



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 09:25 AM EDT

PDB ID : 8TOW / pdb_00008tow
EMDB ID : EMD-41460
Title : Structure of a mutated photosystem II complex reveals perturbation of the oxygen-evolving complex
Authors : Flesher, D.A.; Liu, J.; Wang, J.; Gisriel, C.J.; Yang, K.R.; Batista, V.S.; Debus, R.J.; Brudvig, G.W.
Deposited on : 2023-08-04
Resolution : 2.14 Å(reported)

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:

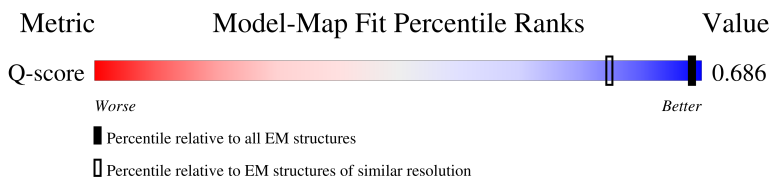
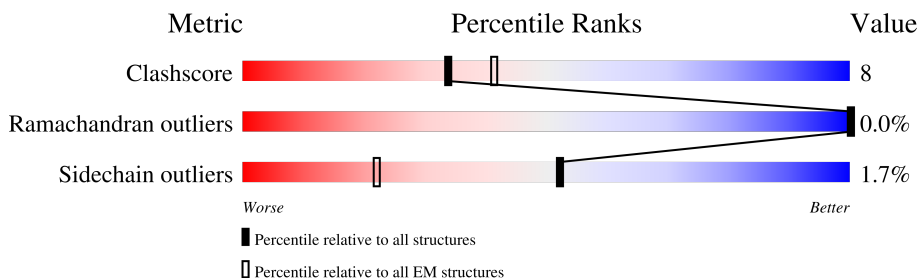
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.14 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2493 (1.66 - 2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	
1	a	360	
2	B	507	
2	b	507	

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Mol	Chain	Length	Quality of chain
3	C	460	
3	c	460	
4	D	352	
4	d	352	
5	E	81	
5	e	81	
6	F	44	
6	f	44	
7	H	64	
7	h	64	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	45	
10	k	45	
11	L	39	
11	l	39	
12	M	35	
12	m	35	
13	O	274	
13	o	274	
14	Q	149	
14	q	149	
15	R	39	

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Mol	Chain	Length	Quality of chain
15	r	39	
16	T	31	
16	t	31	
17	U	131	
17	u	131	
18	V	160	
18	v	160	
19	X	39	
19	x	39	
20	Y	39	
20	y	39	
21	Z	62	
21	z	62	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 54914 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	2	0
			2640	1728	431	466	15		
1	a	334	Total	C	N	O	S	2	0
			2640	1728	431	466	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLU	ASP	conflict	UNP P16033
a	170	GLU	ASP	conflict	UNP P16033

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	506	Total	C	N	O	S	0	0
			3958	2584	662	699	13		
2	b	506	Total	C	N	O	S	0	0
			3958	2584	662	699	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3493	2293	584	603	13		
3	c	450	Total	C	N	O	S	0	0
			3493	2293	584	603	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
			2726	1807	443	464	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	341	Total	C	N	O	S	0	0
			2726	1807	443	464	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	78	Total	C	N	O	S	0	0
			645	419	104	121	1		
5	e	78	Total	C	N	O	S	0	0
			645	419	104	121	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	35	Total	C	N	O	S	0	0
			279	189	46	43	1		
6	f	35	Total	C	N	O	S	0	0
			279	189	46	43	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
			494	328	79	85	2		
7	h	63	Total	C	N	O	S	0	0
			494	328	79	85	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			297	201	46	49	1		
8	i	37	Total	C	N	O	S	0	0
			297	201	46	49	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			279	188	43	46	2		
9	j	39	Total	C	N	O	S	0	0
			279	188	43	46	2		

- 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
			299	210	42	47		
10	k	37	Total	C	N	O	0	0
			299	210	42	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	39	Total	C	N	O	S	0	0
			316	204	54	57	1		
11	l	39	Total	C	N	O	S	0	0
			316	204	54	57	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			245	169	36	39	1		
12	m	31	Total	C	N	O	S	0	0
			245	169	36	39	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	243	Total	C	N	O	S	0	0
			1873	1186	305	379	3		
13	o	243	Total	C	N	O	S	0	0
			1873	1186	305	379	3		

- Molecule 14 is a protein called Sll1638 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	118	Total	C	N	O	S	0	0
			911	573	163	173	2		
14	q	118	Total	C	N	O	S	0	0
			911	573	163	173	2		

- Molecule 15 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	34	Total	C	N	O	0	0
			258	170	45	43		
15	r	34	Total	C	N	O	0	0
			258	170	45	43		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			241	163	36	40	2		
16	t	30	Total	C	N	O	S	0	0
			241	163	36	40	2		

- Molecule 17 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	95	Total	C	N	O	0	0
			740	461	123	156		
17	u	95	Total	C	N	O	0	0
			740	461	123	156		

- Molecule 18 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	135	Total	C	N	O	S	0	0
			1065	665	179	218	3		
18	v	135	Total	C	N	O	S	0	0
			1065	665	179	218	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	38	Total	C	N	O	S	0	0
			288	193	46	48	1		
19	x	38	Total	C	N	O	S	0	0
			288	193	46	48	1		

- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	32	Total	C	N	O	0	0
			242	165	37	40		

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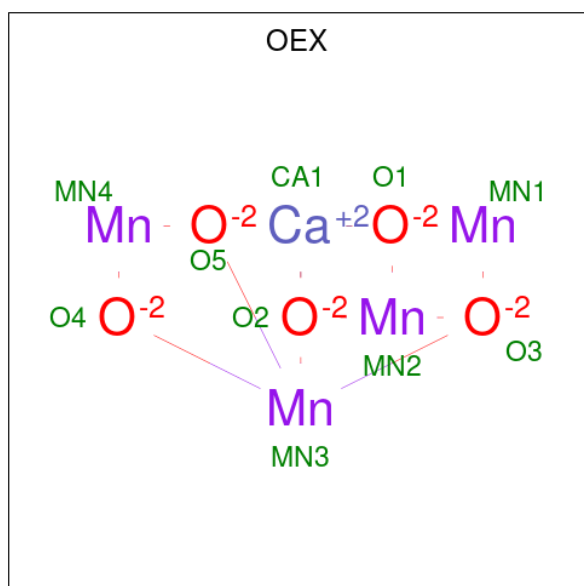
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Mol	Chain	Residues	Atoms				AltConf	Trace
20	y	32	Total	C	N	O	0	0
			242	165	37	40		

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Z	60	Total	C	N	O	S	0
			460	317	70	72	1	0
21	z	60	Total	C	N	O	S	0
			460	317	70	72	1	0

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Fe	0
			1	1	

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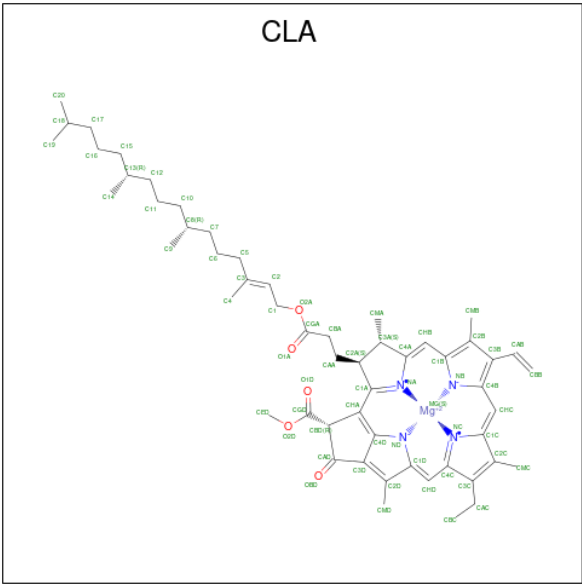
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Mol	Chain	Residues	Atoms		AltConf
23	a	1	Total	Fe	0
			1	1	

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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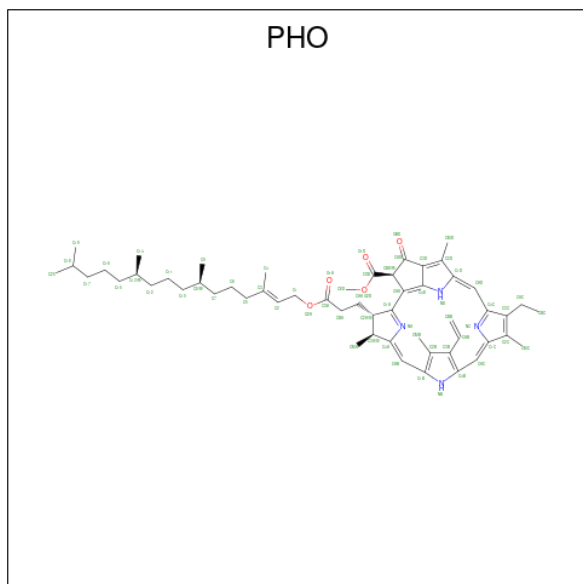
Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	d	1	Total 65	C 55	Mg 1	N 4	O 5	0

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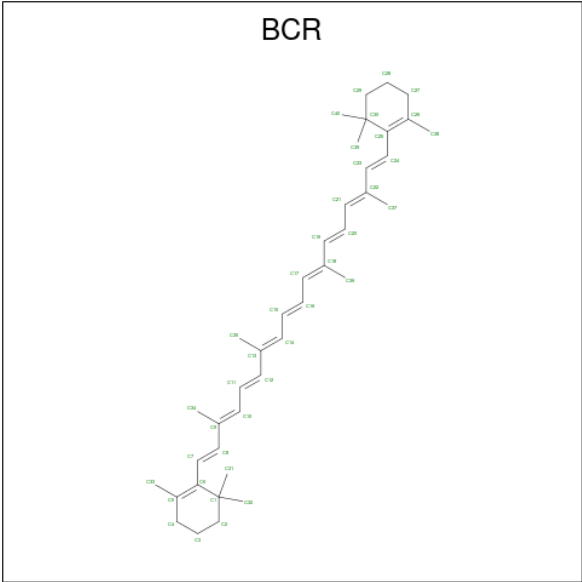
Mol	Chain	Residues	Atoms					AltConf
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



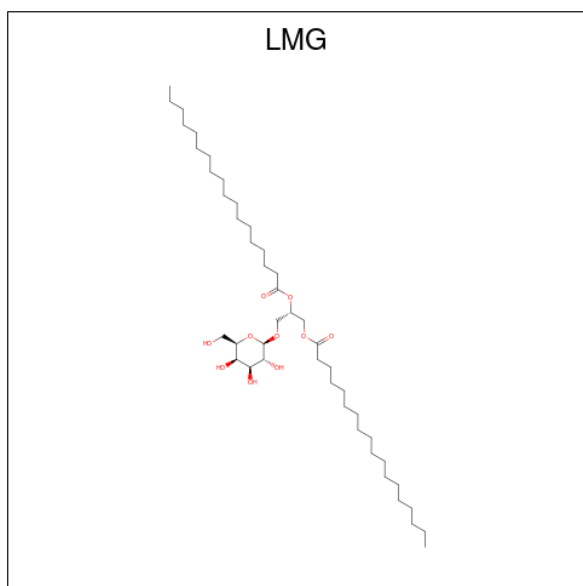
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	Z	1	Total C 40 40	0
27	a	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	c	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
27	f	1	Total C 40 40	0
27	k	1	Total C 40 40	0
27	k	1	Total C 40 40	0
27	z	1	Total C 40 40	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



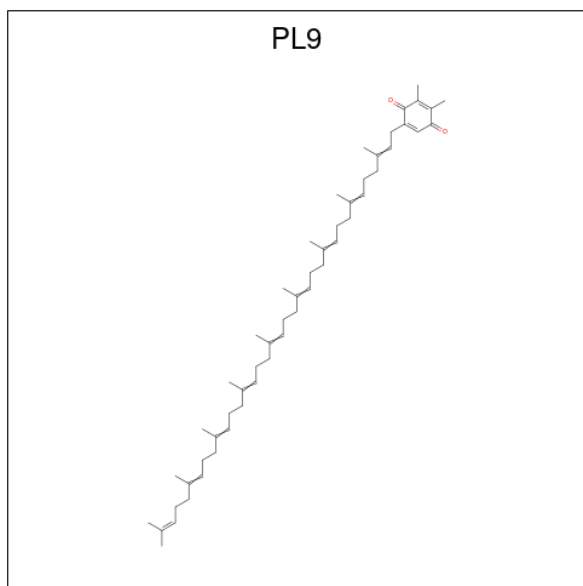
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C O 51 41 10	0
28	A	1	Total C O 36 26 10	0
28	B	1	Total C O 51 41 10	0
28	C	1	Total C O 51 41 10	0
28	C	1	Total C O 49 39 10	0
28	D	1	Total C O 44 34 10	0
28	H	1	Total C O 47 37 10	0

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Mol	Chain	Residues	Atoms			AltConf
28	a	1	Total	C	O	0
			51	41	10	
28	a	1	Total	C	O	0
			36	26	10	
28	b	1	Total	C	O	0
			51	41	10	
28	c	1	Total	C	O	0
			51	41	10	
28	c	1	Total	C	O	0
			49	39	10	
28	d	1	Total	C	O	0
			44	34	10	
28	h	1	Total	C	O	0
			47	37	10	

- Molecule 29 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).



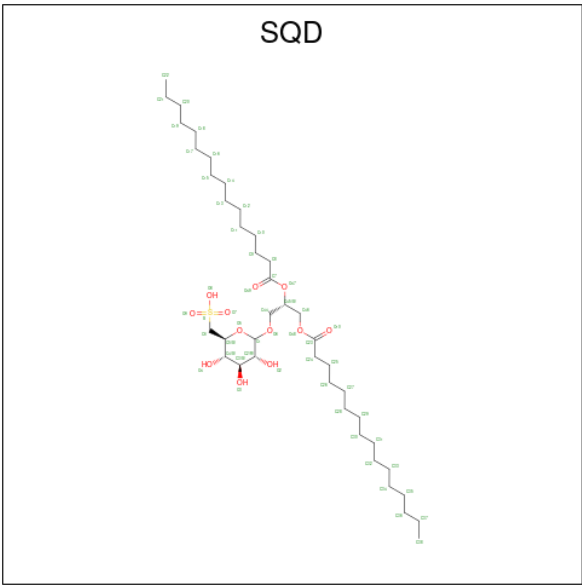
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			55	53	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			55	53	2	

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Mol	Chain	Residues	Atoms			AltConf
29	d	1	Total	C	O	0
			55	53	2	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



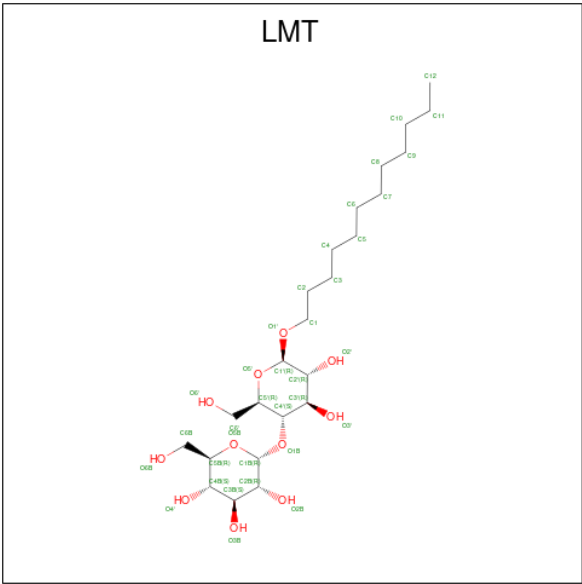
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	A	1	Total	C	O	S	0
			48	35	12	1	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	C	1	Total	C	O	S	0
			54	41	12	1	
30	F	1	Total	C	O	S	0
			34	21	12	1	
30	H	1	Total	C	O	S	0
			54	41	12	1	
30	K	1	Total	C	O		0
			41	32	9		
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			48	35	12	1	
30	b	1	Total	C	O	S	0
			54	41	12	1	

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Mol	Chain	Residues	Atoms				AltConf
30	c	1	Total	C	O	S	0
			54	41	12	1	
30	f	1	Total	C	O	S	0
			34	21	12	1	
30	h	1	Total	C	O	S	0
			54	41	12	1	
30	k	1	Total	C	O		0
			41	32	9		

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O		0
			35	24	11		
31	A	1	Total	C	O		0
			24	18	6		
31	B	1	Total	C	O		0
			35	24	11		
31	B	1	Total	C	O		0
			24	18	6		
31	B	1	Total	C	O		0
			35	24	11		
31	B	1	Total	C	O		0
			24	18	6		
31	B	1	Total	C	O		0
			35	24	11		

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Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			24	18	6	
31	C	1	Total	C	O	0
			35	24	11	
31	C	1	Total	C	O	0
			21	15	6	
31	D	1	Total	C	O	0
			24	18	6	
31	D	1	Total	C	O	0
			35	24	11	
31	D	1	Total	C	O	0
			35	24	11	
31	E	1	Total	C	O	0
			22	16	6	
31	E	1	Total	C	O	0
			35	24	11	
31	F	1	Total	C	O	0
			35	24	11	
31	H	1	Total	C	O	0
			24	18	6	
31	I	1	Total	C	O	0
			24	18	6	
31	I	1	Total	C	O	0
			24	18	6	
31	I	1	Total	C	O	0
			35	24	11	
31	I	1	Total	C	O	0
			22	16	6	
31	J	1	Total	C	O	0
			24	18	6	
31	K	1	Total	C	O	0
			35	24	11	
31	M	1	Total	C	O	0
			35	24	11	
31	M	1	Total	C	O	0
			24	18	6	
31	T	1	Total	C	O	0
			24	18	6	
31	X	1	Total	C	O	0
			24	18	6	
31	X	1	Total	C	O	0
			22	17	5	

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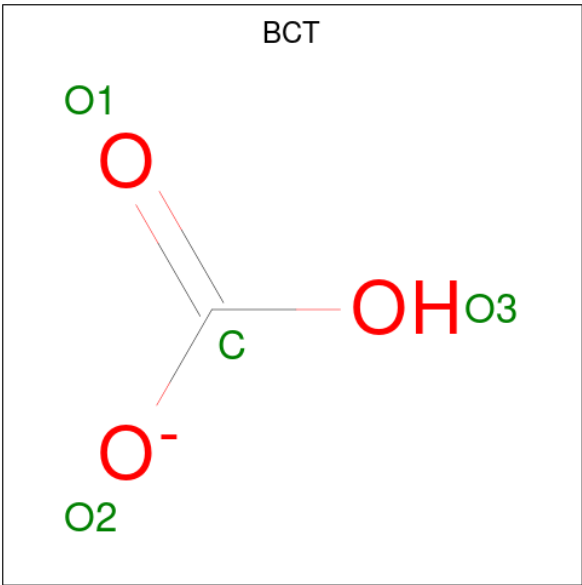
Mol	Chain	Residues	Atoms			AltConf
31	X	1	Total	C	O	0
			22	16	6	
31	X	1	Total	C	O	0
			19	13	6	
31	X	1	Total	C	O	0
			19	13	6	
31	Y	1	Total	C	O	0
			21	15	6	
31	a	1	Total	C	O	0
			35	24	11	
31	a	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	b	1	Total	C	O	0
			24	18	6	
31	b	1	Total	C	O	0
			35	24	11	
31	c	1	Total	C	O	0
			24	18	6	
31	c	1	Total	C	O	0
			35	24	11	
31	c	1	Total	C	O	0
			21	15	6	
31	d	1	Total	C	O	0
			24	18	6	
31	d	1	Total	C	O	0
			35	24	11	
31	d	1	Total	C	O	0
			35	24	11	
31	e	1	Total	C	O	0
			22	16	6	
31	e	1	Total	C	O	0
			35	24	11	
31	f	1	Total	C	O	0
			35	24	11	
31	h	1	Total	C	O	0
			24	18	6	

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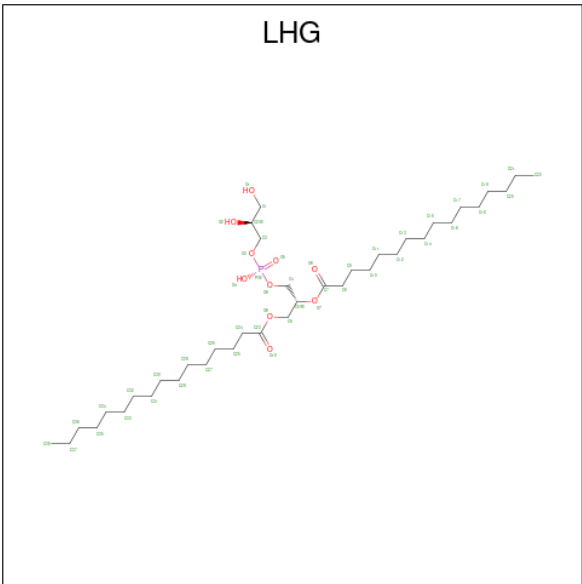
Mol	Chain	Residues	Atoms			AltConf
31	i	1	Total	C	O	0
			24	18	6	
31	i	1	Total	C	O	0
			24	18	6	
31	i	1	Total	C	O	0
			35	24	11	
31	i	1	Total	C	O	0
			22	16	6	
31	j	1	Total	C	O	0
			24	18	6	
31	k	1	Total	C	O	0
			35	24	11	
31	m	1	Total	C	O	0
			35	24	11	
31	m	1	Total	C	O	0
			24	18	6	
31	t	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			24	18	6	
31	x	1	Total	C	O	0
			22	17	5	
31	x	1	Total	C	O	0
			22	16	6	
31	x	1	Total	C	O	0
			19	13	6	
31	x	1	Total	C	O	0
			19	13	6	
31	y	1	Total	C	O	0
			21	15	6	

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



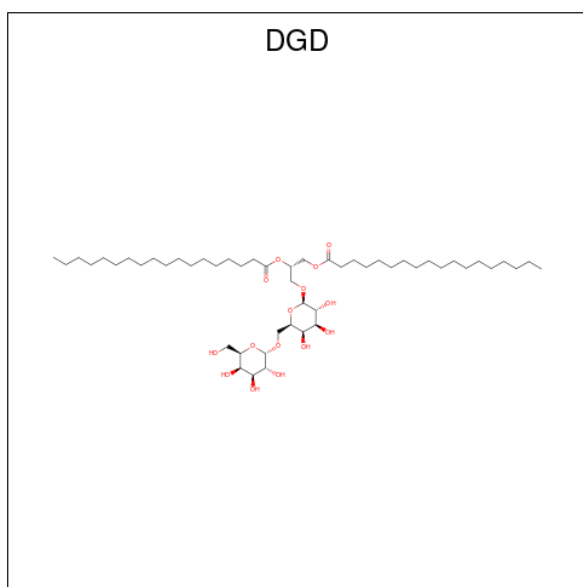
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	P	0
			49	38	10	1	

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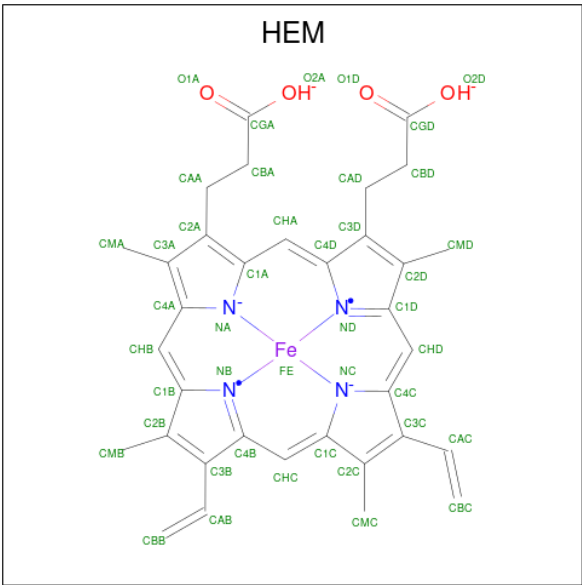
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	E	1	Total	C	O	P	0
			40	29	10	1	
33	Z	1	Total	C	O	P	0
			36	27	8	1	
33	b	1	Total	C	O	P	0
			49	38	10	1	
33	b	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	e	1	Total	C	O	P	0
			40	29	10	1	
33	z	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



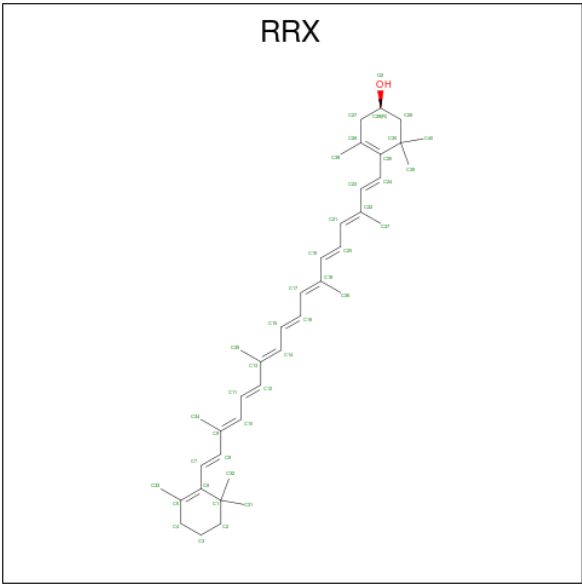
Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	C	1	Total	C	O	0
			62	47	15	
34	H	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	c	1	Total	C	O	0
			62	47	15	
34	h	1	Total	C	O	0
			62	47	15	

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 36 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



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

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
37	K	1	Total	Ca	0
			1	1	
37	U	1	Total	Ca	0
			1	1	
37	V	1	Total	Ca	0
			1	1	
37	k	1	Total	Ca	0
			1	1	
37	u	1	Total	Ca	0
			1	1	
37	v	1	Total	Ca	0
			1	1	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	A	127	Total	O	0
			127	127	
38	B	127	Total	O	0
			127	127	
38	C	107	Total	O	0
			107	107	
38	D	132	Total	O	0
			132	132	
38	E	8	Total	O	0
			8	8	
38	F	4	Total	O	0
			4	4	
38	H	17	Total	O	0
			17	17	
38	I	1	Total	O	0
			1	1	
38	J	2	Total	O	0
			2	2	
38	L	14	Total	O	0
			14	14	

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Mol	Chain	Residues	Atoms		AltConf
38	M	6	Total 6	O 6	0
38	O	37	Total 37	O 37	0
38	T	12	Total 12	O 12	0
38	U	21	Total 21	O 21	0
38	V	17	Total 17	O 17	0
38	X	3	Total 3	O 3	0
38	a	127	Total 127	O 127	0
38	b	127	Total 127	O 127	0
38	c	107	Total 107	O 107	0
38	d	132	Total 132	O 132	0
38	e	8	Total 8	O 8	0
38	f	4	Total 4	O 4	0
38	h	17	Total 17	O 17	0
38	i	1	Total 1	O 1	0
38	j	2	Total 2	O 2	0
38	l	14	Total 14	O 14	0
38	m	6	Total 6	O 6	0
38	o	37	Total 37	O 37	0
38	t	12	Total 12	O 12	0
38	u	21	Total 21	O 21	0
38	v	17	Total 17	O 17	0

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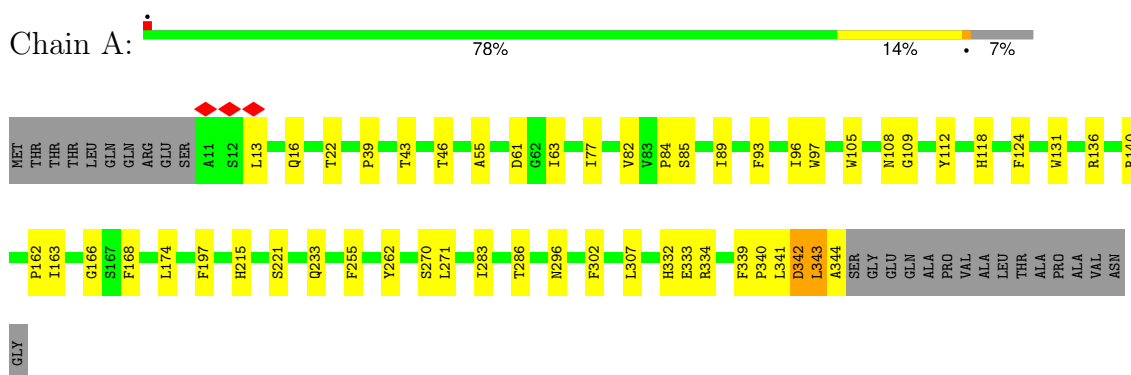
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Mol	Chain	Residues	Atoms		AltConf
38	x	3	Total	O	0
			3	3	

