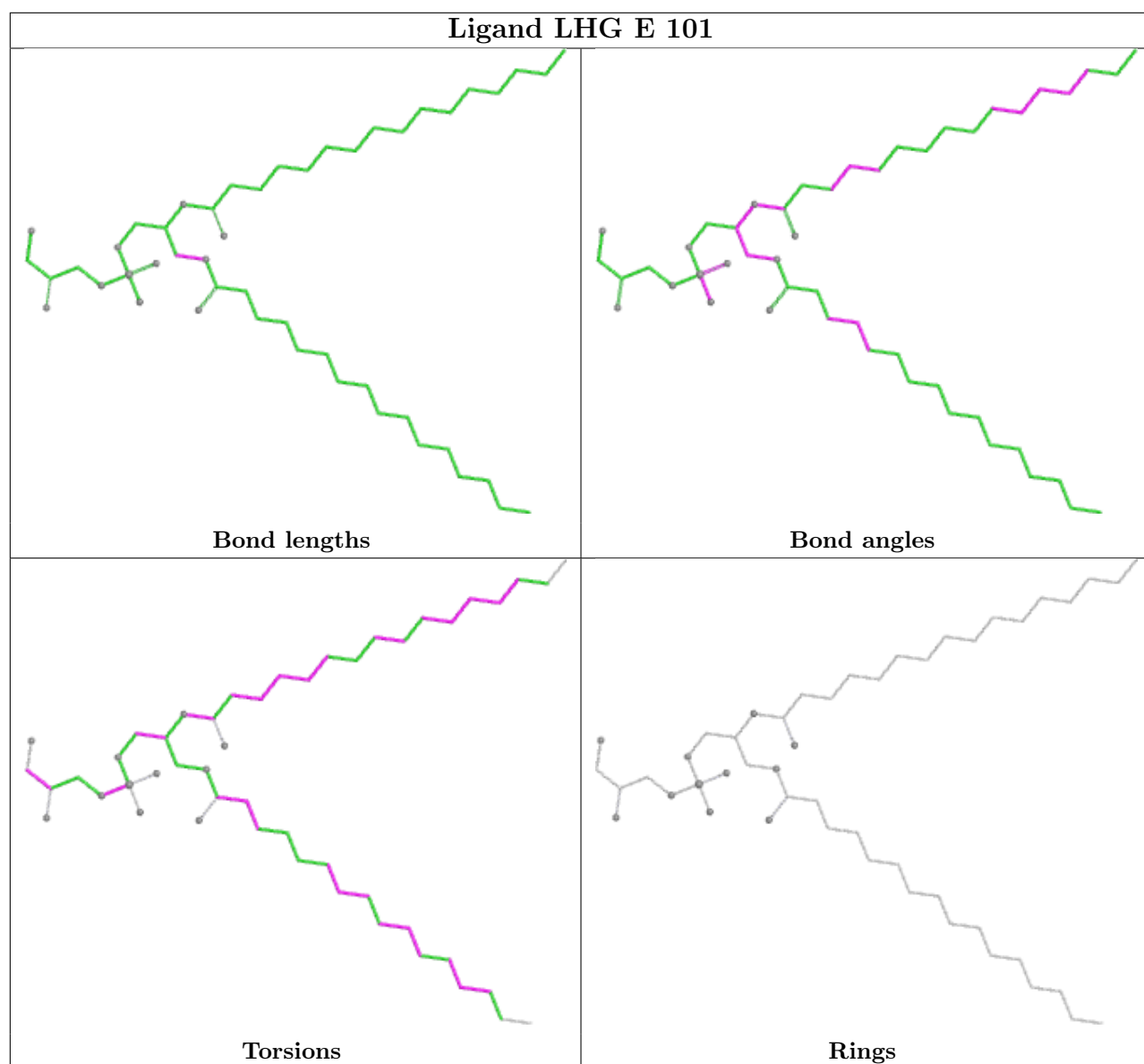
Ligand CLA b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 523	
 Bond lengths	 Bond angles
 Torsions	 Rings

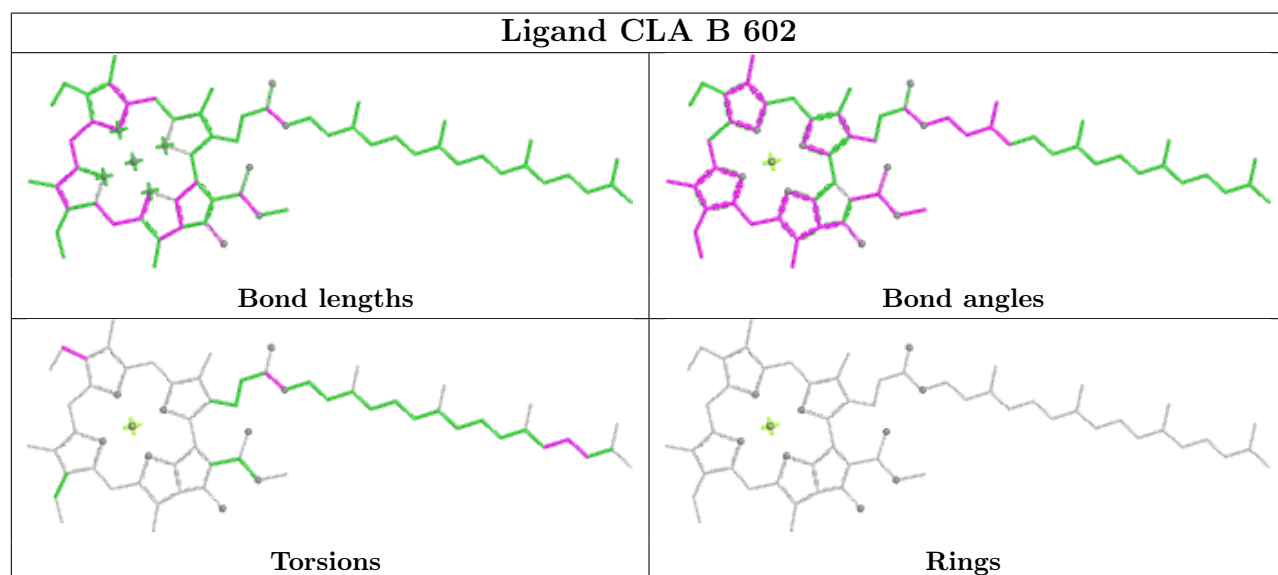
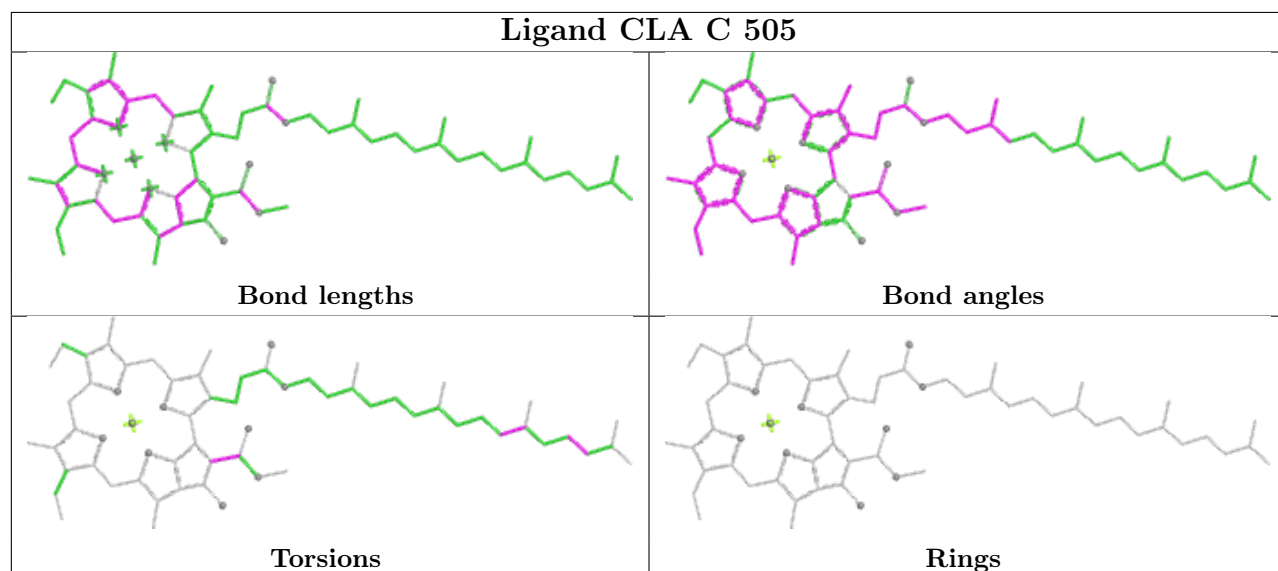
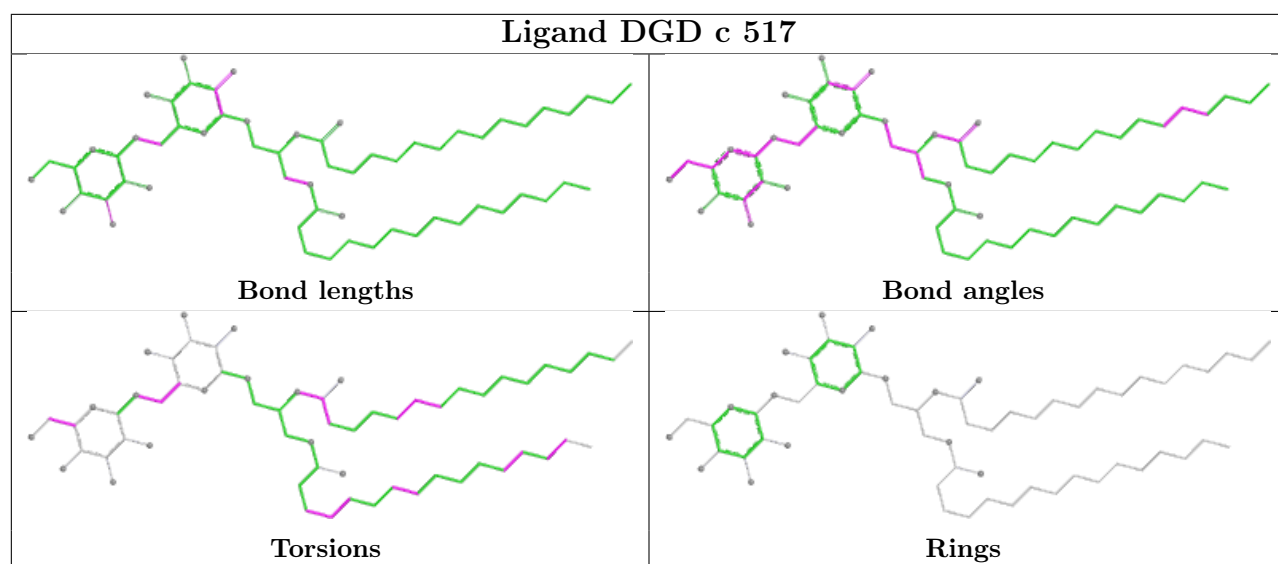


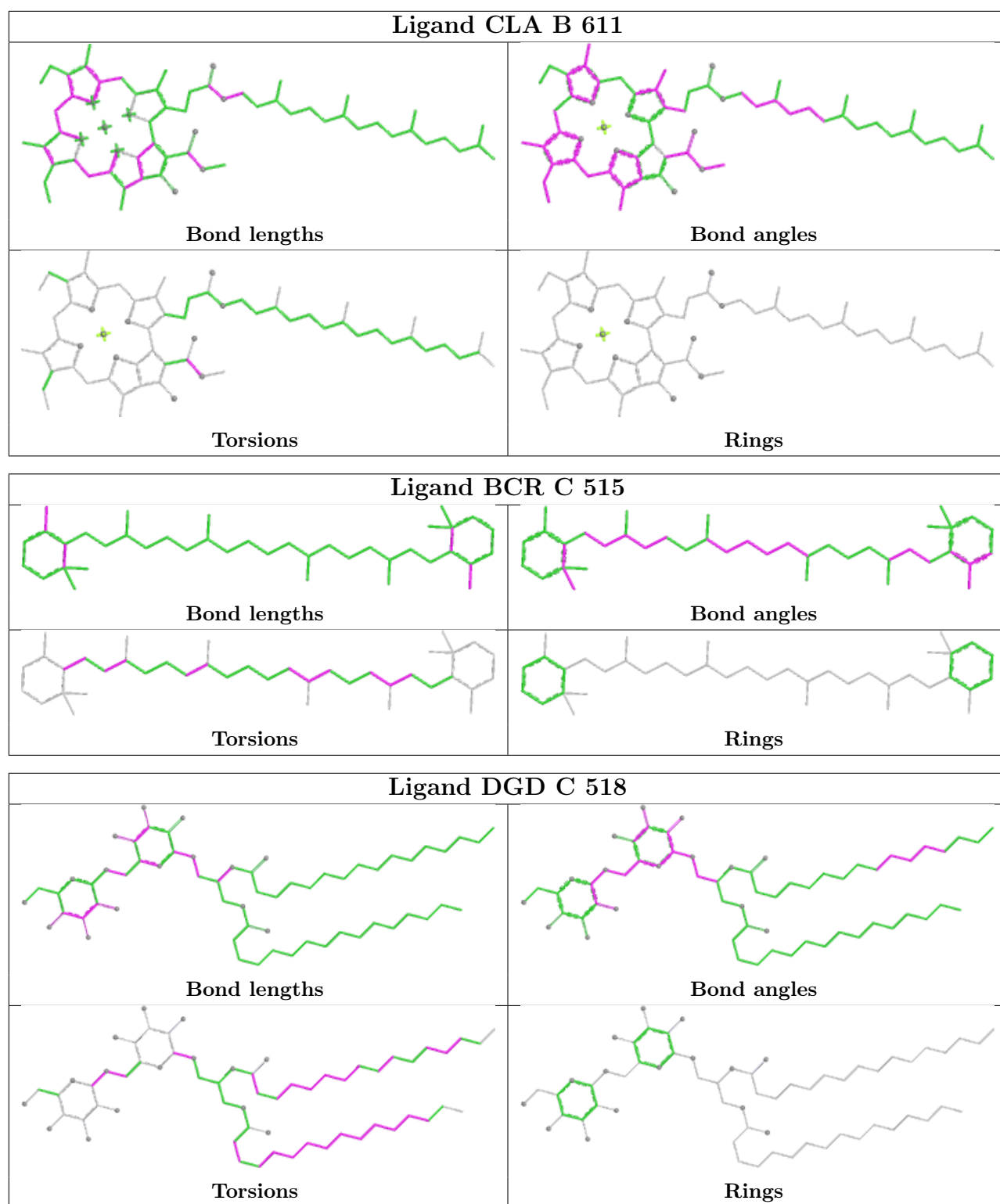


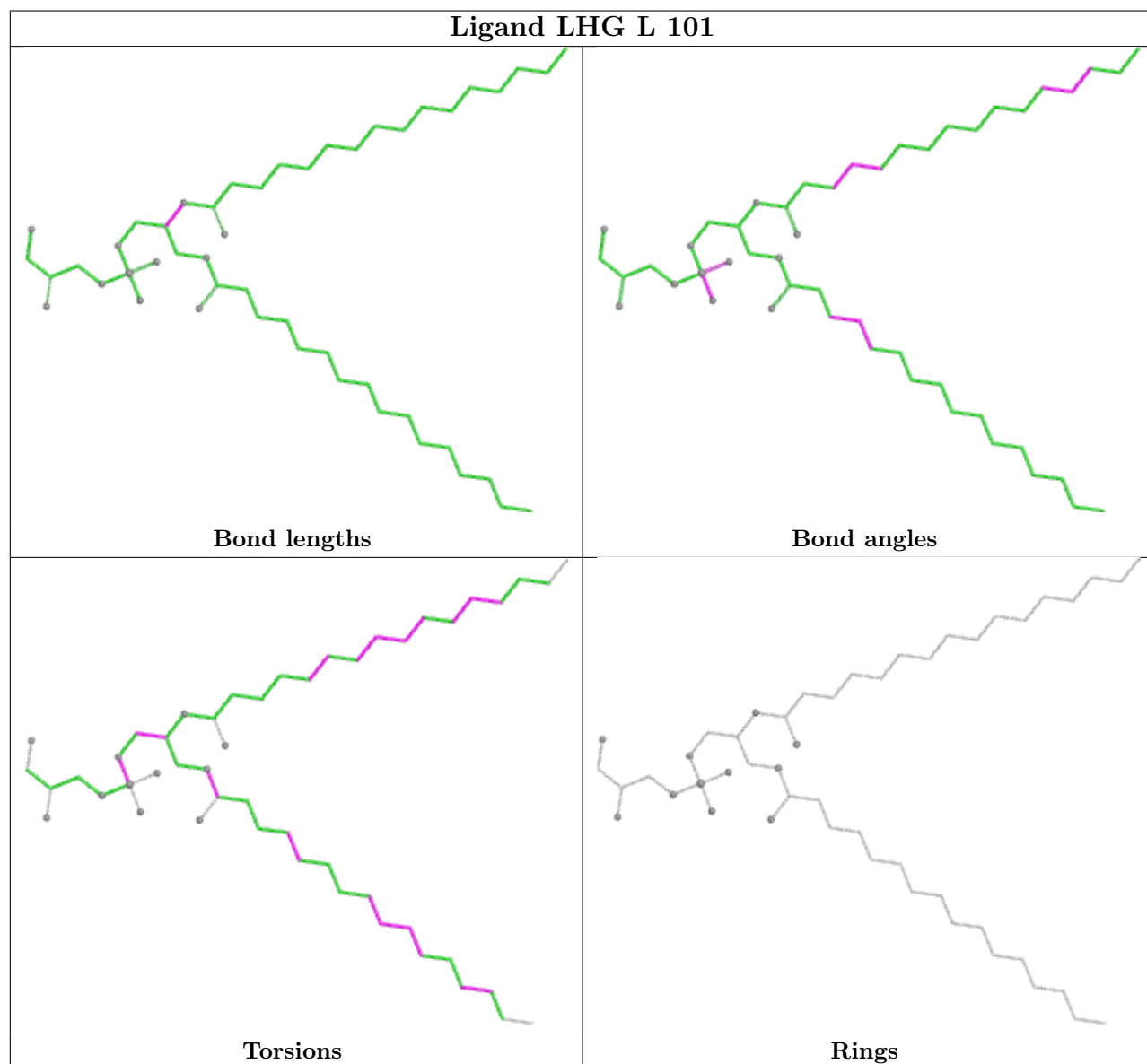
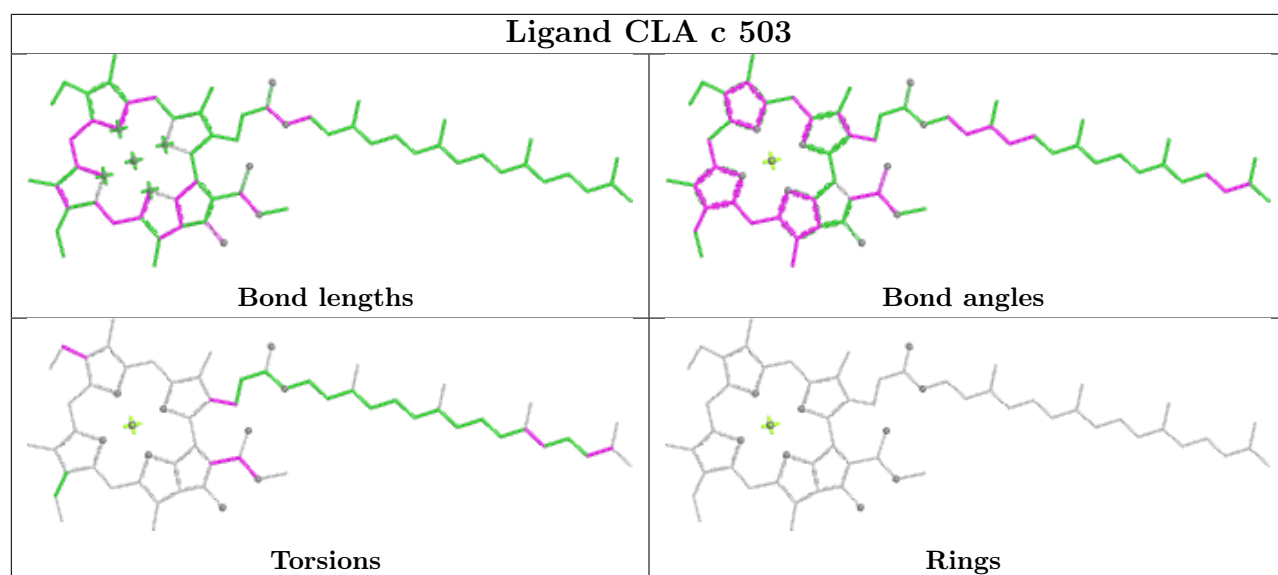


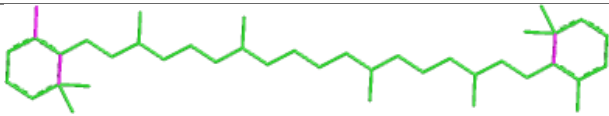
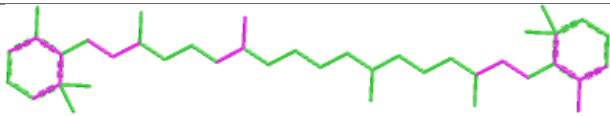
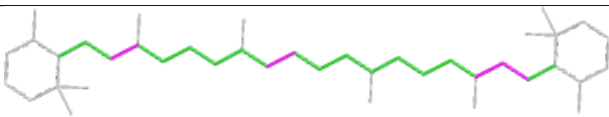
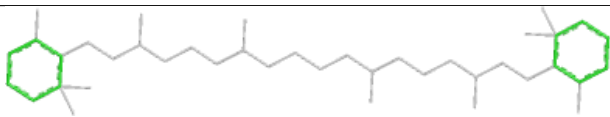


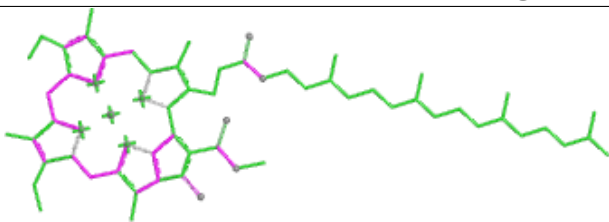
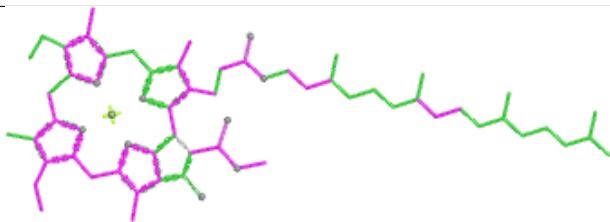
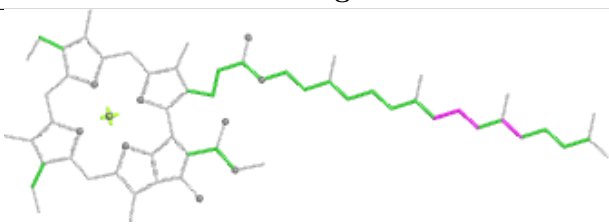
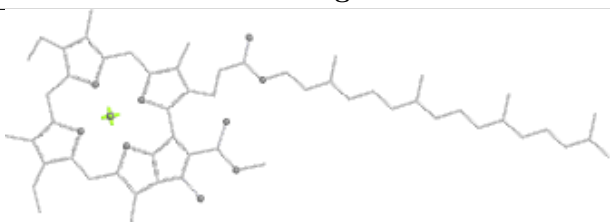


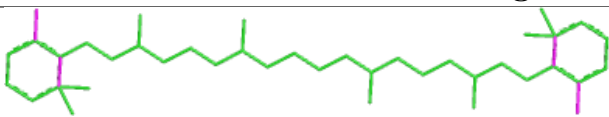
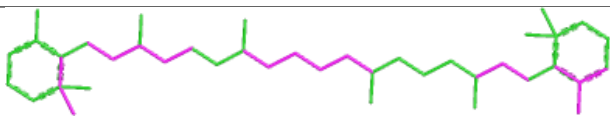
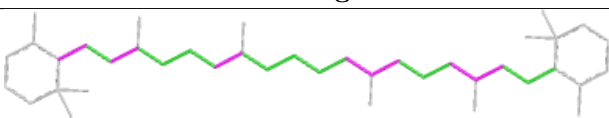
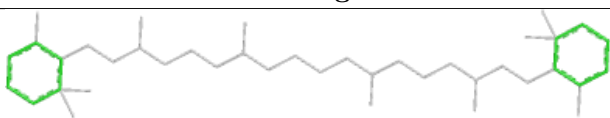