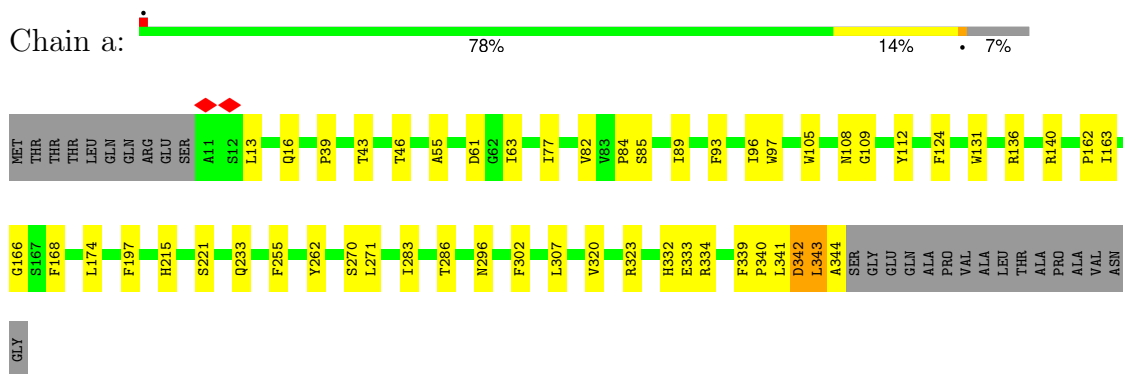
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

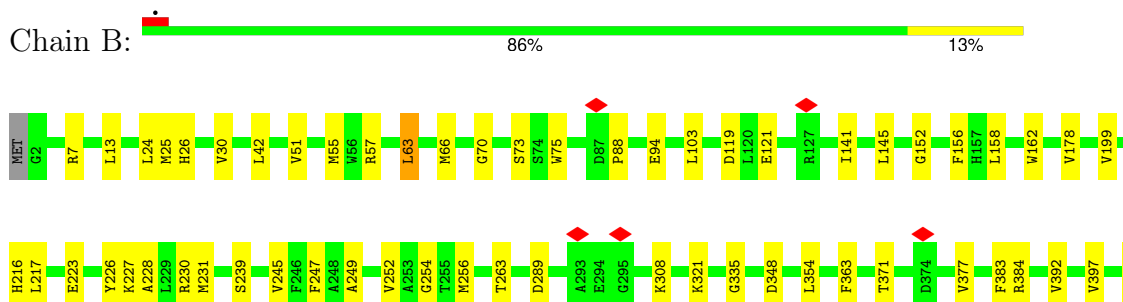
- Molecule 1: Photosystem II protein D1 2

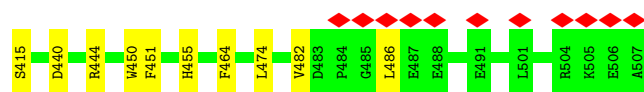


- Molecule 1: Photosystem II protein D1 2



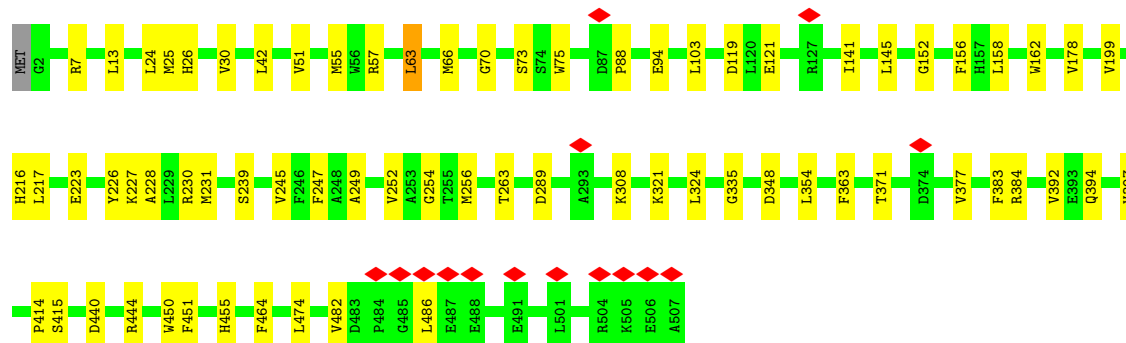
- Molecule 2: Photosystem II CP47 reaction center protein





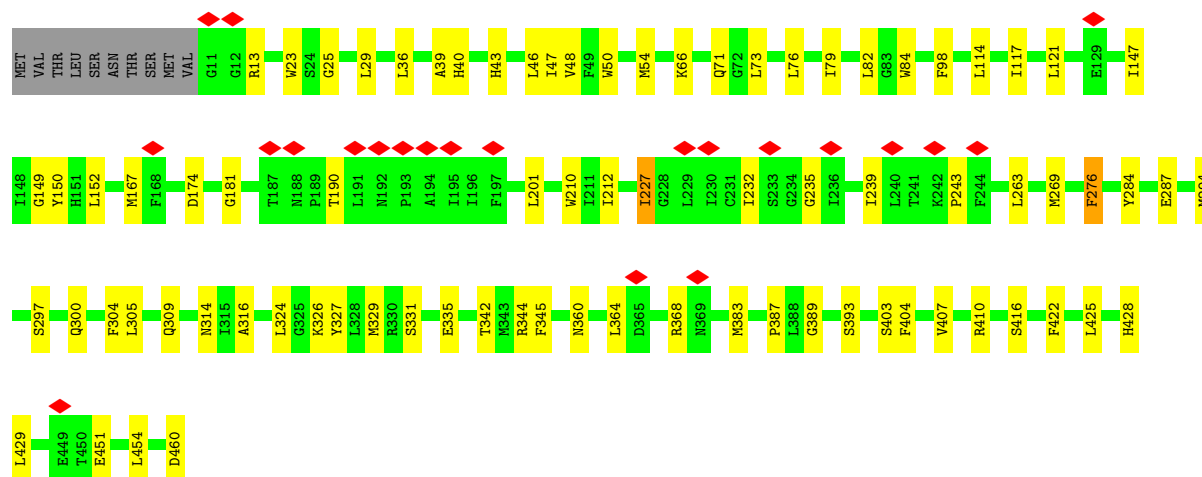
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 86% 14%



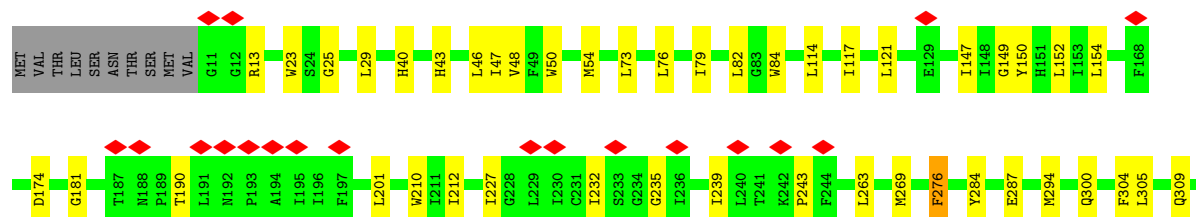
• Molecule 3: Photosystem II CP43 reaction center protein

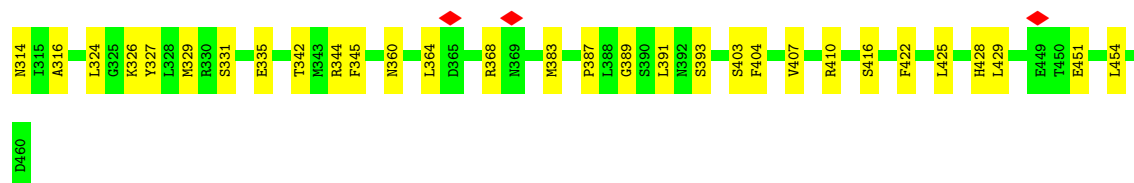
Chain C: 5% 80% 17%



• Molecule 3: Photosystem II CP43 reaction center protein

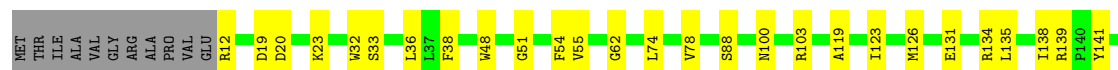
Chain c: 5% 82% 16%





• Molecule 4: Photosystem II D2 protein

Chain D: 83% 13% .



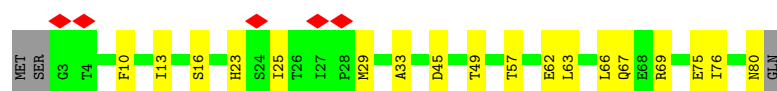
• Molecule 4: Photosystem II D2 protein

Chain d: 84% 12% .



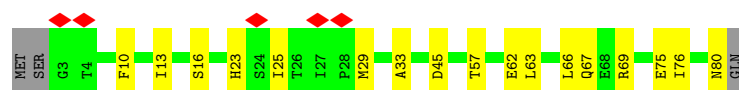
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 6% 74% 22% .



• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 6% 75% 21% .

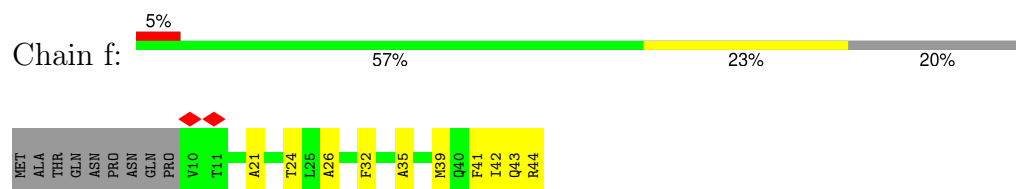


• Molecule 6: Cytochrome b559 subunit beta

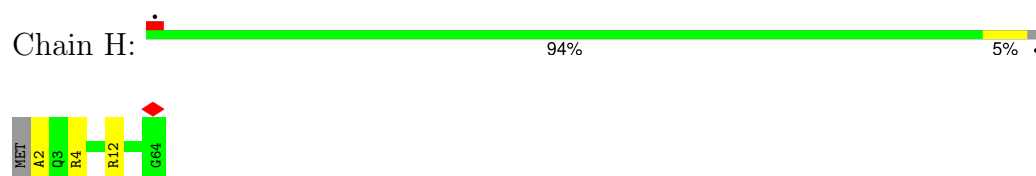
Chain F: 5% 57% 23% 20% .



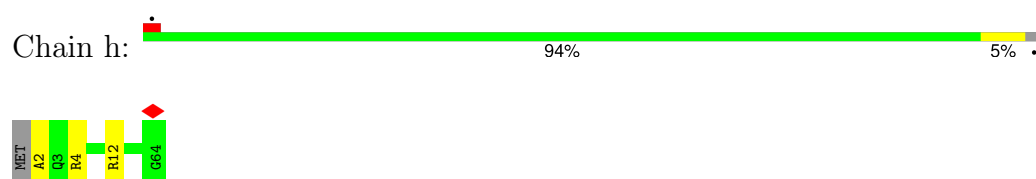
- Molecule 6: Cytochrome b559 subunit beta



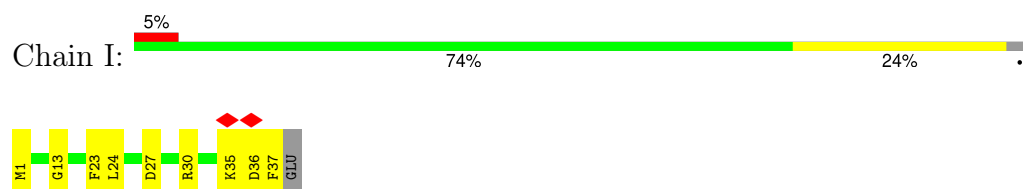
- Molecule 7: Photosystem II reaction center protein H



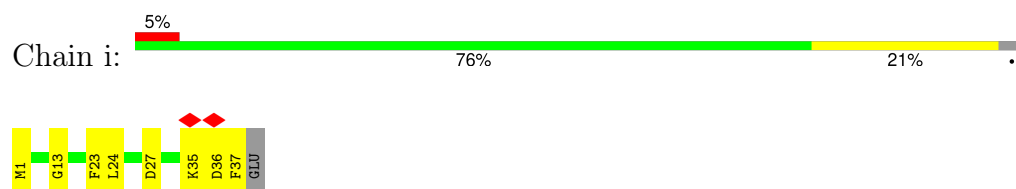
- Molecule 7: Photosystem II reaction center protein H



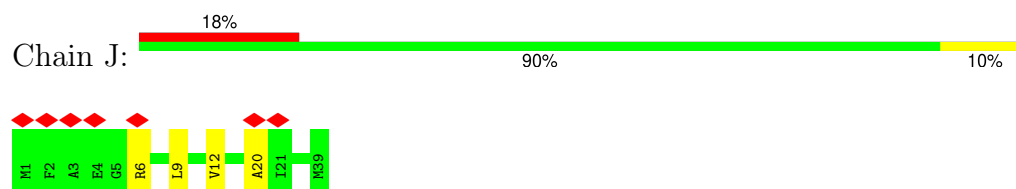
- Molecule 8: Photosystem II reaction center protein I



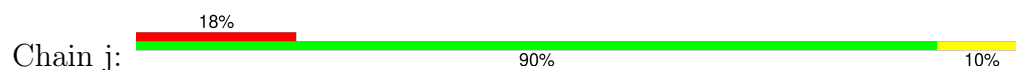
- Molecule 8: Photosystem II reaction center protein I

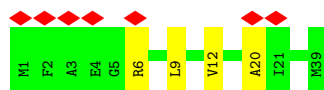


- Molecule 9: Photosystem II reaction center protein J

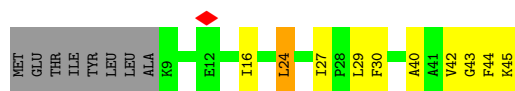


- Molecule 9: Photosystem II reaction center protein J

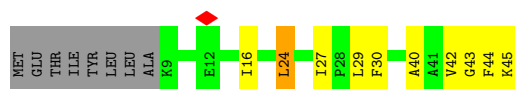




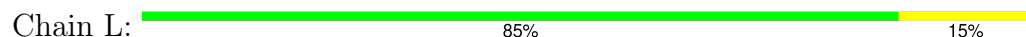
- Molecule 10: Photosystem II reaction center protein K



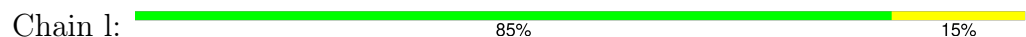
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



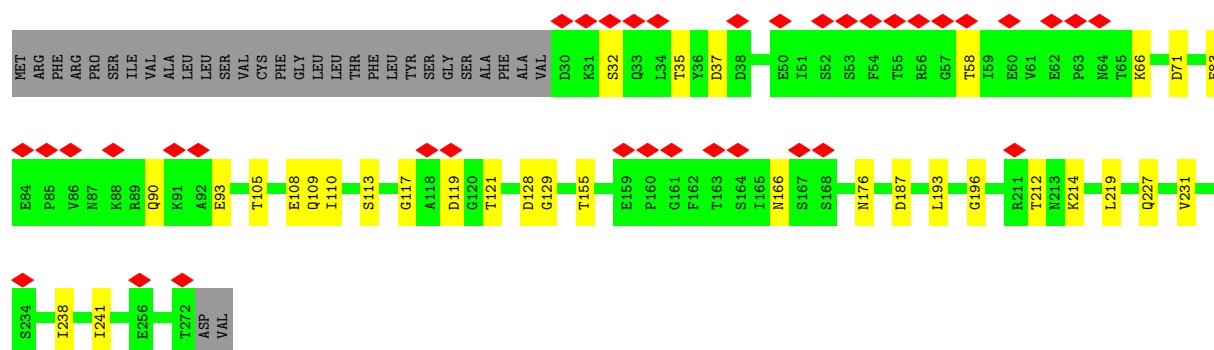
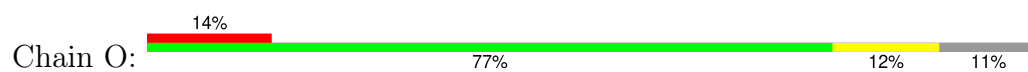
- Molecule 12: Photosystem II reaction center protein M



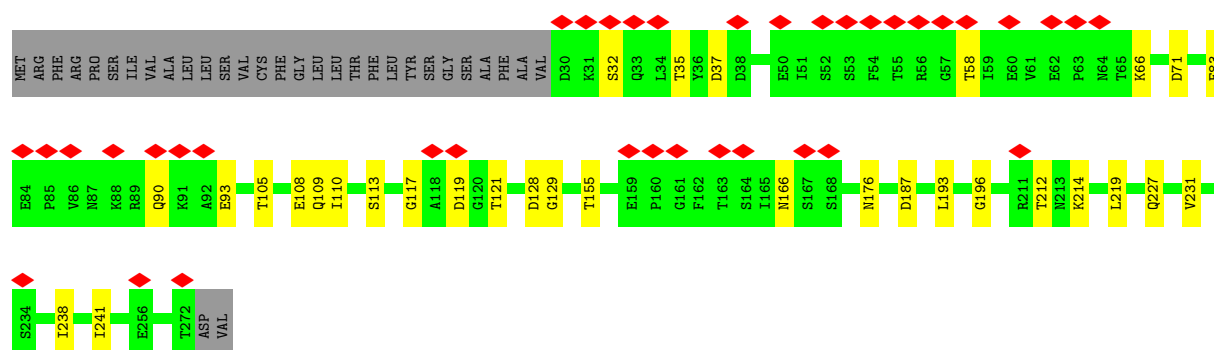
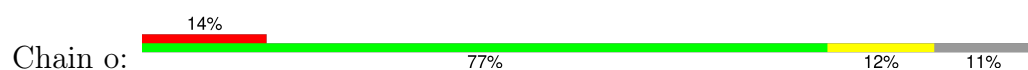
- Molecule 12: Photosystem II reaction center protein M



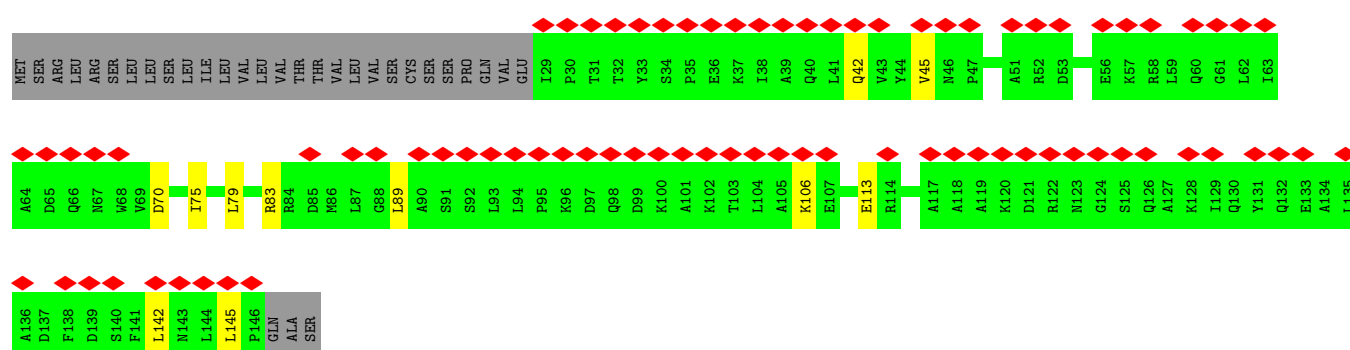
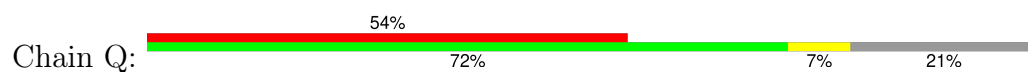
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



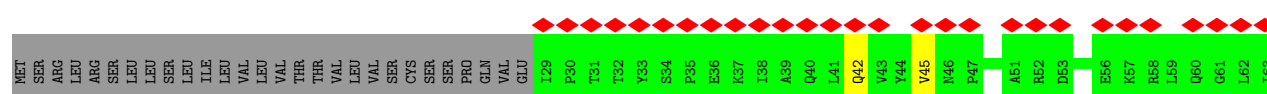
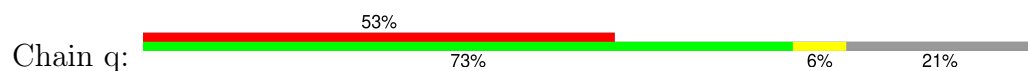
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

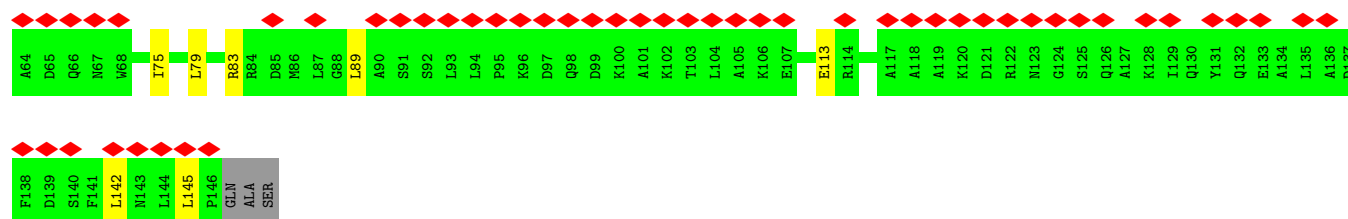


• Molecule 14: Sll1638 protein

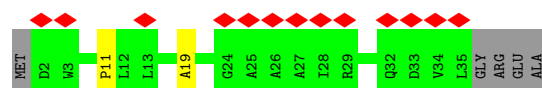
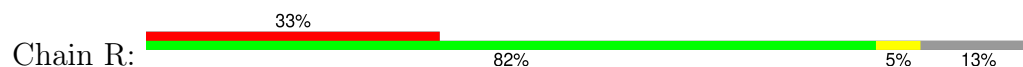


• Molecule 14: Sll1638 protein

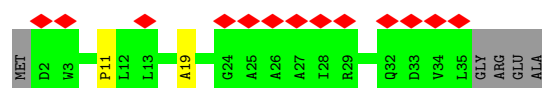
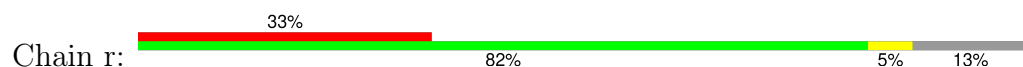




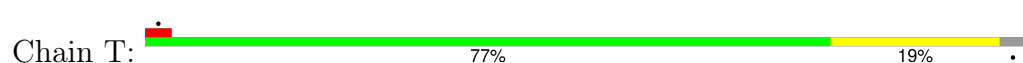
• Molecule 15: Photosystem II protein Y



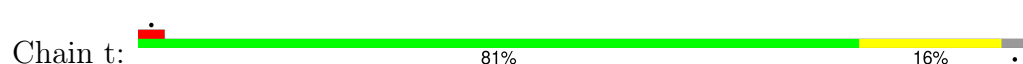
• Molecule 15: Photosystem II protein Y



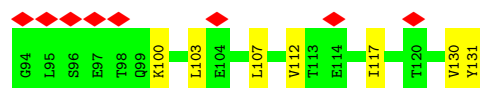
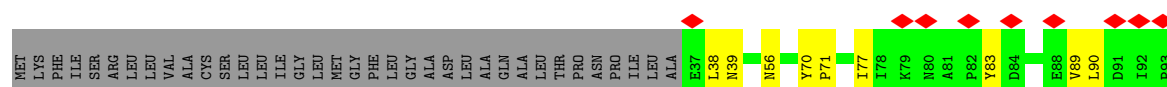
• Molecule 16: Photosystem II reaction center protein T



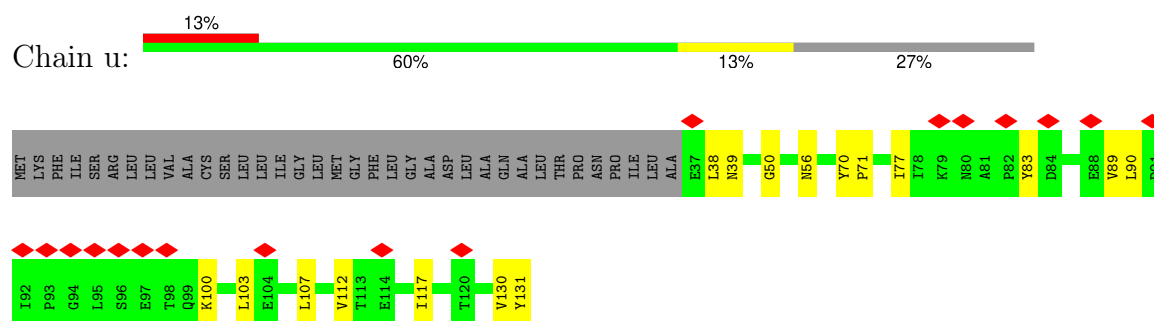
• Molecule 16: Photosystem II reaction center protein T



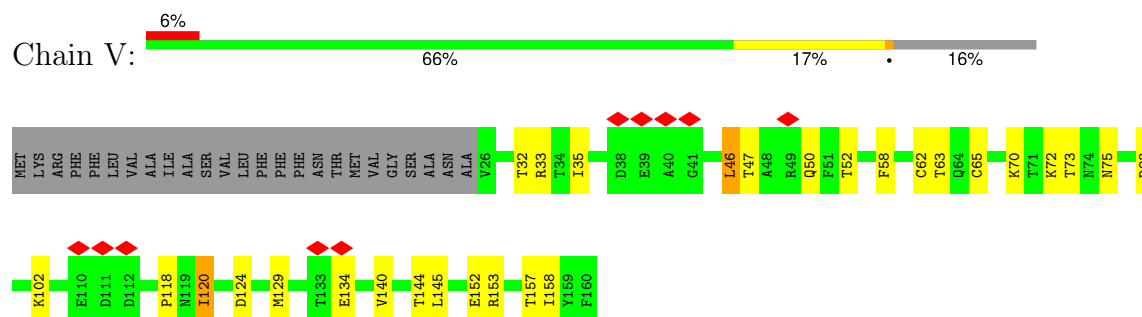
• Molecule 17: Photosystem II 12 kDa extrinsic protein



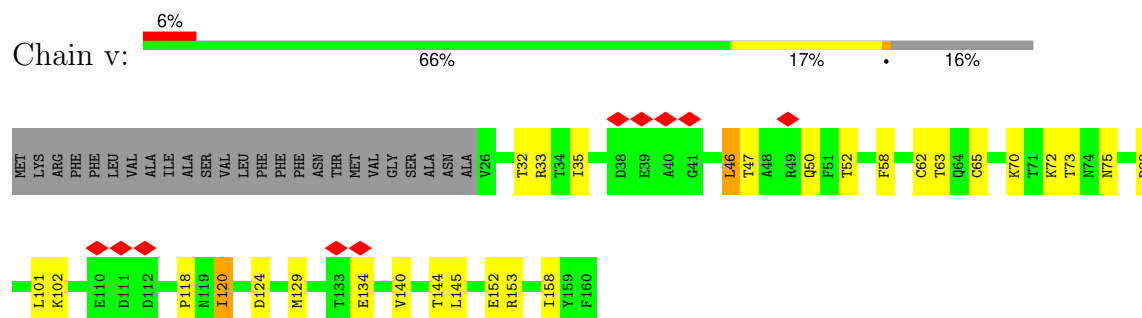
• Molecule 17: Photosystem II 12 kDa extrinsic protein



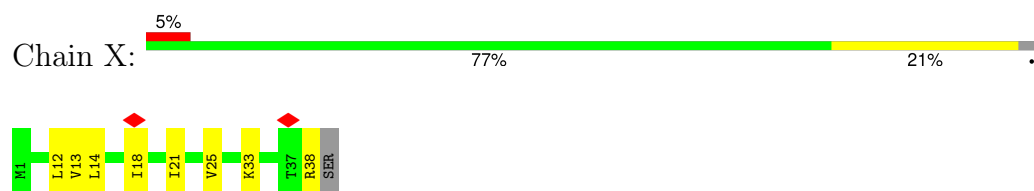
- Molecule 18: Cytochrome c-550



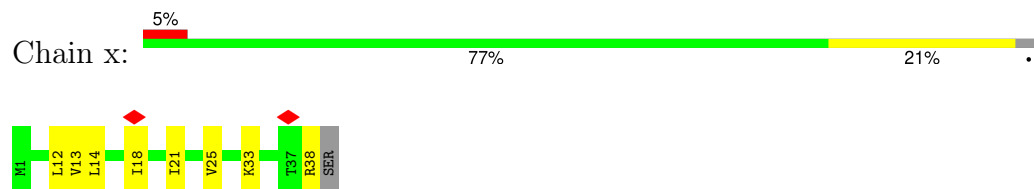
- Molecule 18: Cytochrome c-550



- Molecule 19: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center X protein