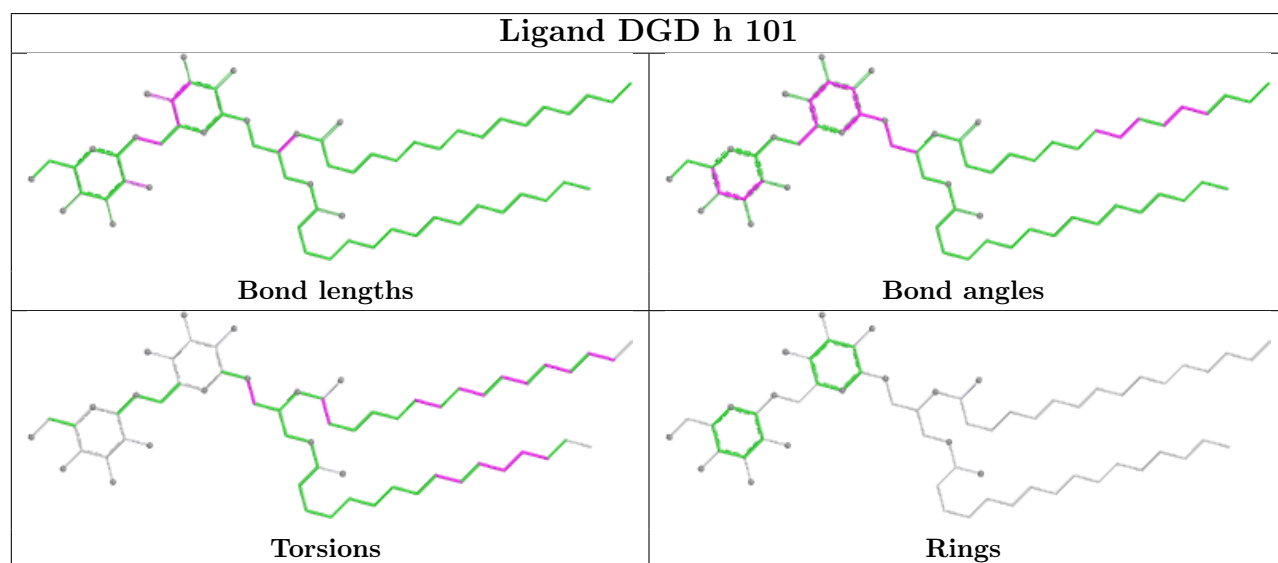
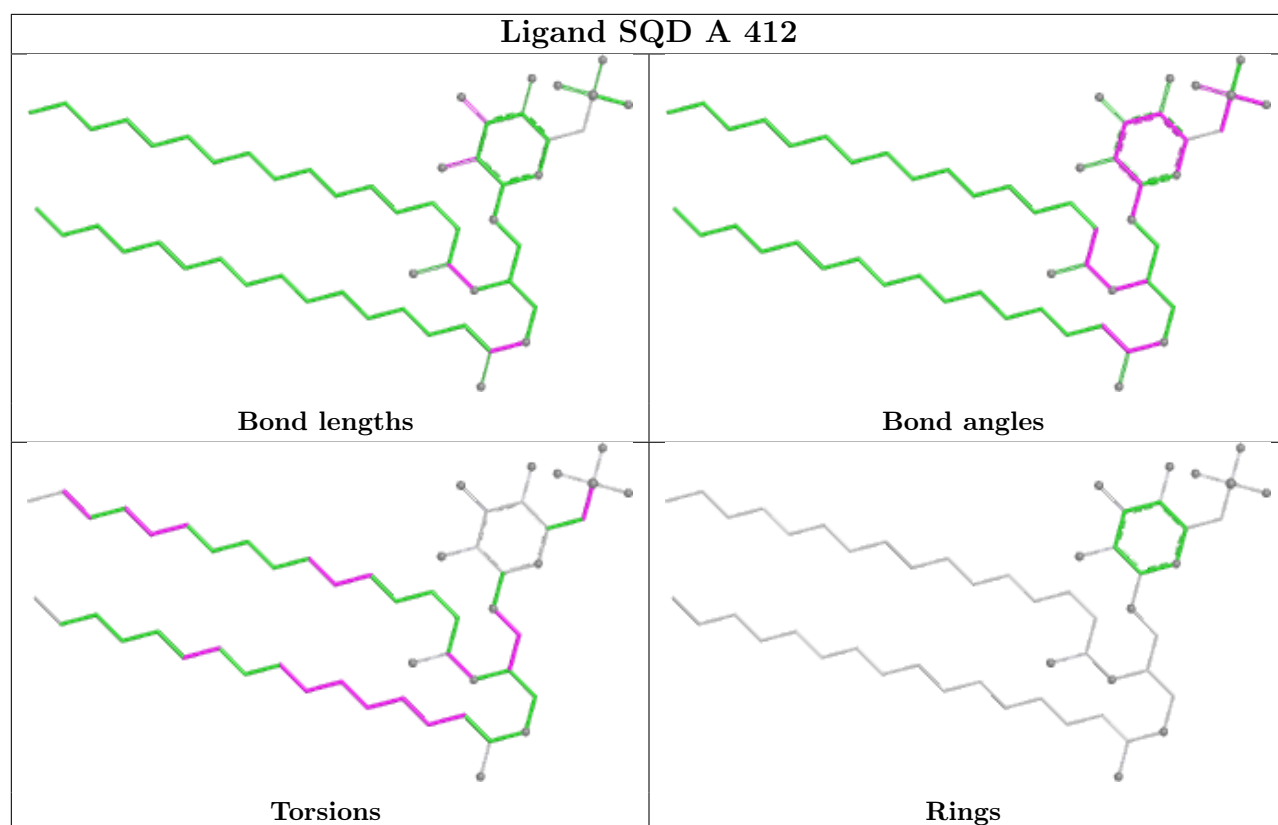


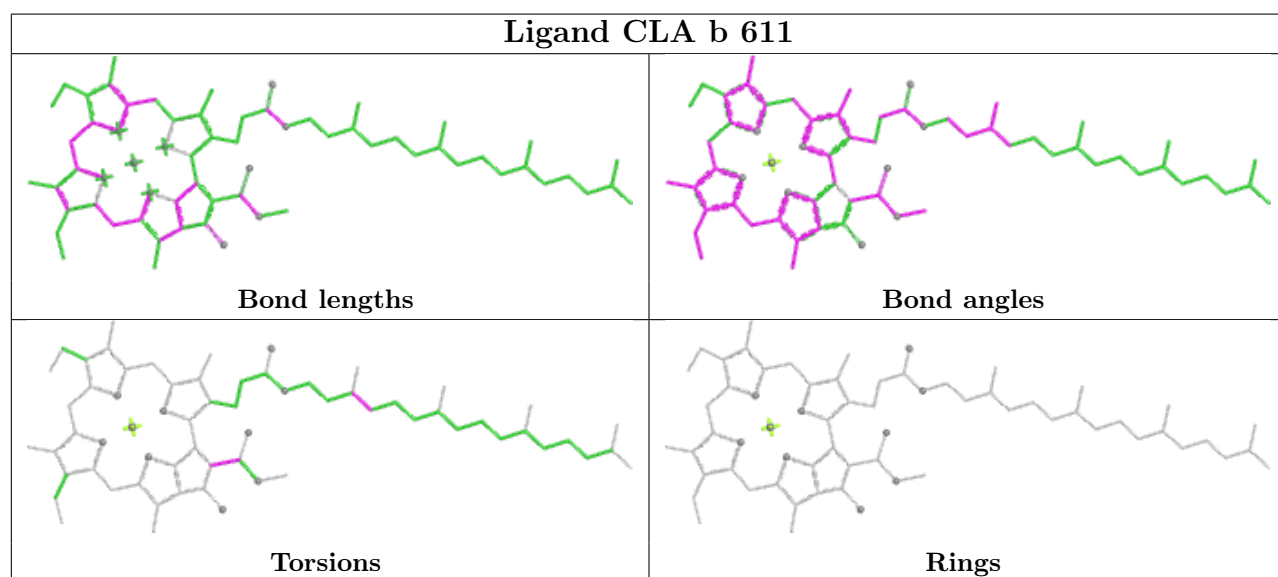
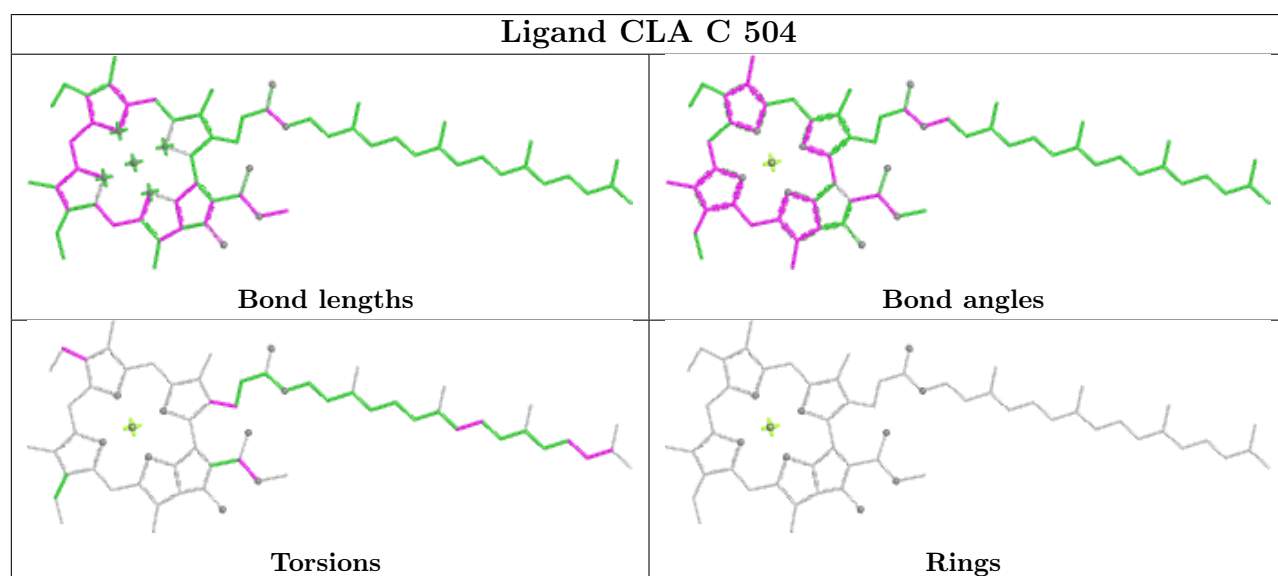
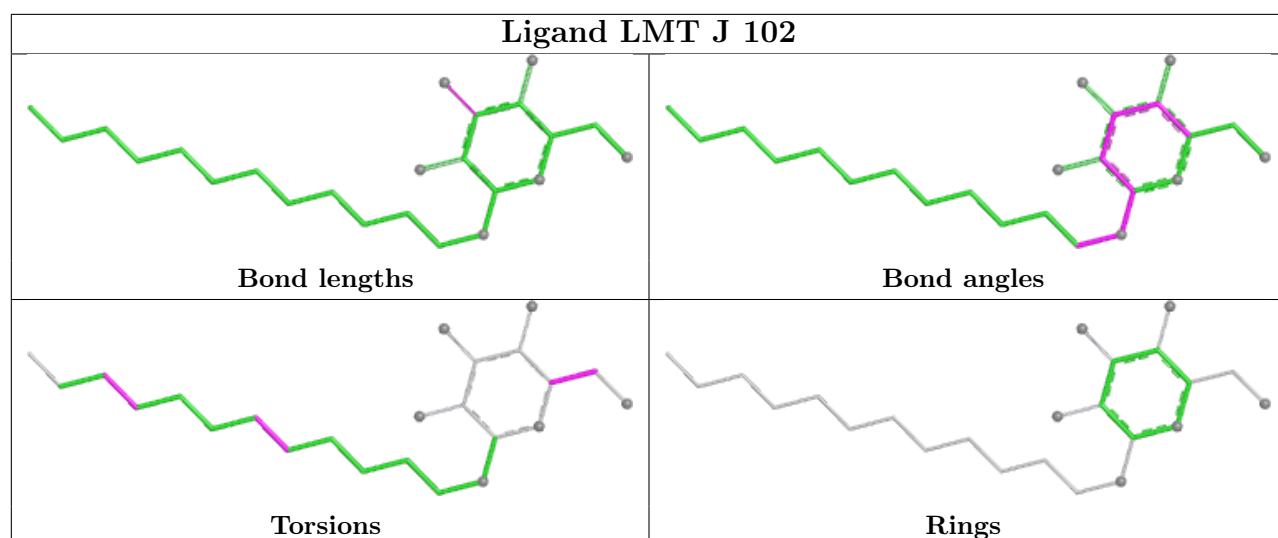


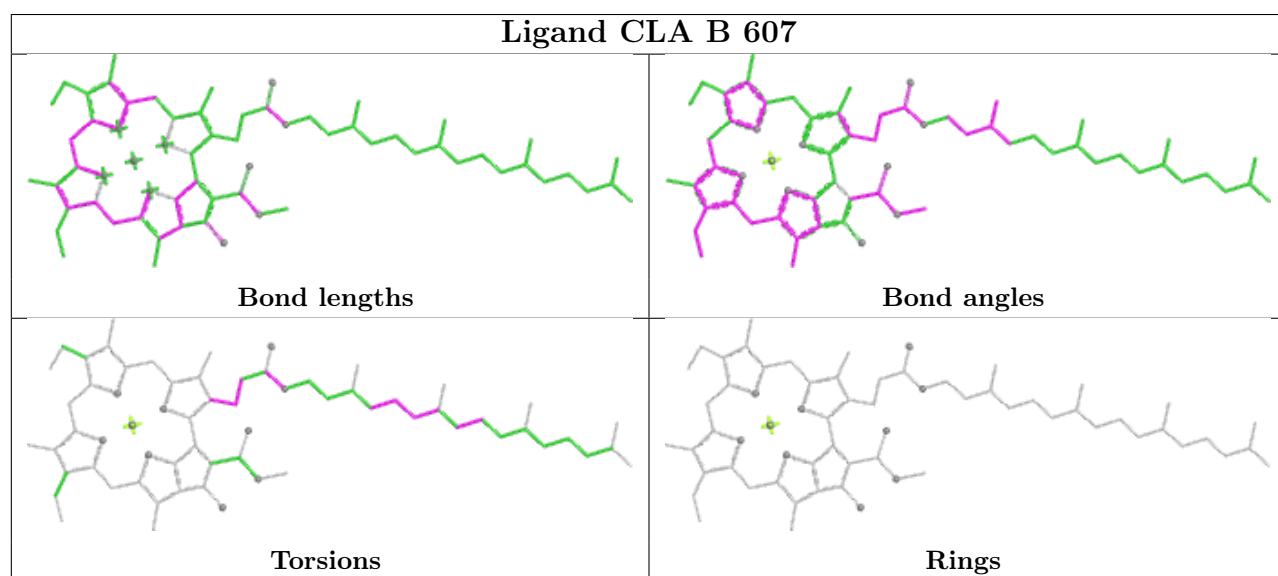
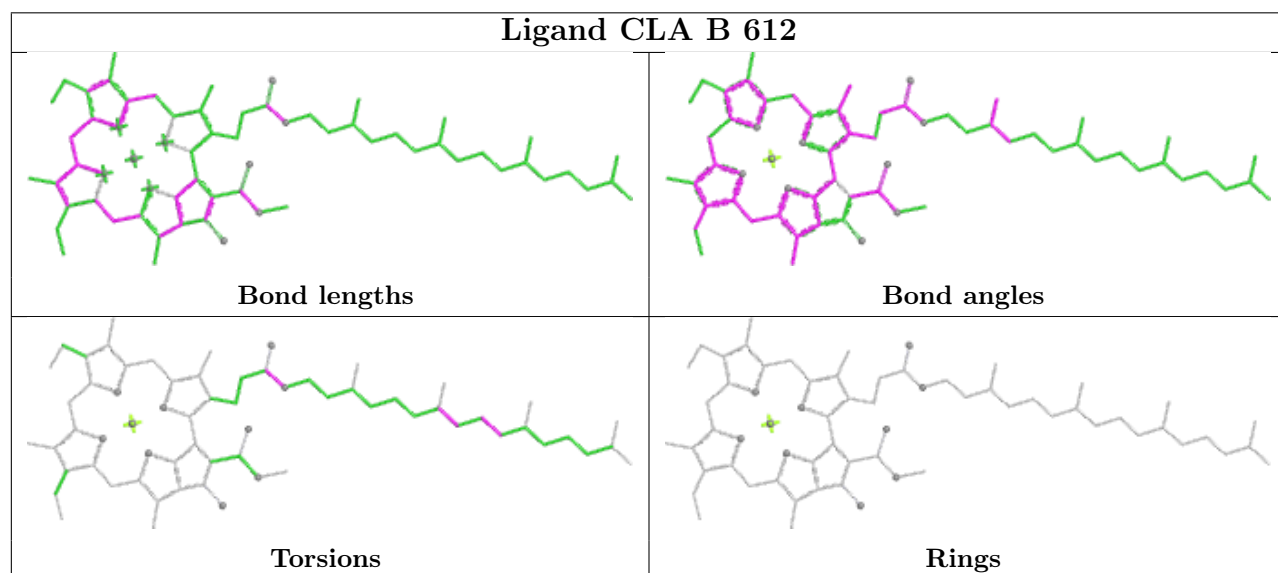
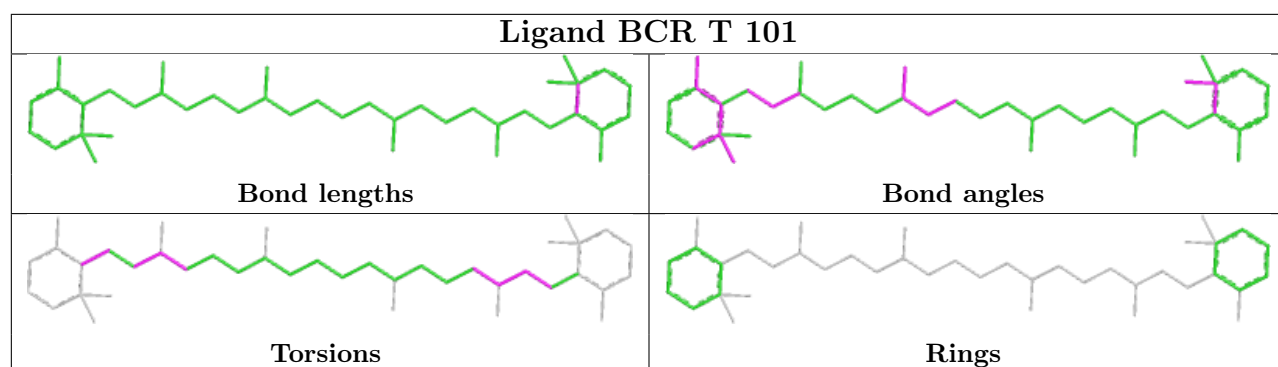
Ligand BCR d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

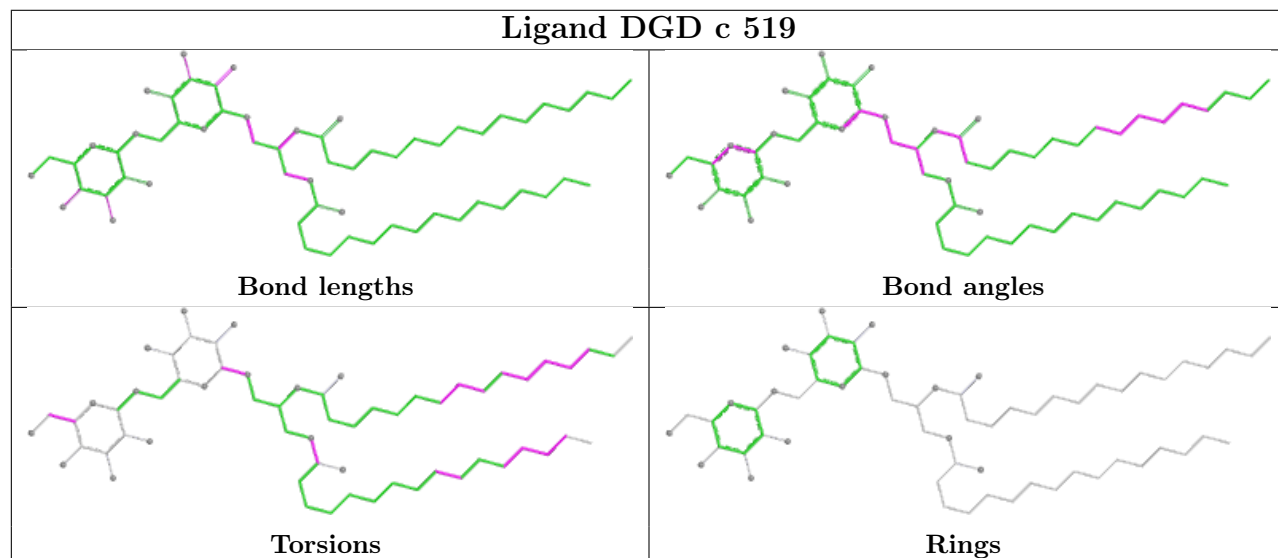
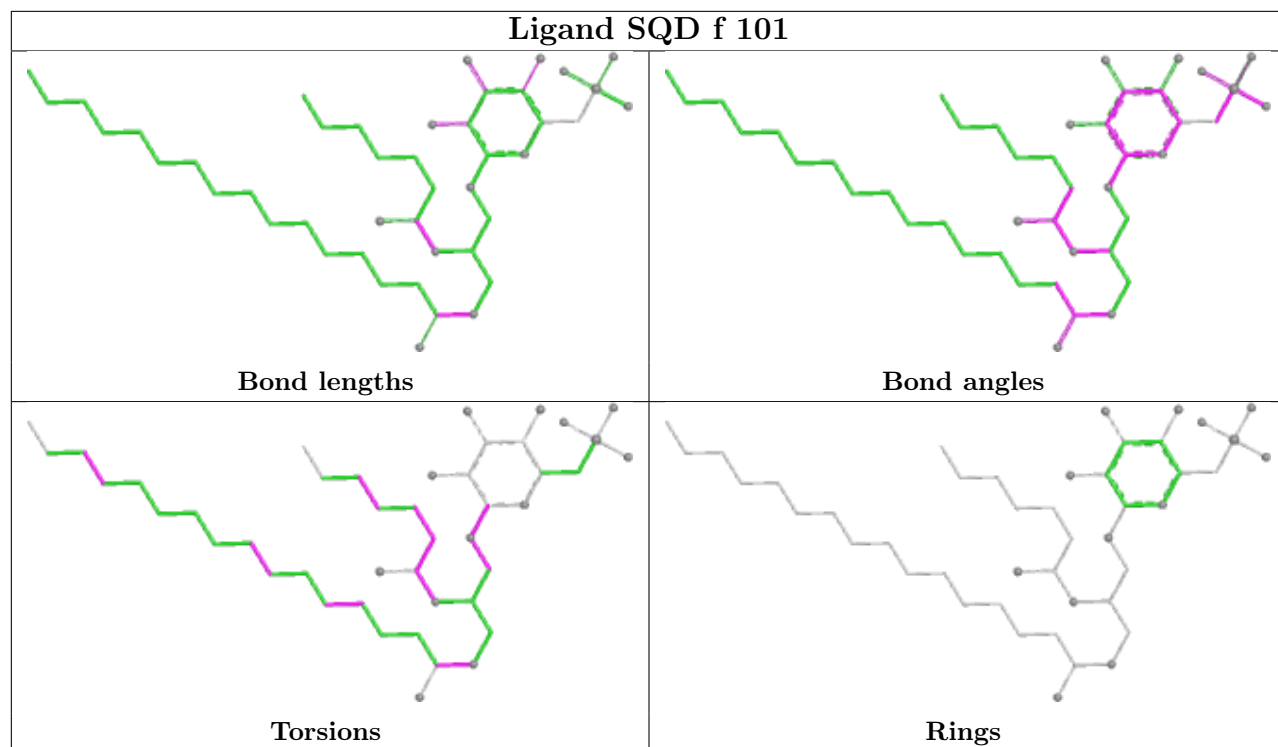
Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

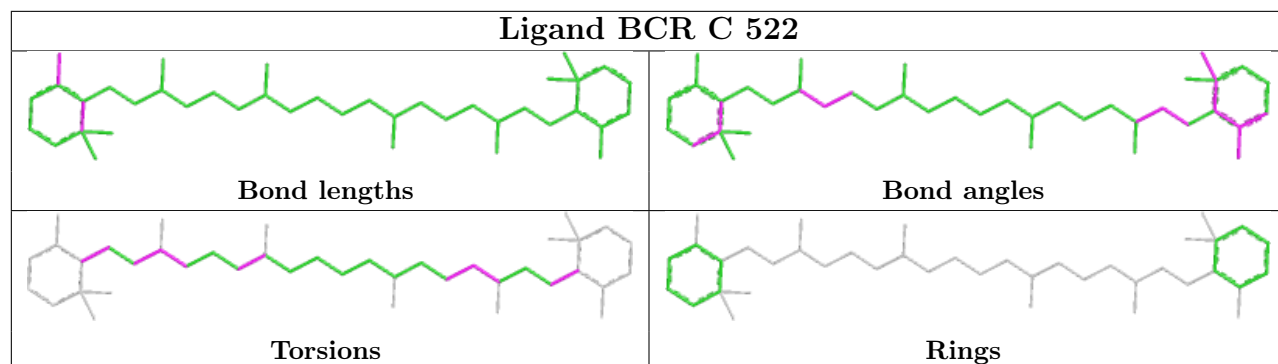
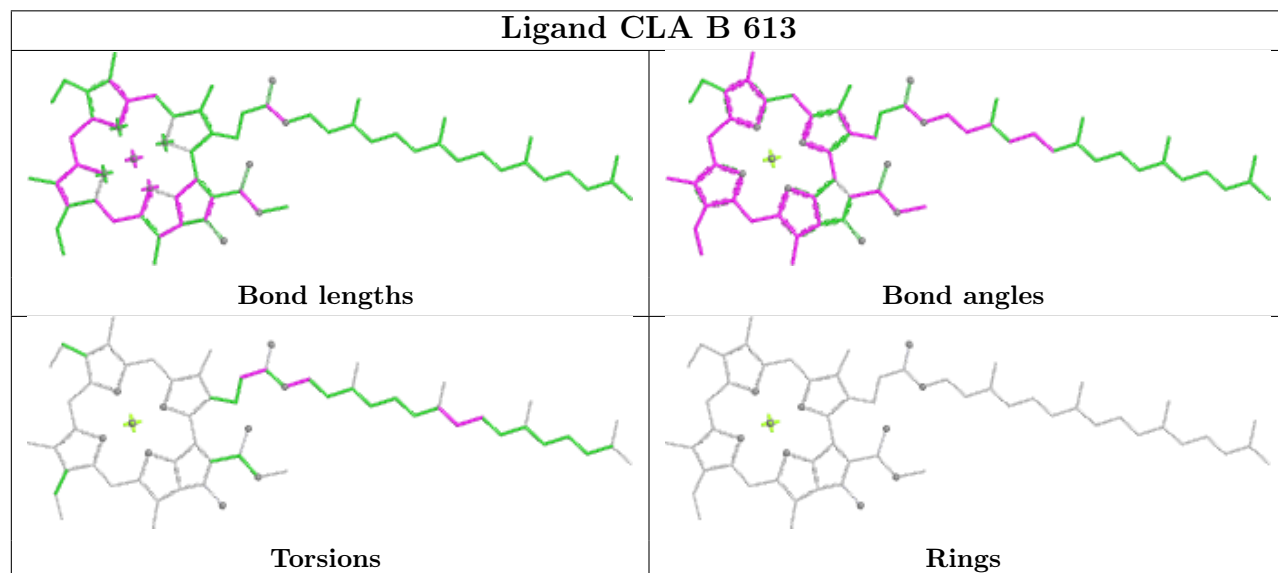
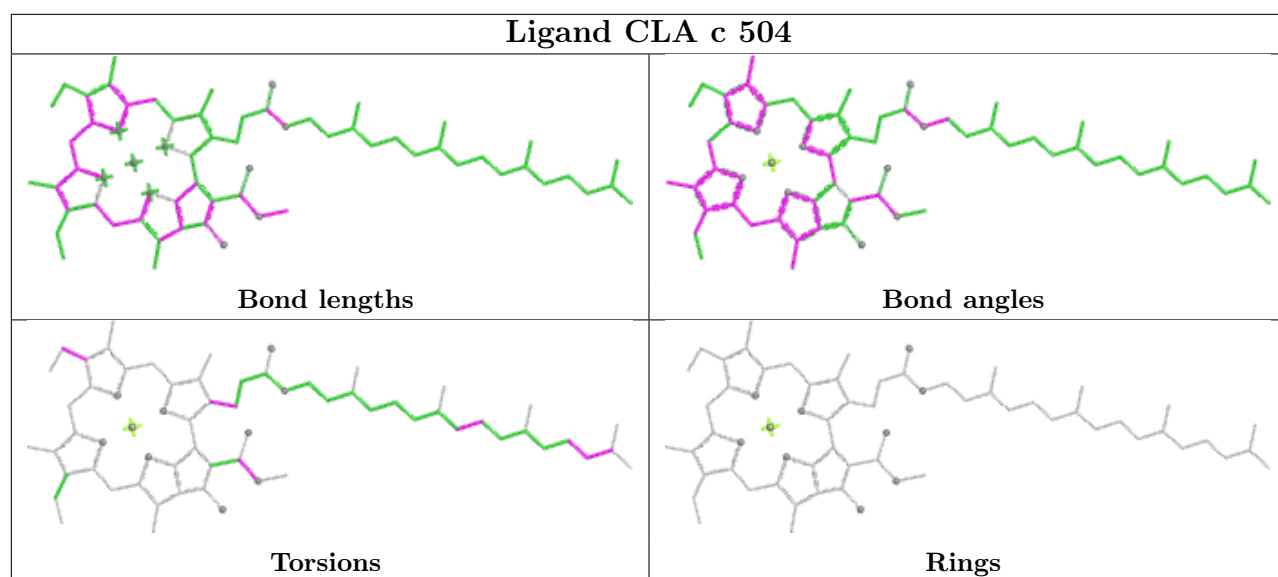
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

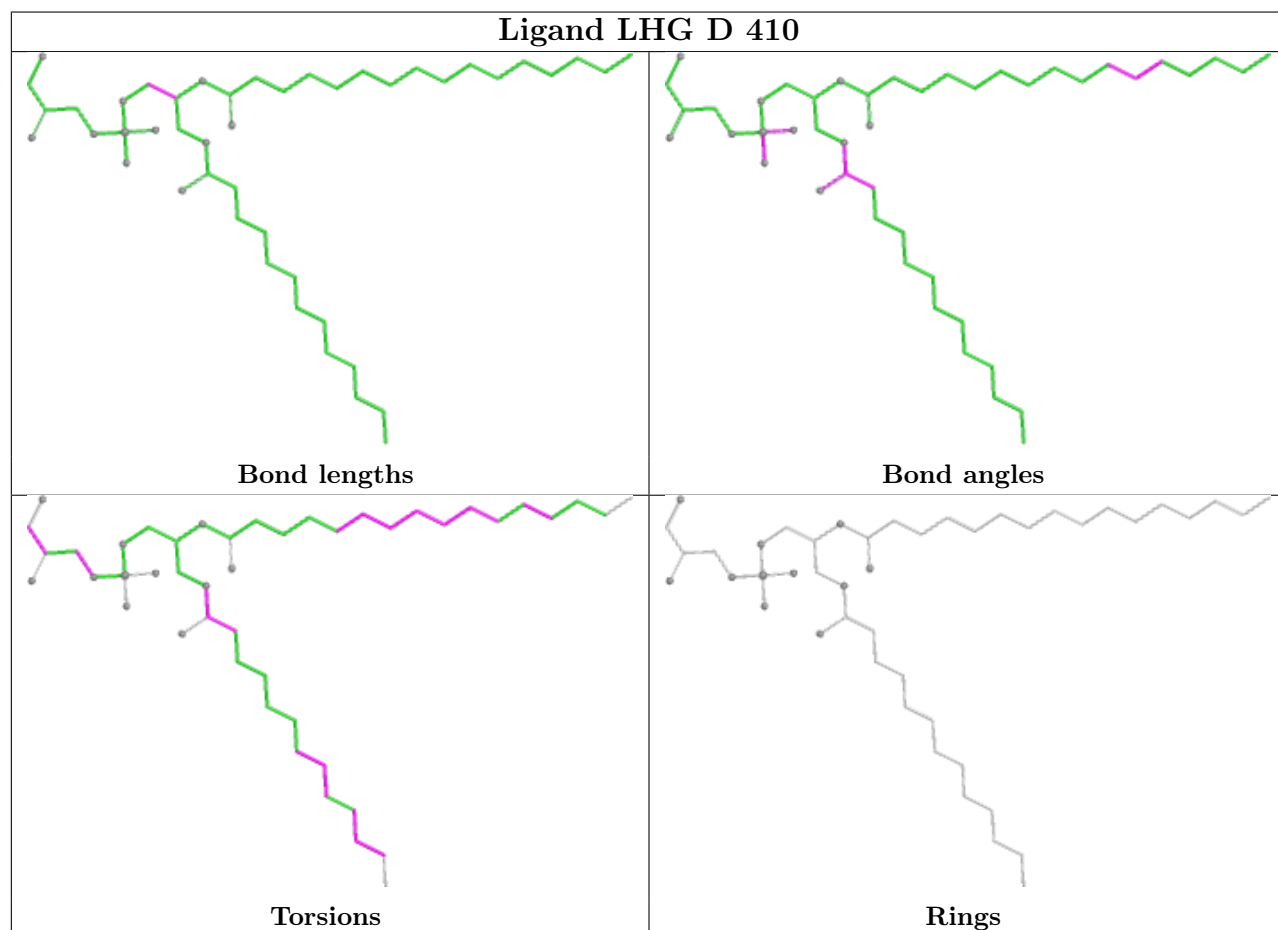
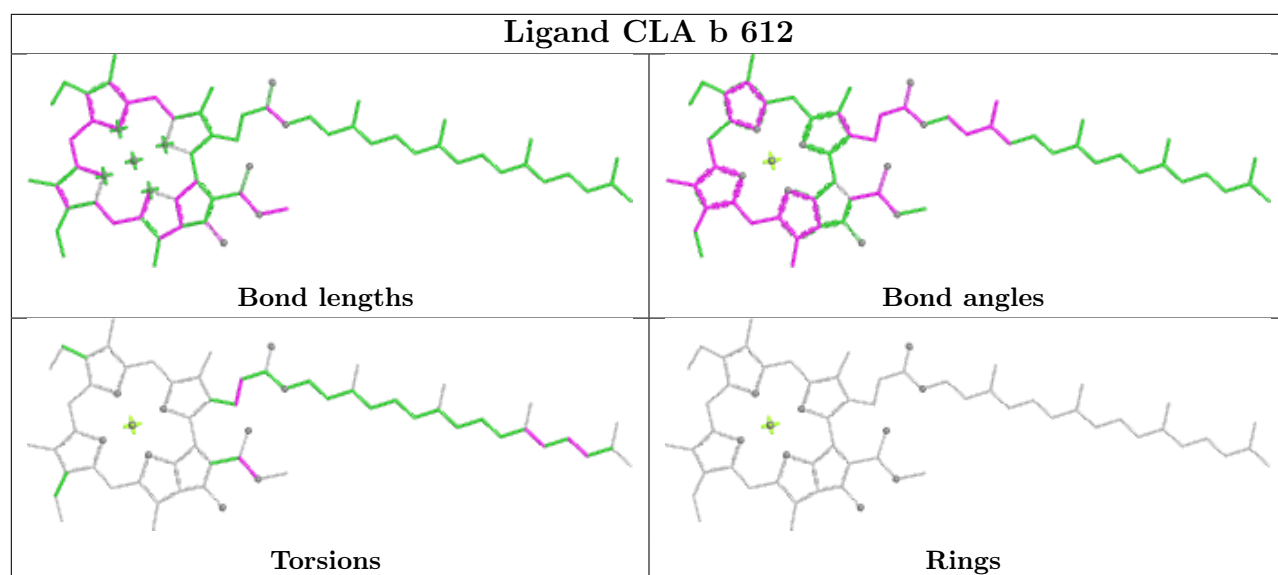


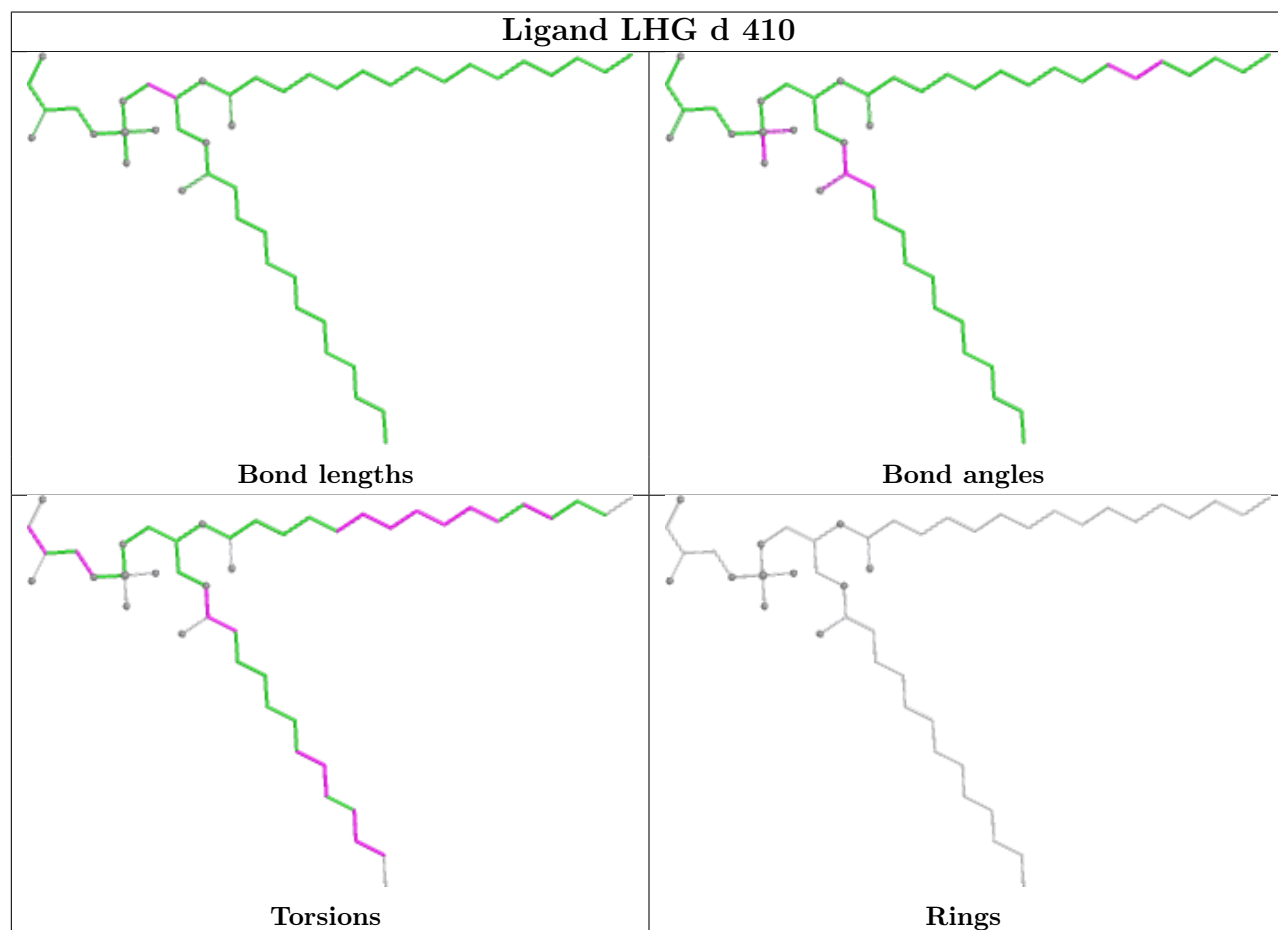
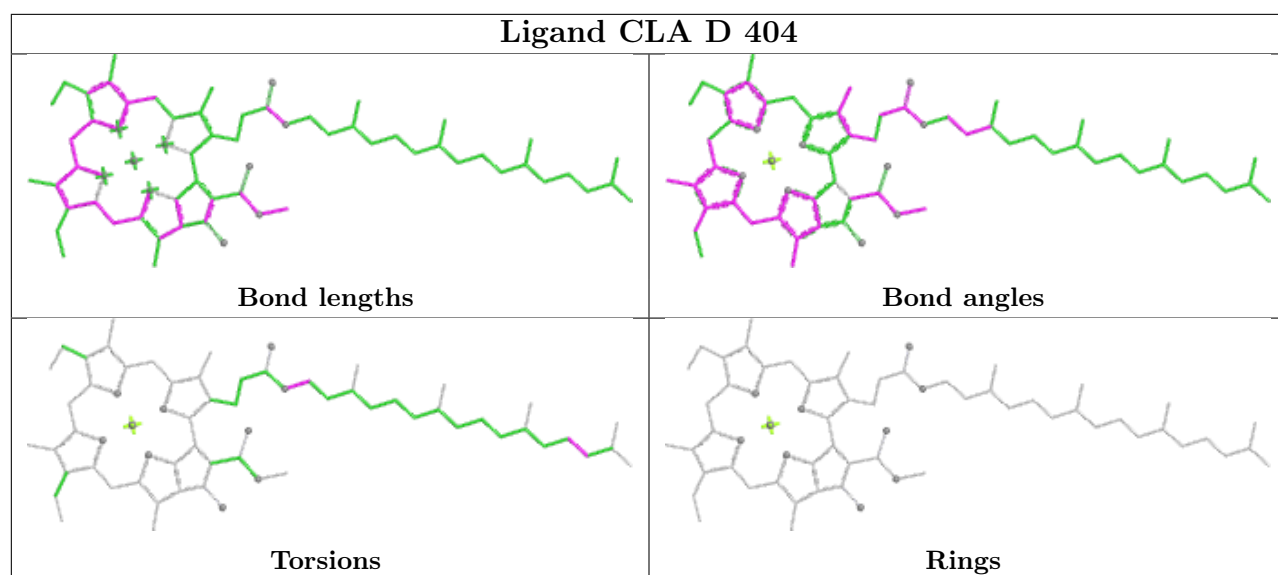