- Molecule 20: Photosystem II reaction center protein Ycf12

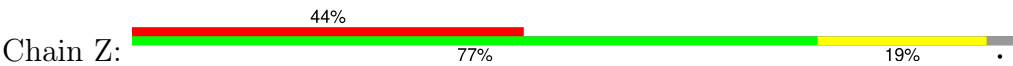




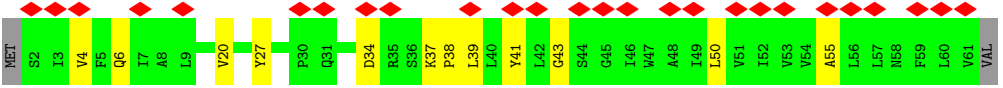
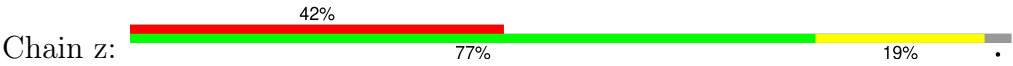
• Molecule 20: Photosystem II reaction center protein Ycf12



• Molecule 21: Photosystem II reaction center protein Z



• Molecule 21: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129229	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00432	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	0/2724	0.69	1/3710 (0.0%)
1	a	0.45	0/2724	0.69	1/3710 (0.0%)
2	B	0.36	0/4091	0.58	0/5568
2	b	0.36	0/4091	0.58	0/5568
3	C	0.40	0/3608	0.66	0/4912
3	c	0.40	0/3608	0.66	0/4912
4	D	0.36	0/2823	0.60	1/3843 (0.0%)
4	d	0.36	0/2823	0.60	1/3843 (0.0%)
5	E	0.40	0/664	0.73	2/906 (0.2%)
5	e	0.40	0/664	0.73	2/906 (0.2%)
6	F	0.41	0/288	0.70	0/393
6	f	0.41	0/288	0.70	0/393
7	H	0.29	0/506	0.52	0/687
7	h	0.29	0/506	0.52	0/687
8	I	0.31	0/294	0.64	0/397
8	i	0.31	0/294	0.64	0/397
9	J	0.22	0/278	0.46	0/375
9	j	0.22	0/278	0.46	0/375
10	K	0.40	0/310	0.84	1/424 (0.2%)
10	k	0.40	0/310	0.84	1/424 (0.2%)
11	L	0.31	0/322	0.53	0/435
11	l	0.31	0/322	0.53	0/435
12	M	0.33	0/239	0.67	0/325
12	m	0.33	0/239	0.67	0/325
13	O	0.27	0/1911	0.59	0/2590
13	o	0.27	0/1911	0.59	0/2590
14	Q	0.25	0/925	0.65	0/1250
14	q	0.25	0/925	0.65	0/1250
15	R	0.27	0/262	0.61	0/361
15	r	0.27	0/262	0.61	0/361
16	T	0.30	0/236	0.55	0/321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.30	0/236	0.55	0/321
17	U	0.26	0/751	0.54	0/1018
17	u	0.26	0/751	0.54	0/1018
18	V	0.32	0/1086	0.58	0/1476
18	v	0.32	0/1086	0.58	0/1476
19	X	0.28	0/293	0.60	0/399
19	x	0.28	0/293	0.60	0/399
20	Y	0.30	0/247	0.56	0/335
20	y	0.30	0/247	0.56	0/335
21	Z	0.32	0/472	0.62	0/649
21	z	0.32	0/472	0.62	0/649
All	All	0.36	0/44660	0.62	10/60748 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	a	0	2
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	24	LEU	N-CA-C	6.18	122.10	113.57
10	k	24	LEU	N-CA-C	6.16	122.08	113.57
4	D	214	HIS	CA-CB-CG	-5.74	108.06	113.80
4	d	214	HIS	CA-CB-CG	-5.74	108.06	113.80
5	e	29	MET	CB-CG-SD	5.49	129.16	112.70
5	E	29	MET	CB-CG-SD	5.48	129.15	112.70
1	a	342	ASP	CA-C-O	-5.34	116.23	122.37
1	A	342	ASP	CA-C-O	-5.31	116.27	122.37
5	E	67	GLN	N-CA-C	-5.06	108.13	114.56
5	e	67	GLN	N-CA-C	-5.03	108.17	114.56