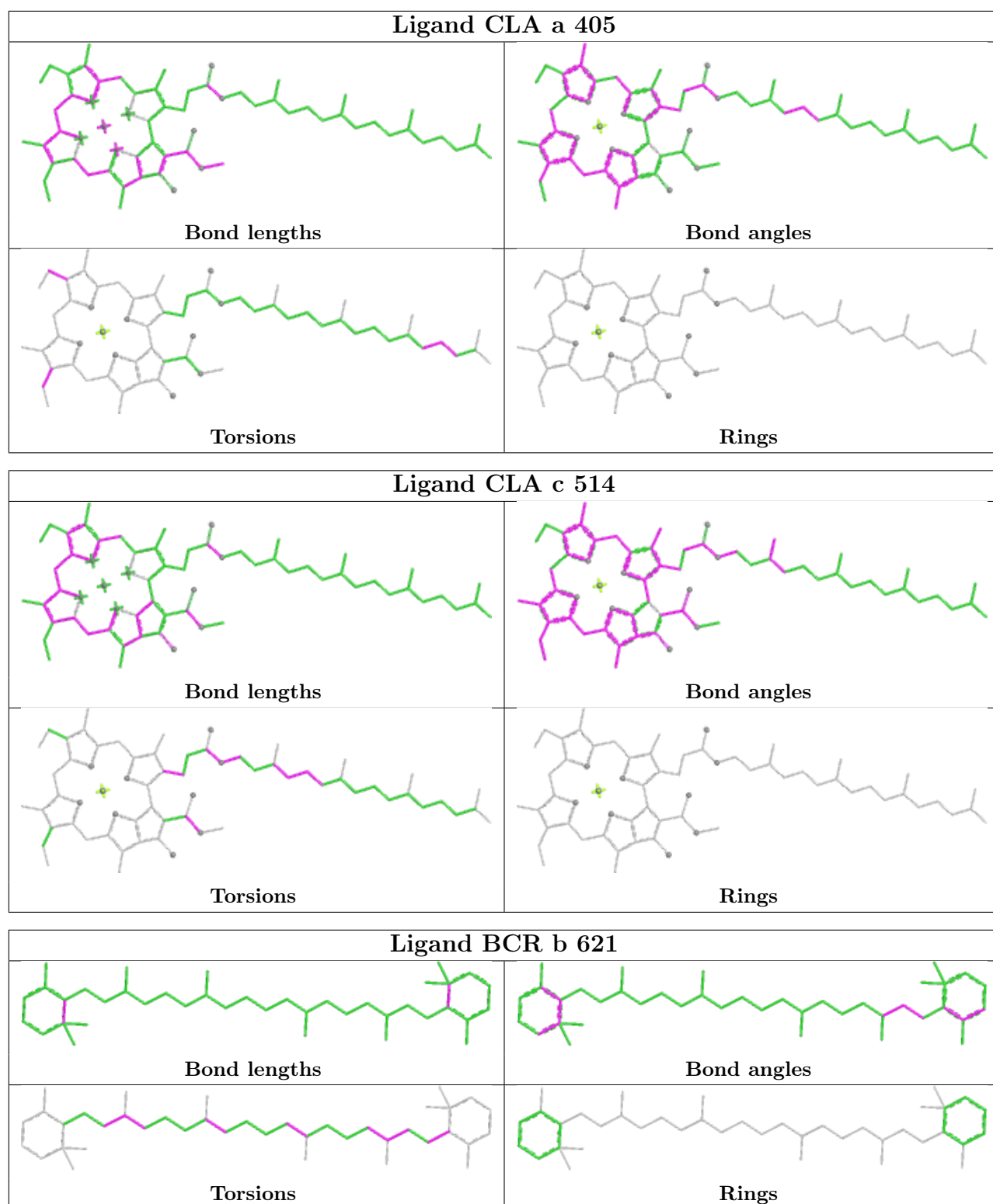


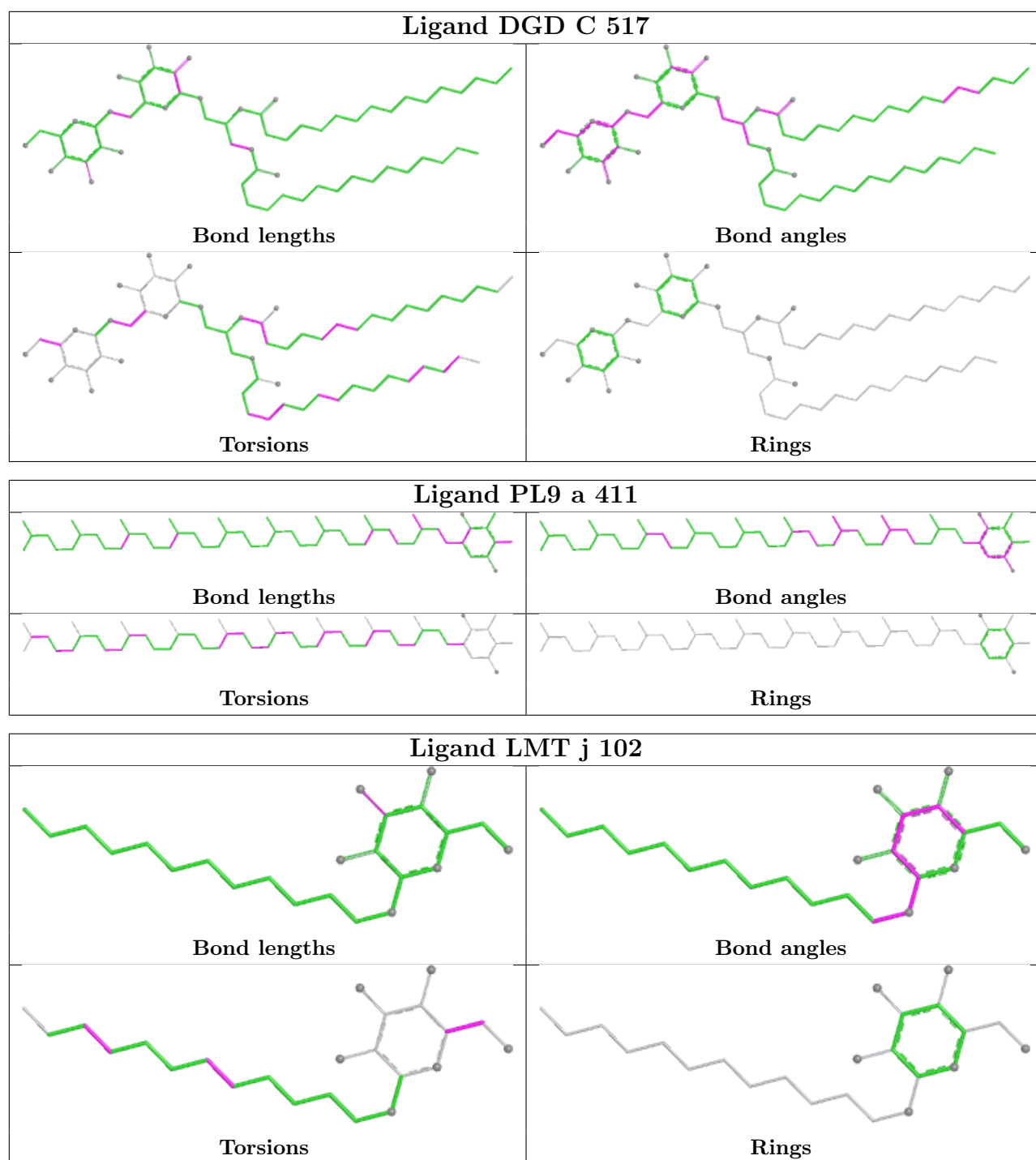


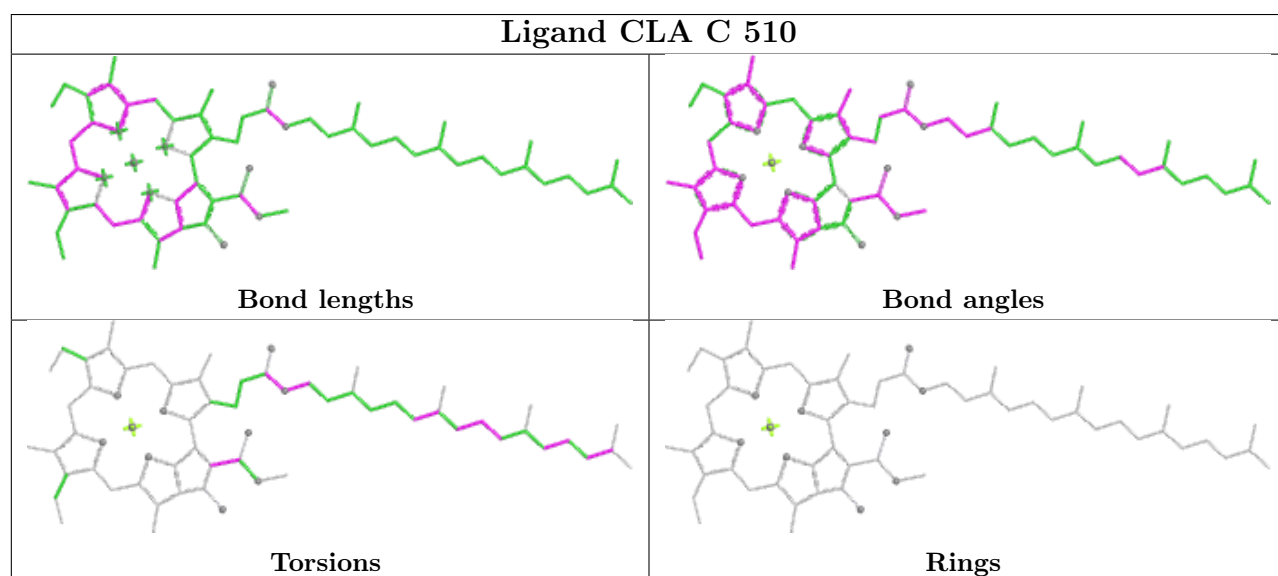
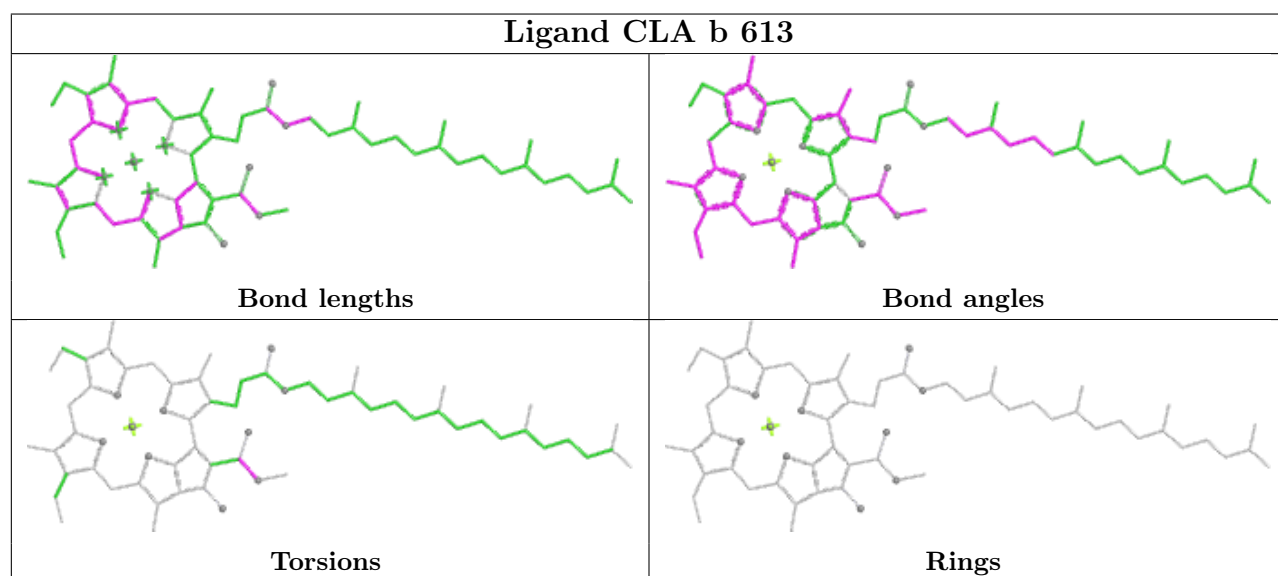
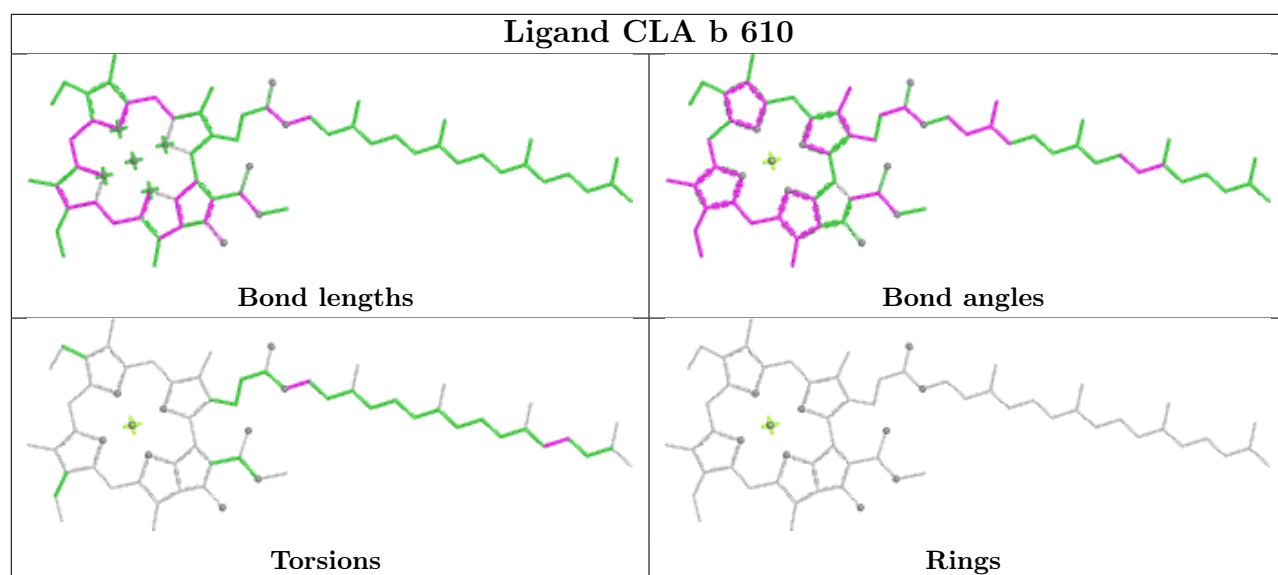


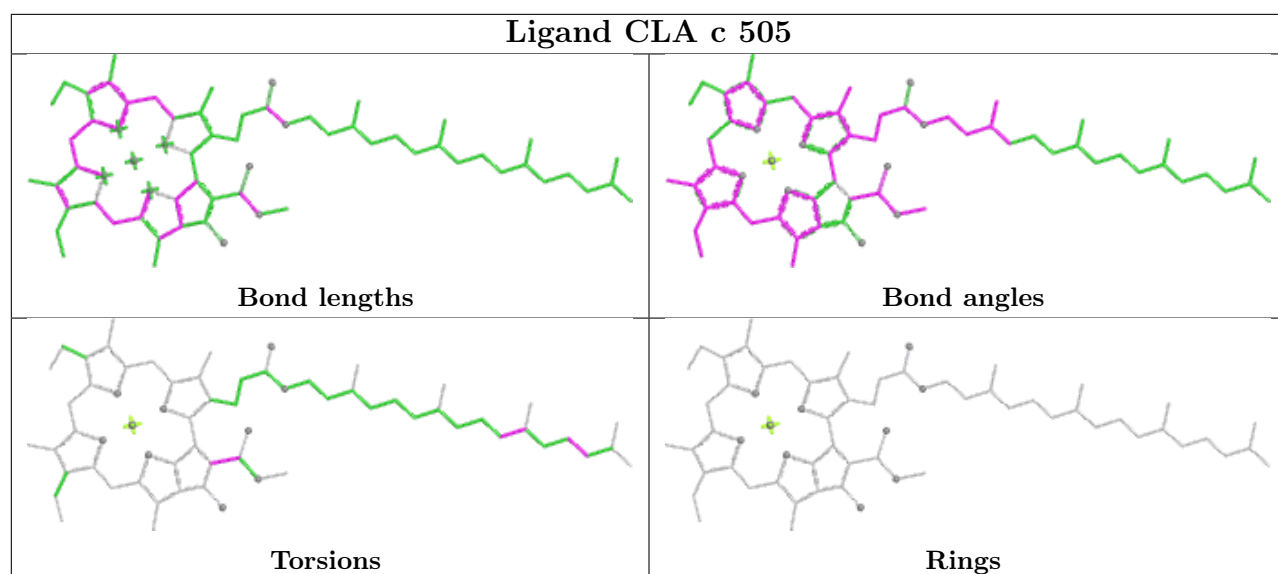
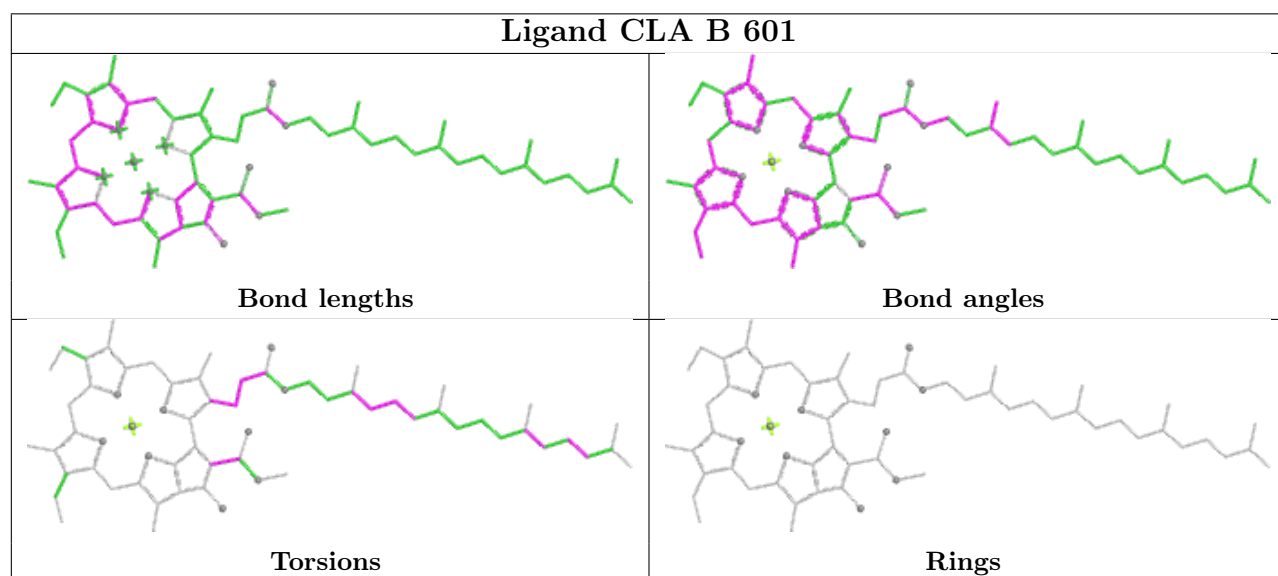
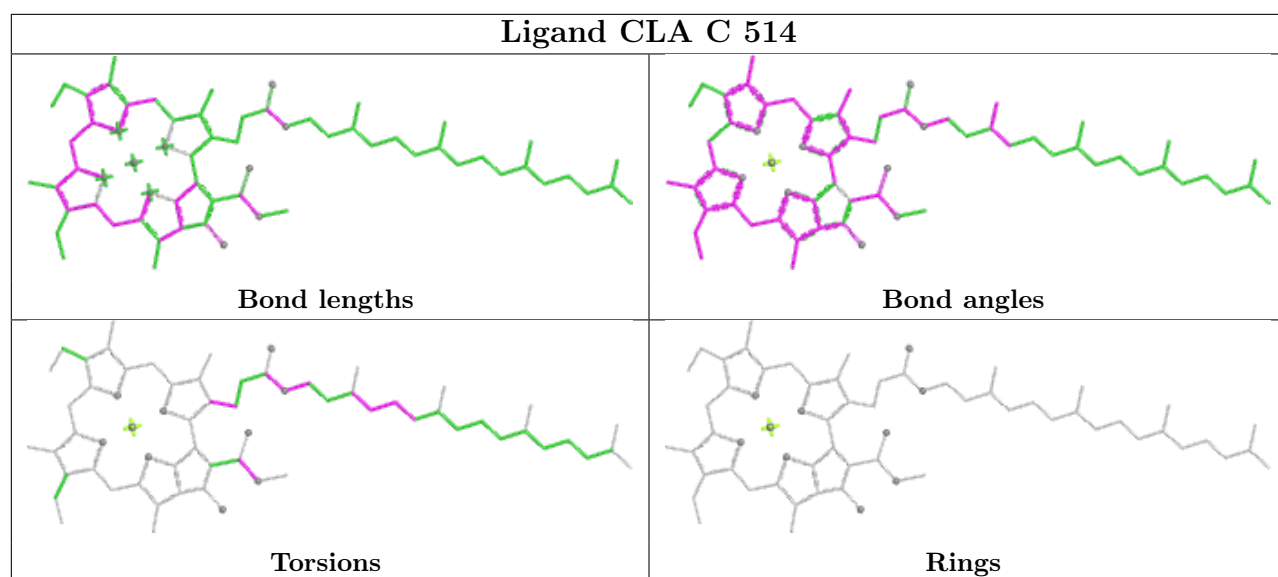


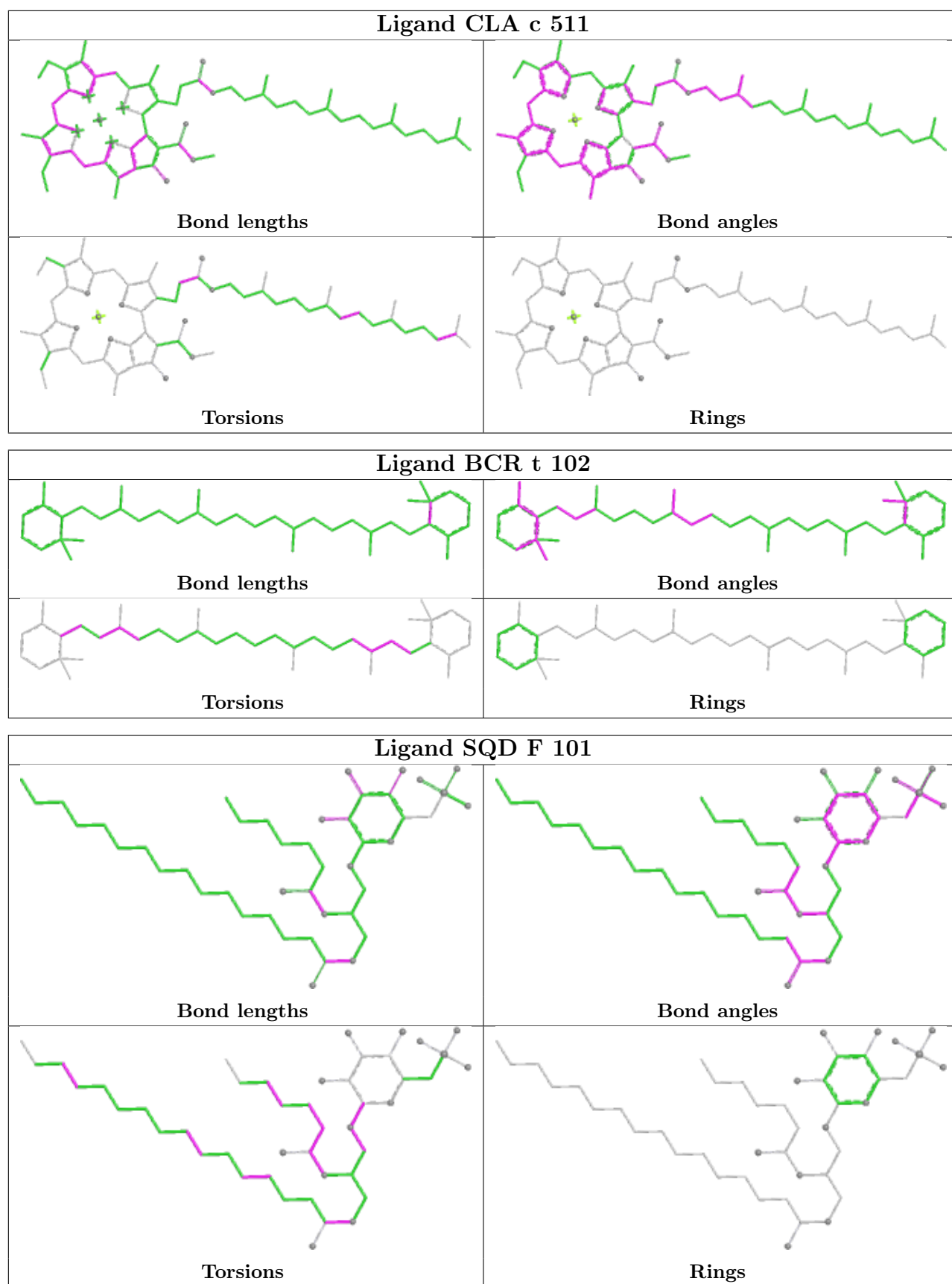


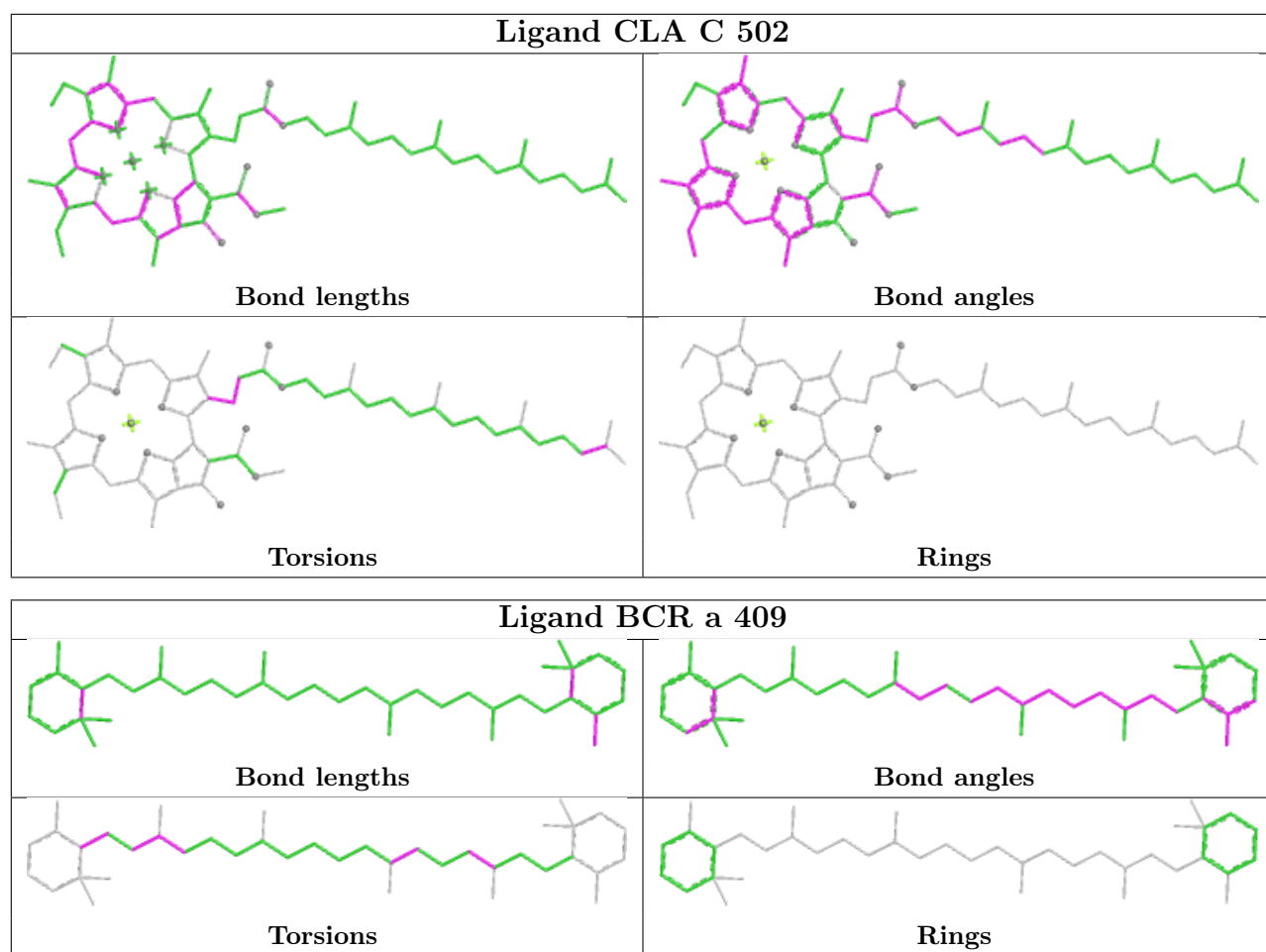


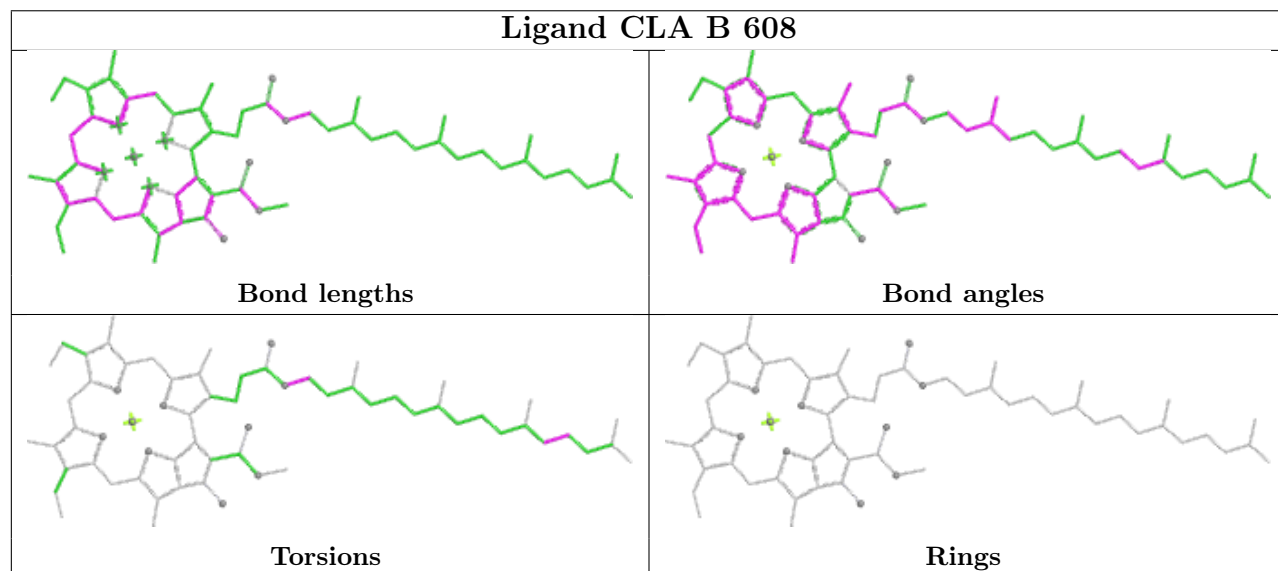
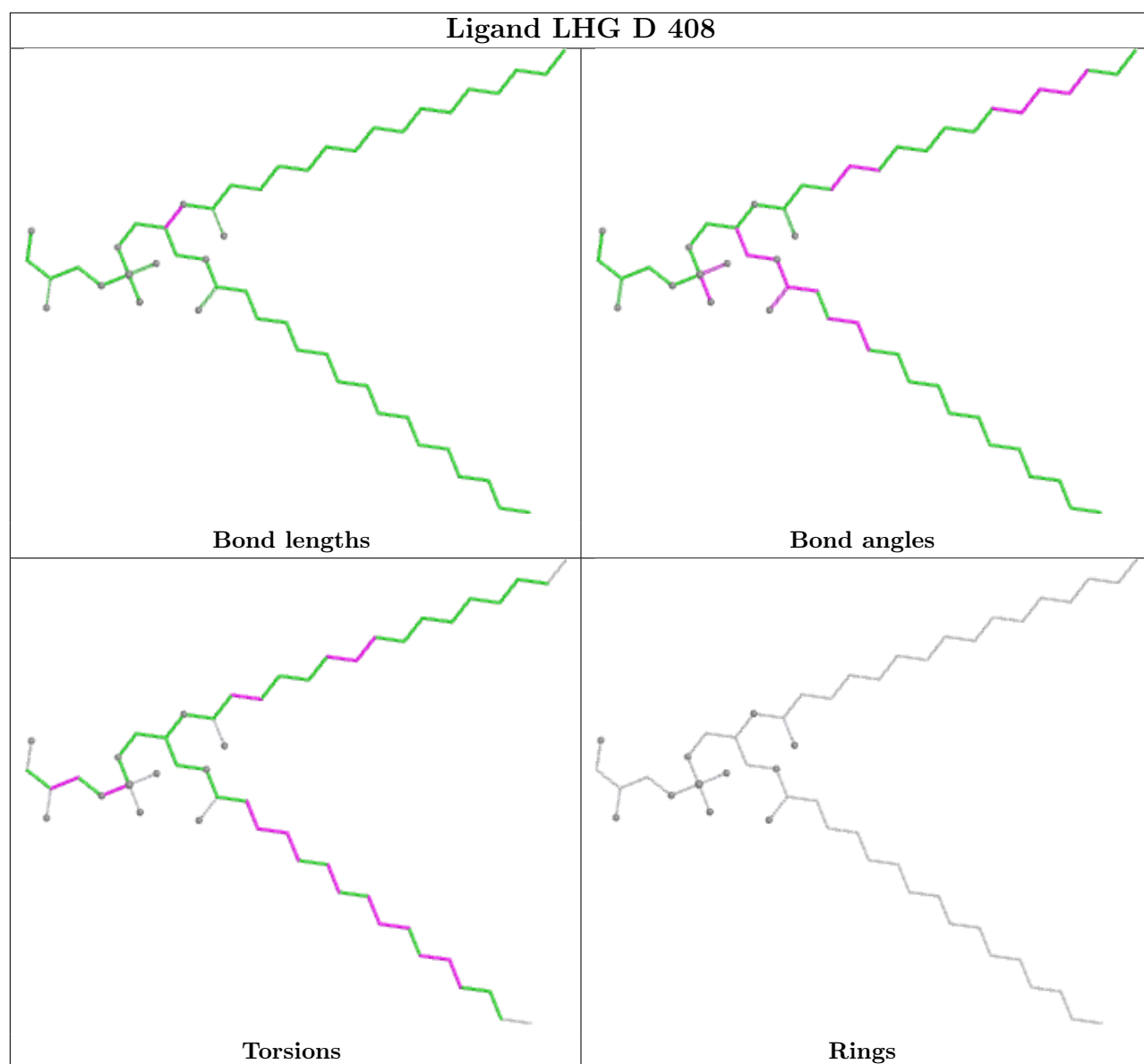


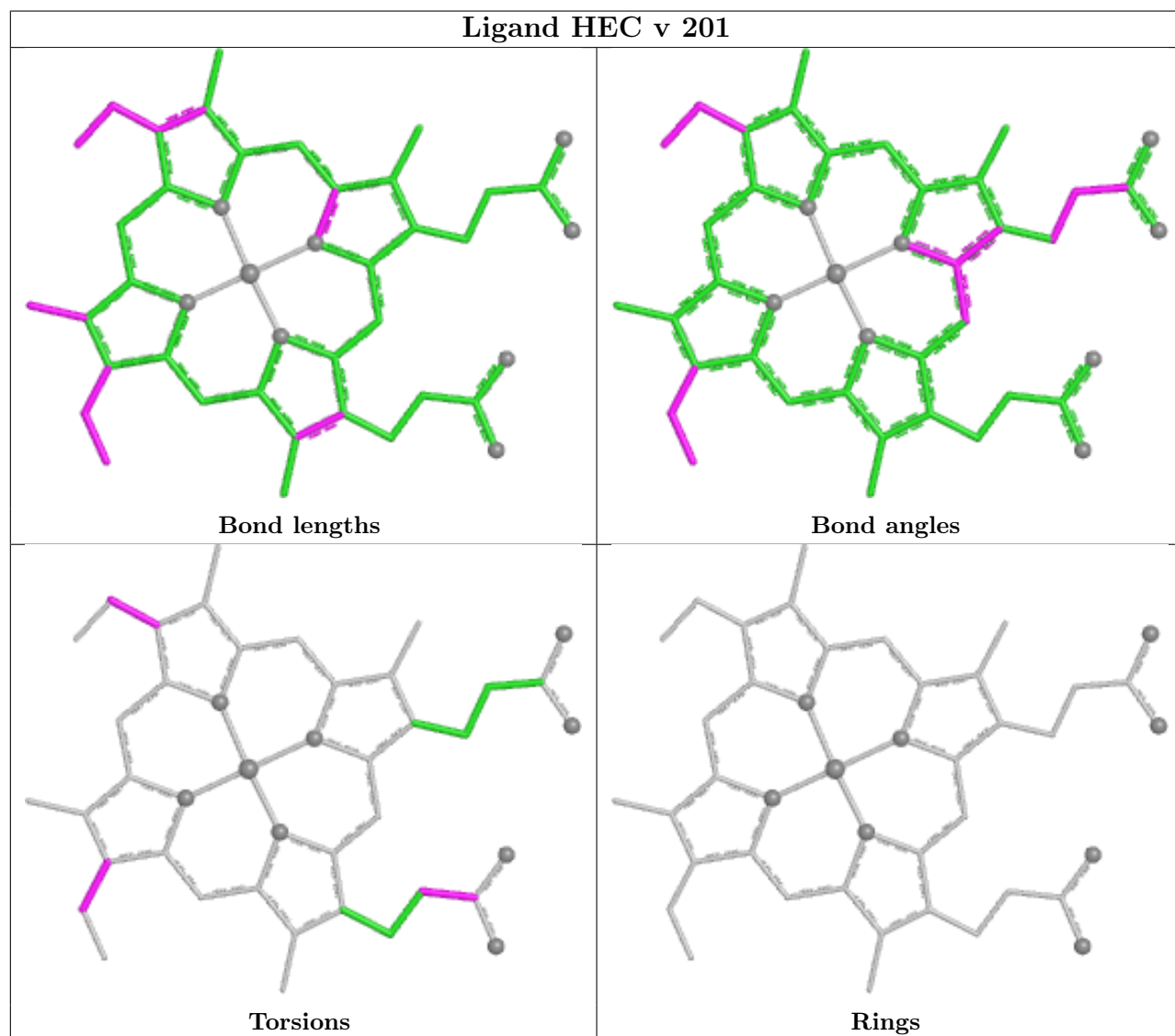
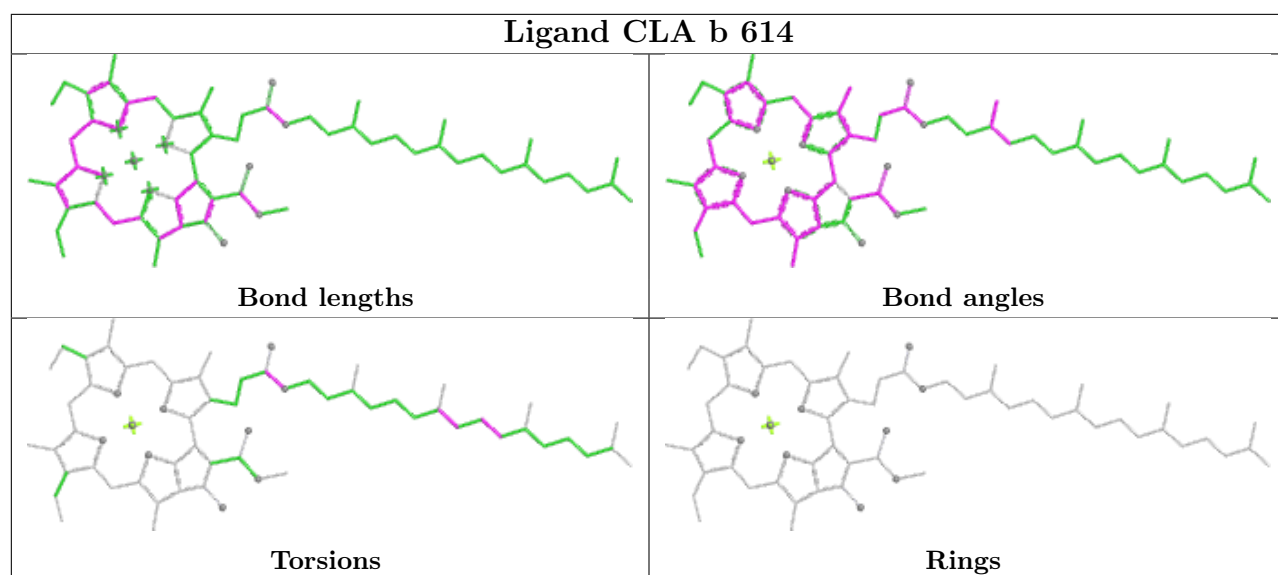


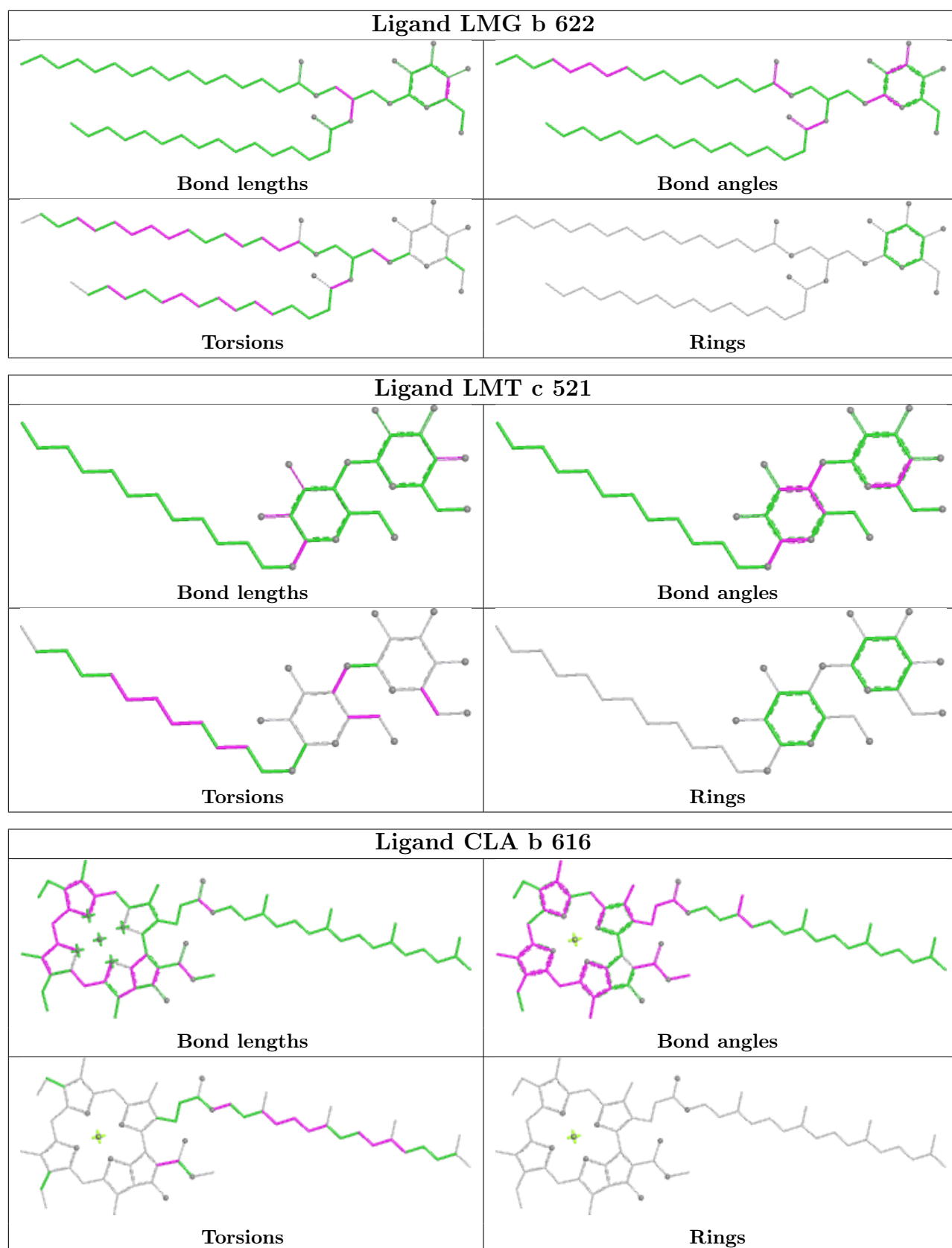


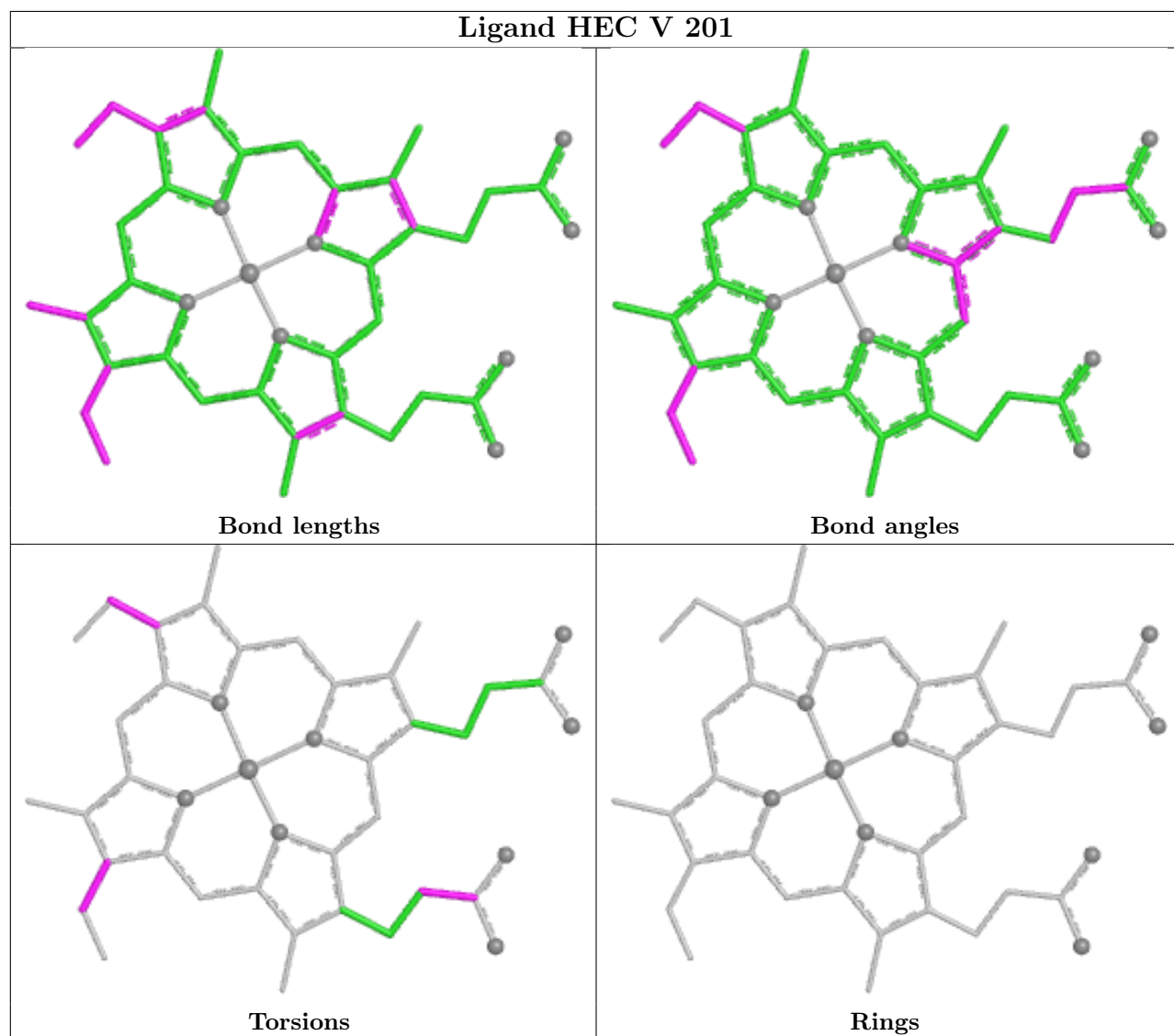
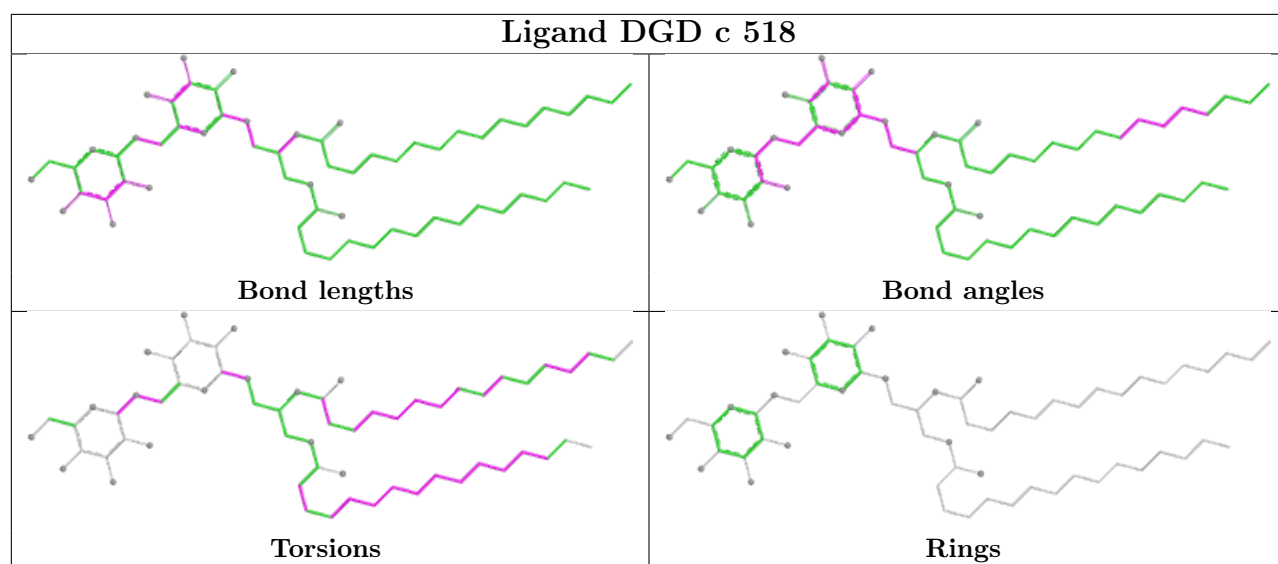