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	ASP	Mainchain
1	a	342	ASP	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2640	0	2535	49	0
1	a	2640	0	2535	47	0
2	B	3958	0	3799	54	0
2	b	3958	0	3799	55	0
3	C	3493	0	3417	65	0
3	c	3493	0	3417	58	0
4	D	2726	0	2617	38	0
4	d	2726	0	2617	36	0
5	E	645	0	616	15	0
5	e	645	0	616	14	0
6	F	279	0	282	12	0
6	f	279	0	282	12	0
7	H	494	0	508	3	0
7	h	494	0	508	3	0
8	I	297	0	313	6	0
8	i	297	0	313	5	0
9	J	279	0	282	4	0
9	j	279	0	282	4	0
10	K	299	0	308	10	0
10	k	299	0	308	9	0
11	L	316	0	321	8	0
11	l	316	0	321	8	0
12	M	245	0	270	7	0
12	m	245	0	270	7	0
13	O	1873	0	1829	17	0
13	o	1873	0	1829	17	0
14	Q	911	0	903	7	0
14	q	911	0	903	5	0
15	R	258	0	276	2	0
15	r	258	0	276	2	0
16	T	241	0	254	5	0
16	t	241	0	254	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	U	740	0	718	10	0
17	u	740	0	718	11	0
18	V	1065	0	1021	21	0
18	v	1065	0	1021	22	0
19	X	288	0	320	8	0
19	x	288	0	320	8	0
20	Y	242	0	255	6	0
20	y	242	0	255	6	0
21	Z	460	0	491	9	0
21	z	460	0	491	9	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	1	0
24	a	2	0	0	1	0
25	A	190	0	203	13	0
25	B	1010	0	1084	51	0
25	C	820	0	878	46	0
25	D	195	0	216	13	0
25	a	190	0	203	10	0
25	b	1010	0	1084	48	0
25	c	820	0	878	45	0
25	d	195	0	216	15	0
26	A	64	0	74	5	0
26	D	64	0	74	1	0
26	a	64	0	74	6	0
26	d	64	0	74	1	0
27	A	40	0	49	4	0
27	B	120	0	147	7	0
27	C	40	0	49	4	0
27	F	40	0	49	3	0
27	K	80	0	98	9	0
27	Z	40	0	49	2	0
27	a	40	0	49	4	0
27	b	120	0	147	6	0
27	c	40	0	49	4	0
27	f	40	0	49	4	0
27	k	80	0	98	9	0
27	z	40	0	49	3	0
28	A	87	0	114	5	0
28	B	51	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	C	100	0	140	7	0
28	D	44	0	56	1	0
28	H	47	0	64	0	0
28	a	87	0	114	6	0
28	b	51	0	72	1	0
28	c	100	0	140	6	0
28	d	44	0	56	0	0
28	h	47	0	64	0	0
29	A	55	0	80	8	0
29	D	55	0	80	2	0
29	a	55	0	80	8	0
29	d	55	0	80	2	0
30	A	102	0	136	5	0
30	B	54	0	78	2	0
30	C	54	0	77	4	0
30	F	34	0	31	0	0
30	H	54	0	77	3	0
30	K	41	0	51	4	0
30	a	102	0	136	4	0
30	b	54	0	78	2	0
30	c	54	0	77	4	0
30	f	34	0	31	0	0
30	h	54	0	77	2	0
30	k	41	0	51	4	0
31	A	59	0	78	0	0
31	B	153	0	203	5	0
31	C	80	0	106	1	0
31	D	94	0	123	4	0
31	E	57	0	74	4	0
31	F	35	0	44	2	0
31	H	24	0	34	1	0
31	I	105	0	140	5	0
31	J	24	0	34	0	0
31	K	35	0	45	8	0
31	M	59	0	80	8	0
31	T	24	0	34	1	0
31	X	106	0	129	5	0
31	Y	21	0	26	2	0
31	a	59	0	78	0	0
31	b	153	0	203	4	0
31	c	80	0	106	1	0
31	d	94	0	123	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	e	57	0	74	4	0
31	f	35	0	44	2	0
31	h	24	0	34	2	0
31	i	105	0	140	3	0
31	j	24	0	34	0	0
31	k	35	0	45	8	0
31	m	59	0	80	9	0
31	t	24	0	34	1	0
31	x	106	0	129	5	0
31	y	21	0	25	2	0
32	A	4	0	1	0	0
32	a	4	0	1	0	0
33	B	98	0	148	12	0
33	D	147	0	222	14	0
33	E	40	0	53	2	0
33	Z	36	0	48	1	0
33	b	98	0	148	11	0
33	d	147	0	222	15	0
33	e	40	0	53	2	0
33	z	36	0	48	1	0
34	C	186	0	246	18	0
34	H	62	0	82	4	0
34	c	186	0	246	15	0
34	h	62	0	82	4	0
35	E	43	0	30	7	0
35	V	43	0	30	3	0
35	e	43	0	30	7	0
35	v	43	0	30	3	0
36	H	41	0	56	2	0
36	h	41	0	56	2	0
37	K	1	0	0	0	0
37	U	1	0	0	0	0
37	V	1	0	0	0	0
37	k	1	0	0	0	0
37	u	1	0	0	0	0
37	v	1	0	0	0	0
38	A	127	0	0	1	0
38	B	127	0	0	0	0
38	C	107	0	0	2	0
38	D	132	0	0	9	0
38	E	8	0	0	0	0
38	F	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	17	0	0	0	0
38	I	1	0	0	0	0
38	J	2	0	0	0	0
38	L	14	0	0	0	0
38	M	6	0	0	0	0
38	O	37	0	0	0	0
38	T	12	0	0	0	0
38	U	21	0	0	2	0
38	V	17	0	0	3	0
38	X	3	0	0	0	0
38	a	127	0	0	0	0
38	b	127	0	0	0	0
38	c	107	0	0	2	0
38	d	132	0	0	8	0
38	e	8	0	0	0	0
38	f	4	0	0	1	0
38	h	17	0	0	0	0
38	i	1	0	0	0	0
38	j	2	0	0	0	0
38	l	14	0	0	0	0
38	m	6	0	0	0	0
38	o	37	0	0	0	0
38	t	12	0	0	0	0
38	u	21	0	0	2	0
38	v	17	0	0	3	0
38	x	3	0	0	0	0
All	All	54914	0	54853	889	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (889) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:102:LYS:HG2	18:V:120:ILE:HD11	1.52	0.91
18:v:102:LYS:HG2	18:v:120:ILE:HD11	1.52	0.89
27:B:617:BCR:H383	30:B:620:SQD:H101	1.61	0.81
27:b:617:BCR:H383	30:b:620:SQD:H101	1.61	0.81
3:C:263:LEU:HD21	25:C:509:CLA:HAB	1.65	0.78
3:c:263:LEU:HD21	25:c:509:CLA:HAB	1.65	0.78
1:A:140:ARG:HH22	33:D:408:LHG:HC41	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:140:ARG:HH22	33:d:408:LHG:HC41	1.49	0.77
3:c:326:LYS:HE2	38:u:303:HOH:O	1.85	0.77
4:d:192:THR:HG23	25:d:403:CLA:HBC2	1.68	0.76
5:E:10:PHE:HE1	35:E:104:HEM:HBD2	1.52	0.75
5:e:10:PHE:HE1	35:e:104:HEM:HBD2	1.52	0.75
4:D:192:THR:HG23	25:D:403:CLA:HBC2	1.68	0.74
3:C:326:LYS:HE2	38:U:303:HOH:O	1.85	0.74
33:d:407:LHG:H282	16:t:17:LEU:HD22	1.69	0.74
27:F:101:BCR:H401	9:J:20:ALA:HB1	1.70	0.73
18:v:62:CYS:SG	35:v:201:HEM:CAB	2.77	0.73
27:f:101:BCR:H401	9:j:20:ALA:HB1	1.70	0.73
33:D:407:LHG:H282	16:T:17:LEU:HD22	1.69	0.72
18:V:62:CYS:SG	35:V:201:HEM:CAB	2.77	0.72
25:c:504:CLA:H172	25:c:511:CLA:HBB2	1.72	0.72
2:B:141:ILE:HG13	2:B:217:LEU:HD21	1.72	0.71
2:b:141:ILE:HG13	2:b:217:LEU:HD21	1.72	0.71
18:v:73:THR:HG21	38:v:311:HOH:O	1.91	0.71
25:C:504:CLA:H172	25:C:511:CLA:HBB2	1.72	0.71
4:D:23:LYS:HD2	4:D:135:LEU:HD11	1.73	0.70
18:V:73:THR:HG21	38:V:311:HOH:O	1.91	0.70
4:d:23:LYS:HD2	4:d:135:LEU:HD11	1.73	0.70
5:e:10:PHE:CE1	35:e:104:HEM:HBD2	2.26	0.70
25:c:506:CLA:HBB1	25:c:506:CLA:H71	1.74	0.70
5:E:10:PHE:CE1	35:E:104:HEM:HBD2	2.26	0.69
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.75	0.68
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.75	0.68
25:C:506:CLA:HBB1	25:C:506:CLA:H71	1.74	0.68
14:Q:142:LEU:HA	14:Q:145:LEU:HD12	1.75	0.68
14:q:142:LEU:HA	14:q:145:LEU:HD12	1.75	0.67
28:C:519:LMG:H341	10:K:29:LEU:HD21	1.76	0.67
4:D:352:LEU:HB2	38:D:547:HOH:O	1.94	0.67
1:A:307:LEU:HB2	6:F:44:ARG:HD2	1.78	0.66
28:c:519:LMG:H341	10:k:29:LEU:HD21	1.76	0.66
25:C:503:CLA:HBB2	25:C:511:CLA:H151	1.75	0.66
25:c:503:CLA:HBB2	25:c:511:CLA:H151	1.75	0.66
1:a:307:LEU:HB2	6:f:44:ARG:HD2	1.77	0.66
4:d:352:LEU:HB2	38:d:547:HOH:O	1.94	0.66
35:V:201:HEM:HMC1	35:V:201:HEM:HBC2	1.79	0.65
3:c:309:GLN:HE22	3:c:368:ARG:HA	1.61	0.65
18:v:65:CYS:SG	35:v:201:HEM:CAC	2.85	0.65
18:V:65:CYS:SG	35:V:201:HEM:CAC	2.85	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:LEU:HD21	25:C:507:CLA:HAB	1.79	0.65
3:c:152:LEU:HD21	25:c:507:CLA:HAB	1.79	0.64
2:b:121:GLU:HG3	7:h:4:ARG:HG2	1.78	0.64
6:f:44:ARG:HD3	38:f:202:HOH:O	1.97	0.64
3:C:309:GLN:HE22	3:C:368:ARG:HA	1.61	0.64
35:v:201:HEM:HMC1	35:v:201:HEM:HBC2	1.79	0.64
2:B:121:GLU:HG3	7:H:4:ARG:HG2	1.78	0.63
24:a:403:CL:CL	38:d:590:HOH:O	2.53	0.63
6:F:44:ARG:HD3	38:F:202:HOH:O	1.97	0.62
24:A:403:CL:CL	38:D:590:HOH:O	2.53	0.62
1:a:341:LEU:HD11	18:v:72:LYS:HB3	1.80	0.62
31:B:623:LMT:H2'	31:D:410:LMT:H3'	1.82	0.62
25:d:404:CLA:H43	31:d:412:LMT:H112	1.82	0.62
29:a:411:PL9:H362	4:d:38:PHE:HB3	1.82	0.62
25:D:404:CLA:H43	31:D:412:LMT:H112	1.82	0.62
2:B:25:MET:HG2	27:B:617:BCR:H23C	1.82	0.61
25:B:602:CLA:H12	34:H:104:DGD:HB41	1.82	0.61
1:A:341:LEU:HD11	18:V:72:LYS:HB3	1.80	0.61
31:b:623:LMT:H2'	31:d:410:LMT:H3'	1.82	0.61
2:B:230:ARG:NH2	33:B:627:LHG:O5	2.21	0.61
2:B:464:PHE:HD2	25:B:611:CLA:HAC2	1.65	0.61
30:a:412:SQD:H111	30:a:412:SQD:H462	1.83	0.61
29:A:411:PL9:H362	4:D:38:PHE:HB3	1.82	0.61
30:A:412:SQD:H111	30:A:412:SQD:H462	1.83	0.61
25:B:608:CLA:H172	25:B:609:CLA:H192	1.82	0.61
13:O:108:GLU:HG3	13:O:109:GLN:HG3	1.83	0.61
5:E:66:LEU:HD23	5:E:75:GLU:HG2	1.83	0.61
13:o:108:GLU:HG3	13:o:109:GLN:HG3	1.83	0.61
5:e:66:LEU:HD23	5:e:75:GLU:HG2	1.83	0.61
25:b:602:CLA:H12	34:h:104:DGD:HB41	1.82	0.60
25:b:608:CLA:H172	25:b:609:CLA:H192	1.82	0.60
2:b:25:MET:HG2	27:b:617:BCR:H23C	1.82	0.60
19:x:25:VAL:HG22	31:x:102:LMT:H102	1.83	0.60
2:b:464:PHE:HD2	25:b:611:CLA:HAC2	1.65	0.60
19:X:25:VAL:HG22	31:X:102:LMT:H102	1.83	0.59
1:a:197:PHE:HE1	34:c:518:DGD:HBE1	1.66	0.59
25:D:401:CLA:H52	29:D:405:PL9:H151	1.84	0.59
1:a:85:SER:HA	1:a:109:GLY:HA3	1.85	0.59
1:A:197:PHE:HE1	34:C:518:DGD:HBE1	1.66	0.59
4:D:62:GLY:HA3	5:E:63:LEU:HD13	1.84	0.59
26:D:402:PHO:HBA2	25:D:403:CLA:H142	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:223:GLU:HG2	2:b:227:LYS:HZ2	1.67	0.59
26:d:402:PHO:HBA2	25:d:403:CLA:H142	1.85	0.59
4:d:62:GLY:HA3	5:e:63:LEU:HD13	1.84	0.58
5:E:13:ILE:HG21	35:E:104:HEM:HAD2	1.85	0.58
14:Q:42:GLN:HA	14:Q:45:VAL:HG22	1.85	0.58
35:e:104:HEM:HAC	6:f:26:ALA:HB1	1.85	0.58
25:d:401:CLA:H52	29:d:405:PL9:H151	1.84	0.58
18:v:129:MET:CE	38:v:315:HOH:O	2.52	0.58
18:v:65:CYS:HA	18:v:72:LYS:HD2	1.86	0.58
18:V:65:CYS:HA	18:V:72:LYS:HD2	1.86	0.58
1:A:163:ILE:HG12	34:C:516:DGD:HA22	1.86	0.58
35:E:104:HEM:HAC	6:F:26:ALA:HB1	1.85	0.58
2:b:30:VAL:HG12	25:b:605:CLA:HHD	1.85	0.58
1:A:85:SER:HA	1:A:109:GLY:HA3	1.85	0.58
14:q:42:GLN:HA	14:q:45:VAL:HG22	1.85	0.57
5:e:13:ILE:HG21	35:e:104:HEM:HAD2	1.85	0.57
11:L:9:ARG:NH1	31:M:102:LMT:H4'	2.20	0.57
2:B:30:VAL:HG12	25:B:605:CLA:HHD	1.85	0.57
18:V:129:MET:CE	38:V:315:HOH:O	2.52	0.57
1:a:163:ILE:HG12	34:c:516:DGD:HA22	1.86	0.57
2:b:392:VAL:HG13	2:b:397:VAL:HB	1.87	0.57
3:C:29:LEU:HD21	25:C:512:CLA:H2A	1.87	0.57
1:a:340:PRO:HG3	3:c:304:PHE:CZ	2.40	0.57
34:C:517:DGD:HAF1	34:C:518:DGD:HAT1	1.87	0.56
19:x:13:VAL:HG21	31:x:103:LMT:H72	1.87	0.56
1:A:340:PRO:HG3	3:C:304:PHE:CZ	2.40	0.56
30:K:101:SQD:H101	30:K:101:SQD:H262	1.88	0.56
14:Q:83:ARG:NH2	14:Q:113:GLU:OE2	2.38	0.56
14:q:83:ARG:NH2	14:q:113:GLU:OE2	2.38	0.56
2:B:392:VAL:HG13	2:B:397:VAL:HB	1.87	0.56
31:B:623:LMT:O6'	33:B:627:LHG:O4	2.23	0.56
28:c:519:LMG:H232	10:k:30:PHE:HE1	1.71	0.56
5:e:45:ASP:HB3	31:e:101:LMT:H1'	1.87	0.56
29:a:411:PL9:H38	6:f:21:ALA:HA	1.87	0.56
30:k:101:SQD:H101	30:k:101:SQD:H262	1.88	0.56
29:A:411:PL9:H38	6:F:21:ALA:HA	1.87	0.56
31:b:623:LMT:O6'	33:b:627:LHG:O4	2.23	0.56
5:E:45:ASP:HB3	31:E:101:LMT:H1'	1.86	0.56
11:l:9:ARG:NH1	31:m:102:LMT:H4'	2.20	0.56
34:c:517:DGD:HAF1	34:c:518:DGD:HAT1	1.87	0.56
28:A:410:LMG:H342	3:C:210:TRP:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:410:LMG:H342	3:c:210:TRP:CE2	2.41	0.56
28:A:414:LMG:HC5	2:b:75:TRP:HB3	1.88	0.55
3:C:269:MET:HG2	25:C:502:CLA:H61	1.88	0.55
3:c:79:ILE:HD11	25:c:504:CLA:HED3	1.88	0.55
28:C:519:LMG:H232	10:K:30:PHE:HE1	1.71	0.55
2:b:230:ARG:NH2	33:b:627:LHG:O5	2.21	0.55
2:B:103:LEU:HD22	25:B:606:CLA:H51	1.87	0.55
33:B:628:LHG:H322	12:M:18:PRO:HB3	1.88	0.55
19:X:13:VAL:HG21	31:X:103:LMT:H72	1.87	0.55
1:a:339:PHE:HB3	1:a:340:PRO:HD2	1.89	0.55
3:c:29:LEU:HD21	25:c:512:CLA:H2A	1.87	0.55
18:v:129:MET:HE2	38:v:315:HOH:O	2.07	0.55
3:C:79:ILE:HD11	25:C:504:CLA:HED3	1.88	0.55
30:c:501:SQD:H331	25:c:509:CLA:H102	1.89	0.55
28:A:410:LMG:H391	34:C:516:DGD:HA91	1.88	0.55
18:V:129:MET:HE2	38:V:315:HOH:O	2.07	0.55
28:a:410:LMG:H391	34:c:516:DGD:HA91	1.88	0.55
33:b:628:LHG:H322	12:m:18:PRO:HB3	1.88	0.55
2:b:103:LEU:HD22	25:b:606:CLA:H51	1.87	0.55
33:b:628:LHG:H201	11:l:28:VAL:HG21	1.88	0.55
25:d:401:CLA:H61	33:d:407:LHG:H151	1.88	0.55
30:C:501:SQD:H331	25:C:509:CLA:H102	1.88	0.55
3:c:269:MET:HG2	25:c:502:CLA:H61	1.88	0.55
12:m:23:LEU:HD22	31:m:101:LMT:H41	1.89	0.55
3:C:114:LEU:HD23	33:Z:102:LHG:H312	1.88	0.54
12:M:23:LEU:HD22	31:M:101:LMT:H41	1.89	0.54
13:O:119:ASP:OD1	13:O:119:ASP:N	2.41	0.54
2:b:121:GLU:O	7:h:12:ARG:NH1	2.40	0.54
33:B:628:LHG:H201	11:L:28:VAL:HG21	1.88	0.54
3:C:393:SER:HA	3:C:407:VAL:HG23	1.89	0.54
18:V:102:LYS:NZ	18:V:134:GLU:OE2	2.40	0.54
13:o:119:ASP:OD1	13:o:119:ASP:N	2.41	0.54
25:D:401:CLA:H61	33:D:407:LHG:H151	1.89	0.54
2:B:121:GLU:O	7:H:12:ARG:NH1	2.40	0.54
2:B:247:PHE:HB2	25:B:608:CLA:HBC1	1.90	0.54
29:a:411:PL9:H371	6:f:24:THR:HG21	1.90	0.54
18:v:102:LYS:NZ	18:v:134:GLU:OE2	2.40	0.54
6:F:42:ILE:HG12	31:F:103:LMT:H6'1	1.89	0.54
6:f:42:ILE:HG12	31:f:103:LMT:H6'1	1.89	0.54
1:a:296:ASN:HB2	3:c:387:PRO:O	2.08	0.54
2:b:247:PHE:HB2	25:b:608:CLA:HBC1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:PHE:HB3	1:A:340:PRO:HD2	1.89	0.54
2:B:75:TRP:HB3	28:a:414:LMG:HC5	1.90	0.54
3:c:114:LEU:HD23	33:z:102:LHG:H312	1.88	0.54
1:A:97:TRP:HH2	25:A:408:CLA:HBA2	1.72	0.53
33:d:407:LHG:H282	16:t:17:LEU:CD2	2.38	0.53
4:d:126:MET:HE3	4:d:150:ILE:HD12	1.91	0.53
13:o:227:GLN:HE21	13:o:241:ILE:HD11	1.74	0.53
33:B:627:LHG:H332	4:D:36:LEU:HB2	1.90	0.53
5:e:13:ILE:HG21	35:e:104:HEM:CAD	2.38	0.53
25:c:504:CLA:H203	25:c:511:CLA:HAB	1.90	0.53
10:K:44:PHE:HD2	31:K:105:LMT:H6D	1.73	0.53
1:A:296:ASN:HB2	3:C:387:PRO:O	2.08	0.53
4:D:126:MET:HE3	4:D:150:ILE:HD12	1.91	0.53
2:b:384:ARG:NH1	38:d:615:HOH:O	2.42	0.53
2:B:384:ARG:NH1	38:D:615:HOH:O	2.42	0.53
25:B:603:CLA:HAB	25:B:605:CLA:H162	1.91	0.53
30:K:101:SQD:H141	27:K:102:BCR:H272	1.91	0.53
1:a:97:TRP:HH2	25:a:408:CLA:HBA2	1.72	0.53
10:k:40:ALA:O	31:k:105:LMT:O3'	2.27	0.53
3:c:393:SER:HA	3:c:407:VAL:HG23	1.89	0.52
35:E:104:HEM:HMB1	15:R:19:ALA:CB	2.39	0.52
10:k:27:ILE:HD12	20:y:75:ILE:HG21	1.91	0.52
2:B:414:PRO:HG2	17:U:38:LEU:HD11	1.91	0.52
10:K:40:ALA:O	31:K:105:LMT:O3'	2.27	0.52
25:c:509:CLA:H193	28:c:519:LMG:H371	1.92	0.52
10:k:43:GLY:HA2	31:k:105:LMT:H4'	1.92	0.52
29:A:411:PL9:H371	6:F:24:THR:HG21	1.90	0.52
1:a:344[A]:ALA:O	3:c:344:ARG:NH1	2.43	0.52
1:A:344[A]:ALA:O	3:C:344:ARG:NH1	2.43	0.52
5:E:13:ILE:HG21	35:E:104:HEM:CAD	2.38	0.52
33:D:407:LHG:H282	16:T:17:LEU:CD2	2.38	0.52
30:a:412:SQD:H223	33:d:407:LHG:H372	1.92	0.52
10:k:44:PHE:HD2	31:k:105:LMT:H6D	1.73	0.52
10:K:27:ILE:HD12	20:Y:75:ILE:HG21	1.91	0.52
10:K:43:GLY:HA2	31:K:105:LMT:H4'	1.92	0.52
3:c:416:SER:HB3	34:c:517:DGD:HBT2	1.91	0.52
33:b:627:LHG:H332	4:d:36:LEU:HB2	1.90	0.52
2:B:254:GLY:HA2	34:H:104:DGD:HBW1	1.92	0.52
25:C:509:CLA:H193	28:C:519:LMG:H371	1.92	0.52
13:O:227:GLN:HE21	13:O:241:ILE:HD11	1.74	0.52
2:b:254:GLY:HA2	34:h:104:DGD:HBW1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:504:CLA:H203	25:C:511:CLA:HAB	1.90	0.51
25:c:506:CLA:HMD2	25:c:508:CLA:HAB	1.91	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
4:d:20:ASP:OD2	19:x:38:ARG:NH1	2.43	0.51
2:B:474:LEU:HD11	25:B:608:CLA:HAA2	1.92	0.51
25:C:506:CLA:HMD2	25:C:508:CLA:HAB	1.91	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.51
25:c:512:CLA:H71	27:k:103:BCR:H282	1.93	0.51
35:e:104:HEM:HMB1	15:r:19:ALA:CB	2.39	0.51
33:b:627:LHG:HC2	4:d:134:ARG:HH21	1.75	0.51
13:O:231:VAL:HG13	13:O:238:ILE:HG22	1.93	0.51
3:c:305:LEU:HD12	3:c:327:TYR:HB3	1.93	0.51
17:u:56:ASN:HD21	17:u:83:TYR:H	1.59	0.51
3:C:416:SER:HB3	34:C:517:DGD:HBT2	1.92	0.51
4:D:88:SER:HB2	5:E:69:ARG:HH22	1.75	0.51
3:C:305:LEU:HD12	3:C:327:TYR:HB3	1.93	0.51
30:k:101:SQD:H141	27:k:102:BCR:H272	1.91	0.51
30:A:412:SQD:H223	33:D:407:LHG:H372	1.92	0.51
25:b:603:CLA:HAB	25:b:605:CLA:H162	1.91	0.51
3:c:403:SER:HB3	18:v:63:THR:HG21	1.93	0.51
1:A:215:HIS:CE1	1:A:271:LEU:HD21	2.46	0.51
25:B:612:CLA:H171	25:B:613:CLA:HBB2	1.93	0.50
3:C:403:SER:HB3	18:V:63:THR:HG21	1.93	0.50
25:C:503:CLA:HAB	25:C:511:CLA:H141	1.93	0.50
17:U:90:LEU:HD11	17:U:107:LEU:HD11	1.93	0.50
25:c:505:CLA:H43	34:c:518:DGD:HB32	1.93	0.50
3:C:425:LEU:O	3:C:429:LEU:HG	2.11	0.50
13:O:176:ASN:HB3	13:O:219:LEU:HD11	1.92	0.50
2:b:414:PRO:HG2	17:u:38:LEU:HD11	1.91	0.50
2:b:474:LEU:HD11	25:b:608:CLA:HAA2	1.92	0.50
5:e:16:SER:OG	9:j:6:ARG:NH1	2.44	0.50
4:D:141:TYR:OH	33:D:406:LHG:O4	2.26	0.50
17:u:90:LEU:HD11	17:u:107:LEU:HD11	1.93	0.50
33:B:627:LHG:HC2	4:D:134:ARG:HH21	1.75	0.50
13:o:176:ASN:HB3	13:o:219:LEU:HD11	1.92	0.50
25:C:512:CLA:H71	27:K:103:BCR:H282	1.93	0.50
2:B:223:GLU:HG2	2:B:227:LYS:HZ2	1.75	0.50
2:B:256:MET:HA	2:B:263:THR:HG21	1.94	0.50
25:C:505:CLA:H43	34:C:518:DGD:HB32	1.93	0.50
2:b:256:MET:HA	2:b:263:THR:HG21	1.94	0.50
3:c:149:GLY:HA3	3:c:239:ILE:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:425:LEU:O	3:c:429:LEU:HG	2.11	0.50
25:c:503:CLA:HAB	25:c:511:CLA:H141	1.93	0.50
3:C:149:GLY:HA3	3:C:239:ILE:HG13	1.94	0.50
25:D:404:CLA:H51	19:X:12:LEU:HA	1.94	0.50
4:d:88:SER:HB2	5:e:69:ARG:HH22	1.75	0.50
1:a:215:HIS:CE1	1:a:271:LEU:HD21	2.46	0.50
36:h:101:RRX:H21	36:h:101:RRX:H17	1.92	0.50
3:C:212:ILE:HG23	3:C:276:PHE:HA	1.94	0.49
34:C:517:DGD:HB21	28:C:519:LMG:H302	1.94	0.49
36:H:101:RRX:H21	36:H:101:RRX:H17	1.92	0.49
17:U:77:ILE:HD11	17:U:103:LEU:HD21	1.94	0.49
2:b:26:HIS:CE1	25:b:612:CLA:HMA2	2.47	0.49
25:d:404:CLA:H51	19:x:12:LEU:HA	1.94	0.49
3:C:425:LEU:HD23	34:C:516:DGD:HBF1	1.94	0.49
25:b:601:CLA:HAC1	36:h:101:RRX:H17	1.94	0.49
13:o:231:VAL:HG13	13:o:238:ILE:HG22	1.92	0.49
30:C:501:SQD:O7	4:D:230:ASN:ND2	2.46	0.49
5:E:16:SER:OG	9:J:6:ARG:NH1	2.44	0.49
17:U:56:ASN:HD21	17:U:83:TYR:H	1.59	0.49
25:c:506:CLA:CMD	25:c:508:CLA:HAB	2.42	0.49
4:D:186:GLN:HB2	25:D:403:CLA:HBC1	1.95	0.49
3:c:451:GLU:OE2	4:d:245:SER:OG	2.30	0.49
34:c:517:DGD:HB21	28:c:519:LMG:H302	1.94	0.49
4:d:186:GLN:HB2	25:d:403:CLA:HBC1	1.95	0.49
13:o:214:LYS:HE3	17:u:39:ASN:HA	1.95	0.49
17:u:77:ILE:HD11	17:u:103:LEU:HD21	1.94	0.49
2:B:26:HIS:CE1	25:B:612:CLA:HMA2	2.47	0.49
25:B:605:CLA:H161	25:B:609:CLA:HBB2	1.95	0.49
3:c:212:ILE:HG23	3:c:276:PHE:HA	1.94	0.49
25:b:612:CLA:H171	25:b:613:CLA:HBB2	1.93	0.49
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.95	0.49
1:A:233:GLN:OE1	2:B:7:ARG:NH2	2.41	0.49
11:L:9:ARG:HH12	31:M:102:LMT:H4'	1.78	0.49
2:b:228:ALA:HA	31:b:623:LMT:H6E	1.95	0.49
3:c:13:ARG:NH2	20:y:92:ASP:OD1	2.40	0.49
3:c:425:LEU:HD23	34:c:516:DGD:HBF1	1.94	0.49
11:l:9:ARG:HH12	31:m:102:LMT:H4'	1.78	0.49
3:C:23:TRP:CZ3	33:D:408:LHG:HC92	2.48	0.48
25:C:506:CLA:CMD	25:C:508:CLA:HAB	2.42	0.48
13:O:214:LYS:HE3	17:U:39:ASN:HA	1.95	0.48
1:a:262:TYR:CG	33:e:102:LHG:HC62	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:q:45:VAL:HG12	14:q:89:LEU:HD11	1.95	0.48
2:B:228:ALA:HA	31:B:623:LMT:H6E	1.95	0.48
25:B:604:CLA:H62	25:B:604:CLA:H41	1.57	0.48
4:D:20:ASP:OD2	19:X:38:ARG:NH1	2.43	0.48
19:X:25:VAL:HG13	31:X:102:LMT:H82	1.94	0.48
1:A:283:ILE:HA	1:A:286:THR:HG22	1.95	0.48
2:B:42:LEU:HD13	2:B:94:GLU:HG3	1.94	0.48
4:D:241:GLU:OE2	38:D:632:HOH:O	2.20	0.48
1:a:93:PHE:HZ	25:a:408:CLA:HAA1	1.78	0.48
19:x:25:VAL:HG13	31:x:102:LMT:H82	1.94	0.48
1:A:221:SER:HB3	4:D:138:ILE:HD12	1.96	0.48
1:A:270:SER:HB3	30:C:501:SQD:H442	1.95	0.48
25:B:610:CLA:H201	25:B:612:CLA:HMD2	1.95	0.48
17:U:131:TYR:OXT	18:V:75:ASN:ND2	2.37	0.48
1:A:262:TYR:CG	33:E:102:LHG:HC62	2.48	0.48
25:B:601:CLA:OBD	31:H:102:LMT:O2'	2.31	0.48
31:M:101:LMT:H91	30:b:620:SQD:H332	1.94	0.48
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.94	0.48
25:b:605:CLA:H161	25:b:609:CLA:HBB2	1.95	0.48
3:c:389:GLY:HA3	3:c:407:VAL:HG22	1.96	0.48
17:u:90:LEU:O	17:u:100:LYS:NZ	2.37	0.48
1:a:283:ILE:HA	1:a:286:THR:HG22	1.95	0.48
27:k:103:BCR:H24C	27:k:103:BCR:H371	1.64	0.48
1:A:93:PHE:HZ	25:A:408:CLA:HAA1	1.78	0.48
30:B:620:SQD:H332	31:m:101:LMT:H91	1.94	0.48
3:C:13:ARG:NH2	20:Y:92:ASP:OD1	2.40	0.48
13:O:35:THR:HG22	13:O:37:ASP:H	1.79	0.48
14:Q:45:VAL:HG12	14:Q:89:LEU:HD11	1.95	0.48
25:d:401:CLA:H91	29:d:405:PL9:H402	1.96	0.48
31:m:101:LMT:H3'	31:m:101:LMT:H1B	1.72	0.48
30:c:501:SQD:O7	4:d:230:ASN:ND2	2.46	0.48
1:a:221:SER:HB3	4:d:138:ILE:HD12	1.96	0.48
18:v:35:ILE:HD12	18:v:145:LEU:HD12	1.95	0.48
27:C:515:BCR:HC31	8:I:24:LEU:HG	1.95	0.48
30:H:103:SQD:H102	30:H:103:SQD:H131	1.73	0.48
1:a:43:THR:HG23	27:a:409:BCR:H362	1.96	0.48
1:a:270:SER:HB3	30:c:501:SQD:H442	1.95	0.48
25:b:601:CLA:OBD	31:h:102:LMT:O2'	2.31	0.48
3:c:23:TRP:CZ3	33:d:408:LHG:HC92	2.48	0.48
13:o:35:THR:HG22	13:o:37:ASP:H	1.79	0.48
3:c:73:LEU:HD13	3:c:76:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:601:CLA:HAC1	36:H:101:RRX:H17	1.94	0.47
3:C:73:LEU:HD13	3:C:76:LEU:HD12	1.96	0.47
17:U:90:LEU:O	17:U:100:LYS:NZ	2.37	0.47
25:a:405:CLA:H102	26:a:407:PHO:HAA1	1.96	0.47
4:d:141:TYR:OH	33:d:406:LHG:O4	2.26	0.47
1:A:16:GLN:HB3	30:A:413:SQD:H1	1.96	0.47
25:D:401:CLA:H91	29:D:405:PL9:H402	1.96	0.47
18:V:35:ILE:HD12	18:V:145:LEU:HD12	1.95	0.47
25:b:609:CLA:H42	33:b:627:LHG:H121	1.97	0.47
3:c:117:ILE:HD13	25:c:512:CLA:H122	1.96	0.47
27:c:515:BCR:HC31	8:i:24:LEU:HG	1.95	0.47
2:b:55:MET:HE2	2:b:63:LEU:HD23	1.97	0.47
2:B:226:TYR:HA	2:B:231:MET:HG3	1.97	0.47
25:B:607:CLA:H102	28:B:621:LMG:H232	1.97	0.47
2:b:51:VAL:HG13	2:b:308:LYS:HB2	1.96	0.47
25:b:602:CLA:H112	25:b:602:CLA:H152	1.61	0.47
25:b:610:CLA:H201	25:b:612:CLA:HMD2	1.95	0.47
28:c:519:LMG:H182	28:c:519:LMG:H151	1.64	0.47
19:x:33:LYS:HE2	31:x:102:LMT:O2'	2.15	0.47
27:K:102:BCR:H363	20:Y:76:VAL:HG23	1.97	0.47
16:T:22:ALA:HB1	27:b:619:BCR:H272	1.96	0.47
25:B:609:CLA:H42	33:B:627:LHG:H121	1.97	0.47
3:C:117:ILE:CD1	25:C:512:CLA:H122	2.44	0.47
3:C:389:GLY:HA3	3:C:407:VAL:HG22	1.96	0.47
4:D:12:ARG:HD2	4:D:12:ARG:HA	1.73	0.47
31:E:103:LMT:H5B	31:K:105:LMT:H2B	1.97	0.47
13:O:66:LYS:HZ2	13:O:113:SER:HB3	1.80	0.47
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.95	0.47
1:a:136:ARG:NH2	8:i:27:ASP:OD1	2.48	0.47
1:a:233:GLN:OE1	2:b:7:ARG:NH2	2.41	0.47
27:b:618:BCR:H15C	27:b:618:BCR:H351	1.69	0.47
3:c:47:ILE:HG22	25:c:504:CLA:HHD	1.97	0.47
25:A:405:CLA:H102	26:A:407:PHO:HAA1	1.96	0.47
25:C:509:CLA:H92	33:D:408:LHG:H371	1.97	0.47
3:c:316:ALA:HB2	3:c:364:LEU:HD21	1.97	0.47
31:e:103:LMT:H5B	31:k:105:LMT:H2B	1.97	0.47
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.48	0.47
11:L:1:MET:HE3	11:L:1:MET:HB2	1.74	0.47
25:b:603:CLA:H2	25:b:605:CLA:H91	1.96	0.47
18:v:152:GLU:OE2	18:v:153:ARG:HG3	2.15	0.47
25:A:408:CLA:H92	25:A:408:CLA:H61	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:611:CLA:H142	33:B:628:LHG:H361	1.97	0.47
3:C:47:ILE:HG22	25:C:504:CLA:HHD	1.97	0.47
1:a:16:GLN:HB3	30:a:413:SQD:H1	1.97	0.47
2:b:226:TYR:HA	2:b:231:MET:HG3	1.97	0.47
3:c:84:TRP:HH2	25:c:503:CLA:H162	1.80	0.47
3:c:300:GLN:HB2	3:c:383:MET:HG3	1.97	0.47
4:d:241:GLU:OE2	38:d:632:HOH:O	2.20	0.47
1:A:332:HIS:O	1:A:333:GLU:C	2.58	0.46
1:A:343[A]:LEU:HG	3:C:300:GLN:NE2	2.30	0.46
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.46
3:C:117:ILE:HD13	25:C:512:CLA:H122	1.96	0.46
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.76	0.46
1:a:343[A]:LEU:HG	3:c:300:GLN:NE2	2.30	0.46
3:c:117:ILE:CD1	25:c:512:CLA:H122	2.44	0.46
30:k:101:SQD:H272	30:k:101:SQD:H241	1.63	0.46
3:C:147:ILE:HA	3:C:150:TYR:CD2	2.50	0.46
3:C:316:ALA:HB2	3:C:364:LEU:HD21	1.97	0.46
25:C:514:CLA:H13	25:C:514:CLA:H172	1.60	0.46
25:b:611:CLA:H112	25:b:611:CLA:H72	1.76	0.46
27:c:515:BCR:H24C	27:c:515:BCR:H371	1.74	0.46
6:f:32:PHE:HB3	27:f:101:BCR:H363	1.96	0.46
4:D:123:ILE:HD11	34:H:104:DGD:HAW1	1.97	0.46
26:a:407:PHO:HAB	4:d:205:LEU:HD13	1.97	0.46
12:m:27:ILE:HA	31:m:101:LMT:H6D	1.97	0.46
26:A:407:PHO:HAB	4:D:205:LEU:HD13	1.97	0.46
25:B:603:CLA:H2	25:B:605:CLA:H91	1.96	0.46
27:K:103:BCR:H24C	27:K:103:BCR:H371	1.64	0.46
5:e:23:HIS:C	5:e:25:ILE:N	2.73	0.46
33:e:102:LHG:H122	33:e:102:LHG:H152	1.68	0.46
27:k:102:BCR:H363	20:y:76:VAL:HG23	1.97	0.46
16:t:26:PRO:HB2	16:t:28:ARG:HE	1.81	0.46
19:X:33:LYS:HE2	31:X:102:LMT:O2'	2.15	0.46
25:c:509:CLA:H92	33:d:408:LHG:H371	1.97	0.46
3:C:117:ILE:HG23	3:C:121:LEU:HD12	1.97	0.46
6:F:35:ALA:O	6:F:39:MET:HG3	2.16	0.46
31:M:101:LMT:H32	25:b:614:CLA:H2	1.98	0.46
18:V:152:GLU:OE2	18:V:153:ARG:HG3	2.15	0.46
29:a:411:PL9:H351	6:f:24:THR:CG2	2.46	0.46
25:b:607:CLA:H102	28:b:621:LMG:H232	1.97	0.46
25:c:502:CLA:C2D	25:c:504:CLA:H2	2.46	0.46
27:k:102:BCR:H24C	27:k:102:BCR:H371	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:THR:HG23	27:A:409:BCR:H362	1.96	0.46
2:B:55:MET:HE2	2:B:63:LEU:HD23	1.97	0.46
30:C:501:SQD:H312	25:C:509:CLA:H93	1.98	0.46
5:E:23:HIS:C	5:E:25:ILE:N	2.73	0.46
2:b:482:VAL:HB	2:b:486:LEU:HD22	1.97	0.46
25:b:611:CLA:H142	33:b:628:LHG:H361	1.97	0.46
3:C:300:GLN:HB2	3:C:383:MET:HG3	1.97	0.46
26:a:407:PHO:H71	25:d:401:CLA:H203	1.97	0.46
3:c:147:ILE:HA	3:c:150:TYR:CD2	2.50	0.46
26:A:407:PHO:H71	25:D:401:CLA:H203	1.97	0.46
27:B:619:BCR:H272	16:t:22:ALA:HB1	1.97	0.46
25:C:502:CLA:C2D	25:C:504:CLA:H2	2.46	0.46
6:f:35:ALA:O	6:f:39:MET:HG3	2.16	0.46
1:A:61:ASP:HB2	1:A:63:ILE:HG12	1.98	0.46
3:C:287:GLU:HG3	38:C:686:HOH:O	2.16	0.46
25:C:512:CLA:H111	27:K:103:BCR:H23C	1.98	0.46
6:F:32:PHE:HB3	27:F:101:BCR:H363	1.96	0.46
1:a:332:HIS:O	1:a:333:GLU:C	2.58	0.46
4:d:123:ILE:HD11	34:h:104:DGD:HAW1	1.97	0.46
33:D:407:LHG:HC82	33:D:407:LHG:H112	1.75	0.45
1:a:61:ASP:HB2	1:a:63:ILE:HG12	1.98	0.45
1:a:124:PHE:HZ	34:c:516:DGD:HBH2	1.81	0.45
25:c:514:CLA:H13	25:c:514:CLA:H172	1.60	0.45
3:C:84:TRP:HH2	25:C:503:CLA:H162	1.80	0.45
30:c:501:SQD:H312	25:c:509:CLA:H93	1.98	0.45
25:c:512:CLA:H192	21:z:20:VAL:HA	1.98	0.45
30:h:103:SQD:H102	30:h:103:SQD:H131	1.73	0.45
27:z:101:BCR:H351	27:z:101:BCR:H15C	1.65	0.45
25:C:512:CLA:H192	21:Z:20:VAL:HA	1.98	0.45
27:K:103:BCR:H15C	27:K:103:BCR:H351	1.64	0.45
10:k:16:ILE:HG13	21:z:6:GLN:HG2	1.99	0.45
2:B:145:LEU:HD22	25:B:604:CLA:H162	1.98	0.45
34:C:517:DGD:HAH1	34:C:517:DGD:HAT2	1.72	0.45
10:K:16:ILE:HG13	21:Z:6:GLN:HG2	1.99	0.45
12:M:31:LYS:HA	12:m:31:LYS:HA	1.98	0.45
3:c:117:ILE:HG23	3:c:121:LEU:HD12	1.97	0.45
1:A:77:ILE:HD13	11:L:31:ILE:HG23	1.98	0.45
26:A:407:PHO:HBB2	38:D:630:HOH:O	2.16	0.45
2:B:440:ASP:OD1	2:B:444:ARG:NH1	2.45	0.45
25:C:511:CLA:H112	25:C:511:CLA:H152	1.71	0.45
1:a:166:GLY:HA3	3:c:345:PHE:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:613:CLA:OBD	25:b:614:CLA:HAB	2.17	0.45
5:e:66:LEU:HD21	5:e:76:ILE:HD11	1.99	0.45
6:f:43:GLN:HB2	31:f:103:LMT:O3B	2.17	0.45
8:i:36:ASP:OD1	8:i:37:PHE:N	2.49	0.45
27:k:102:BCR:H363	20:y:76:VAL:CG2	2.47	0.45
18:v:140:VAL:O	18:v:144:THR:OG1	2.29	0.45
25:B:608:CLA:H43	25:B:609:CLA:H101	1.98	0.45
18:V:140:VAL:O	18:V:144:THR:OG1	2.29	0.45
21:Z:39:LEU:O	21:Z:43:GLY:N	2.42	0.45
2:b:145:LEU:HD22	25:b:604:CLA:H162	1.98	0.45
3:c:287:GLU:HG3	38:c:686:HOH:O	2.16	0.45
4:d:233:ARG:HH12	30:k:101:SQD:H2	1.82	0.45
1:A:124:PHE:HZ	34:C:516:DGD:HBH2	1.81	0.45
29:A:411:PL9:H351	6:F:24:THR:CG2	2.46	0.45
2:B:482:VAL:HB	2:B:486:LEU:HD22	1.97	0.45
25:B:613:CLA:OBD	25:B:614:CLA:HAB	2.17	0.45
12:M:27:ILE:HA	31:M:101:LMT:H6D	1.97	0.45
2:b:73:SER:HB2	2:b:88:PRO:HB3	1.99	0.45
25:b:608:CLA:H43	25:b:609:CLA:H101	1.98	0.45
3:c:451:GLU:HB3	3:c:454:LEU:HD12	1.99	0.45
1:A:131:TRP:CZ3	25:C:506:CLA:HAA2	2.52	0.45
3:C:243:PRO:HA	25:C:507:CLA:HED3	1.98	0.45
3:C:404:PHE:HE1	38:C:668:HOH:O	2.00	0.45
5:E:57:THR:HG21	5:E:80:ASN:HB2	1.99	0.45
16:T:26:PRO:HB2	16:T:28:ARG:HE	1.81	0.45
1:a:131:TRP:CZ3	25:c:506:CLA:HAA2	2.52	0.45
2:B:70:GLY:HA2	2:B:178:VAL:HG11	1.99	0.45
2:B:119:ASP:OD2	11:L:4:ASN:ND2	2.43	0.45
25:B:614:CLA:H2	31:m:101:LMT:H32	1.98	0.45
3:C:43:HIS:O	3:C:46:LEU:HB2	2.17	0.45
3:C:284:TYR:O	3:C:410:ARG:NH2	2.43	0.45
25:C:505:CLA:H91	25:C:505:CLA:H112	1.84	0.45
25:c:512:CLA:H111	27:k:103:BCR:H23C	1.98	0.45
34:C:516:DGD:HA52	34:C:516:DGD:HA21	1.71	0.45
6:F:43:GLN:HB2	31:F:103:LMT:O3B	2.17	0.45
3:c:43:HIS:O	3:c:46:LEU:HB2	2.17	0.45
3:c:154:LEU:HD12	3:c:154:LEU:HA	1.85	0.45
11:l:1:MET:HB2	11:l:1:MET:HE3	1.74	0.45
27:A:409:BCR:H24C	27:A:409:BCR:H371	1.77	0.44
3:C:36:LEU:HD12	3:C:36:LEU:HA	1.79	0.44
27:C:515:BCR:H24C	27:C:515:BCR:H371	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:C:518:DGD:HAH1	34:C:518:DGD:HAT2	1.59	0.44
5:E:66:LEU:HD21	5:E:76:ILE:HD11	1.99	0.44
31:I:101:LMT:H61	31:I:101:LMT:H32	1.77	0.44
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.99	0.44
2:b:216:HIS:CE1	25:b:609:CLA:NA	2.84	0.44
3:c:404:PHE:HE1	38:c:668:HOH:O	2.00	0.44
18:v:47:THR:H	18:v:50:GLN:HE21	1.65	0.44
2:b:57:ARG:NH2	2:b:335:GLY:O	2.50	0.44
4:d:51:GLY:HA2	4:d:55:VAL:HB	2.00	0.44
1:A:89:ILE:HD11	1:A:108:ASN:HB3	2.00	0.44
2:B:73:SER:HB2	2:B:88:PRO:HB3	1.99	0.44
2:B:216:HIS:CE1	25:B:609:CLA:NA	2.84	0.44
27:Z:101:BCR:H15C	27:Z:101:BCR:H351	1.65	0.44
27:a:409:BCR:H351	27:a:409:BCR:H15C	1.70	0.44
2:b:440:ASP:OD1	2:b:444:ARG:NH1	2.45	0.44
5:e:57:THR:HG21	5:e:80:ASN:HB2	1.99	0.44
1:A:166:GLY:HA3	3:C:345:PHE:HE1	1.82	0.44
25:B:604:CLA:CMB	25:B:607:CLA:HAB	2.47	0.44
1:a:77:ILE:HD13	11:l:31:ILE:HG23	1.98	0.44
26:a:407:PHO:HBB2	38:d:630:HOH:O	2.16	0.44
2:b:70:GLY:HA2	2:b:178:VAL:HG11	1.99	0.44
2:b:348:ASP:HB3	2:b:354:LEU:HD11	2.00	0.44
27:b:617:BCR:H15C	27:b:617:BCR:H351	1.76	0.44
3:c:243:PRO:HA	25:c:507:CLA:HED3	1.98	0.44
34:c:517:DGD:HA92	34:c:517:DGD:HA62	1.82	0.44
2:B:121:GLU:HA	7:H:2:ALA:HB1	2.00	0.44
4:D:233:ARG:HH12	30:K:101:SQD:H2	1.82	0.44
13:O:83:GLU:HG3	13:O:93:GLU:O	2.18	0.44
2:b:119:ASP:OD2	11:l:4:ASN:ND2	2.43	0.44
25:b:604:CLA:CMB	25:b:607:CLA:HAB	2.47	0.44
2:B:57:ARG:NH2	2:B:335:GLY:O	2.50	0.44
2:B:450:TRP:CE2	25:B:607:CLA:HBA1	2.53	0.44
31:E:103:LMT:H6'2	9:J:9:LEU:HD22	2.00	0.44
10:K:44:PHE:CD2	31:K:105:LMT:H6D	2.52	0.44
1:a:162:PRO:HB3	1:a:168:PHE:HA	2.00	0.44
1:a:221:SER:HA	4:d:139:ARG:HB2	2.00	0.44
12:m:31:LYS:HB3	12:m:31:LYS:HE2	1.71	0.44
1:A:334:ARG:HH21	13:O:187:ASP:C	2.26	0.44
2:B:24:LEU:HD21	25:B:616:CLA:CAB	2.48	0.44
3:C:227:ILE:HD13	3:C:227:ILE:HA	1.85	0.44
9:J:12:VAL:HG12	31:K:105:LMT:H81	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:47:THR:H	18:V:50:GLN:HE21	1.65	0.44
3:c:50:TRP:O	3:c:54:MET:HB2	2.18	0.44
18:v:101:LEU:HD23	18:v:101:LEU:HA	1.81	0.44
21:z:37:LYS:HE2	21:z:41:TYR:HE2	1.83	0.44
1:A:221:SER:HA	4:D:139:ARG:HB2	2.00	0.44
25:A:408:CLA:HAA2	28:A:410:LMG:H121	1.99	0.44
2:B:162:TRP:HE1	31:B:624:LMT:H6E	1.83	0.44
25:B:615:CLA:H172	25:B:615:CLA:H13	1.79	0.44
33:B:628:LHG:H142	11:L:25:LEU:HB2	2.00	0.44
30:a:412:SQD:H441	30:a:412:SQD:H2	1.73	0.44
33:b:627:LHG:HC41	31:d:410:LMT:H22	2.00	0.44
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.53	0.44
25:A:408:CLA:H62	25:A:408:CLA:H41	1.74	0.44
3:C:117:ILE:HG22	21:Z:27:TYR:HD2	1.83	0.44
34:C:516:DGD:HAT2	34:C:516:DGD:HA71	1.81	0.44
4:D:51:GLY:HA2	4:D:55:VAL:HB	2.00	0.44
27:a:409:BCR:H24C	27:a:409:BCR:H371	1.77	0.44
2:b:24:LEU:HD21	25:b:616:CLA:CAB	2.48	0.44
38:d:615:HOH:O	17:u:130:VAL:HG13	2.18	0.44
13:o:83:GLU:HG3	13:o:93:GLU:O	2.18	0.44
18:v:58:PHE:HA	18:v:62:CYS:SG	2.58	0.44
30:A:412:SQD:S	30:A:412:SQD:O4	2.65	0.43
3:C:451:GLU:HB3	3:C:454:LEU:HD12	1.99	0.43
33:E:102:LHG:H152	33:E:102:LHG:H122	1.68	0.43
9:j:12:VAL:HG12	31:k:105:LMT:H81	1.99	0.43
21:z:39:LEU:O	21:z:43:GLY:N	2.42	0.43
38:D:615:HOH:O	17:U:130:VAL:HG13	2.18	0.43
8:I:13:GLY:HA3	31:I:103:LMT:H111	1.99	0.43
27:K:102:BCR:H363	20:Y:76:VAL:CG2	2.47	0.43
31:K:105:LMT:H1B	31:K:105:LMT:H3'	1.56	0.43
2:b:450:TRP:CE2	25:b:607:CLA:HBA1	2.53	0.43
3:c:25:GLY:HA3	25:c:512:CLA:HMD2	2.00	0.43
25:c:509:CLA:HBC3	25:c:511:CLA:H71	2.00	0.43
34:c:518:DGD:HAE1	34:c:518:DGD:HA82	1.81	0.43
18:v:118:PRO:HB3	18:v:129:MET:HE1	1.99	0.43
19:x:21:ILE:O	19:x:25:VAL:HG23	2.18	0.43
1:A:334:ARG:NH2	38:D:597:HOH:O	2.52	0.43
27:B:618:BCR:H351	27:B:618:BCR:H15C	1.69	0.43
3:C:149:GLY:HA2	3:C:235:GLY:HA2	2.01	0.43
18:V:33:ARG:NH1	18:V:46:LEU:O	2.42	0.43
2:b:30:VAL:HG22	25:b:613:CLA:C3C	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:k:105:LMT:H3'	31:k:105:LMT:H1B	1.56	0.43
18:v:129:MET:HE3	18:v:129:MET:HB2	1.81	0.43
2:B:249:ALA:HA	2:B:252:VAL:HG22	2.01	0.43
25:B:611:CLA:H112	25:B:611:CLA:H72	1.77	0.43
3:C:50:TRP:O	3:C:54:MET:HB2	2.18	0.43
3:C:174:ASP:O	3:C:181:GLY:HA2	2.19	0.43
4:D:19:ASP:OD1	4:D:32:TRP:NE1	2.45	0.43
27:K:102:BCR:H15C	27:K:102:BCR:H351	1.75	0.43
21:Z:37:LYS:HE2	21:Z:41:TYR:HE2	1.83	0.43
25:c:514:CLA:H143	25:c:514:CLA:H111	1.86	0.43
18:v:70:LYS:H	18:v:70:LYS:HG2	1.67	0.43
13:O:105:THR:O	13:O:105:THR:OG1	2.35	0.43
19:X:21:ILE:O	19:X:25:VAL:HG23	2.18	0.43
25:a:408:CLA:HAA2	28:a:410:LMG:H121	1.99	0.43
25:b:604:CLA:H62	25:b:604:CLA:H41	1.57	0.43
3:c:284:TYR:O	3:c:410:ARG:NH2	2.43	0.43
25:c:511:CLA:H152	25:c:511:CLA:H112	1.71	0.43
8:i:13:GLY:HA3	31:i:103:LMT:H111	1.99	0.43
2:B:383:PHE:N	4:D:344:GLU:O	2.50	0.43
25:B:602:CLA:H112	25:B:602:CLA:H152	1.61	0.43
4:D:263:ASN:HB3	4:D:266:TRP:HB3	2.01	0.43
31:I:103:LMT:H51	31:I:103:LMT:H22	1.88	0.43
21:Z:38:PRO:O	21:Z:41:TYR:HB2	2.18	0.43
27:B:619:BCR:H15C	27:B:619:BCR:H351	1.78	0.43
3:C:451:GLU:OE2	4:D:245:SER:OG	2.29	0.43
18:V:118:PRO:HB3	18:V:129:MET:HE1	1.99	0.43
1:a:334:ARG:HH21	13:o:187:ASP:C	2.26	0.43
2:b:121:GLU:HA	7:h:2:ALA:HB1	2.00	0.43
2:b:162:TRP:HE1	31:b:624:LMT:H6E	1.83	0.43
3:c:314:ASN:HD21	13:o:128:ASP:HB3	1.84	0.43
4:d:263:ASN:HB3	4:d:266:TRP:HB3	2.01	0.43
31:e:103:LMT:H6'2	9:j:9:LEU:HD22	2.00	0.43
27:k:102:BCR:H351	27:k:102:BCR:H15C	1.75	0.43
2:B:450:TRP:NE1	25:B:607:CLA:HBA1	2.34	0.43
28:C:519:LMG:H182	28:C:519:LMG:H151	1.64	0.43
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.43
12:M:25:LEU:HD23	12:M:25:LEU:HA	1.81	0.43
12:M:31:LYS:HB3	12:M:31:LYS:HE2	1.71	0.43
14:Q:106:LYS:HA	14:Q:106:LYS:HD2	1.79	0.43
21:Z:50:LEU:HD23	21:Z:50:LEU:HA	1.91	0.43
2:b:216:HIS:HD1	25:b:609:CLA:HED2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:d:404:CLA:H192	25:d:404:CLA:H162	1.90	0.43
33:d:408:LHG:H131	33:d:408:LHG:H102	1.75	0.43
5:e:10:PHE:HE1	35:e:104:HEM:CBD	2.28	0.43
21:z:38:PRO:O	21:z:41:TYR:HB2	2.18	0.43
27:A:409:BCR:H351	27:A:409:BCR:H15C	1.70	0.43
2:B:348:ASP:HB3	2:B:354:LEU:HD11	2.00	0.43
4:D:319:ILE:O	4:D:323:GLU:HG3	2.19	0.43
10:K:42:VAL:HB	10:K:45:LYS:HE2	2.01	0.43
18:V:58:PHE:HA	18:V:62:CYS:SG	2.58	0.43
25:b:614:CLA:H41	25:b:614:CLA:H62	1.74	0.43
25:b:614:CLA:H8	27:b:617:BCR:H362	2.01	0.43
3:c:117:ILE:HG22	21:z:27:TYR:HD2	1.83	0.43
4:d:19:ASP:OD1	4:d:32:TRP:NE1	2.45	0.43
20:y:69:LEU:HD11	31:y:101:LMT:H61	2.01	0.43
2:B:239:SER:OG	25:B:608:CLA:O1D	2.34	0.43
3:C:331:SER:OG	3:C:335:GLU:OE1	2.37	0.43
34:C:517:DGD:HA62	34:C:517:DGD:HA92	1.82	0.43
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.53	0.43
4:d:185:LEU:HD22	25:d:403:CLA:HMD1	2.01	0.43
13:o:66:LYS:HZ2	13:o:113:SER:HB3	1.83	0.43
13:o:105:THR:O	13:o:105:THR:OG1	2.35	0.43
33:D:408:LHG:H241	38:D:628:HOH:O	2.20	0.42
28:D:409:LMG:H352	28:D:409:LMG:H382	1.83	0.42
1:a:340:PRO:HB2	18:v:158:ILE:HG13	2.01	0.42
33:b:628:LHG:H142	11:l:25:LEU:HB2	2.00	0.42
3:c:174:ASP:O	3:c:181:GLY:HA2	2.19	0.42
4:d:100:ASN:HB3	4:d:103:ARG:HB2	2.01	0.42
1:A:55:ALA:HA	27:A:409:BCR:H272	2.01	0.42
2:B:30:VAL:HG22	25:B:613:CLA:C3C	2.48	0.42
2:B:216:HIS:HD1	25:B:609:CLA:HED2	1.84	0.42
3:C:314:ASN:HD21	13:O:128:ASP:HB3	1.84	0.42
25:C:507:CLA:H192	25:C:507:CLA:H161	1.83	0.42
25:C:509:CLA:HBC3	25:C:511:CLA:H71	2.00	0.42
25:b:615:CLA:H2	25:b:616:CLA:HBB2	2.00	0.42
3:c:331:SER:OG	3:c:335:GLU:OE1	2.37	0.42
25:d:403:CLA:H193	25:d:403:CLA:H162	1.80	0.42
31:h:102:LMT:O1B	31:h:102:LMT:O6'	2.35	0.42
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.42
25:B:608:CLA:H193	25:B:608:CLA:H162	1.90	0.42
20:Y:69:LEU:HD11	31:Y:101:LMT:H61	2.01	0.42
2:b:450:TRP:NE1	25:b:607:CLA:HBA1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:51:GLY:HA3	4:d:78:VAL:HG22	2.01	0.42
4:d:319:ILE:O	4:d:323:GLU:HG3	2.19	0.42
10:k:44:PHE:CD2	31:k:105:LMT:H6D	2.52	0.42
17:u:130:VAL:HG23	38:u:304:HOH:O	2.20	0.42
1:A:39:PRO:HB2	25:A:408:CLA:HAB	2.01	0.42
30:A:412:SQD:H2	30:A:412:SQD:H441	1.73	0.42
18:V:70:LYS:H	18:V:70:LYS:HG2	1.68	0.42
1:a:55:ALA:HA	27:a:409:BCR:H272	2.01	0.42
25:a:405:CLA:H191	33:d:407:LHG:H331	2.01	0.42
33:d:407:LHG:H112	33:d:407:LHG:HC82	1.75	0.42
27:f:101:BCR:H371	27:f:101:BCR:H24C	1.79	0.42
25:B:612:CLA:H61	25:B:612:CLA:H102	1.74	0.42
25:B:614:CLA:H8	27:B:617:BCR:H362	2.01	0.42
4:D:185:LEU:HD22	25:D:403:CLA:HMD1	2.01	0.42
30:K:101:SQD:H241	30:K:101:SQD:H272	1.63	0.42
27:K:102:BCR:H24C	27:K:102:BCR:H371	1.79	0.42
25:b:613:CLA:H143	25:b:613:CLA:H111	1.87	0.42
34:c:518:DGD:HAH1	34:c:518:DGD:HAT2	1.59	0.42
25:A:405:CLA:H193	25:A:405:CLA:H161	1.97	0.42
29:A:411:PL9:H261	25:D:403:CLA:H141	2.02	0.42
25:B:607:CLA:H203	33:D:406:LHG:H161	2.02	0.42
33:B:627:LHG:HC41	31:D:410:LMT:H22	2.00	0.42
3:C:25:GLY:HA3	25:C:512:CLA:HMD2	2.00	0.42
12:M:27:ILE:O	12:m:31:LYS:NZ	2.49	0.42
2:b:216:HIS:ND1	25:b:609:CLA:HED2	2.34	0.42
25:b:614:CLA:H141	25:b:614:CLA:H162	1.86	0.42
25:c:502:CLA:H122	25:c:508:CLA:H61	2.02	0.42
1:A:46:THR:HG21	28:A:414:LMG:H162	2.02	0.42
2:B:152:GLY:HA2	2:B:156:PHE:HD2	1.85	0.42
11:L:9:ARG:NH1	31:m:101:LMT:H6'1	2.35	0.42
3:c:50:TRP:CZ2	3:c:54:MET:HG2	2.55	0.42
3:c:149:GLY:HA2	3:c:235:GLY:HA2	2.01	0.42
25:c:503:CLA:H141	25:c:503:CLA:H161	1.84	0.42
1:A:255:PHE:CE2	29:A:411:PL9:H13	2.55	0.42
1:A:283:ILE:HA	1:A:283:ILE:HD13	1.92	0.42
2:B:216:HIS:ND1	25:B:609:CLA:HED2	2.34	0.42
3:C:167:MET:HE2	3:C:167:MET:HB3	1.84	0.42
30:H:103:SQD:H292	30:H:103:SQD:H262	1.86	0.42
13:O:58:THR:HG22	13:O:166:ASN:HB3	2.02	0.42
2:b:383:PHE:CZ	13:o:196:GLY:HA2	2.55	0.42
25:c:507:CLA:H203	25:c:507:CLA:H122	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:508:CLA:H62	25:c:508:CLA:H41	1.83	0.42
34:c:517:DGD:HAT2	34:c:517:DGD:HAH1	1.72	0.42
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.84	0.42
17:u:131:TYR:OXT	18:v:75:ASN:ND2	2.37	0.42
8:I:36:ASP:OD1	8:I:37:PHE:N	2.49	0.42
1:a:39:PRO:HB2	25:a:408:CLA:HAB	2.01	0.42
1:a:255:PHE:CE2	29:a:411:PL9:H13	2.55	0.42
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.08	0.42
25:b:615:CLA:H172	25:b:615:CLA:H13	1.79	0.42
31:c:525:LMT:H6D	31:c:525:LMT:H21	2.02	0.42
1:A:340:PRO:HB2	18:V:158:ILE:HG13	2.01	0.42
25:A:405:CLA:H201	33:D:407:LHG:H322	2.02	0.42
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.08	0.42
25:C:502:CLA:H122	25:C:508:CLA:H61	2.02	0.42
34:C:518:DGD:HA82	34:C:518:DGD:HAE1	1.81	0.42
1:a:46:THR:HG21	28:a:414:LMG:H162	2.02	0.42
1:a:334:ARG:NH2	38:d:597:HOH:O	2.52	0.42
10:k:42:VAL:HB	10:k:45:LYS:HE2	2.01	0.42
25:B:613:CLA:H143	25:B:613:CLA:H111	1.87	0.41
25:B:615:CLA:H2	25:B:616:CLA:HBB2	2.01	0.41
31:T:101:LMT:H91	31:T:101:LMT:H61	1.90	0.41
2:b:249:ALA:HA	2:b:252:VAL:HG22	2.01	0.41
2:b:321:LYS:NZ	2:b:363:PHE:O	2.52	0.41
3:c:428:HIS:CE1	25:c:506:CLA:ND	2.87	0.41
13:o:58:THR:HG22	13:o:166:ASN:HB3	2.02	0.41
21:z:34:ASP:OD1	21:z:34:ASP:N	2.53	0.41
1:A:302:PHE:HE2	4:D:74:LEU:HD12	1.85	0.41
3:C:50:TRP:CZ2	3:C:54:MET:HG2	2.55	0.41
25:C:509:CLA:H162	25:C:509:CLA:H122	1.71	0.41
5:E:10:PHE:HE1	35:E:104:HEM:CBD	2.28	0.41
31:M:101:LMT:H6'1	11:l:9:ARG:NH1	2.34	0.41
14:Q:75:ILE:HA	14:Q:79:LEU:HD12	2.01	0.41
4:d:149:PRO:HB3	25:d:403:CLA:H62	2.02	0.41
31:d:410:LMT:H92	30:h:103:SQD:H282	2.02	0.41
1:A:215:HIS:HA	29:A:411:PL9:O1	2.20	0.41
25:A:405:CLA:H72	25:A:405:CLA:H111	1.83	0.41
25:A:405:CLA:H191	33:D:407:LHG:H331	2.01	0.41
25:B:604:CLA:C2B	25:B:607:CLA:HAB	2.51	0.41
25:C:512:CLA:H203	25:C:512:CLA:H162	1.88	0.41
21:Z:34:ASP:OD1	21:Z:34:ASP:N	2.53	0.41
25:c:505:CLA:H62	25:c:505:CLA:H41	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:41:PHE:HE1	31:y:101:LMT:H22	1.85	0.41
12:m:25:LEU:HD23	12:m:25:LEU:HA	1.80	0.41
25:B:605:CLA:H92	25:B:605:CLA:H62	1.91	0.41
3:C:422:PHE:HD1	34:C:516:DGD:HBF2	1.86	0.41
3:C:428:HIS:CE1	25:C:506:CLA:ND	2.87	0.41
25:b:615:CLA:H2	25:b:616:CLA:CBB	2.51	0.41
4:d:12:ARG:HD2	4:d:12:ARG:HA	1.73	0.41
2:B:24:LEU:HD21	25:B:616:CLA:C3B	2.50	0.41
2:B:321:LYS:NZ	2:B:363:PHE:O	2.52	0.41
2:B:383:PHE:CZ	13:O:196:GLY:HA2	2.55	0.41
25:B:615:CLA:H2	25:B:616:CLA:CBB	2.51	0.41
3:c:324:LEU:HD22	3:c:329:MET:HE3	2.02	0.41
34:c:516:DGD:HAT2	34:c:516:DGD:HA71	1.81	0.41
33:d:408:LHG:H241	38:d:628:HOH:O	2.20	0.41
31:i:101:LMT:H61	31:i:101:LMT:H32	1.77	0.41
3:C:364:LEU:HA	3:C:364:LEU:HD23	1.87	0.41
27:C:515:BCR:HC32	8:I:23:PHE:HB3	2.02	0.41
34:C:518:DGD:HA62	34:C:518:DGD:HA91	1.97	0.41
4:D:33:SER:OG	4:D:131:GLU:OE1	2.34	0.41
4:D:219:GLU:HB3	33:D:408:LHG:HC62	2.03	0.41
21:Z:55:ALA:HB2	27:Z:101:BCR:HC8	2.03	0.41
25:a:408:CLA:H62	25:a:408:CLA:H41	1.74	0.41
3:c:391:LEU:HD12	3:c:391:LEU:HA	1.93	0.41
4:d:219:GLU:HB3	33:d:408:LHG:HC62	2.03	0.41
31:t:101:LMT:H91	31:t:101:LMT:H61	1.90	0.41
1:A:118:HIS:HE1	25:A:408:CLA:C4D	2.34	0.41
1:A:166:GLY:CA	38:A:587:HOH:O	2.69	0.41
29:A:411:PL9:H351	6:F:24:THR:HG21	2.02	0.41
25:B:610:CLA:H51	25:B:610:CLA:H8	1.89	0.41
34:C:517:DGD:HBF2	34:C:517:DGD:HBE2	1.91	0.41
28:C:519:LMG:H232	10:K:30:PHE:CE1	2.55	0.41
4:D:100:ASN:HB3	4:D:103:ARG:HB2	2.01	0.41
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.84	0.41
31:E:103:LMT:H31	31:K:105:LMT:H61	2.02	0.41
27:F:101:BCR:H351	27:F:101:BCR:H15C	1.85	0.41
20:Y:73:GLY:HA2	20:Y:76:VAL:HG12	2.02	0.41
1:a:215:HIS:HA	29:a:411:PL9:O1	2.20	0.41
2:b:66:MET:HE2	25:b:605:CLA:HED3	2.03	0.41
2:b:152:GLY:HA2	2:b:156:PHE:HD2	1.85	0.41
25:b:604:CLA:C2B	25:b:607:CLA:HAB	2.51	0.41
25:b:604:CLA:H142	25:b:604:CLA:H111	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:515:BCR:HC32	8:i:23:PHE:HB3	2.02	0.41
27:f:101:BCR:H15C	27:f:101:BCR:H351	1.85	0.41
31:i:103:LMT:H51	31:i:103:LMT:H22	1.88	0.41
13:o:110:ILE:HA	13:o:129:GLY:HA3	2.03	0.41
17:u:70:TYR:HA	17:u:71:PRO:HA	1.84	0.41
25:A:405:CLA:H122	26:A:407:PHO:H3A	2.03	0.41
25:B:614:CLA:H62	25:B:614:CLA:H41	1.74	0.41
33:B:627:LHG:H331	33:B:627:LHG:H302	1.82	0.41
25:C:505:CLA:HMC1	28:C:519:LMG:H402	2.03	0.41
31:C:525:LMT:H6D	31:C:525:LMT:H21	2.02	0.41
25:D:401:CLA:H92	25:D:401:CLA:H62	1.95	0.41
5:E:33:ALA:HB2	15:R:11:PRO:HB2	2.03	0.41
13:O:83:GLU:OE1	13:O:93:GLU:HB2	2.20	0.41
17:U:130:VAL:HG23	38:U:304:HOH:O	2.20	0.41
2:b:24:LEU:HD21	25:b:616:CLA:C3B	2.50	0.41
2:b:371:THR:HG22	2:b:377:VAL:HG22	2.02	0.41
25:c:505:CLA:HMC1	28:c:519:LMG:H402	2.03	0.41
25:d:404:CLA:H72	25:d:404:CLA:H111	1.79	0.41
31:e:103:LMT:H31	31:k:105:LMT:H61	2.02	0.41
20:y:73:GLY:HA2	20:y:76:VAL:HG12	2.02	0.41
1:A:344[B]:ALA:HB3	3:C:345:PHE:HE2	1.86	0.41
31:B:623:LMT:H81	33:B:627:LHG:H131	2.03	0.41
3:C:66:LYS:HB3	3:C:71:GLN:NE2	2.36	0.41
3:C:324:LEU:HD22	3:C:329:MET:HE3	2.02	0.41
25:C:503:CLA:H141	25:C:503:CLA:H161	1.84	0.41
4:D:54:PHE:O	5:E:49:THR:OG1	2.30	0.41
31:D:410:LMT:H92	30:H:103:SQD:H282	2.03	0.41
16:T:26:PRO:HA	16:T:27:PRO:HD3	1.98	0.41
1:a:344[B]:ALA:HB3	3:c:345:PHE:HE2	1.86	0.41
31:m:101:LMT:O1B	31:m:101:LMT:O6'	2.39	0.41
14:q:75:ILE:HA	14:q:79:LEU:HD12	2.01	0.41
18:v:33:ARG:NH1	18:v:46:LEU:O	2.42	0.41
25:B:614:CLA:H141	25:B:614:CLA:H162	1.86	0.41
27:B:617:BCR:H15C	27:B:617:BCR:H351	1.76	0.41
25:C:507:CLA:H203	25:C:507:CLA:H122	2.02	0.41
31:I:102:LMT:H122	31:I:102:LMT:H92	1.91	0.41
31:I:102:LMT:H92	31:I:102:LMT:H62	1.88	0.41
14:Q:70:ASP:OD1	14:Q:70:ASP:N	2.54	0.41
2:b:239:SER:OG	25:b:608:CLA:O1D	2.34	0.41
2:b:394:GLN:HG2	17:u:50:GLY:HA3	2.03	0.41
25:b:607:CLA:H203	33:d:406:LHG:H161	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:48:TRP:HA	4:d:78:VAL:HG21	2.03	0.41
13:o:83:GLU:OE1	13:o:93:GLU:HB2	2.20	0.41
1:A:343[B]:LEU:HD12	3:C:297:SER:HA	2.03	0.40
25:B:614:CLA:H91	25:B:614:CLA:H111	1.82	0.40
3:C:76:LEU:HD22	3:C:98:PHE:HB3	2.03	0.40
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.03	0.40
25:a:405:CLA:H122	26:a:407:PHO:H3A	2.03	0.40
29:a:411:PL9:H261	25:d:403:CLA:H141	2.02	0.40
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.03	0.40
25:b:612:CLA:H122	25:b:612:CLA:H162	1.82	0.40
33:b:627:LHG:H331	33:b:627:LHG:H302	1.83	0.40
3:c:82:LEU:HD11	25:c:504:CLA:HBA1	2.02	0.40
4:d:119:ALA:HB1	34:h:104:DGD:HAE2	2.02	0.40
21:z:50:LEU:HD23	21:z:50:LEU:HA	1.91	0.40
2:B:371:THR:HG22	2:B:377:VAL:HG22	2.02	0.40
3:C:40:HIS:HB3	25:C:513:CLA:OBD	2.22	0.40
25:C:504:CLA:H193	25:C:504:CLA:H161	1.94	0.40
25:C:505:CLA:H62	25:C:505:CLA:H41	1.92	0.40
4:D:48:TRP:HA	4:D:78:VAL:HG21	2.03	0.40
13:O:110:ILE:HA	13:O:129:GLY:HA3	2.03	0.40
1:a:323:ARG:HD2	1:a:323:ARG:HA	1.93	0.40
26:a:407:PHO:H2	26:a:407:PHO:H61	1.90	0.40
25:a:408:CLA:H61	25:a:408:CLA:H92	1.80	0.40
25:c:502:CLA:H72	25:c:502:CLA:H111	1.91	0.40
25:c:508:CLA:H101	27:c:515:BCR:H362	2.04	0.40
25:c:514:CLA:H52	27:z:101:BCR:H281	2.03	0.40
5:e:33:ALA:HB2	15:r:11:PRO:HB2	2.03	0.40
3:C:39:ALA:HB2	25:C:512:CLA:HMA2	2.04	0.40
3:C:82:LEU:HD11	25:C:504:CLA:HBA1	2.02	0.40
38:D:612:HOH:O	18:V:157:THR:HG22	2.22	0.40
6:F:41:PHE:HE1	31:Y:101:LMT:H22	1.85	0.40
31:M:101:LMT:O1B	31:M:101:LMT:O6'	2.39	0.40
17:U:70:TYR:HA	17:U:71:PRO:HA	1.84	0.40
28:a:414:LMG:H131	28:a:414:LMG:H161	1.88	0.40
2:b:321:LYS:HA	2:b:321:LYS:HD2	1.90	0.40
2:b:324:LEU:HA	4:d:293:LEU:HG	2.04	0.40
27:k:103:BCR:H351	27:k:103:BCR:H15C	1.64	0.40
19:x:14:LEU:O	19:x:18:ILE:HB	2.22	0.40
21:z:55:ALA:HB2	27:z:101:BCR:HC8	2.03	0.40
1:A:22:THR:HG21	8:I:30:ARG:HD2	2.04	0.40
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:HIS:HE1	25:B:609:CLA:C1A	2.34	0.40
3:C:326:LYS:HB2	3:C:326:LYS:HE3	1.78	0.40
4:D:119:ALA:HB1	34:H:104:DGD:HAE2	2.02	0.40
4:D:149:PRO:HB3	25:D:403:CLA:H62	2.02	0.40
19:X:14:LEU:O	19:X:18:ILE:HB	2.22	0.40
1:a:302:PHE:HE2	4:d:74:LEU:HD12	1.85	0.40
1:a:320:VAL:HG12	4:d:329:MET:HE3	2.03	0.40
1:a:341:LEU:HD12	3:c:383:MET:HE3	2.03	0.40
25:a:405:CLA:H201	33:d:407:LHG:H322	2.02	0.40
29:a:411:PL9:H351	6:f:24:THR:HG21	2.02	0.40
3:c:40:HIS:HB3	25:c:513:CLA:OBD	2.21	0.40
31:x:103:LMT:H22	31:x:103:LMT:H51	1.80	0.40
2:B:66:MET:HE2	25:B:605:CLA:HED3	2.03	0.40
3:C:460:ASP:OD1	3:C:460:ASP:N	2.54	0.40
25:C:508:CLA:H62	25:C:508:CLA:H41	1.83	0.40
13:O:117:GLY:N	13:O:121:THR:O	2.45	0.40
31:X:103:LMT:H22	31:X:103:LMT:H51	1.80	0.40
25:b:615:CLA:HBA1	25:b:615:CLA:H3A	1.95	0.40
3:c:422:PHE:HD1	34:c:516:DGD:HBF2	1.86	0.40
25:c:509:CLA:H122	25:c:509:CLA:H162	1.71	0.40
13:o:117:GLY:N	13:o:121:THR:O	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	327 (98%)	6 (2%)	0	100	100
1	a	333/360 (92%)	327 (98%)	6 (2%)	0	100	100
2	B	504/507 (99%)	497 (99%)	7 (1%)	0	100	100
2	b	504/507 (99%)	497 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	448/460 (97%)	439 (98%)	9 (2%)	0	100	100
3	c	448/460 (97%)	439 (98%)	9 (2%)	0	100	100
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
5	E	76/81 (94%)	74 (97%)	2 (3%)	0	100	100
5	e	76/81 (94%)	74 (97%)	2 (3%)	0	100	100
6	F	33/44 (75%)	33 (100%)	0	0	100	100
6	f	33/44 (75%)	33 (100%)	0	0	100	100
7	H	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
7	h	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
8	I	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
8	i	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
9	J	37/39 (95%)	37 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
10	k	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
11	L	37/39 (95%)	37 (100%)	0	0	100	100
11	l	37/39 (95%)	37 (100%)	0	0	100	100
12	M	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
12	m	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
13	O	241/274 (88%)	225 (93%)	15 (6%)	1 (0%)	30	26
13	o	241/274 (88%)	225 (93%)	15 (6%)	1 (0%)	30	26
14	Q	116/149 (78%)	112 (97%)	4 (3%)	0	100	100
14	q	116/149 (78%)	112 (97%)	4 (3%)	0	100	100
15	R	32/39 (82%)	32 (100%)	0	0	100	100
15	r	32/39 (82%)	32 (100%)	0	0	100	100
16	T	28/31 (90%)	28 (100%)	0	0	100	100
16	t	28/31 (90%)	28 (100%)	0	0	100	100
17	U	93/131 (71%)	91 (98%)	2 (2%)	0	100	100
17	u	93/131 (71%)	91 (98%)	2 (2%)	0	100	100
18	V	133/160 (83%)	128 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	v	133/160 (83%)	128 (96%)	5 (4%)	0	100	100
19	X	36/39 (92%)	36 (100%)	0	0	100	100
19	x	36/39 (92%)	36 (100%)	0	0	100	100
20	Y	30/39 (77%)	30 (100%)	0	0	100	100
20	y	30/39 (77%)	30 (100%)	0	0	100	100
21	Z	58/62 (94%)	58 (100%)	0	0	100	100
21	z	58/62 (94%)	58 (100%)	0	0	100	100
All	All	5468/5976 (92%)	5340 (98%)	126 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	32	SER
13	o	32	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/293 (94%)	271 (99%)	3 (1%)	65	71
1	a	274/293 (94%)	271 (99%)	3 (1%)	65	71
2	B	403/404 (100%)	398 (99%)	5 (1%)	63	69
2	b	403/404 (100%)	398 (99%)	5 (1%)	63	69
3	C	351/361 (97%)	342 (97%)	9 (3%)	40	42
3	c	351/361 (97%)	342 (97%)	9 (3%)	40	42
4	D	277/285 (97%)	276 (100%)	1 (0%)	84	88
4	d	277/285 (97%)	275 (99%)	2 (1%)	76	81
5	E	70/73 (96%)	69 (99%)	1 (1%)	59	65
5	e	70/73 (96%)	69 (99%)	1 (1%)	59	65
6	F	28/37 (76%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	28/37 (76%)	28 (100%)	0	100	100
7	H	53/54 (98%)	53 (100%)	0	100	100
7	h	53/54 (98%)	53 (100%)	0	100	100
8	I	32/33 (97%)	31 (97%)	1 (3%)	35	35
8	i	32/33 (97%)	31 (97%)	1 (3%)	35	35
9	J	24/24 (100%)	24 (100%)	0	100	100
9	j	24/24 (100%)	24 (100%)	0	100	100
10	K	31/38 (82%)	30 (97%)	1 (3%)	34	35
10	k	31/38 (82%)	30 (97%)	1 (3%)	34	35
11	L	36/36 (100%)	36 (100%)	0	100	100
11	l	36/36 (100%)	36 (100%)	0	100	100
12	M	27/31 (87%)	26 (96%)	1 (4%)	30	29
12	m	27/31 (87%)	26 (96%)	1 (4%)	30	29
13	O	207/233 (89%)	202 (98%)	5 (2%)	43	45
13	o	207/233 (89%)	202 (98%)	5 (2%)	43	45
14	Q	93/128 (73%)	93 (100%)	0	100	100
14	q	93/128 (73%)	93 (100%)	0	100	100
15	R	26/29 (90%)	26 (100%)	0	100	100
15	r	26/29 (90%)	26 (100%)	0	100	100
16	T	24/25 (96%)	24 (100%)	0	100	100
16	t	24/25 (96%)	24 (100%)	0	100	100
17	U	83/111 (75%)	80 (96%)	3 (4%)	31	30
17	u	83/111 (75%)	80 (96%)	3 (4%)	31	30
18	V	117/137 (85%)	111 (95%)	6 (5%)	21	17
18	v	117/137 (85%)	111 (95%)	6 (5%)	21	17
19	X	32/33 (97%)	32 (100%)	0	100	100
19	x	32/33 (97%)	32 (100%)	0	100	100
20	Y	25/30 (83%)	24 (96%)	1 (4%)	28	25
20	y	25/30 (83%)	24 (96%)	1 (4%)	28	25
21	Z	49/52 (94%)	48 (98%)	1 (2%)	48	53
21	z	49/52 (94%)	48 (98%)	1 (2%)	48	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4524/4894 (92%)	4447 (98%)	77 (2%)	52 58