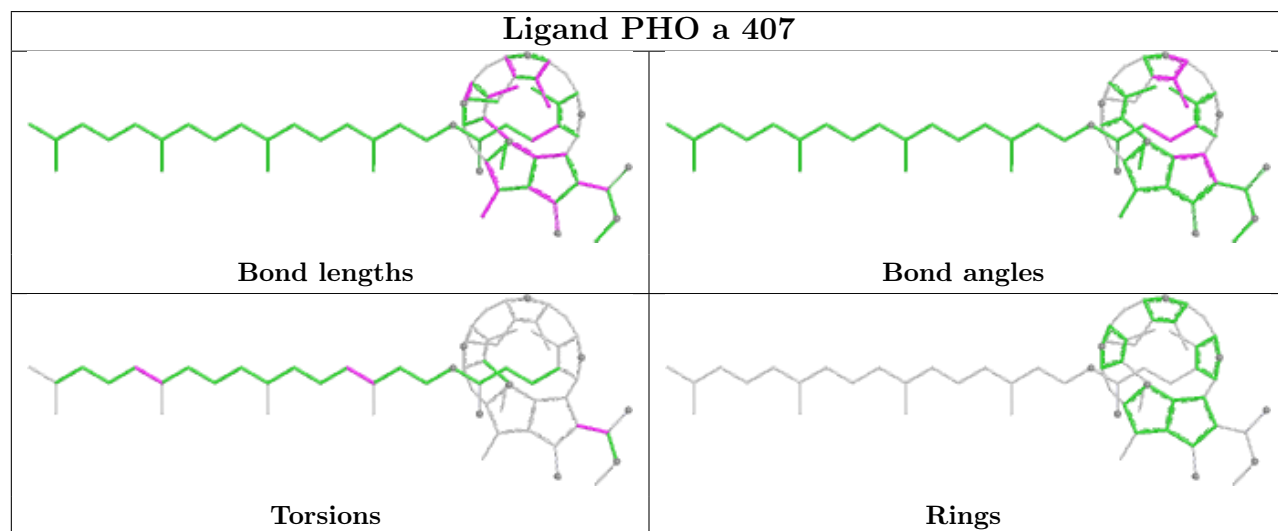
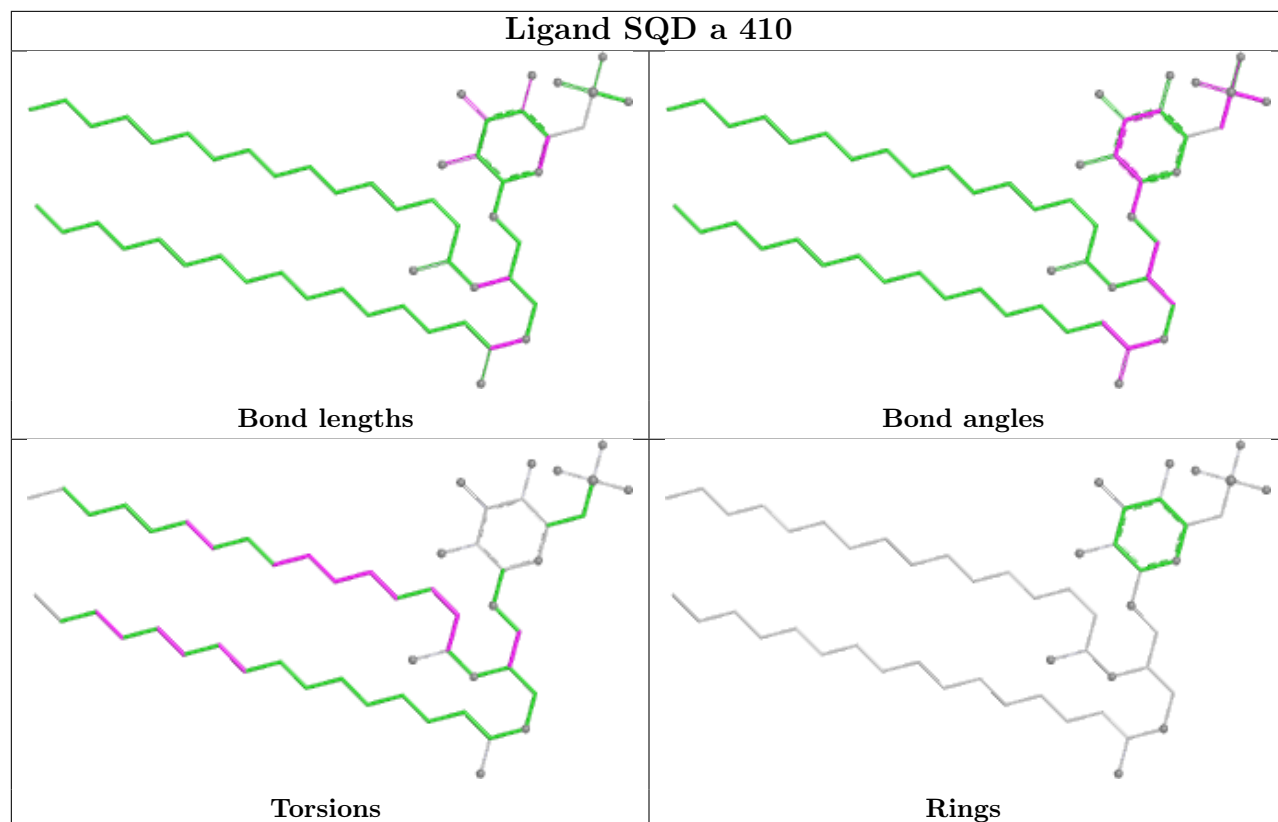


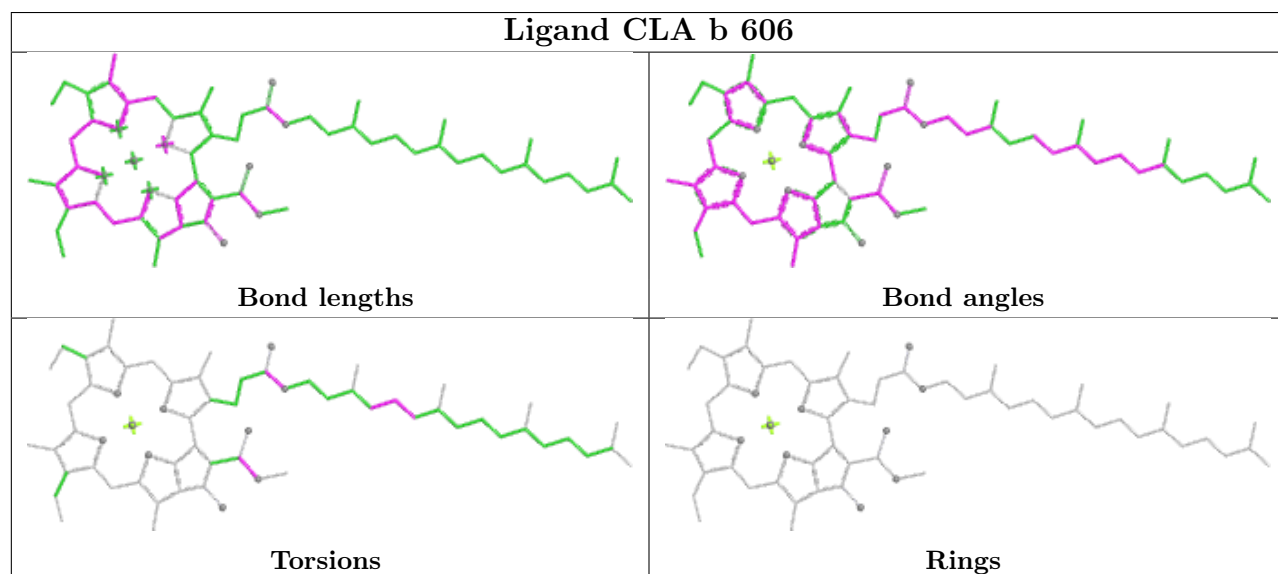
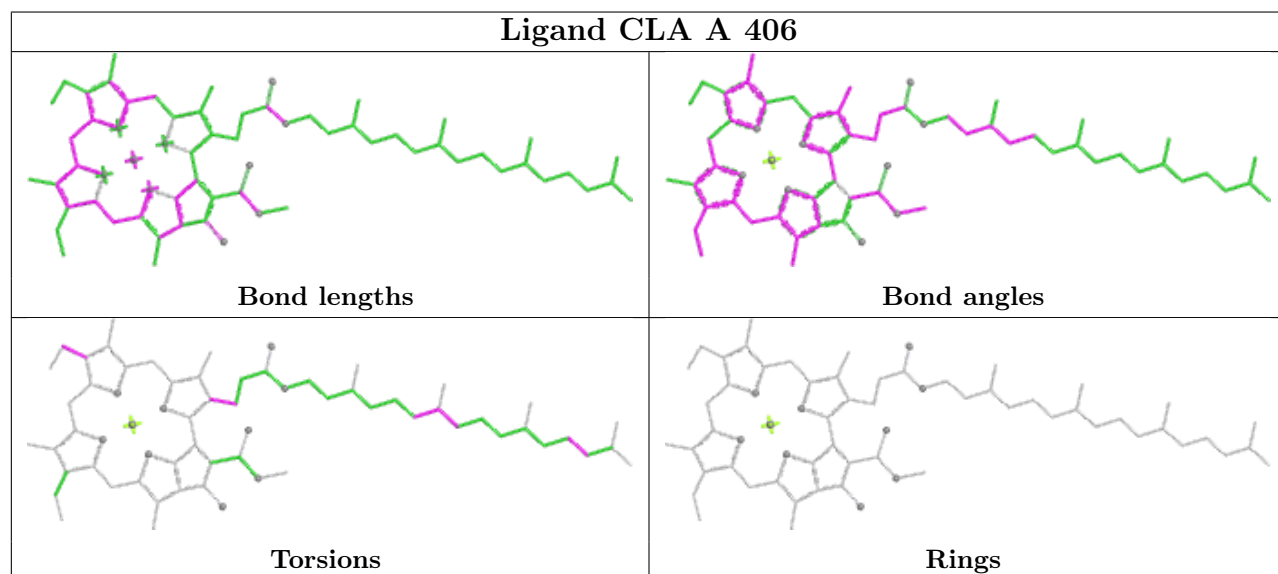
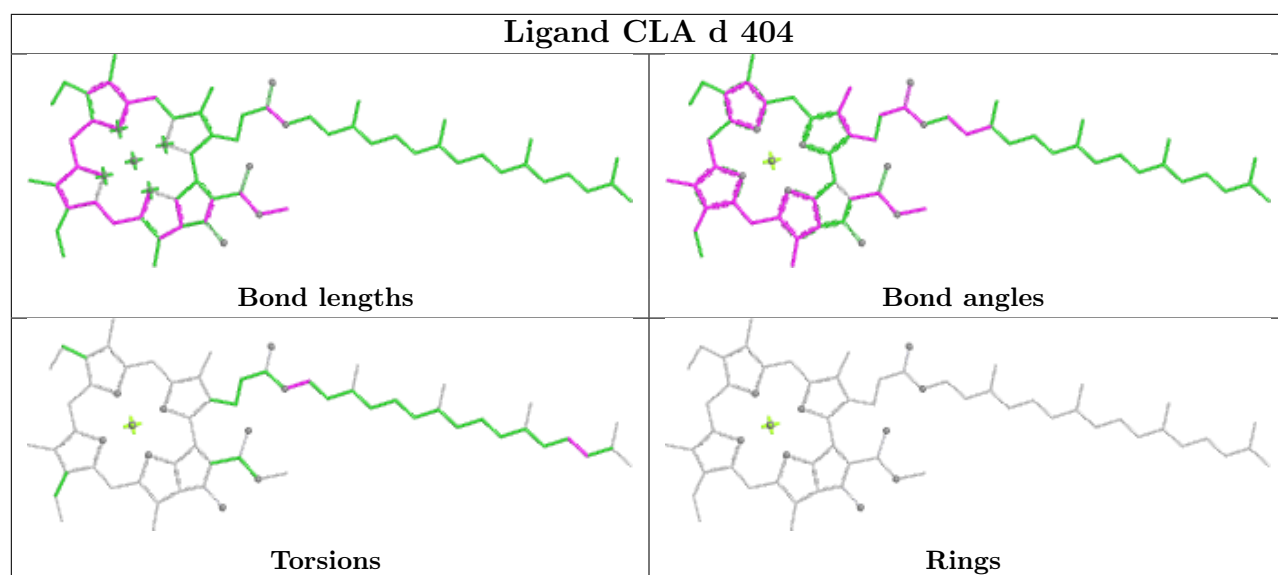


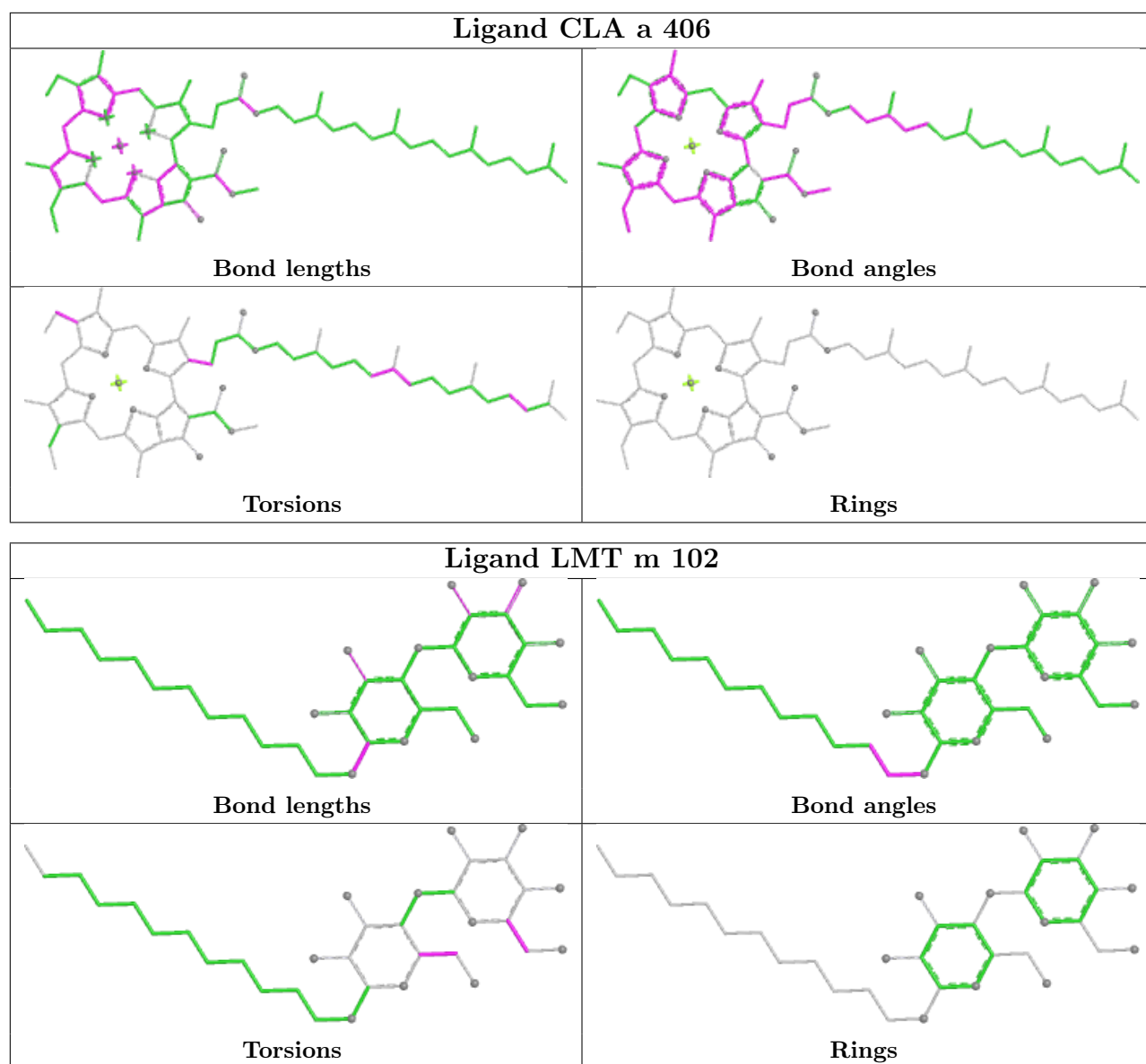


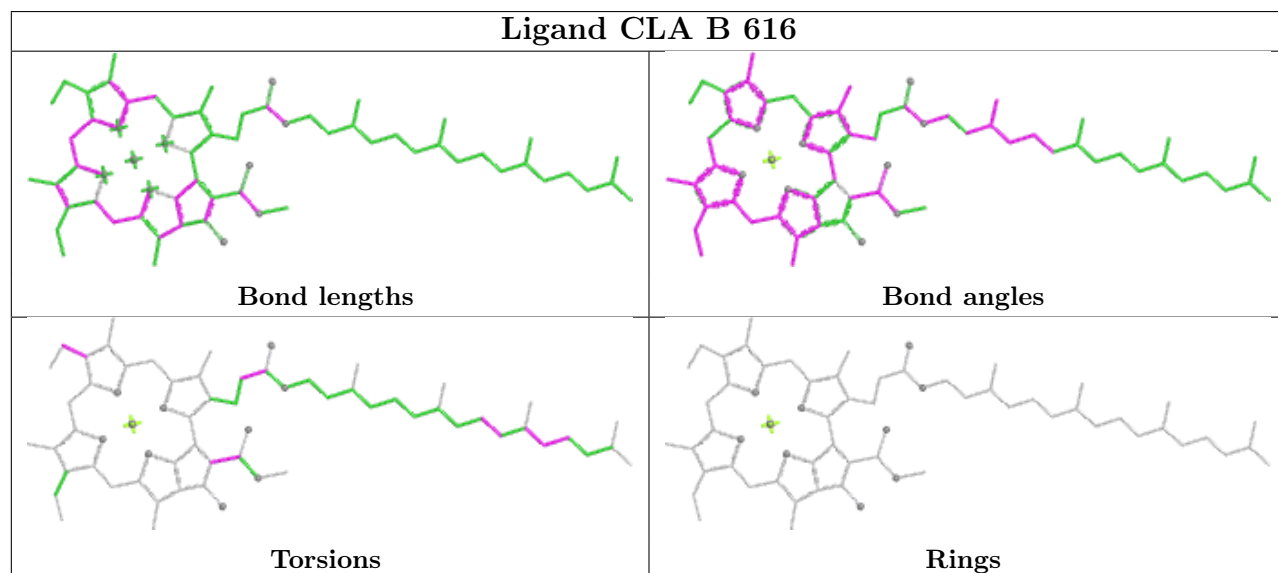
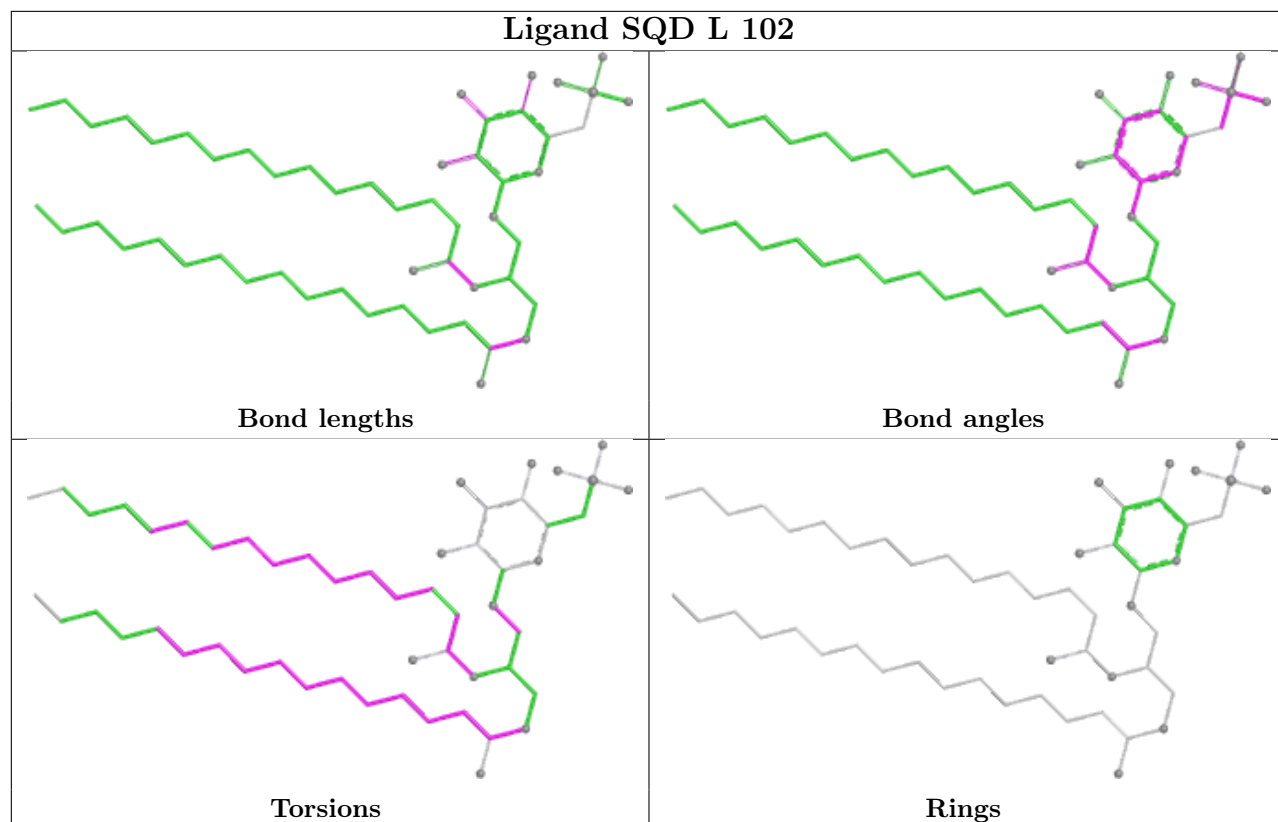