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	343[A]	LEU
1	A	343[B]	LEU
2	B	13	LEU
2	B	63	LEU
2	B	245	VAL
2	B	289	ASP
2	B	415	SER
3	C	48	VAL
3	C	190	THR
3	C	201	LEU
3	C	227	ILE
3	C	232	ILE
3	C	276	PHE
3	C	294	MET
3	C	342	THR
3	C	360	ASN
4	D	192	THR
5	E	62	GLU
8	I	35	LYS
10	K	24	LEU
12	M	15	VAL
13	O	71	ASP
13	O	90	GLN
13	O	155	THR
13	O	193	LEU
13	O	212	THR
17	U	89	VAL
17	U	112	VAL
17	U	117	ILE
18	V	32	THR
18	V	46	LEU
18	V	52	THR
18	V	83	ASP
18	V	120	ILE
18	V	124	ASP
20	Y	64	GLU

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Mol	Chain	Res	Type
21	Z	4	VAL
1	a	13	LEU
1	a	343[A]	LEU
1	a	343[B]	LEU
2	b	13	LEU
2	b	63	LEU
2	b	245	VAL
2	b	289	ASP
2	b	415	SER
3	c	48	VAL
3	c	190	THR
3	c	201	LEU
3	c	227	ILE
3	c	232	ILE
3	c	276	PHE
3	c	294	MET
3	c	342	THR
3	c	360	ASN
4	d	25	ASP
4	d	192	THR
5	e	62	GLU
8	i	35	LYS
10	k	24	LEU
12	m	15	VAL
13	o	71	ASP
13	o	90	GLN
13	o	155	THR
13	o	193	LEU
13	o	212	THR
17	u	89	VAL
17	u	112	VAL
17	u	117	ILE
18	v	32	THR
18	v	46	LEU
18	v	52	THR
18	v	83	ASP
18	v	120	ILE
18	v	124	ASP
20	y	64	GLU
21	z	4	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	303	ASN
1	A	304	GLN
2	B	177	HIS
2	B	291	GLN
2	B	455	HIS
3	C	309	GLN
3	C	314	ASN
4	D	100	ASN
4	D	334	GLN
8	I	31	ASN
12	M	2	GLN
13	O	103	GLN
13	O	153	ASN
13	O	227	GLN
14	Q	143	ASN
15	R	22	ASN
17	U	56	ASN
17	U	72	ASN
18	V	50	GLN
18	V	93	ASN
1	a	25	ASN
1	a	187	GLN
1	a	303	ASN
1	a	304	GLN
2	b	177	HIS
2	b	291	GLN
2	b	455	HIS
3	c	309	GLN
3	c	314	ASN
4	d	100	ASN
4	d	334	GLN
5	e	74	GLN
6	f	43	GLN
8	i	31	ASN
12	m	2	GLN
13	o	103	GLN
13	o	153	ASN
13	o	227	GLN
14	q	143	ASN
15	r	22	ASN
17	u	56	ASN
17	u	72	ASN

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Mol	Chain	Res	Type
17	u	80	ASN
18	v	50	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	0.99	0	8,9,11	0.93	0
8	FME	I	1	8	8,9,10	0.99	0	8,9,11	1.13	1 (12%)
9	FME	J	1	9	6,7,10	0.82	0	2,7,11	0.67	0
16	FME	T	1	16	8,9,10	0.88	0	8,9,11	1.04	1 (12%)
9	FME	j	1	9	6,7,10	0.83	0	2,7,11	0.67	0
12	FME	m	1	12	8,9,10	0.98	0	8,9,11	0.93	0
16	FME	t	1	16	8,9,10	0.88	0	8,9,11	1.04	1 (12%)
8	FME	i	1	8	8,9,10	0.98	0	8,9,11	1.13	1 (12%)

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
12	FME	M	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
9	FME	J	1	9	-	3/5/6/11	-
16	FME	T	1	16	-	4/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FME	j	1	9	-	3/5/6/11	-
12	FME	m	1	12	-	0/7/9/11	-
16	FME	t	1	16	-	4/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.50	114.31	109.50
8	I	1	FME	C-CA-N	2.48	114.28	109.50
16	T	1	FME	C-CA-N	2.10	113.55	109.50
16	t	1	FME	C-CA-N	2.10	113.55	109.50

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1	FME	N-CA-CB-CG
9	J	1	FME	C-CA-CB-CG
16	T	1	FME	N-CA-CB-CG
9	j	1	FME	N-CA-CB-CG
9	j	1	FME	C-CA-CB-CG
16	t	1	FME	N-CA-CB-CG
9	J	1	FME	CA-CB-CG-SD
9	j	1	FME	CA-CB-CG-SD
16	T	1	FME	CA-CB-CG-SD
16	t	1	FME	CA-CB-CG-SD
16	T	1	FME	C-CA-CB-CG
16	t	1	FME	C-CA-CB-CG
8	I	1	FME	CA-CB-CG-SD
8	i	1	FME	CA-CB-CG-SD
8	I	1	FME	C-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
16	T	1	FME	CB-CG-SD-CE
16	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 12 are monoatomic - leaving 220 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$
28	LMG	d	409	-	43,43,55	1.30	5 (11%)	51,51,63	1.11	3 (5%)
33	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
30	SQD	b	620	-	52,54,54	0.41	0	62,65,65	0.44	0
25	CLA	b	614	2	69,73,73	2.23	21 (30%)	82,113,113	2.50	26 (31%)
29	PL9	D	405	-	55,55,55	1.20	5 (9%)	68,69,69	1.41	11 (16%)
25	CLA	c	514	3	69,73,73	2.25	22 (31%)	82,113,113	2.41	26 (31%)
31	LMT	c	524	-	36,36,36	1.18	4 (11%)	47,47,47	1.18	3 (6%)
25	CLA	c	504	3	69,73,73	2.25	23 (33%)	82,113,113	2.51	28 (34%)
27	BCR	b	618	-	41,41,41	2.68	6 (14%)	56,56,56	6.46	20 (35%)
25	CLA	b	608	2	69,73,73	2.24	21 (30%)	82,113,113	2.39	27 (32%)
31	LMT	e	101	-	22,22,36	1.09	2 (9%)	27,27,47	1.16	3 (11%)
25	CLA	c	502	3	69,73,73	2.22	22 (31%)	82,113,113	2.50	28 (34%)
31	LMT	X	103	-	22,22,36	1.01	2 (9%)	27,27,47	1.28	3 (11%)
31	LMT	x	105	-	19,19,36	1.12	2 (10%)	24,24,47	1.00	0
33	LHG	z	102	-	35,35,48	1.15	2 (5%)	38,40,54	1.16	3 (7%)
31	LMT	M	102	-	24,24,36	1.06	2 (8%)	29,29,47	1.08	1 (3%)
25	CLA	d	401	38	69,73,73	2.19	22 (31%)	82,113,113	2.50	26 (31%)
25	CLA	b	616	2	64,68,73	2.26	21 (32%)	76,107,113	2.62	27 (35%)
25	CLA	c	506	3	59,63,73	2.40	22 (37%)	70,101,113	2.74	28 (40%)
27	BCR	C	515	-	41,41,41	2.66	6 (14%)	56,56,56	6.60	16 (28%)
31	LMT	E	103	-	36,36,36	1.23	6 (16%)	47,47,47	1.57	6 (12%)
25	CLA	c	512	3	69,73,73	2.24	23 (33%)	82,113,113	2.60	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	C	522	-	24,24,36	1.15	5 (20%)	29,29,47	1.32	5 (17%)
33	LHG	B	627	-	48,48,48	0.95	2 (4%)	51,54,54	1.06	2 (3%)
31	LMT	i	104	-	22,22,36	1.05	2 (9%)	27,27,47	1.05	0
25	CLA	C	506	3	59,63,73	2.40	22 (37%)	70,101,113	2.74	28 (40%)
27	BCR	B	618	-	41,41,41	2.68	6 (14%)	56,56,56	6.46	20 (35%)
25	CLA	B	613	2	69,73,73	2.16	22 (31%)	82,113,113	2.52	26 (31%)
25	CLA	b	607	38	69,73,73	2.18	22 (31%)	82,113,113	2.49	28 (34%)
28	LMG	D	409	-	43,43,55	1.30	5 (11%)	51,51,63	1.11	3 (5%)
32	BCT	a	417	-	3,3,3	1.15	0	2,3,3	4.17	2 (100%)
25	CLA	C	512	3	69,73,73	2.24	23 (33%)	82,113,113	2.60	28 (34%)
31	LMT	y	101	-	21,21,36	1.10	2 (9%)	26,26,47	1.05	1 (3%)
30	SQD	A	413	-	46,48,54	1.00	3 (6%)	56,59,65	1.86	12 (21%)
25	CLA	C	508	38	69,73,73	2.21	22 (31%)	82,113,113	2.55	29 (35%)
25	CLA	C	505	38	69,73,73	2.18	21 (30%)	82,113,113	2.54	29 (35%)
33	LHG	B	628	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
30	SQD	B	620	-	52,54,54	0.41	0	62,65,65	0.44	0
31	LMT	E	101	-	22,22,36	1.08	2 (9%)	27,27,47	1.16	3 (11%)
31	LMT	X	105	-	19,19,36	1.12	2 (10%)	24,24,47	1.00	0
25	CLA	B	604	2	69,73,73	2.19	20 (28%)	82,113,113	2.49	30 (36%)
31	LMT	i	102	-	24,24,36	1.04	3 (12%)	29,29,47	1.07	1 (3%)
31	LMT	x	101	-	24,24,36	1.04	2 (8%)	29,29,47	1.06	1 (3%)
33	LHG	Z	102	-	35,35,48	1.15	2 (5%)	38,40,54	1.16	3 (7%)
27	BCR	F	101	-	41,41,41	2.60	6 (14%)	56,56,56	6.63	22 (39%)
28	LMG	C	523	-	49,49,55	1.44	6 (12%)	57,57,63	1.22	4 (7%)
25	CLA	b	612	2	69,73,73	2.23	21 (30%)	82,113,113	2.44	27 (32%)
31	LMT	x	104	-	19,19,36	1.20	3 (15%)	24,24,47	1.06	1 (4%)
28	LMG	A	414	-	36,36,55	1.11	2 (5%)	44,44,63	1.19	3 (6%)
31	LMT	A	416	-	24,24,36	1.07	3 (12%)	29,29,47	1.00	1 (3%)
31	LMT	h	102	-	24,24,36	1.07	2 (8%)	29,29,47	1.11	2 (6%)
25	CLA	B	605	2	69,73,73	2.18	21 (30%)	82,113,113	2.58	26 (31%)
31	LMT	B	624	-	24,24,36	1.04	3 (12%)	29,29,47	0.90	0
25	CLA	B	614	2	69,73,73	2.22	21 (30%)	82,113,113	2.50	26 (31%)
25	CLA	A	408	1	64,68,73	2.31	22 (34%)	76,107,113	2.61	25 (32%)
25	CLA	b	605	2	69,73,73	2.18	21 (30%)	82,113,113	2.58	25 (30%)
25	CLA	b	601	38	49,53,73	2.53	23 (46%)	58,89,113	2.86	24 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	D	406	-	48,48,48	0.91	3 (6%)	51,54,54	0.99	3 (5%)
31	LMT	X	102	-	22,22,36	1.09	2 (9%)	27,27,47	1.05	1 (3%)
26	PHO	a	407	-	58,69,69	2.16	10 (17%)	55,99,99	1.62	7 (12%)
31	LMT	H	102	-	24,24,36	1.07	2 (8%)	29,29,47	1.12	2 (6%)
27	BCR	k	103	-	41,41,41	2.64	6 (14%)	56,56,56	6.56	26 (46%)
31	LMT	e	103	-	36,36,36	1.22	6 (16%)	47,47,47	1.57	6 (12%)
25	CLA	C	513	3	54,58,73	2.52	21 (38%)	64,95,113	2.75	21 (32%)
30	SQD	k	101	-	41,41,54	1.04	3 (7%)	49,49,65	1.77	9 (18%)
31	LMT	I	101	-	24,24,36	1.06	2 (8%)	29,29,47	1.06	2 (6%)
31	LMT	x	103	-	22,22,36	1.01	2 (9%)	27,27,47	1.28	3 (11%)
30	SQD	a	413	-	46,48,54	1.00	3 (6%)	56,59,65	1.86	12 (21%)
31	LMT	b	625	-	36,36,36	1.23	6 (16%)	47,47,47	1.06	1 (2%)
31	LMT	t	101	-	24,24,36	1.09	2 (8%)	29,29,47	1.16	2 (6%)
27	BCR	b	619	-	41,41,41	2.70	6 (14%)	56,56,56	6.55	22 (39%)
27	BCR	B	617	-	41,41,41	2.69	6 (14%)	56,56,56	6.53	16 (28%)
31	LMT	C	524	-	36,36,36	1.18	4 (11%)	47,47,47	1.18	3 (6%)
35	HEM	v	201	18	50,50,50	1.78	14 (28%)	67,82,82	1.90	12 (17%)
31	LMT	d	410	-	24,24,36	0.99	2 (8%)	29,29,47	1.21	4 (13%)
27	BCR	K	102	-	41,41,41	2.61	6 (14%)	56,56,56	6.89	21 (37%)
25	CLA	c	510	3	69,73,73	2.24	23 (33%)	82,113,113	2.50	26 (31%)
25	CLA	c	507	3	69,73,73	2.23	22 (31%)	82,113,113	2.43	26 (31%)
31	LMT	I	102	-	24,24,36	1.03	3 (12%)	29,29,47	1.06	1 (3%)
36	RRX	H	101	-	42,42,42	1.33	8 (19%)	56,58,58	1.39	9 (16%)
28	LMG	A	410	-	51,51,55	1.48	8 (15%)	59,59,63	1.11	3 (5%)
31	LMT	M	101	-	36,36,36	1.17	6 (16%)	47,47,47	1.04	2 (4%)
27	BCR	c	515	-	41,41,41	2.66	6 (14%)	56,56,56	6.60	16 (28%)
31	LMT	m	102	-	24,24,36	1.07	2 (8%)	29,29,47	1.08	1 (3%)
25	CLA	d	403	4	69,73,73	2.19	21 (30%)	82,113,113	2.55	25 (30%)
25	CLA	C	510	3	69,73,73	2.24	23 (33%)	82,113,113	2.50	26 (31%)
25	CLA	c	508	38	69,73,73	2.21	21 (30%)	82,113,113	2.55	29 (35%)
28	LMG	a	410	-	51,51,55	1.48	8 (15%)	59,59,63	1.11	3 (5%)
31	LMT	c	522	-	24,24,36	1.14	4 (16%)	29,29,47	1.33	5 (17%)
31	LMT	I	103	-	36,36,36	1.18	5 (13%)	47,47,47	0.93	1 (2%)
28	LMG	B	621	-	51,51,55	1.46	8 (15%)	59,59,63	1.03	2 (3%)
25	CLA	B	610	38	69,73,73	2.25	23 (33%)	82,113,113	2.47	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	d	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	4 (7%)
25	CLA	d	404	4	69,73,73	2.22	23 (33%)	82,113,113	2.49	26 (31%)
31	LMT	Y	101	-	21,21,36	1.10	2 (9%)	26,26,47	1.05	1 (3%)
27	BCR	z	101	-	41,41,41	2.64	6 (14%)	56,56,56	6.49	20 (35%)
31	LMT	d	412	-	36,36,36	1.17	5 (13%)	47,47,47	0.95	1 (2%)
31	LMT	x	102	-	22,22,36	1.10	2 (9%)	27,27,47	1.05	1 (3%)
25	CLA	B	608	2	69,73,73	2.24	21 (30%)	82,113,113	2.39	27 (32%)
25	CLA	c	511	3	69,73,73	2.21	22 (31%)	82,113,113	2.52	30 (36%)
30	SQD	K	101	-	41,41,54	1.04	3 (7%)	49,49,65	1.77	9 (18%)
31	LMT	j	101	-	24,24,36	1.04	3 (12%)	29,29,47	1.19	4 (13%)
25	CLA	b	609	2	69,73,73	2.25	21 (30%)	82,113,113	2.41	24 (29%)
34	DGD	H	104	-	63,63,67	1.34	8 (12%)	77,77,81	0.97	3 (3%)
34	DGD	c	516	-	63,63,67	1.33	8 (12%)	77,77,81	0.93	2 (2%)
34	DGD	c	518	-	63,63,67	1.33	8 (12%)	77,77,81	1.05	3 (3%)
30	SQD	C	501	-	52,54,54	0.93	4 (7%)	62,65,65	1.62	9 (14%)
28	LMG	h	105	-	47,47,55	1.41	6 (12%)	55,55,63	1.39	7 (12%)
26	PHO	A	407	-	58,69,69	2.15	10 (17%)	55,99,99	1.63	7 (12%)
31	LMT	J	101	-	24,24,36	1.04	3 (12%)	29,29,47	1.19	4 (13%)
31	LMT	i	101	-	24,24,36	1.06	2 (8%)	29,29,47	1.06	2 (6%)
30	SQD	F	102	-	32,34,54	1.20	4 (12%)	42,45,65	1.97	11 (26%)
30	SQD	f	102	-	32,34,54	1.20	4 (12%)	42,45,65	1.97	11 (26%)
34	DGD	c	517	-	63,63,67	1.33	8 (12%)	77,77,81	1.08	5 (6%)
27	BCR	a	409	-	41,41,41	2.64	6 (14%)	56,56,56	6.48	20 (35%)
31	LMT	B	629	-	36,36,36	1.18	5 (13%)	47,47,47	1.00	1 (2%)
25	CLA	B	615	2	69,73,73	2.17	21 (30%)	82,113,113	2.55	28 (34%)
31	LMT	b	629	-	36,36,36	1.18	5 (13%)	47,47,47	1.00	1 (2%)
25	CLA	b	602	2	69,73,73	2.21	21 (30%)	82,113,113	2.45	26 (31%)
27	BCR	b	617	-	41,41,41	2.69	6 (14%)	56,56,56	6.53	16 (28%)
31	LMT	X	104	-	19,19,36	1.20	3 (15%)	24,24,47	1.06	1 (4%)
31	LMT	b	623	-	36,36,36	1.18	4 (11%)	47,47,47	1.10	4 (8%)
31	LMT	K	105	-	36,36,36	1.20	6 (16%)	47,47,47	1.22	5 (10%)
33	LHG	e	102	-	39,39,48	1.03	2 (5%)	42,45,54	1.12	3 (7%)
34	DGD	C	516	-	63,63,67	1.33	8 (12%)	77,77,81	0.93	2 (2%)
30	SQD	h	103	-	52,54,54	0.94	3 (5%)	62,65,65	1.53	8 (12%)
25	CLA	b	606	2	64,68,73	2.34	23 (35%)	76,107,113	2.49	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	C	525	-	21,21,36	1.01	1 (4%)	26,26,47	1.28	2 (7%)
31	LMT	f	103	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	2 (4%)
25	CLA	c	503	3	69,73,73	2.19	20 (28%)	82,113,113	2.42	28 (34%)
33	LHG	b	628	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
26	PHO	d	402	-	58,69,69	2.18	10 (17%)	55,99,99	1.71	10 (18%)
25	CLA	b	604	2	69,73,73	2.19	20 (28%)	82,113,113	2.49	30 (36%)
27	BCR	B	619	-	41,41,41	2.70	6 (14%)	56,56,56	6.55	22 (39%)
25	CLA	a	406	38	69,73,73	2.24	23 (33%)	82,113,113	2.53	26 (31%)
32	BCT	A	417	-	3,3,3	1.15	0	2,3,3	4.18	2 (100%)
33	LHG	E	102	-	39,39,48	1.03	2 (5%)	42,45,54	1.12	3 (7%)
30	SQD	c	501	-	52,54,54	0.94	4 (7%)	62,65,65	1.63	9 (14%)
25	CLA	B	609	2	69,73,73	2.25	21 (30%)	82,113,113	2.42	24 (29%)
31	LMT	d	411	-	36,36,36	1.17	5 (13%)	47,47,47	0.92	0
25	CLA	C	507	3	69,73,73	2.23	22 (31%)	82,113,113	2.44	26 (31%)
31	LMT	A	415	-	36,36,36	1.19	5 (13%)	47,47,47	1.01	3 (6%)
25	CLA	B	612	2	69,73,73	2.23	21 (30%)	82,113,113	2.44	27 (32%)
31	LMT	B	625	-	36,36,36	1.23	6 (16%)	47,47,47	1.06	1 (2%)
25	CLA	b	603	2	69,73,73	2.24	20 (28%)	82,113,113	2.41	27 (32%)
25	CLA	b	613	2	69,73,73	2.15	22 (31%)	82,113,113	2.53	26 (31%)
31	LMT	b	624	-	24,24,36	1.04	3 (12%)	29,29,47	0.90	0
27	BCR	Z	101	-	41,41,41	2.64	6 (14%)	56,56,56	6.49	20 (35%)
25	CLA	B	607	38	69,73,73	2.18	22 (31%)	82,113,113	2.50	28 (34%)
25	CLA	B	603	2	69,73,73	2.24	20 (28%)	82,113,113	2.41	27 (32%)
31	LMT	B	626	-	24,24,36	1.01	2 (8%)	29,29,47	0.91	0
28	LMG	C	519	-	51,51,55	1.47	8 (15%)	59,59,63	1.12	3 (5%)
27	BCR	f	101	-	41,41,41	2.60	6 (14%)	56,56,56	6.63	22 (39%)
31	LMT	m	101	-	36,36,36	1.17	6 (16%)	47,47,47	1.04	2 (4%)
31	LMT	X	101	-	24,24,36	1.05	2 (8%)	29,29,47	1.06	1 (3%)
30	SQD	a	412	-	52,54,54	0.96	3 (5%)	62,65,65	1.69	15 (24%)
31	LMT	b	626	-	24,24,36	1.01	2 (8%)	29,29,47	0.90	0
25	CLA	b	611	2	69,73,73	2.19	20 (28%)	82,113,113	2.40	26 (31%)
25	CLA	c	505	38	69,73,73	2.18	21 (30%)	82,113,113	2.54	29 (35%)
25	CLA	c	513	3	54,58,73	2.51	21 (38%)	64,95,113	2.75	21 (32%)
29	PL9	a	411	-	55,55,55	1.10	4 (7%)	68,69,69	1.46	11 (16%)
25	CLA	B	602	2	69,73,73	2.20	21 (30%)	82,113,113	2.45	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	B	623	-	36,36,36	1.18	4 (11%)	47,47,47	1.10	4 (8%)
31	LMT	k	105	-	36,36,36	1.20	6 (16%)	47,47,47	1.22	5 (10%)
35	HEM	V	201	18	50,50,50	1.78	14 (28%)	67,82,82	1.90	12 (17%)
25	CLA	C	502	3	69,73,73	2.22	22 (31%)	82,113,113	2.50	28 (34%)
31	LMT	F	103	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	2 (4%)
31	LMT	a	416	-	24,24,36	1.06	3 (12%)	29,29,47	1.00	1 (3%)
25	CLA	c	509	3	69,73,73	2.22	22 (31%)	82,113,113	2.33	26 (31%)
25	CLA	A	406	38	69,73,73	2.24	22 (31%)	82,113,113	2.53	26 (31%)
29	PL9	A	411	-	55,55,55	1.10	4 (7%)	68,69,69	1.46	11 (16%)
31	LMT	c	525	-	21,21,36	1.00	1 (4%)	26,26,47	1.28	2 (7%)
27	BCR	A	409	-	41,41,41	2.64	6 (14%)	56,56,56	6.48	20 (35%)
25	CLA	C	511	3	69,73,73	2.21	21 (30%)	82,113,113	2.52	30 (36%)
33	LHG	D	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	4 (7%)
25	CLA	B	606	2	64,68,73	2.34	23 (35%)	76,107,113	2.48	28 (36%)
28	LMG	c	523	-	49,49,55	1.44	6 (12%)	57,57,63	1.22	4 (7%)
25	CLA	C	504	3	69,73,73	2.25	23 (33%)	82,113,113	2.51	28 (34%)
27	BCR	k	102	-	41,41,41	2.61	6 (14%)	56,56,56	6.89	21 (37%)
33	LHG	d	406	-	48,48,48	0.92	3 (6%)	51,54,54	0.99	3 (5%)
34	DGD	h	104	-	63,63,67	1.34	8 (12%)	77,77,81	0.97	3 (3%)
35	HEM	E	104	5,6	50,50,50	1.62	9 (18%)	67,82,82	1.68	13 (19%)
25	CLA	D	403	4	69,73,73	2.19	21 (30%)	82,113,113	2.55	25 (30%)
33	LHG	b	627	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	2 (3%)
25	CLA	D	404	4	69,73,73	2.22	23 (33%)	82,113,113	2.49	26 (31%)
25	CLA	B	601	38	49,53,73	2.53	23 (46%)	58,89,113	2.86	23 (39%)
34	DGD	C	518	-	63,63,67	1.33	8 (12%)	77,77,81	1.05	3 (3%)
25	CLA	a	405	1	69,73,73	2.16	21 (30%)	82,113,113	2.48	27 (32%)
33	LHG	D	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	C	514	3	69,73,73	2.25	22 (31%)	82,113,113	2.41	26 (31%)
31	LMT	i	103	-	36,36,36	1.19	5 (13%)	47,47,47	0.93	1 (2%)
25	CLA	b	615	2	69,73,73	2.18	21 (30%)	82,113,113	2.56	28 (34%)
35	HEM	e	104	5,6	50,50,50	1.62	9 (18%)	67,82,82	1.68	13 (19%)
25	CLA	C	503	3	69,73,73	2.19	20 (28%)	82,113,113	2.42	28 (34%)
28	LMG	b	621	-	51,51,55	1.46	8 (15%)	59,59,63	1.03	2 (3%)
29	PL9	d	405	-	55,55,55	1.20	5 (9%)	68,69,69	1.42	11 (16%)
30	SQD	H	103	-	52,54,54	0.94	3 (5%)	62,65,65	1.53	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	K	103	-	41,41,41	2.64	6 (14%)	56,56,56	6.56	26 (46%)
25	CLA	a	408	1	64,68,73	2.31	22 (34%)	76,107,113	2.61	25 (32%)
25	CLA	B	616	2	64,68,73	2.26	21 (32%)	76,107,113	2.62	27 (35%)
25	CLA	C	509	3	69,73,73	2.22	22 (31%)	82,113,113	2.33	26 (31%)
25	CLA	D	401	38	69,73,73	2.20	22 (31%)	82,113,113	2.50	26 (31%)
26	PHO	D	402	-	58,69,69	2.18	10 (17%)	55,99,99	1.70	10 (18%)
36	RRX	h	101	-	42,42,42	1.33	8 (19%)	56,58,58	1.39	9 (16%)
31	LMT	D	412	-	36,36,36	1.17	5 (13%)	47,47,47	0.95	1 (2%)
31	LMT	D	410	-	24,24,36	0.99	2 (8%)	29,29,47	1.21	4 (13%)
28	LMG	H	105	-	47,47,55	1.41	6 (12%)	55,55,63	1.39	7 (12%)
31	LMT	I	104	-	22,22,36	1.05	2 (9%)	27,27,47	1.05	0
22	OEX	A	401	3,1,38	0,14,14	-	-	-	-	-
25	CLA	A	405	1	69,73,73	2.16	21 (30%)	82,113,113	2.48	27 (32%)
28	LMG	c	519	-	51,51,55	1.47	8 (15%)	59,59,63	1.12	3 (5%)
30	SQD	A	412	-	52,54,54	0.96	3 (5%)	62,65,65	1.69	15 (24%)
31	LMT	D	411	-	36,36,36	1.17	5 (13%)	47,47,47	0.92	0
22	OEX	a	401	3,1,38	0,14,14	-	-	-	-	-
25	CLA	B	611	2	69,73,73	2.19	20 (28%)	82,113,113	2.40	26 (31%)
34	DGD	C	517	-	63,63,67	1.33	8 (12%)	77,77,81	1.08	5 (6%)
31	LMT	T	101	-	24,24,36	1.09	2 (8%)	29,29,47	1.16	2 (6%)
31	LMT	a	415	-	36,36,36	1.19	5 (13%)	47,47,47	1.01	3 (6%)
28	LMG	a	414	-	36,36,55	1.12	2 (5%)	44,44,63	1.19	3 (6%)
25	CLA	b	610	38	69,73,73	2.26	22 (31%)	82,113,113	2.47	32 (39%)

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
28	LMG	d	409	-	-	14/38/58/70	0/1/1/1
33	LHG	d	408	-	-	24/53/53/53	-
30	SQD	b	620	-	-	24/49/69/69	0/1/1/1
25	CLA	b	614	2	-	14/39/115/115	-
29	PL9	D	405	-	-	9/53/73/73	0/1/1/1
25	CLA	c	514	3	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	c	524	-	-	10/21/61/61	0/2/2/2
25	CLA	c	504	3	-	5/39/115/115	-
27	BCR	b	618	-	-	6/29/63/63	0/2/2/2
25	CLA	b	608	2	-	8/39/115/115	-
31	LMT	e	101	-	-	5/13/33/61	0/1/1/2
25	CLA	c	502	3	-	12/39/115/115	-
31	LMT	X	103	-	-	3/13/33/61	0/1/1/2
31	LMT	x	105	-	-	6/10/30/61	0/1/1/2
33	LHG	z	102	-	-	24/37/37/53	-
31	LMT	M	102	-	-	4/15/35/61	0/1/1/2
25	CLA	d	401	38	-	10/39/115/115	-
25	CLA	b	616	2	-	16/33/109/115	-
25	CLA	c	506	3	-	11/27/103/115	-
27	BCR	C	515	-	-	9/29/63/63	0/2/2/2
31	LMT	E	103	-	-	9/21/61/61	0/2/2/2
25	CLA	c	512	3	-	19/39/115/115	-
31	LMT	C	522	-	-	7/15/35/61	0/1/1/2
33	LHG	B	627	-	-	30/53/53/53	-
31	LMT	i	104	-	-	9/13/33/61	0/1/1/2
25	CLA	C	506	3	-	11/27/103/115	-
27	BCR	B	618	-	-	6/29/63/63	0/2/2/2
25	CLA	B	613	2	-	8/39/115/115	-
25	CLA	b	607	38	-	11/39/115/115	-
28	LMG	D	409	-	-	14/38/58/70	0/1/1/1
25	CLA	C	512	3	-	19/39/115/115	-
31	LMT	y	101	-	-	7/12/32/61	0/1/1/2
30	SQD	A	413	-	-	22/43/63/69	0/1/1/1
25	CLA	C	508	38	-	12/39/115/115	-
25	CLA	C	505	38	-	13/39/115/115	-
33	LHG	B	628	-	-	24/53/53/53	-
30	SQD	B	620	-	-	24/49/69/69	0/1/1/1
31	LMT	E	101	-	-	5/13/33/61	0/1/1/2
31	LMT	X	105	-	-	6/10/30/61	0/1/1/2
25	CLA	B	604	2	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	i	102	-	-	8/15/35/61	0/1/1/2
31	LMT	x	101	-	-	6/15/35/61	0/1/1/2
33	LHG	Z	102	-	-	24/37/37/53	-
27	BCR	F	101	-	-	9/29/63/63	0/2/2/2
28	LMG	C	523	-	-	17/44/64/70	0/1/1/1
25	CLA	b	612	2	-	10/39/115/115	-
31	LMT	x	104	-	-	7/10/30/61	0/1/1/2
28	LMG	A	414	-	-	6/31/51/70	0/1/1/1
31	LMT	A	416	-	-	5/15/35/61	0/1/1/2
31	LMT	h	102	-	-	9/15/35/61	0/1/1/2
25	CLA	B	605	2	-	11/39/115/115	-
31	LMT	B	624	-	-	9/15/35/61	0/1/1/2
25	CLA	B	614	2	-	14/39/115/115	-
25	CLA	A	408	1	-	14/33/109/115	-
25	CLA	b	605	2	-	11/39/115/115	-
25	CLA	b	601	38	-	3/15/91/115	-
33	LHG	D	406	-	-	24/53/53/53	-
31	LMT	X	102	-	-	9/12/32/61	0/1/1/2
26	PHO	a	407	-	-	7/37/103/103	0/5/6/6
31	LMT	H	102	-	-	9/15/35/61	0/1/1/2
27	BCR	k	103	-	-	8/29/63/63	0/2/2/2
31	LMT	e	103	-	-	9/21/61/61	0/2/2/2
25	CLA	C	513	3	-	7/21/97/115	-
30	SQD	k	101	-	-	21/35/55/69	0/1/1/1
31	LMT	I	101	-	-	11/15/35/61	0/1/1/2
31	LMT	x	103	-	-	3/13/33/61	0/1/1/2
30	SQD	a	413	-	-	22/43/63/69	0/1/1/1
31	LMT	b	625	-	-	11/21/61/61	0/2/2/2
31	LMT	t	101	-	-	11/15/35/61	0/1/1/2
27	BCR	b	619	-	-	11/29/63/63	0/2/2/2
27	BCR	B	617	-	-	6/29/63/63	0/2/2/2
31	LMT	C	524	-	-	10/21/61/61	0/2/2/2
35	HEM	v	201	18	-	2/14/54/54	-
31	LMT	d	410	-	-	8/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	K	102	-	-	15/29/63/63	0/2/2/2
25	CLA	c	510	3	-	11/39/115/115	-
25	CLA	c	507	3	-	16/39/115/115	-
31	LMT	I	102	-	-	8/15/35/61	0/1/1/2
36	RRX	H	101	-	-	15/29/65/65	0/2/2/2
28	LMG	A	410	-	-	22/46/66/70	0/1/1/1
31	LMT	M	101	-	-	10/21/61/61	0/2/2/2
27	BCR	c	515	-	-	9/29/63/63	0/2/2/2
31	LMT	m	102	-	-	4/15/35/61	0/1/1/2
25	CLA	d	403	4	-	9/39/115/115	-
25	CLA	C	510	3	-	11/39/115/115	-
25	CLA	c	508	38	-	12/39/115/115	-
28	LMG	a	410	-	-	22/46/66/70	0/1/1/1
31	LMT	c	522	-	-	7/15/35/61	0/1/1/2
31	LMT	I	103	-	-	7/21/61/61	0/2/2/2
28	LMG	B	621	-	-	7/46/66/70	0/1/1/1
25	CLA	B	610	38	-	10/39/115/115	-
33	LHG	d	407	-	-	25/53/53/53	-
25	CLA	d	404	4	-	13/39/115/115	-
31	LMT	Y	101	-	-	7/12/32/61	0/1/1/2
27	BCR	z	101	-	-	8/29/63/63	0/2/2/2
31	LMT	d	412	-	-	7/21/61/61	0/2/2/2
31	LMT	x	102	-	-	9/12/32/61	0/1/1/2
25	CLA	B	608	2	-	8/39/115/115	-
25	CLA	c	511	3	-	11/39/115/115	-
30	SQD	K	101	-	-	21/35/55/69	0/1/1/1
31	LMT	j	101	-	-	11/15/35/61	0/1/1/2
25	CLA	b	609	2	-	14/39/115/115	-
34	DGD	H	104	-	-	11/51/91/95	0/2/2/2
34	DGD	c	516	-	-	14/51/91/95	0/2/2/2
34	DGD	c	518	-	-	16/51/91/95	0/2/2/2
30	SQD	C	501	-	-	28/49/69/69	0/1/1/1
28	LMG	h	105	-	-	17/42/62/70	0/1/1/1
26	PHO	A	407	-	-	7/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	J	101	-	-	11/15/35/61	0/1/1/2
31	LMT	i	101	-	-	11/15/35/61	0/1/1/2
30	SQD	F	102	-	-	16/29/49/69	0/1/1/1
30	SQD	f	102	-	-	16/29/49/69	0/1/1/1
34	DGD	c	517	-	-	17/51/91/95	0/2/2/2
27	BCR	a	409	-	-	9/29/63/63	0/2/2/2
31	LMT	B	629	-	-	10/21/61/61	0/2/2/2
25	CLA	B	615	2	-	12/39/115/115	-
31	LMT	b	629	-	-	10/21/61/61	0/2/2/2
25	CLA	b	602	2	-	17/39/115/115	-
27	BCR	b	617	-	-	6/29/63/63	0/2/2/2
31	LMT	X	104	-	-	7/10/30/61	0/1/1/2
31	LMT	b	623	-	-	11/21/61/61	0/2/2/2
31	LMT	K	105	-	-	13/21/61/61	0/2/2/2
33	LHG	e	102	-	-	29/44/44/53	-
34	DGD	C	516	-	-	14/51/91/95	0/2/2/2
30	SQD	h	103	-	-	16/49/69/69	0/1/1/1
25	CLA	b	606	2	-	9/33/109/115	-
31	LMT	C	525	-	-	8/12/32/61	0/1/1/2
31	LMT	f	103	-	-	11/21/61/61	0/2/2/2
25	CLA	c	503	3	-	9/39/115/115	-
33	LHG	b	628	-	-	24/53/53/53	-
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
25	CLA	b	604	2	-	11/39/115/115	-
27	BCR	B	619	-	-	11/29/63/63	0/2/2/2
25	CLA	a	406	38	-	11/39/115/115	-
33	LHG	E	102	-	-	29/44/44/53	-
30	SQD	c	501	-	-	28/49/69/69	0/1/1/1
25	CLA	B	609	2	-	14/39/115/115	-
31	LMT	d	411	-	-	10/21/61/61	0/2/2/2
25	CLA	C	507	3	-	16/39/115/115	-
31	LMT	A	415	-	-	10/21/61/61	0/2/2/2
25	CLA	B	612	2	-	10/39/115/115	-
31	LMT	B	625	-	-	11/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	603	2	-	17/39/115/115	-
25	CLA	b	613	2	-	8/39/115/115	-
31	LMT	b	624	-	-	9/15/35/61	0/1/1/2
27	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
25	CLA	B	607	38	-	11/39/115/115	-
25	CLA	B	603	2	-	17/39/115/115	-
31	LMT	B	626	-	-	5/15/35/61	0/1/1/2
28	LMG	C	519	-	-	17/46/66/70	0/1/1/1
27	BCR	f	101	-	-	9/29/63/63	0/2/2/2
31	LMT	m	101	-	-	10/21/61/61	0/2/2/2
31	LMT	X	101	-	-	6/15/35/61	0/1/1/2
30	SQD	a	412	-	-	26/49/69/69	0/1/1/1
31	LMT	b	626	-	-	5/15/35/61	0/1/1/2
25	CLA	b	611	2	-	9/39/115/115	-
25	CLA	c	505	38	-	13/39/115/115	-
25	CLA	c	513	3	-	7/21/97/115	-
29	PL9	a	411	-	-	18/53/73/73	0/1/1/1
25	CLA	B	602	2	-	17/39/115/115	-
31	LMT	B	623	-	-	11/21/61/61	0/2/2/2
31	LMT	k	105	-	-	13/21/61/61	0/2/2/2
35	HEM	V	201	18	-	2/14/54/54	-
25	CLA	C	502	3	-	12/39/115/115	-
31	LMT	F	103	-	-	11/21/61/61	0/2/2/2
31	LMT	a	416	-	-	5/15/35/61	0/1/1/2
25	CLA	c	509	3	-	9/39/115/115	-
25	CLA	A	406	38	-	11/39/115/115	-
29	PL9	A	411	-	-	18/53/73/73	0/1/1/1
31	LMT	c	525	-	-	8/12/32/61	0/1/1/2
27	BCR	A	409	-	-	9/29/63/63	0/2/2/2
25	CLA	C	511	3	-	11/39/115/115	-
33	LHG	D	407	-	-	25/53/53/53	-
25	CLA	B	606	2	-	9/33/109/115	-
28	LMG	c	523	-	-	17/44/64/70	0/1/1/1
25	CLA	C	504	3	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	k	102	-	-	15/29/63/63	0/2/2/2
33	LHG	d	406	-	-	24/53/53/53	-
34	DGD	h	104	-	-	11/51/91/95	0/2/2/2
35	HEM	E	104	5,6	-	7/14/54/54	-
25	CLA	D	403	4	-	9/39/115/115	-
33	LHG	b	627	-	-	30/53/53/53	-
25	CLA	D	404	4	-	13/39/115/115	-
25	CLA	B	601	38	-	3/15/91/115	-
34	DGD	C	518	-	-	16/51/91/95	0/2/2/2
25	CLA	a	405	1	-	9/39/115/115	-
33	LHG	D	408	-	-	24/53/53/53	-
25	CLA	C	514	3	-	17/39/115/115	-
31	LMT	i	103	-	-	7/21/61/61	0/2/2/2
25	CLA	b	615	2	-	12/39/115/115	-
35	HEM	e	104	5,6	-	7/14/54/54	-
25	CLA	C	503	3	-	9/39/115/115	-
28	LMG	b	621	-	-	7/46/66/70	0/1/1/1
29	PL9	d	405	-	-	9/53/73/73	0/1/1/1
30	SQD	H	103	-	-	16/49/69/69	0/1/1/1
27	BCR	K	103	-	-	8/29/63/63	0/2/2/2
25	CLA	a	408	1	-	14/33/109/115	-
25	CLA	B	616	2	-	16/33/109/115	-
25	CLA	C	509	3	-	9/39/115/115	-
25	CLA	D	401	38	-	9/39/115/115	-
26	PHO	D	402	-	-	4/37/103/103	0/5/6/6
36	RRX	h	101	-	-	15/29/65/65	0/2/2/2
31	LMT	D	412	-	-	7/21/61/61	0/2/2/2
31	LMT	D	410	-	-	8/15/35/61	0/1/1/2
28	LMG	H	105	-	-	17/42/62/70	0/1/1/1
31	LMT	I	104	-	-	9/13/33/61	0/1/1/2
25	CLA	A	405	1	-	9/39/115/115	-
28	LMG	c	519	-	-	17/46/66/70	0/1/1/1
30	SQD	A	412	-	-	26/49/69/69	0/1/1/1
31	LMT	D	411	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	611	2	-	9/39/115/115	-
34	DGD	C	517	-	-	17/51/91/95	0/2/2/2
31	LMT	T	101	-	-	11/15/35/61	0/1/1/2
31	LMT	a	415	-	-	10/21/61/61	0/2/2/2
28	LMG	a	414	-	-	6/31/51/70	0/1/1/1
25	CLA	b	610	38	-	10/39/115/115	-