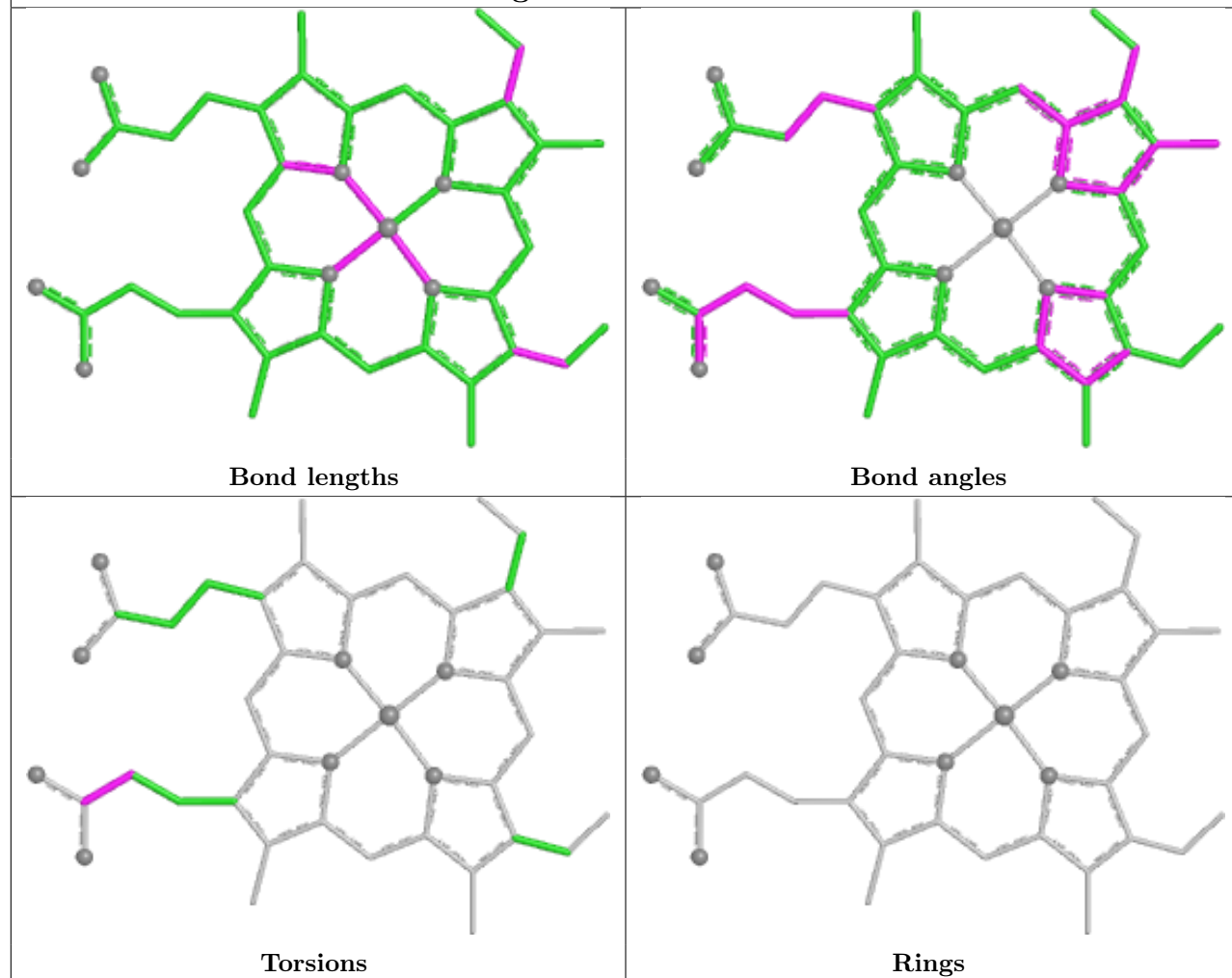




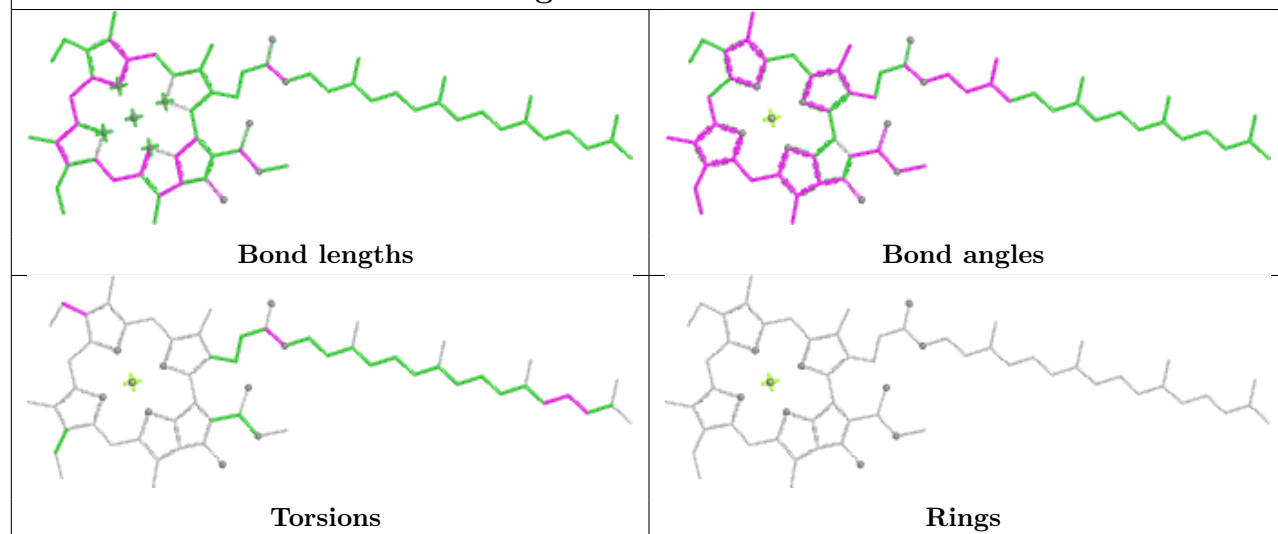


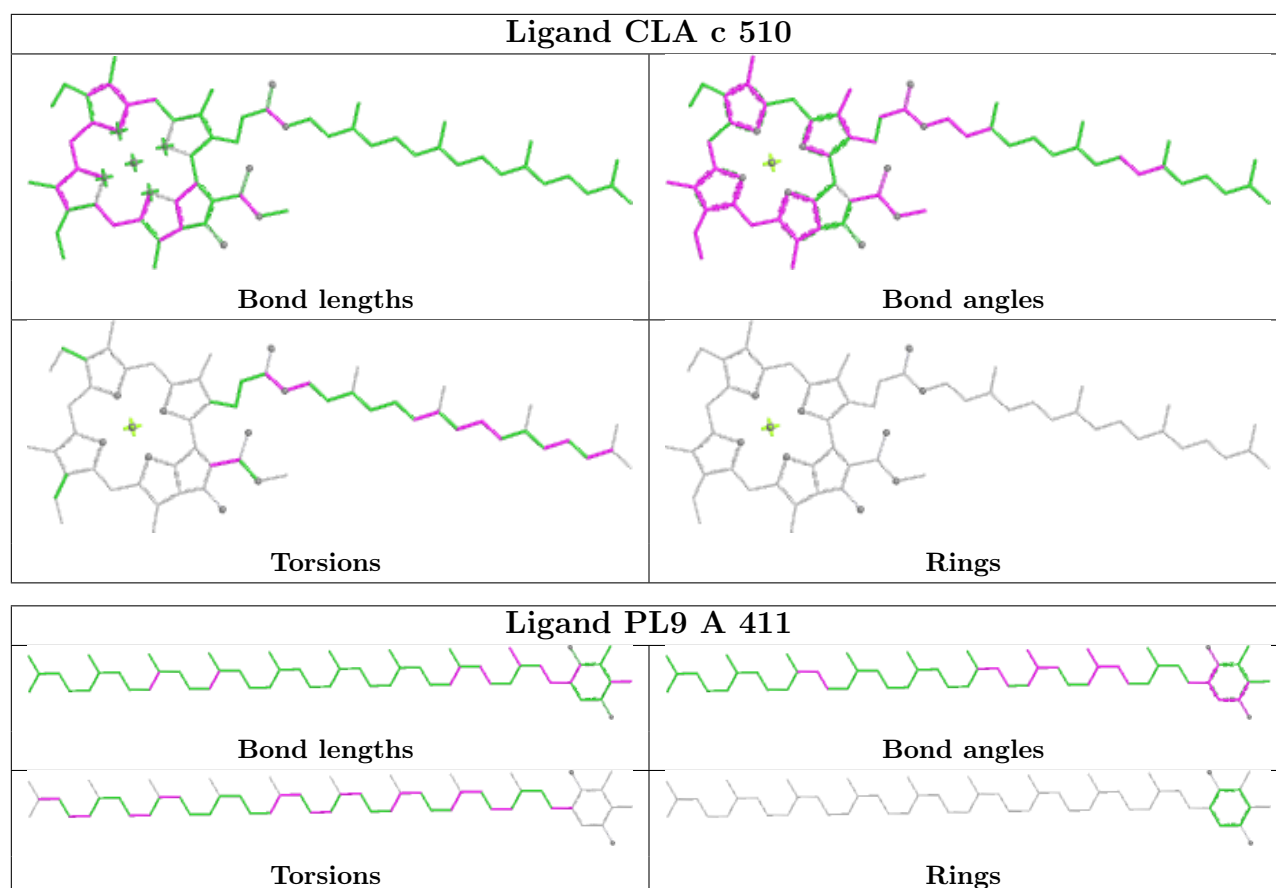


Ligand HEM e 103



Ligand CLA b 604





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

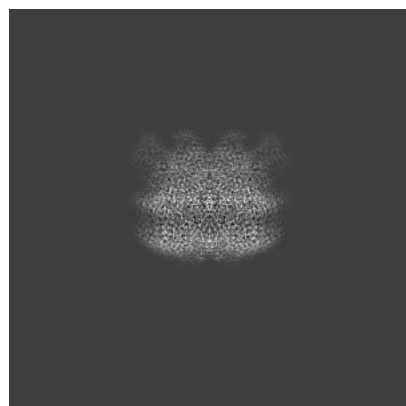
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30547. These allow visual inspection of the internal detail of the map and identification of artifacts.

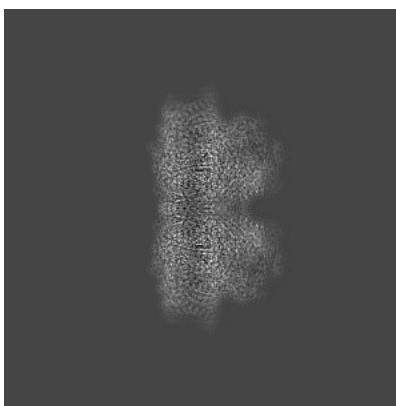
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

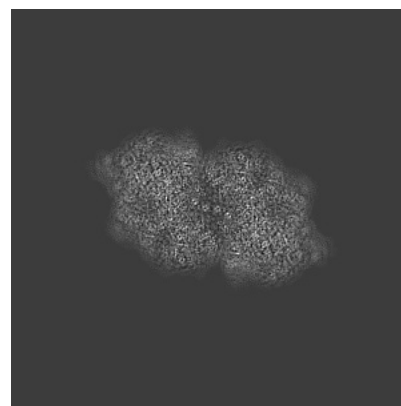
5.1.1 Primary map



X

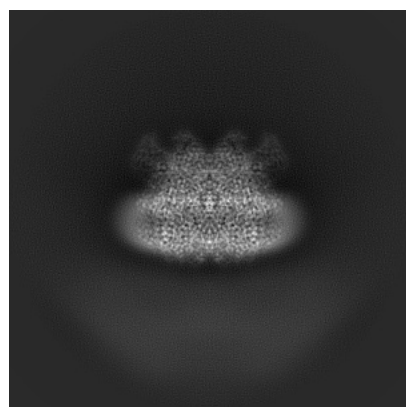


Y

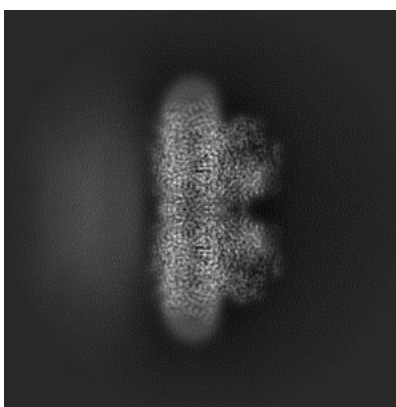


Z

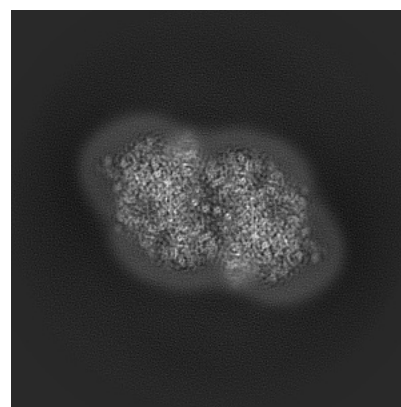
5.1.2 Raw map



X



Y

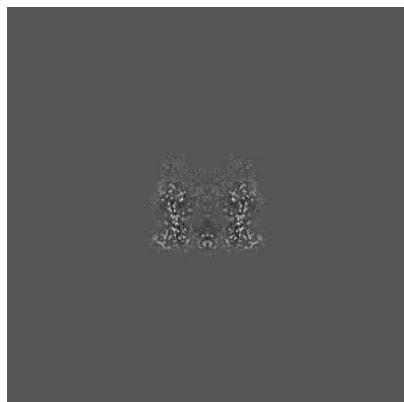


Z

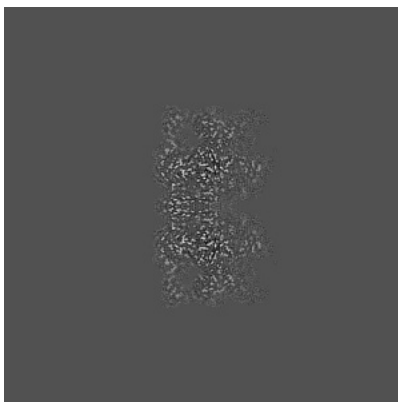
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

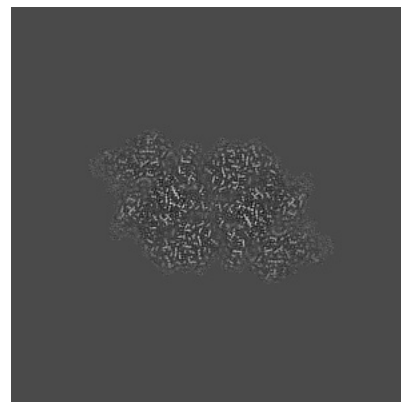
5.2.1 Primary map



X Index: 200

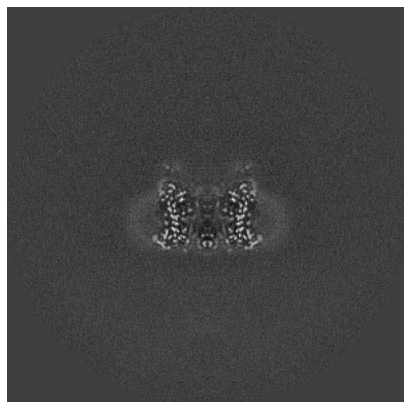


Y Index: 200

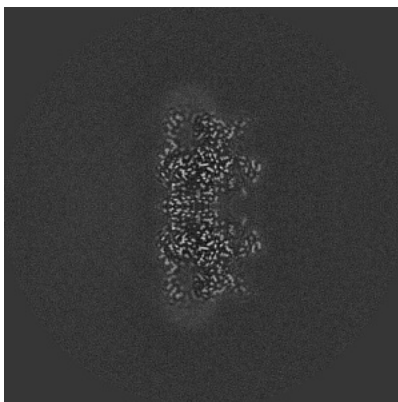


Z Index: 200

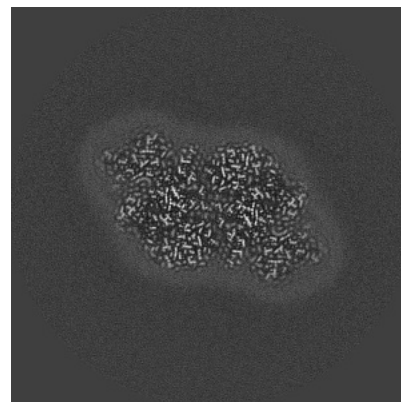
5.2.2 Raw map



X Index: 200



Y Index: 200

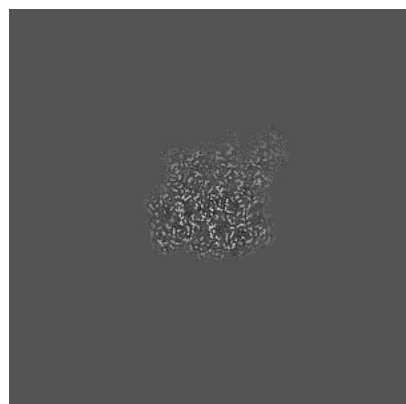


Z Index: 200

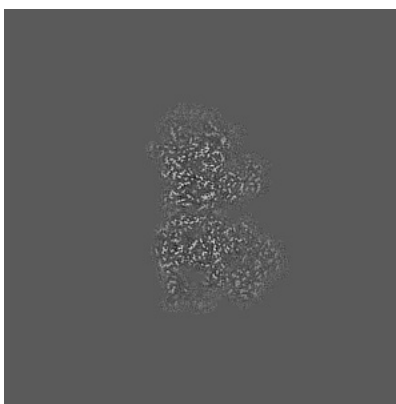
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

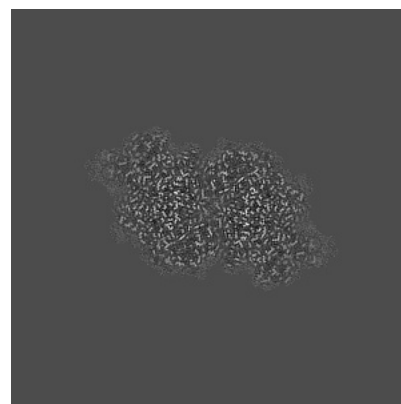
5.3.1 Primary map



X Index: 167

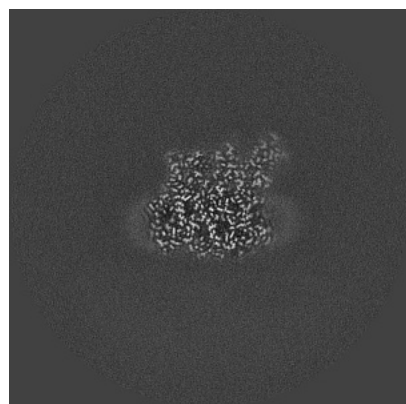


Y Index: 218

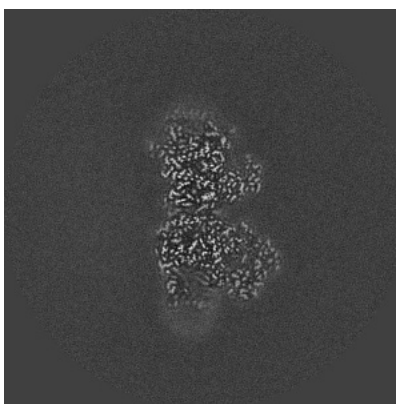


Z Index: 207

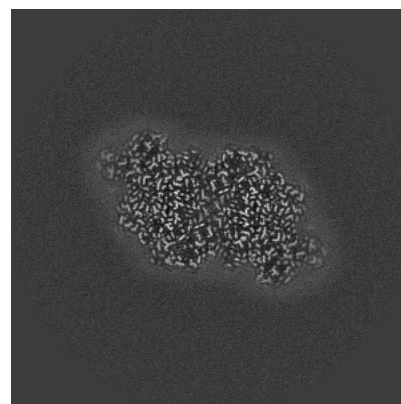
5.3.2 Raw map



X Index: 167



Y Index: 218

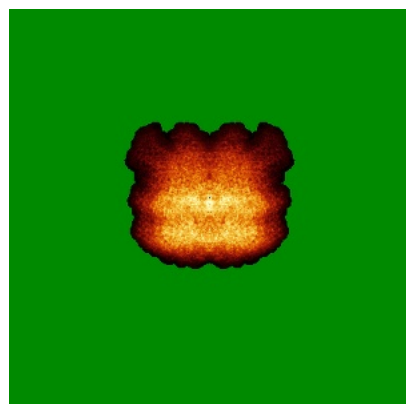


Z Index: 207

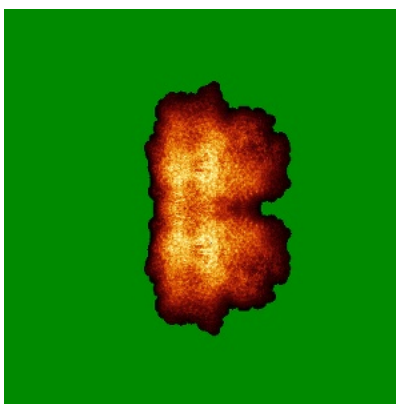
The images above show the largest variance slices of the map in three orthogonal directions.

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

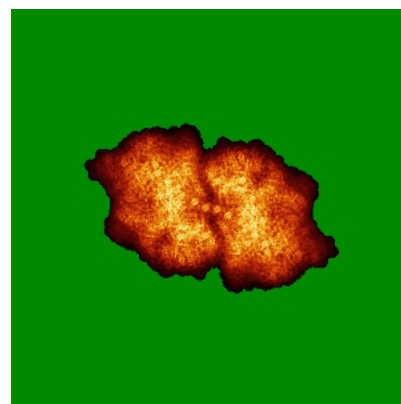
5.4.1 Primary map



X

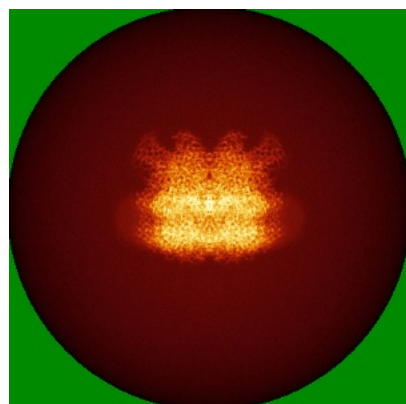


Y

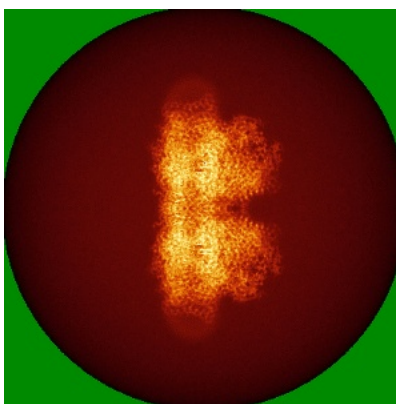


Z

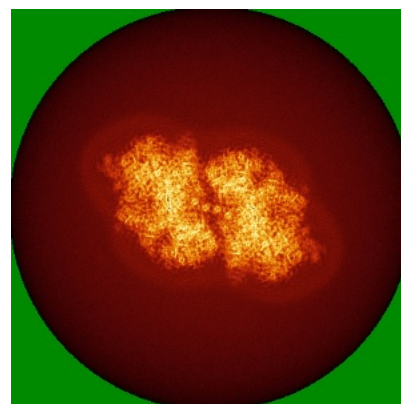
5.4.2 Raw map



X



Y

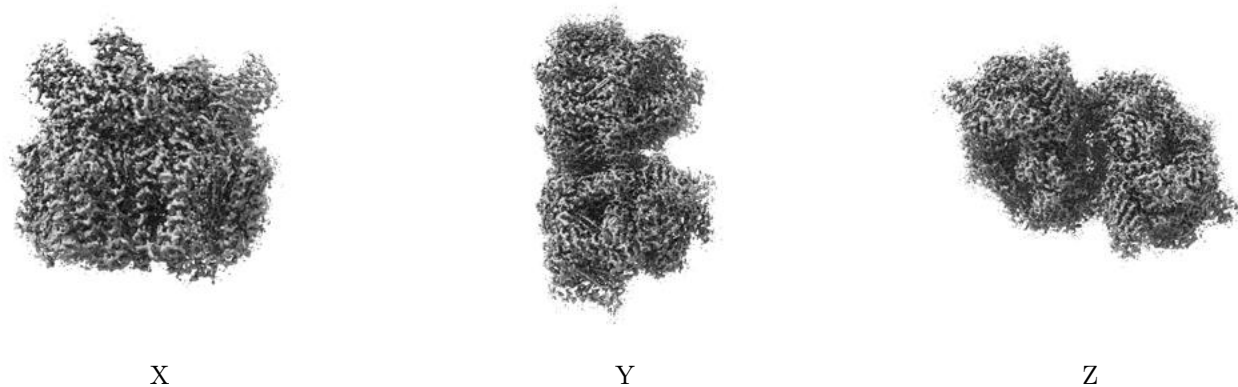


Z

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.

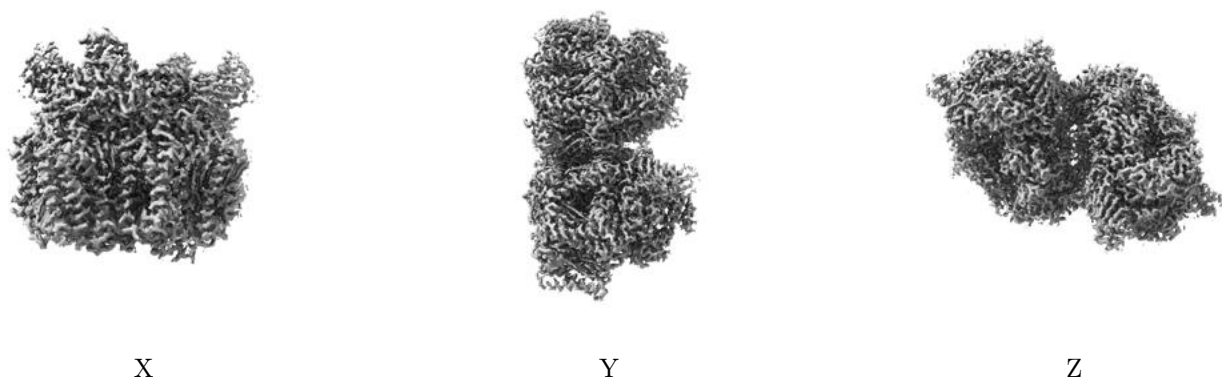
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

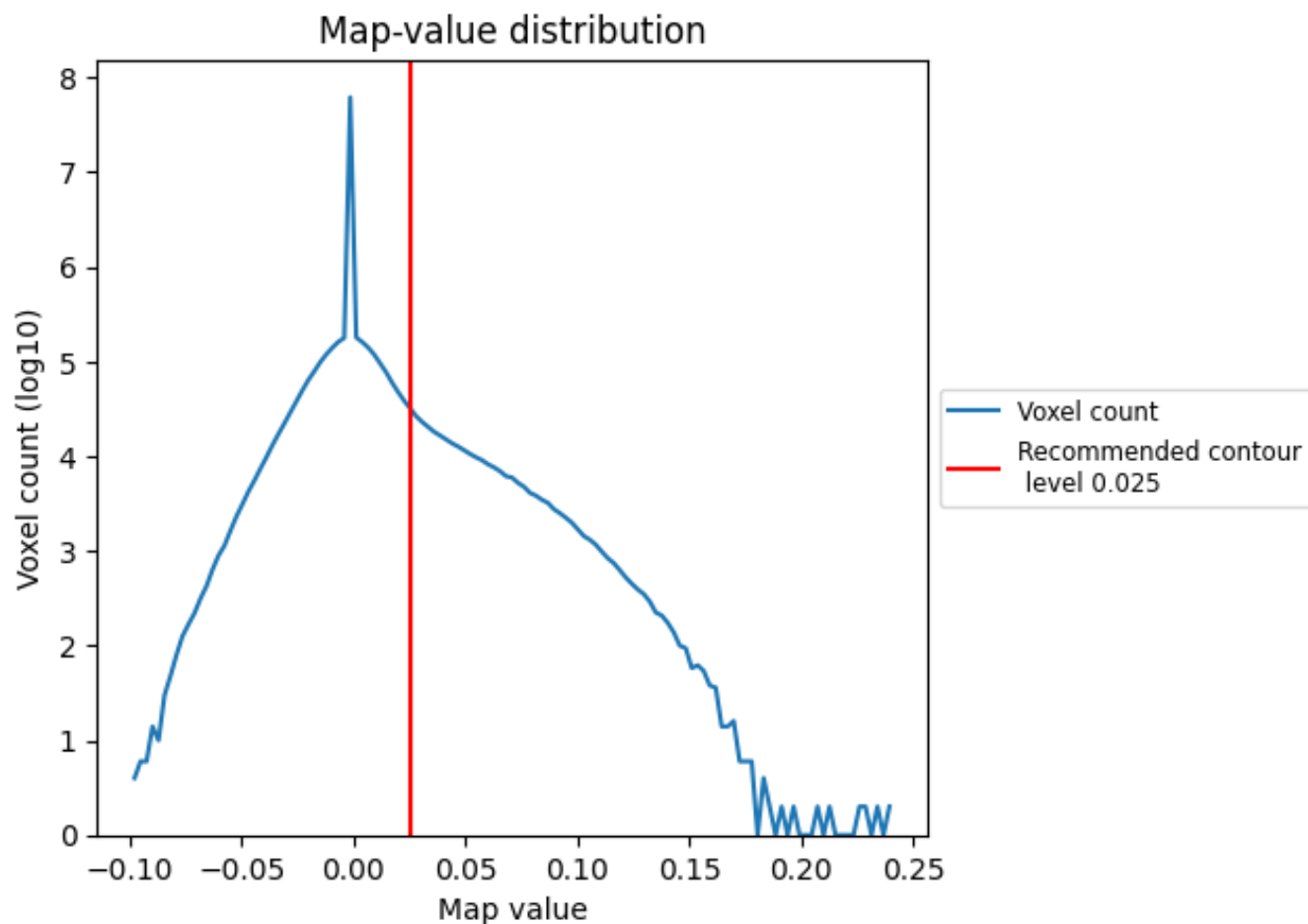
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

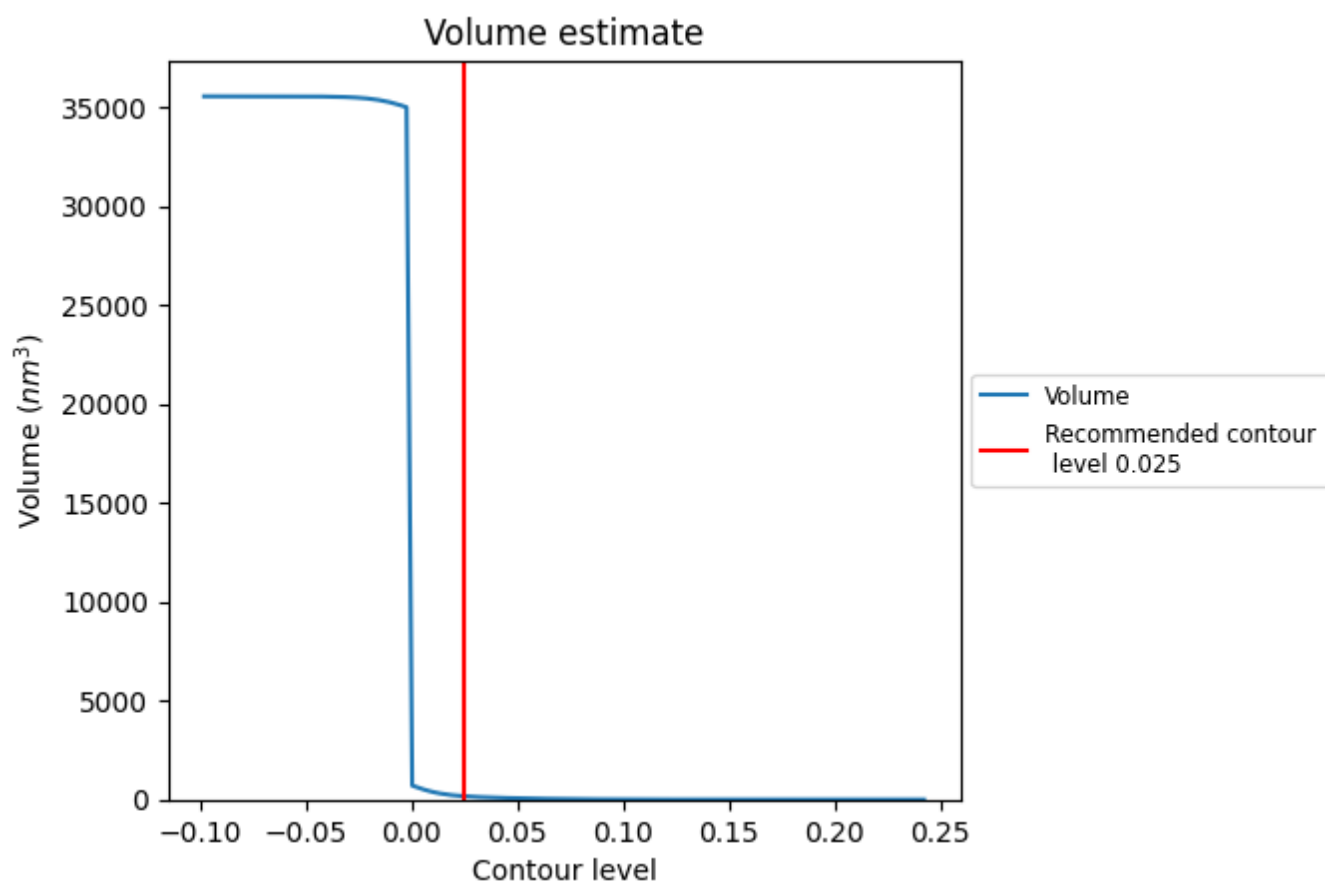
This section contains the results of statistical analysis of the map.

6.1 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.

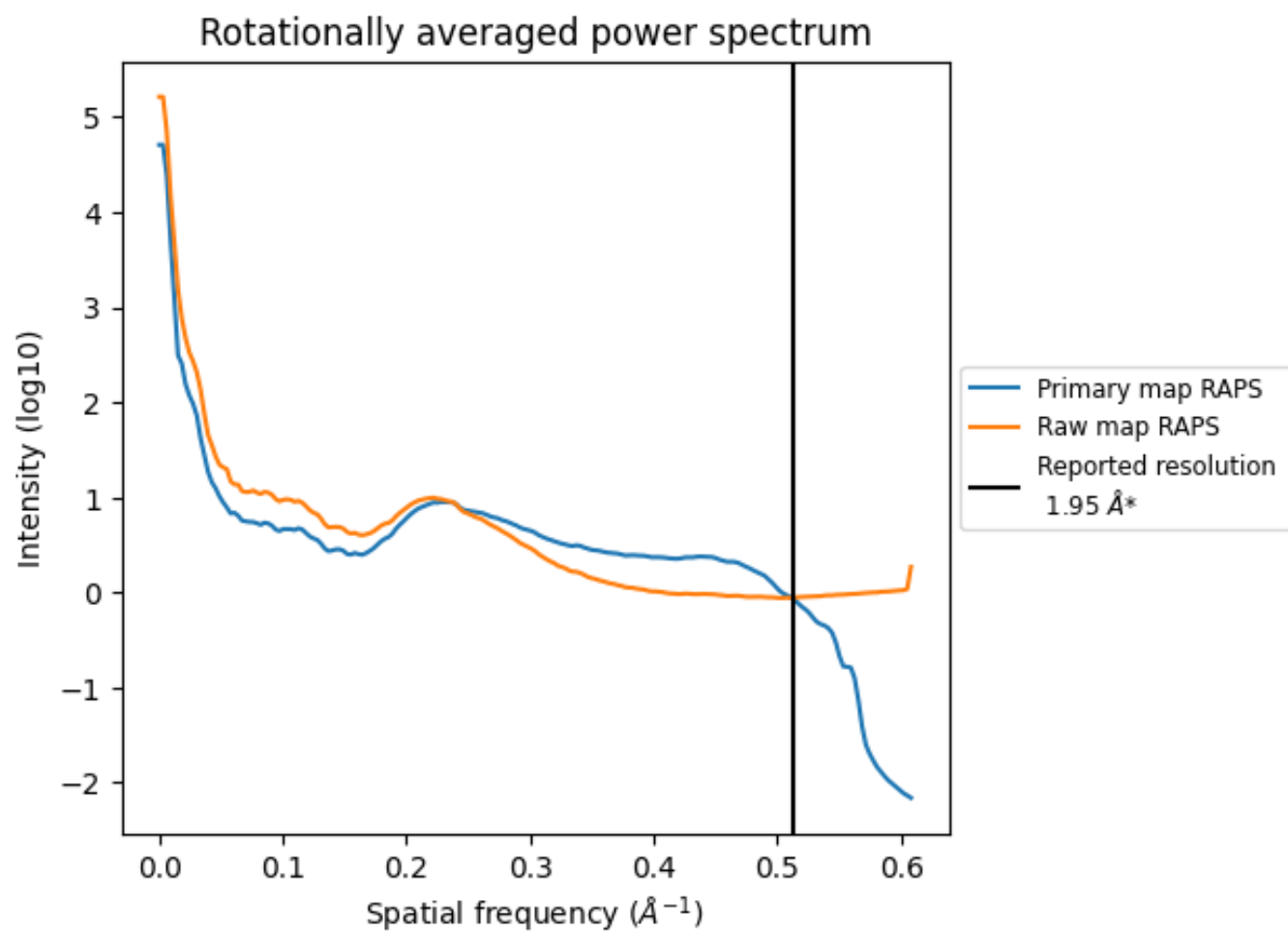
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm^3 ; this corresponds to an approximate mass of 152 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.

6.3 Rotationally averaged power spectrum ⓘ

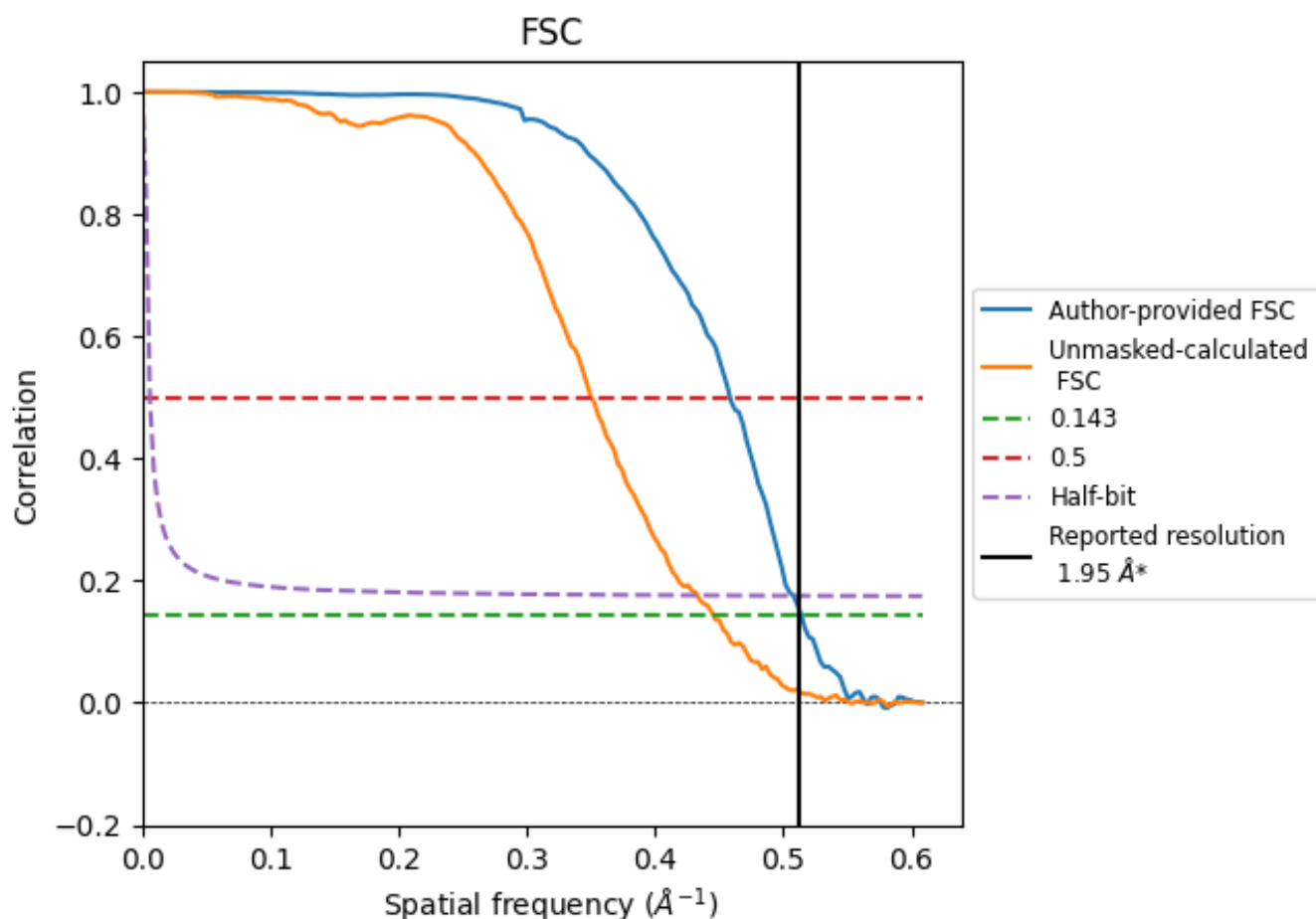


*Reported resolution corresponds to spatial frequency of 0.513 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.513 Å⁻¹

7.2 Resolution estimates [i](#)

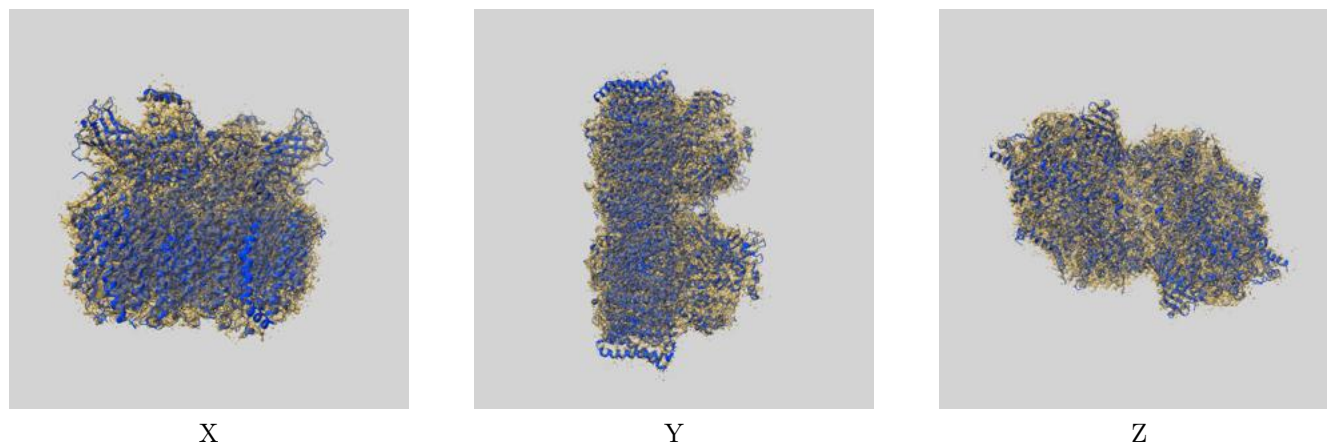
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.95	-	-
Author-provided FSC curve	1.95	2.18	1.97
Unmasked-calculated*	2.24	2.86	2.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.24 differs from the reported value 1.95 by more than 10 %

8 Map-model fit [i](#)

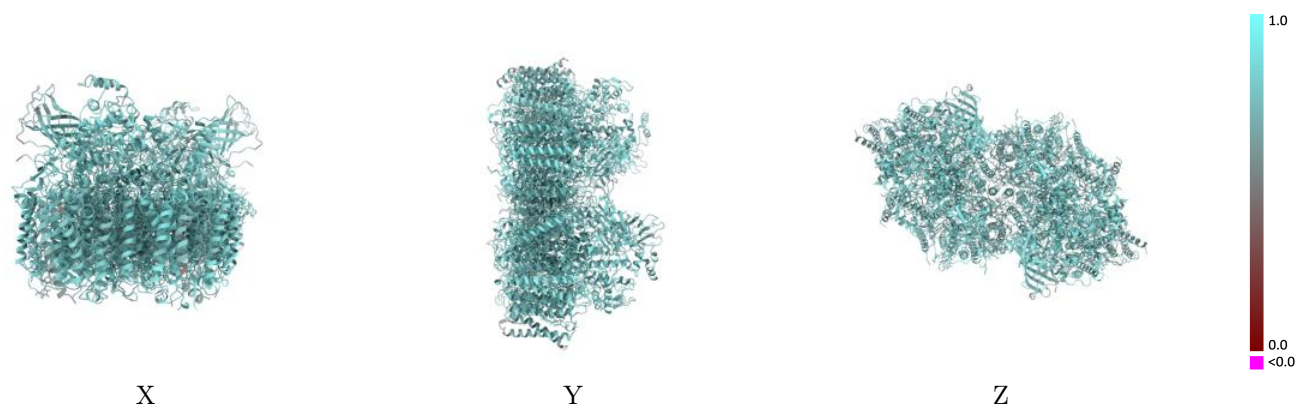
This section contains information regarding the fit between EMDB map EMD-30547 and PDB model 7D1T. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



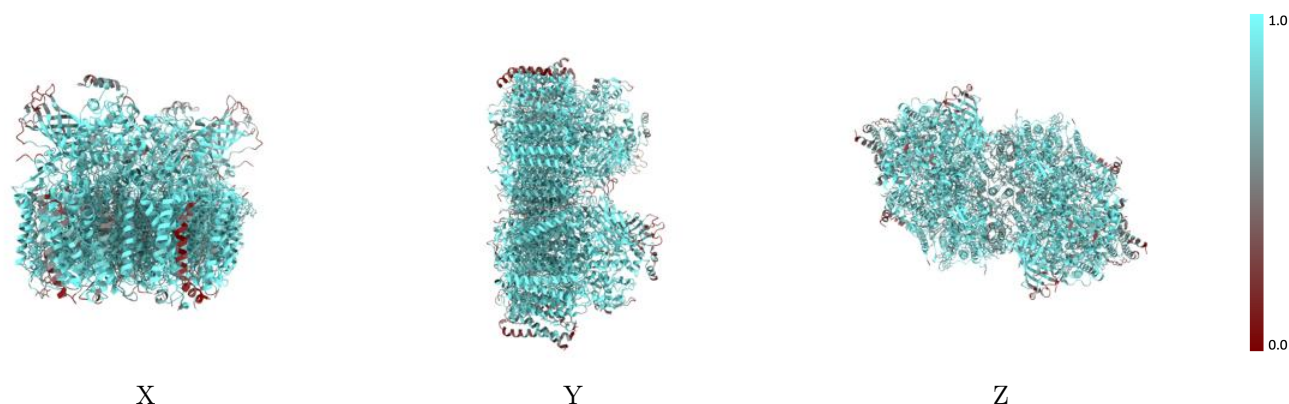
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



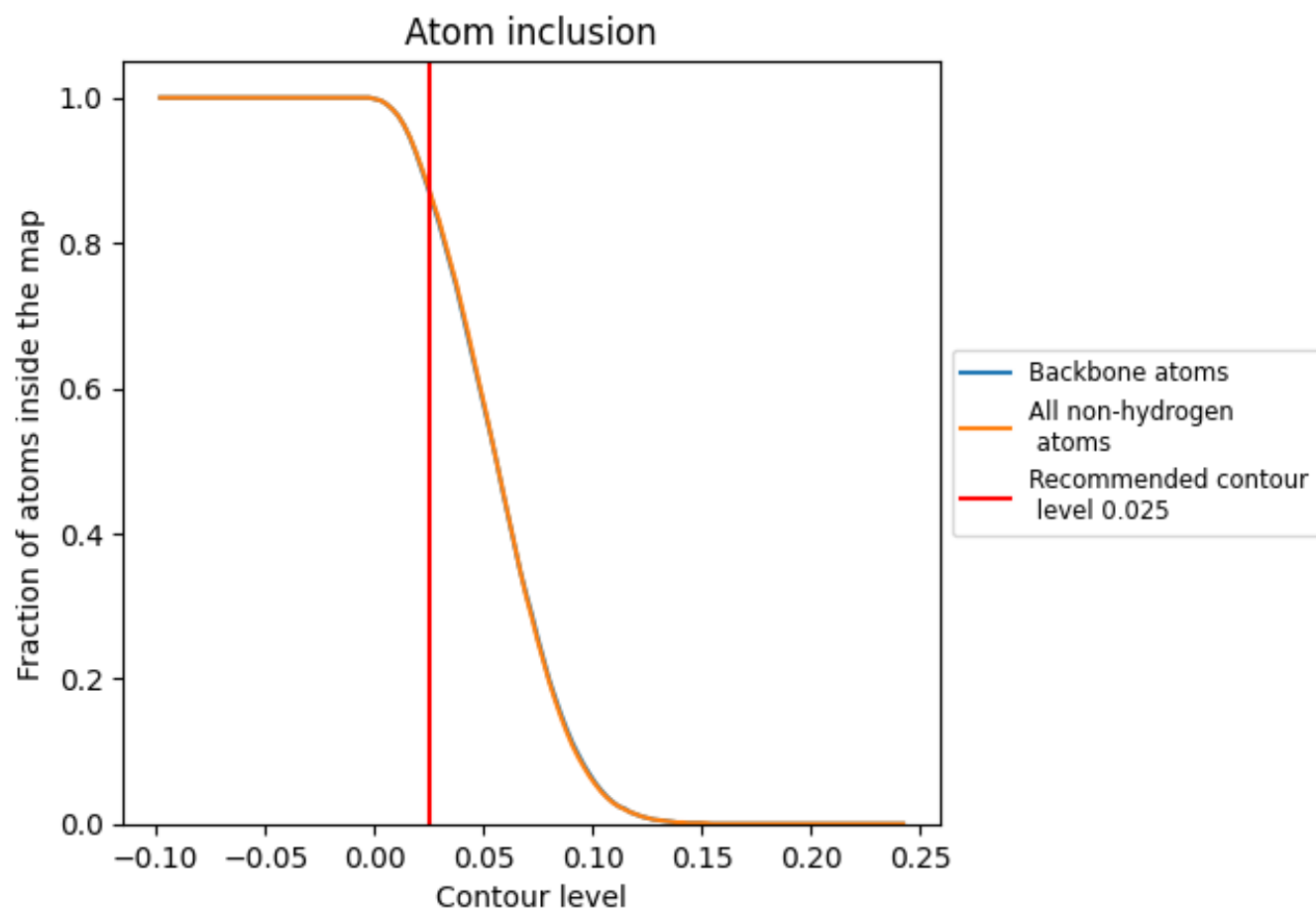
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.025).

8.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8750	 0.7760
A	 0.9330	 0.8060
B	 0.9180	 0.7910
C	 0.9010	 0.7770
D	 0.9450	 0.8080
E	 0.8350	 0.7550
F	 0.8600	 0.7660
H	 0.9200	 0.7810
I	 0.8990	 0.7730
J	 0.8410	 0.7630
K	 0.8080	 0.7400
L	 0.8830	 0.7850
M	 0.8750	 0.7860
O	 0.7410	 0.7210
R	 0.1990	 0.6150
T	 0.9000	 0.7970
U	 0.7840	 0.7400
V	 0.8660	 0.7580
X	 0.8730	 0.7610
Y	 0.6680	 0.6940
Z	 0.5480	 0.6450
a	 0.9330	 0.8070
b	 0.9220	 0.7920
c	 0.9010	 0.7780
d	 0.9450	 0.8080
e	 0.8350	 0.7550
f	 0.8600	 0.7660
h	 0.9200	 0.7820
i	 0.8990	 0.7780
j	 0.8410	 0.7630
k	 0.8080	 0.7410
l	 0.9280	 0.8030
m	 0.8750	 0.7870
o	 0.7410	 0.7210
r	 0.1990	 0.6080



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Chain	Atom inclusion	Q-score
t	 0.9000	 0.7970
u	 0.7840	 0.7410
v	 0.8660	 0.7610
x	 0.8730	 0.7590
y	 0.6680	 0.6900
z	 0.5480	 0.6410