All (2179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	402	PHO	C3B-C4B	9.27	1.50	1.41
26	d	402	PHO	C3B-C4B	9.27	1.50	1.41
26	D	402	PHO	C1B-C2B	9.24	1.49	1.39
26	d	402	PHO	C1B-C2B	9.24	1.49	1.39
26	A	407	PHO	C1B-C2B	9.12	1.49	1.39
26	a	407	PHO	C1B-C2B	9.12	1.49	1.39
26	a	407	PHO	C3B-C4B	8.74	1.50	1.41
27	Z	101	BCR	C8-C9	-8.72	1.27	1.46
27	z	101	BCR	C8-C9	-8.72	1.27	1.46
26	A	407	PHO	C3B-C4B	8.69	1.50	1.41
27	B	619	BCR	C8-C9	-8.48	1.27	1.46
27	b	619	BCR	C8-C9	-8.48	1.27	1.46
27	B	617	BCR	C8-C9	-8.48	1.27	1.46
27	b	617	BCR	C8-C9	-8.48	1.27	1.46
27	B	618	BCR	C8-C9	-8.47	1.27	1.46
27	b	618	BCR	C8-C9	-8.47	1.27	1.46
27	C	515	BCR	C8-C9	-8.36	1.28	1.46
27	c	515	BCR	C8-C9	-8.36	1.28	1.46
27	K	103	BCR	C8-C9	-8.25	1.28	1.46
27	k	103	BCR	C8-C9	-8.25	1.28	1.46
27	A	409	BCR	C8-C9	-8.21	1.28	1.46
27	a	409	BCR	C8-C9	-8.21	1.28	1.46
27	B	619	BCR	C11-C10	-8.20	1.17	1.43
27	b	619	BCR	C11-C10	-8.20	1.17	1.43
27	B	617	BCR	C11-C10	-8.14	1.17	1.43
27	b	617	BCR	C11-C10	-8.14	1.17	1.43
27	B	618	BCR	C11-C10	-8.08	1.18	1.43
27	b	618	BCR	C11-C10	-8.08	1.18	1.43
27	K	102	BCR	C8-C9	-8.08	1.28	1.46
27	k	102	BCR	C8-C9	-8.08	1.28	1.46
27	C	515	BCR	C11-C10	-8.07	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	515	BCR	C11-C10	-8.06	1.18	1.43
27	K	103	BCR	C11-C10	-8.06	1.18	1.43
27	k	103	BCR	C11-C10	-8.06	1.18	1.43
27	F	101	BCR	C8-C9	-8.04	1.28	1.46
27	f	101	BCR	C8-C9	-8.04	1.28	1.46
25	C	504	CLA	MG-NA	8.01	2.25	2.06
25	c	504	CLA	MG-NA	8.01	2.25	2.06
27	A	409	BCR	C11-C10	-7.98	1.18	1.43
27	a	409	BCR	C11-C10	-7.98	1.18	1.43
27	F	101	BCR	C11-C10	-7.88	1.18	1.43
27	f	101	BCR	C11-C10	-7.88	1.18	1.43
27	Z	101	BCR	C11-C10	-7.85	1.18	1.43
27	z	101	BCR	C11-C10	-7.85	1.18	1.43
27	K	102	BCR	C11-C10	-7.82	1.18	1.43
27	k	102	BCR	C11-C10	-7.82	1.18	1.43
25	B	609	CLA	MG-NA	7.76	2.24	2.06
25	b	609	CLA	MG-NA	7.76	2.24	2.06
27	K	102	BCR	C20-C21	-7.69	1.19	1.43
27	k	102	BCR	C20-C21	-7.69	1.19	1.43
25	B	606	CLA	MG-NA	7.68	2.24	2.06
25	b	606	CLA	MG-NA	7.67	2.24	2.06
25	C	508	CLA	MG-NA	7.64	2.24	2.06
25	c	508	CLA	MG-NA	7.64	2.24	2.06
25	B	601	CLA	MG-NA	7.60	2.24	2.06
25	b	601	CLA	MG-NA	7.60	2.24	2.06
25	B	610	CLA	MG-NA	7.58	2.24	2.06
25	b	610	CLA	MG-NA	7.58	2.24	2.06
27	B	618	BCR	C20-C21	-7.51	1.19	1.43
27	b	618	BCR	C20-C21	-7.51	1.19	1.43
25	B	604	CLA	MG-NA	7.47	2.24	2.06
27	B	617	BCR	C20-C21	-7.47	1.20	1.43
27	b	617	BCR	C20-C21	-7.47	1.20	1.43
25	c	507	CLA	MG-NA	7.46	2.24	2.06
25	C	507	CLA	MG-NA	7.46	2.24	2.06
27	B	619	BCR	C20-C21	-7.46	1.20	1.43
27	b	619	BCR	C20-C21	-7.46	1.20	1.43
25	b	603	CLA	MG-NA	7.46	2.24	2.06
27	A	409	BCR	C20-C21	-7.45	1.20	1.43
27	a	409	BCR	C20-C21	-7.45	1.20	1.43
27	B	618	BCR	C16-C17	-7.45	1.20	1.43
27	b	618	BCR	C16-C17	-7.45	1.20	1.43
25	B	603	CLA	MG-NA	7.45	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	604	CLA	MG-NA	7.45	2.24	2.06
25	B	608	CLA	MG-NA	7.44	2.23	2.06
25	C	509	CLA	MG-NA	7.44	2.23	2.06
25	b	608	CLA	MG-NA	7.43	2.23	2.06
25	c	509	CLA	MG-NA	7.42	2.23	2.06
27	C	515	BCR	C20-C21	-7.42	1.20	1.43
27	c	515	BCR	C20-C21	-7.42	1.20	1.43
25	c	512	CLA	MG-NA	7.39	2.23	2.06
25	C	512	CLA	MG-NA	7.39	2.23	2.06
25	B	602	CLA	MG-NA	7.39	2.23	2.06
25	b	602	CLA	MG-NA	7.39	2.23	2.06
27	B	619	BCR	C16-C17	-7.38	1.20	1.43
27	b	619	BCR	C16-C17	-7.38	1.20	1.43
25	C	510	CLA	MG-NA	7.37	2.23	2.06
25	C	513	CLA	MG-NA	7.36	2.23	2.06
25	c	513	CLA	MG-NA	7.36	2.23	2.06
25	C	502	CLA	MG-NA	7.35	2.23	2.06
25	c	510	CLA	MG-NA	7.34	2.23	2.06
27	C	515	BCR	C16-C17	-7.34	1.20	1.43
27	k	103	BCR	C20-C21	-7.34	1.20	1.43
27	c	515	BCR	C16-C17	-7.33	1.20	1.43
27	B	617	BCR	C16-C17	-7.33	1.20	1.43
27	b	617	BCR	C16-C17	-7.33	1.20	1.43
25	B	611	CLA	MG-NA	7.33	2.23	2.06
25	b	611	CLA	MG-NA	7.33	2.23	2.06
27	z	101	BCR	C16-C17	-7.33	1.20	1.43
25	c	502	CLA	MG-NA	7.33	2.23	2.06
25	a	406	CLA	MG-NA	7.32	2.23	2.06
27	K	103	BCR	C20-C21	-7.31	1.20	1.43
27	A	409	BCR	C16-C17	-7.31	1.20	1.43
25	C	511	CLA	MG-NA	7.31	2.23	2.06
25	c	511	CLA	MG-NA	7.31	2.23	2.06
27	a	409	BCR	C16-C17	-7.30	1.20	1.43
27	Z	101	BCR	C16-C17	-7.30	1.20	1.43
27	K	103	BCR	C16-C17	-7.30	1.20	1.43
27	k	103	BCR	C16-C17	-7.30	1.20	1.43
25	A	406	CLA	MG-NA	7.28	2.23	2.06
27	Z	101	BCR	C20-C21	-7.26	1.20	1.43
27	z	101	BCR	C20-C21	-7.26	1.20	1.43
25	B	615	CLA	MG-NA	7.24	2.23	2.06
25	b	615	CLA	MG-NA	7.24	2.23	2.06
25	C	514	CLA	MG-NA	7.24	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	514	CLA	MG-NA	7.24	2.23	2.06
27	F	101	BCR	C20-C21	-7.23	1.20	1.43
27	f	101	BCR	C20-C21	-7.23	1.20	1.43
25	c	506	CLA	MG-NA	7.22	2.23	2.06
25	D	404	CLA	MG-NA	7.22	2.23	2.06
25	d	404	CLA	MG-NA	7.22	2.23	2.06
25	a	408	CLA	MG-NA	7.21	2.23	2.06
25	C	506	CLA	MG-NA	7.21	2.23	2.06
25	B	614	CLA	MG-NA	7.20	2.23	2.06
25	b	614	CLA	MG-NA	7.20	2.23	2.06
25	A	408	CLA	MG-NA	7.18	2.23	2.06
27	F	101	BCR	C16-C17	-7.18	1.20	1.43
27	f	101	BCR	C16-C17	-7.18	1.20	1.43
25	B	612	CLA	MG-NA	7.15	2.23	2.06
25	b	612	CLA	MG-NA	7.15	2.23	2.06
25	C	503	CLA	MG-NA	7.14	2.23	2.06
25	c	503	CLA	MG-NA	7.14	2.23	2.06
27	k	102	BCR	C16-C17	-7.13	1.21	1.43
27	K	102	BCR	C16-C17	-7.13	1.21	1.43
25	B	613	CLA	MG-NA	7.05	2.23	2.06
25	b	613	CLA	MG-NA	7.05	2.23	2.06
25	B	605	CLA	MG-NA	7.03	2.23	2.06
25	b	605	CLA	MG-NA	7.03	2.23	2.06
25	B	607	CLA	MG-NA	6.95	2.22	2.06
25	b	607	CLA	MG-NA	6.95	2.22	2.06
25	D	403	CLA	MG-NA	6.95	2.22	2.06
25	d	403	CLA	MG-NA	6.95	2.22	2.06
25	C	505	CLA	MG-NA	6.94	2.22	2.06
25	D	401	CLA	MG-NA	6.93	2.22	2.06
25	c	505	CLA	MG-NA	6.93	2.22	2.06
25	d	401	CLA	MG-NA	6.89	2.22	2.06
25	B	616	CLA	MG-NA	6.85	2.22	2.06
25	b	616	CLA	MG-NA	6.85	2.22	2.06
25	A	405	CLA	MG-NA	6.78	2.22	2.06
25	a	405	CLA	MG-NA	6.78	2.22	2.06
25	C	505	CLA	O2A-C1	5.45	1.60	1.46
25	a	408	CLA	O2A-C1	5.45	1.60	1.46
25	A	408	CLA	O2A-C1	5.44	1.60	1.46
25	D	401	CLA	O2A-C1	5.44	1.60	1.46
25	d	401	CLA	O2A-C1	5.44	1.60	1.46
25	c	505	CLA	O2A-C1	5.43	1.60	1.46
25	b	610	CLA	O2A-C1	5.42	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	610	CLA	O2A-C1	5.41	1.60	1.46
25	B	607	CLA	O2A-C1	5.39	1.60	1.46
25	b	607	CLA	O2A-C1	5.39	1.60	1.46
25	c	510	CLA	O2A-C1	5.39	1.60	1.46
25	C	508	CLA	O2A-C1	5.37	1.60	1.46
25	C	510	CLA	O2A-C1	5.36	1.60	1.46
25	C	513	CLA	O2A-C1	5.36	1.60	1.46
25	c	513	CLA	O2A-C1	5.35	1.60	1.46
25	A	406	CLA	O2A-C1	5.35	1.60	1.46
25	c	508	CLA	O2A-C1	5.35	1.60	1.46
25	b	614	CLA	O2A-C1	5.32	1.60	1.46
25	C	504	CLA	O2A-C1	5.32	1.60	1.46
25	c	504	CLA	O2A-C1	5.32	1.60	1.46
25	B	603	CLA	O2A-C1	5.32	1.60	1.46
25	b	603	CLA	O2A-C1	5.32	1.60	1.46
25	C	514	CLA	O2A-C1	5.31	1.60	1.46
25	a	406	CLA	O2A-C1	5.31	1.60	1.46
25	B	614	CLA	O2A-C1	5.30	1.60	1.46
25	c	514	CLA	O2A-C1	5.30	1.60	1.46
25	C	509	CLA	O2A-C1	5.29	1.60	1.46
25	C	503	CLA	O2A-C1	5.28	1.60	1.46
25	c	503	CLA	O2A-C1	5.28	1.60	1.46
25	c	509	CLA	O2A-C1	5.26	1.60	1.46
25	B	602	CLA	O2A-C1	5.26	1.60	1.46
25	b	602	CLA	O2A-C1	5.26	1.60	1.46
25	b	606	CLA	O2A-C1	5.24	1.60	1.46
25	B	606	CLA	O2A-C1	5.24	1.60	1.46
25	B	608	CLA	O2A-C1	5.24	1.60	1.46
25	b	608	CLA	O2A-C1	5.24	1.60	1.46
25	b	616	CLA	O2A-C1	5.20	1.60	1.46
25	D	404	CLA	O2A-C1	5.20	1.60	1.46
25	d	404	CLA	O2A-C1	5.20	1.60	1.46
25	B	613	CLA	O2A-C1	5.19	1.60	1.46
25	b	613	CLA	O2A-C1	5.19	1.60	1.46
25	C	507	CLA	O2A-C1	5.19	1.60	1.46
25	c	507	CLA	O2A-C1	5.19	1.60	1.46
25	b	609	CLA	O2A-C1	5.18	1.60	1.46
25	B	609	CLA	O2A-C1	5.18	1.60	1.46
35	e	104	HEM	FE-NB	5.18	2.10	1.94
25	C	512	CLA	O2A-C1	5.17	1.60	1.46
25	c	512	CLA	O2A-C1	5.17	1.60	1.46
35	E	104	HEM	FE-NB	5.17	2.10	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	616	CLA	O2A-C1	5.16	1.60	1.46
25	C	514	CLA	O2D-CGD	5.15	1.45	1.33
25	c	514	CLA	O2D-CGD	5.15	1.45	1.33
25	B	615	CLA	O2A-C1	5.15	1.60	1.46
25	b	615	CLA	O2A-C1	5.15	1.60	1.46
25	C	502	CLA	O2A-C1	5.15	1.60	1.46
25	c	502	CLA	O2A-C1	5.13	1.59	1.46
25	B	604	CLA	O2A-C1	5.13	1.59	1.46
25	b	604	CLA	O2A-C1	5.13	1.59	1.46
25	B	605	CLA	O2A-C1	5.11	1.59	1.46
25	b	605	CLA	O2A-C1	5.11	1.59	1.46
25	C	509	CLA	O2D-CGD	5.10	1.45	1.33
25	c	509	CLA	O2D-CGD	5.10	1.45	1.33
25	B	611	CLA	O2D-CGD	5.09	1.45	1.33
25	b	611	CLA	O2D-CGD	5.09	1.45	1.33
25	b	606	CLA	O2D-CGD	5.08	1.45	1.33
25	C	511	CLA	O2A-C1	5.08	1.59	1.46
25	c	511	CLA	O2A-C1	5.08	1.59	1.46
25	A	406	CLA	O2D-CGD	5.07	1.45	1.33
25	a	406	CLA	O2D-CGD	5.07	1.45	1.33
25	A	405	CLA	O2A-C1	5.06	1.59	1.46
25	a	405	CLA	O2A-C1	5.06	1.59	1.46
25	C	506	CLA	O2A-C1	5.06	1.59	1.46
25	B	606	CLA	O2D-CGD	5.06	1.45	1.33
25	c	503	CLA	O2D-CGD	5.05	1.45	1.33
25	c	506	CLA	O2A-C1	5.04	1.59	1.46
25	C	507	CLA	O2D-CGD	5.03	1.45	1.33
25	c	507	CLA	O2D-CGD	5.03	1.45	1.33
25	C	503	CLA	O2D-CGD	5.02	1.45	1.33
25	B	601	CLA	O2D-CGD	5.02	1.45	1.33
25	b	601	CLA	O2D-CGD	5.02	1.45	1.33
25	b	612	CLA	O2A-C1	5.01	1.59	1.46
25	C	512	CLA	O2D-CGD	5.01	1.45	1.33
25	c	512	CLA	O2D-CGD	5.01	1.45	1.33
25	b	612	CLA	O2D-CGD	5.00	1.45	1.33
25	c	502	CLA	O2D-CGD	5.00	1.45	1.33
25	B	612	CLA	O2D-CGD	4.99	1.45	1.33
25	b	607	CLA	O2D-CGD	4.99	1.45	1.33
25	C	506	CLA	O2D-CGD	4.99	1.45	1.33
25	c	506	CLA	O2D-CGD	4.99	1.45	1.33
25	B	612	CLA	O2A-C1	4.99	1.59	1.46
25	A	405	CLA	O2D-CGD	4.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	405	CLA	O2D-CGD	4.99	1.45	1.33
25	d	403	CLA	O2A-C1	4.99	1.59	1.46
25	D	401	CLA	O2D-CGD	4.98	1.45	1.33
25	B	607	CLA	O2D-CGD	4.98	1.45	1.33
25	B	609	CLA	O2D-CGD	4.98	1.45	1.33
25	C	502	CLA	O2D-CGD	4.98	1.45	1.33
25	b	609	CLA	O2D-CGD	4.98	1.45	1.33
25	D	403	CLA	O2A-C1	4.98	1.59	1.46
25	d	401	CLA	O2D-CGD	4.96	1.45	1.33
25	B	605	CLA	O2D-CGD	4.94	1.45	1.33
25	b	605	CLA	O2D-CGD	4.94	1.45	1.33
25	B	608	CLA	O2D-CGD	4.94	1.45	1.33
25	b	608	CLA	O2D-CGD	4.93	1.45	1.33
25	B	616	CLA	O2D-CGD	4.93	1.45	1.33
25	b	616	CLA	O2D-CGD	4.93	1.45	1.33
25	c	505	CLA	O2D-CGD	4.93	1.45	1.33
25	B	604	CLA	O2D-CGD	4.93	1.45	1.33
25	b	604	CLA	O2D-CGD	4.93	1.45	1.33
25	C	505	CLA	O2D-CGD	4.93	1.45	1.33
25	C	513	CLA	O2D-CGD	4.91	1.45	1.33
25	c	513	CLA	O2D-CGD	4.91	1.45	1.33
25	C	514	CLA	CHC-C1C	4.90	1.48	1.38
25	B	610	CLA	O2D-CGD	4.90	1.45	1.33
25	b	610	CLA	O2D-CGD	4.90	1.45	1.33
25	B	611	CLA	O2A-C1	4.89	1.59	1.46
25	b	611	CLA	O2A-C1	4.89	1.59	1.46
25	c	514	CLA	CHC-C1C	4.88	1.48	1.38
25	A	408	CLA	O2D-CGD	4.87	1.45	1.33
25	a	408	CLA	O2D-CGD	4.87	1.45	1.33
25	c	511	CLA	O2D-CGD	4.86	1.45	1.33
25	B	603	CLA	O2D-CGD	4.84	1.45	1.33
25	b	603	CLA	O2D-CGD	4.84	1.45	1.33
25	C	511	CLA	O2D-CGD	4.83	1.45	1.33
25	D	404	CLA	O2D-CGD	4.80	1.45	1.33
25	d	404	CLA	O2D-CGD	4.80	1.45	1.33
25	A	405	CLA	C3D-C4D	-4.79	1.33	1.44
25	a	405	CLA	C3D-C4D	-4.79	1.33	1.44
25	B	613	CLA	O2D-CGD	4.79	1.45	1.33
25	b	613	CLA	O2D-CGD	4.79	1.45	1.33
25	B	615	CLA	O2D-CGD	4.78	1.45	1.33
25	b	615	CLA	O2D-CGD	4.78	1.45	1.33
25	C	508	CLA	O2D-CGD	4.77	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	508	CLA	O2D-CGD	4.77	1.45	1.33
25	B	602	CLA	CHC-C1C	4.76	1.48	1.38
25	b	602	CLA	CHC-C1C	4.76	1.48	1.38
25	B	603	CLA	C3D-C4D	-4.74	1.33	1.44
25	D	403	CLA	C1D-ND	-4.74	1.31	1.37
25	d	403	CLA	C1D-ND	-4.74	1.31	1.37
25	C	506	CLA	C3D-C4D	-4.72	1.33	1.44
25	c	506	CLA	C3D-C4D	-4.72	1.33	1.44
25	c	509	CLA	CHC-C1C	4.72	1.47	1.38
25	B	606	CLA	CHC-C1C	4.72	1.47	1.38
25	b	606	CLA	CHC-C1C	4.72	1.47	1.38
25	C	509	CLA	CHC-C1C	4.71	1.47	1.38
25	b	603	CLA	C3D-C4D	-4.71	1.33	1.44
25	A	405	CLA	CHC-C1C	4.70	1.47	1.38
25	a	405	CLA	CHC-C1C	4.70	1.47	1.38
25	B	614	CLA	O2D-CGD	4.70	1.44	1.33
25	b	614	CLA	O2D-CGD	4.70	1.44	1.33
25	b	612	CLA	C1D-ND	-4.69	1.31	1.37
25	C	504	CLA	CHC-C1C	4.69	1.47	1.38
25	c	504	CLA	CHC-C1C	4.69	1.47	1.38
35	V	201	HEM	FE-NC	4.69	2.10	1.95
35	v	201	HEM	FE-NC	4.69	2.10	1.95
25	B	612	CLA	C1D-ND	-4.69	1.31	1.37
25	B	602	CLA	O2D-CGD	4.67	1.44	1.33
25	b	602	CLA	O2D-CGD	4.67	1.44	1.33
25	D	403	CLA	CHC-C1C	4.66	1.47	1.38
25	d	403	CLA	CHC-C1C	4.66	1.47	1.38
25	D	403	CLA	O2D-CGD	4.66	1.44	1.33
25	D	404	CLA	CHC-C1C	4.66	1.47	1.38
25	d	404	CLA	CHC-C1C	4.66	1.47	1.38
25	d	403	CLA	O2D-CGD	4.65	1.44	1.33
25	C	506	CLA	CHC-C1C	4.63	1.47	1.38
25	c	506	CLA	CHC-C1C	4.63	1.47	1.38
25	b	612	CLA	CHC-C1C	4.62	1.47	1.38
25	B	612	CLA	CHC-C1C	4.62	1.47	1.38
25	C	510	CLA	O2D-CGD	4.62	1.44	1.33
25	c	510	CLA	O2D-CGD	4.62	1.44	1.33
25	A	406	CLA	C3D-C4D	-4.59	1.33	1.44
25	a	406	CLA	C3D-C4D	-4.59	1.33	1.44
25	C	512	CLA	CHC-C1C	4.59	1.47	1.38
25	B	605	CLA	CHC-C1C	4.59	1.47	1.38
25	b	605	CLA	CHC-C1C	4.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	512	CLA	CHC-C1C	4.59	1.47	1.38
25	B	608	CLA	CHD-C1D	4.58	1.47	1.38
25	b	608	CLA	CHD-C1D	4.58	1.47	1.38
27	B	619	BCR	C10-C9	-4.57	1.25	1.35
27	b	619	BCR	C10-C9	-4.57	1.25	1.35
25	B	614	CLA	CHC-C1C	4.57	1.47	1.38
25	b	614	CLA	CHC-C1C	4.57	1.47	1.38
27	b	617	BCR	C10-C9	-4.57	1.25	1.35
25	D	401	CLA	C3C-C2C	4.57	1.46	1.36
25	d	401	CLA	C3C-C2C	4.57	1.46	1.36
25	C	504	CLA	O2D-CGD	4.56	1.44	1.33
25	c	504	CLA	O2D-CGD	4.56	1.44	1.33
25	C	502	CLA	CHC-C1C	4.56	1.47	1.38
27	B	617	BCR	C10-C9	-4.55	1.25	1.35
25	b	606	CLA	CHD-C1D	4.55	1.47	1.38
25	C	504	CLA	C3C-C2C	4.55	1.46	1.36
25	A	408	CLA	CHC-C1C	4.54	1.47	1.38
25	a	408	CLA	CHC-C1C	4.54	1.47	1.38
25	c	504	CLA	C3C-C2C	4.54	1.46	1.36
25	B	612	CLA	C3D-C4D	-4.54	1.34	1.44
25	c	502	CLA	CHC-C1C	4.54	1.47	1.38
25	B	608	CLA	C3D-C4D	-4.54	1.34	1.44
25	b	608	CLA	C3D-C4D	-4.54	1.34	1.44
27	C	515	BCR	C10-C9	-4.53	1.25	1.35
27	c	515	BCR	C10-C9	-4.53	1.25	1.35
25	b	612	CLA	C3D-C4D	-4.53	1.34	1.44
25	B	604	CLA	C3D-C4D	-4.52	1.34	1.44
25	c	508	CLA	C3D-C4D	-4.52	1.34	1.44
25	C	508	CLA	C3D-C4D	-4.51	1.34	1.44
25	B	606	CLA	CHD-C1D	4.51	1.47	1.38
25	d	404	CLA	CHD-C1D	4.51	1.47	1.38
25	b	604	CLA	C3D-C4D	-4.51	1.34	1.44
25	a	406	CLA	CHD-C1D	4.51	1.47	1.38
25	B	606	CLA	C3D-C4D	-4.51	1.34	1.44
25	b	606	CLA	C3D-C4D	-4.51	1.34	1.44
25	D	404	CLA	CHD-C1D	4.50	1.47	1.38
25	C	507	CLA	CHD-C1D	4.49	1.47	1.38
25	c	507	CLA	CHD-C1D	4.49	1.47	1.38
25	A	406	CLA	CHD-C1D	4.49	1.47	1.38
25	C	502	CLA	CHD-C1D	4.49	1.47	1.38
25	c	502	CLA	CHD-C1D	4.49	1.47	1.38
25	B	602	CLA	C3C-C2C	4.49	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	602	CLA	C3C-C2C	4.49	1.46	1.36
25	c	507	CLA	C3C-C2C	4.48	1.46	1.36
25	C	505	CLA	CHD-C1D	4.48	1.47	1.38
25	C	503	CLA	C3D-C4D	-4.48	1.34	1.44
25	c	503	CLA	C3D-C4D	-4.48	1.34	1.44
25	C	511	CLA	C3D-C4D	-4.47	1.34	1.44
25	c	511	CLA	C3D-C4D	-4.47	1.34	1.44
25	B	610	CLA	C3D-C4D	-4.47	1.34	1.44
25	b	610	CLA	C3D-C4D	-4.47	1.34	1.44
25	B	602	CLA	CHD-C1D	4.47	1.47	1.38
25	b	602	CLA	CHD-C1D	4.47	1.47	1.38
25	c	505	CLA	CHD-C1D	4.46	1.47	1.38
25	C	507	CLA	C3C-C2C	4.46	1.46	1.36
25	D	404	CLA	C3D-C4D	-4.46	1.34	1.44
25	d	404	CLA	C3D-C4D	-4.46	1.34	1.44
25	A	406	CLA	C3C-C2C	4.44	1.46	1.36
27	B	618	BCR	C10-C9	-4.43	1.25	1.35
27	b	618	BCR	C10-C9	-4.43	1.25	1.35
27	A	409	BCR	C10-C9	-4.42	1.25	1.35
27	a	409	BCR	C10-C9	-4.42	1.25	1.35
28	H	105	LMG	O8-C28	4.42	1.46	1.33
25	D	404	CLA	C3C-C2C	4.42	1.46	1.36
25	d	404	CLA	C3C-C2C	4.42	1.46	1.36
28	h	105	LMG	O8-C28	4.41	1.46	1.33
25	a	406	CLA	C3C-C2C	4.41	1.46	1.36
25	B	604	CLA	CHD-C1D	4.40	1.47	1.38
27	K	103	BCR	C10-C9	-4.39	1.25	1.35
27	k	103	BCR	C10-C9	-4.39	1.25	1.35
25	c	507	CLA	C3D-C4D	-4.39	1.34	1.44
28	a	410	LMG	O8-C28	4.39	1.46	1.33
25	C	514	CLA	C3C-C2C	4.39	1.46	1.36
25	c	514	CLA	C3C-C2C	4.39	1.46	1.36
25	C	502	CLA	C3D-C4D	-4.39	1.34	1.44
25	c	502	CLA	C3D-C4D	-4.39	1.34	1.44
25	B	614	CLA	C3D-C4D	-4.39	1.34	1.44
25	b	614	CLA	C3D-C4D	-4.39	1.34	1.44
33	Z	102	LHG	O8-C23	4.38	1.46	1.33
33	z	102	LHG	O8-C23	4.38	1.46	1.33
25	C	512	CLA	C3C-C2C	4.38	1.46	1.36
25	c	512	CLA	C3C-C2C	4.38	1.46	1.36
25	B	616	CLA	CHD-C1D	4.38	1.47	1.38
25	b	616	CLA	CHD-C1D	4.38	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	509	CLA	CHD-C1D	4.38	1.47	1.38
25	c	509	CLA	CHD-C1D	4.38	1.47	1.38
28	A	410	LMG	O8-C28	4.38	1.46	1.33
25	B	610	CLA	C3C-C2C	4.37	1.46	1.36
25	b	610	CLA	C3C-C2C	4.37	1.46	1.36
25	D	403	CLA	C3C-C2C	4.37	1.46	1.36
25	d	403	CLA	C3C-C2C	4.37	1.46	1.36
25	B	609	CLA	CHD-C1D	4.37	1.47	1.38
25	b	609	CLA	CHD-C1D	4.37	1.47	1.38
25	C	503	CLA	C3C-C2C	4.37	1.46	1.36
25	c	503	CLA	C3C-C2C	4.37	1.46	1.36
25	b	604	CLA	CHD-C1D	4.36	1.46	1.38
25	C	509	CLA	C3C-C2C	4.36	1.46	1.36
25	c	509	CLA	C3C-C2C	4.36	1.46	1.36
25	B	609	CLA	C3D-C4D	-4.36	1.34	1.44
25	C	506	CLA	C3C-C2C	4.35	1.46	1.36
25	C	507	CLA	C3D-C4D	-4.35	1.34	1.44
25	A	408	CLA	C3C-C2C	4.35	1.46	1.36
25	c	506	CLA	C3C-C2C	4.35	1.46	1.36
25	B	615	CLA	CHC-C1C	4.35	1.47	1.38
25	b	615	CLA	CHC-C1C	4.35	1.47	1.38
25	C	510	CLA	CHD-C1D	4.35	1.46	1.38
25	c	510	CLA	CHD-C1D	4.35	1.46	1.38
25	d	401	CLA	CHD-C1D	4.34	1.46	1.38
27	F	101	BCR	C10-C9	-4.34	1.25	1.35
27	f	101	BCR	C10-C9	-4.34	1.25	1.35
25	B	615	CLA	C3D-C4D	-4.34	1.34	1.44
25	b	615	CLA	C3D-C4D	-4.34	1.34	1.44
25	D	401	CLA	CHD-C1D	4.34	1.46	1.38
25	B	607	CLA	C3D-C4D	-4.33	1.34	1.44
25	b	607	CLA	C3D-C4D	-4.33	1.34	1.44
25	a	408	CLA	C3C-C2C	4.33	1.46	1.36
25	b	609	CLA	C3D-C4D	-4.33	1.34	1.44
25	A	408	CLA	C3D-C4D	-4.33	1.34	1.44
25	B	613	CLA	C3D-C4D	-4.33	1.34	1.44
25	B	601	CLA	C3C-C2C	4.33	1.46	1.36
25	b	601	CLA	C3C-C2C	4.33	1.46	1.36
28	a	414	LMG	O8-C28	4.33	1.46	1.33
25	b	613	CLA	C3D-C4D	-4.33	1.34	1.44
33	B	627	LHG	O7-C7	4.32	1.46	1.34
28	C	523	LMG	O8-C28	4.32	1.45	1.33
28	c	523	LMG	O8-C28	4.32	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	403	CLA	C3D-C4D	-4.32	1.34	1.44
25	d	403	CLA	C3D-C4D	-4.32	1.34	1.44
25	C	511	CLA	CHD-C1D	4.32	1.46	1.38
25	c	511	CLA	CHD-C1D	4.32	1.46	1.38
25	B	603	CLA	C3C-C2C	4.31	1.46	1.36
25	b	603	CLA	C3C-C2C	4.31	1.46	1.36
28	A	414	LMG	O8-C28	4.30	1.45	1.33
25	C	506	CLA	CHD-C1D	4.30	1.46	1.38
25	c	506	CLA	CHD-C1D	4.30	1.46	1.38
25	D	401	CLA	C3D-C4D	-4.30	1.34	1.44
25	b	602	CLA	C3D-C4D	-4.30	1.34	1.44
25	d	401	CLA	C3D-C4D	-4.30	1.34	1.44
25	a	408	CLA	C3D-C4D	-4.30	1.34	1.44
33	b	627	LHG	O7-C7	4.29	1.46	1.34
25	B	608	CLA	CHC-C1C	4.29	1.47	1.38
25	b	606	CLA	C3C-C2C	4.29	1.46	1.36
25	B	606	CLA	C3C-C2C	4.29	1.46	1.36
33	E	102	LHG	O8-C23	4.29	1.45	1.33
25	b	608	CLA	CHC-C1C	4.29	1.47	1.38
25	A	408	CLA	CHD-C1D	4.29	1.46	1.38
25	b	609	CLA	CHC-C1C	4.29	1.47	1.38
25	C	512	CLA	C3D-C4D	-4.29	1.34	1.44
25	c	512	CLA	C3D-C4D	-4.29	1.34	1.44
25	B	602	CLA	C3D-C4D	-4.28	1.34	1.44
28	c	519	LMG	O8-C28	4.28	1.45	1.33
25	C	513	CLA	C3C-C2C	4.27	1.46	1.36
25	C	502	CLA	C3C-C2C	4.27	1.46	1.36
25	B	609	CLA	CHC-C1C	4.27	1.47	1.38
25	c	504	CLA	C3D-C4D	-4.27	1.34	1.44
25	a	408	CLA	CHD-C1D	4.27	1.46	1.38
28	C	519	LMG	O8-C28	4.27	1.45	1.33
25	C	504	CLA	C3D-C4D	-4.26	1.34	1.44
33	e	102	LHG	O8-C23	4.26	1.45	1.33
35	E	104	HEM	FE-NC	4.26	2.09	1.95
25	B	605	CLA	C3D-C4D	-4.26	1.34	1.44
25	b	605	CLA	C3D-C4D	-4.26	1.34	1.44
35	v	201	HEM	FE-NB	4.26	2.08	1.94
25	c	513	CLA	C3C-C2C	4.26	1.46	1.36
25	c	502	CLA	C3C-C2C	4.26	1.46	1.36
25	b	607	CLA	CHC-C1C	4.26	1.47	1.38
35	V	201	HEM	FE-NB	4.25	2.08	1.94
35	e	104	HEM	FE-NC	4.25	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	607	CLA	CHC-C1C	4.25	1.47	1.38
25	B	610	CLA	CHD-C1D	4.25	1.46	1.38
25	b	610	CLA	CHD-C1D	4.25	1.46	1.38
25	B	611	CLA	C3D-C4D	-4.24	1.34	1.44
25	b	611	CLA	C3D-C4D	-4.24	1.34	1.44
25	A	406	CLA	CHC-C1C	4.24	1.47	1.38
25	B	616	CLA	C3D-C4D	-4.24	1.34	1.44
25	b	616	CLA	C3D-C4D	-4.24	1.34	1.44
25	c	503	CLA	CHD-C1D	4.24	1.46	1.38
25	C	508	CLA	C3C-C2C	4.23	1.45	1.36
25	c	505	CLA	C3D-C4D	-4.23	1.34	1.44
25	C	503	CLA	CHD-C1D	4.23	1.46	1.38
25	C	505	CLA	C3D-C4D	-4.23	1.34	1.44
25	B	601	CLA	CHD-C1D	4.23	1.46	1.38
25	b	601	CLA	CHD-C1D	4.23	1.46	1.38
25	C	511	CLA	C3C-C2C	4.23	1.45	1.36
25	c	511	CLA	C3C-C2C	4.23	1.45	1.36
33	B	628	LHG	O8-C23	4.23	1.45	1.33
33	b	628	LHG	O8-C23	4.23	1.45	1.33
25	C	510	CLA	C3C-C2C	4.23	1.45	1.36
25	c	510	CLA	C3C-C2C	4.23	1.45	1.36
25	a	406	CLA	CHC-C1C	4.22	1.46	1.38
28	c	523	LMG	O7-C10	4.22	1.46	1.34
25	c	511	CLA	CHC-C1C	4.22	1.46	1.38
25	B	613	CLA	C3C-C2C	4.21	1.45	1.36
35	V	201	HEM	C1B-NB	-4.21	1.33	1.40
35	v	201	HEM	C1B-NB	-4.21	1.33	1.40
25	B	601	CLA	CHC-C1C	4.21	1.46	1.38
25	b	601	CLA	CHC-C1C	4.21	1.46	1.38
25	b	613	CLA	C3C-C2C	4.21	1.45	1.36
25	C	511	CLA	CHC-C1C	4.21	1.46	1.38
25	c	508	CLA	C3C-C2C	4.21	1.45	1.36
28	B	621	LMG	O8-C28	4.20	1.45	1.33
28	b	621	LMG	O8-C28	4.20	1.45	1.33
25	C	508	CLA	CHD-C1D	4.20	1.46	1.38
25	c	508	CLA	CHD-C1D	4.20	1.46	1.38
28	C	523	LMG	O7-C10	4.20	1.46	1.34
25	C	514	CLA	C3D-C4D	-4.19	1.34	1.44
25	c	514	CLA	C3D-C4D	-4.19	1.34	1.44
25	D	401	CLA	CHC-C1C	4.19	1.46	1.38
25	d	401	CLA	CHC-C1C	4.19	1.46	1.38
25	B	603	CLA	CHC-C1C	4.19	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	414	LMG	O7-C10	4.19	1.46	1.34
25	B	610	CLA	CHC-C1C	4.18	1.46	1.38
25	b	610	CLA	CHC-C1C	4.18	1.46	1.38
25	C	509	CLA	C3D-C4D	-4.18	1.34	1.44
25	c	509	CLA	C3D-C4D	-4.18	1.34	1.44
27	z	101	BCR	C10-C9	-4.18	1.26	1.35
28	A	414	LMG	O7-C10	4.17	1.46	1.34
25	C	512	CLA	CHD-C1D	4.17	1.46	1.38
26	A	407	PHO	C1D-C2D	4.17	1.44	1.39
26	a	407	PHO	C1D-C2D	4.17	1.44	1.39
27	k	102	BCR	C10-C9	-4.17	1.26	1.35
33	z	102	LHG	O7-C7	4.17	1.46	1.34
33	Z	102	LHG	O7-C7	4.16	1.46	1.34
25	B	607	CLA	C3C-C2C	4.16	1.45	1.36
25	b	607	CLA	C3C-C2C	4.16	1.45	1.36
25	b	603	CLA	CHC-C1C	4.16	1.46	1.38
25	B	616	CLA	C1C-NC	-4.16	1.31	1.37
34	c	517	DGD	O1G-C1A	4.16	1.45	1.33
33	B	627	LHG	O8-C23	4.16	1.45	1.33
33	b	627	LHG	O8-C23	4.16	1.45	1.33
27	K	102	BCR	C10-C9	-4.16	1.26	1.35
27	Z	101	BCR	C10-C9	-4.15	1.26	1.35
34	C	517	DGD	O1G-C1A	4.15	1.45	1.33
25	C	503	CLA	CHC-C1C	4.15	1.46	1.38
25	c	503	CLA	CHC-C1C	4.15	1.46	1.38
25	C	513	CLA	CHC-C1C	4.14	1.46	1.38
25	c	513	CLA	CHC-C1C	4.14	1.46	1.38
25	C	508	CLA	CHC-C1C	4.14	1.46	1.38
25	c	508	CLA	CHC-C1C	4.14	1.46	1.38
25	c	512	CLA	CHD-C1D	4.14	1.46	1.38
28	H	105	LMG	O7-C10	4.14	1.46	1.34
25	C	505	CLA	CHC-C1C	4.13	1.46	1.38
25	B	608	CLA	C3C-C2C	4.13	1.45	1.36
25	b	608	CLA	C3C-C2C	4.13	1.45	1.36
28	h	105	LMG	O7-C10	4.13	1.45	1.34
25	c	505	CLA	CHC-C1C	4.13	1.46	1.38
25	b	616	CLA	C1C-NC	-4.13	1.31	1.37
28	A	410	LMG	O7-C10	4.12	1.45	1.34
28	a	410	LMG	O7-C10	4.12	1.45	1.34
25	C	510	CLA	CHC-C1C	4.12	1.46	1.38
25	c	510	CLA	CHC-C1C	4.12	1.46	1.38
25	B	601	CLA	C3D-C4D	-4.11	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	CHC-C1C	4.09	1.46	1.38
25	b	613	CLA	CHC-C1C	4.09	1.46	1.38
25	b	608	CLA	C1B-NB	-4.09	1.32	1.37
25	B	608	CLA	C1B-NB	-4.09	1.32	1.37
25	C	504	CLA	CHD-C1D	4.08	1.46	1.38
25	c	504	CLA	CHD-C1D	4.08	1.46	1.38
25	b	601	CLA	C3D-C4D	-4.08	1.35	1.44
25	B	614	CLA	C3C-C2C	4.08	1.45	1.36
25	b	614	CLA	C3C-C2C	4.08	1.45	1.36
25	C	510	CLA	CHB-C1B	4.07	1.48	1.39
25	c	510	CLA	CHB-C1B	4.07	1.48	1.39
33	D	408	LHG	O7-C7	4.07	1.45	1.34
33	d	408	LHG	O7-C7	4.07	1.45	1.34
34	C	516	DGD	O2G-C1B	4.07	1.45	1.34
25	A	406	CLA	CHD-C4C	4.07	1.48	1.39
25	a	406	CLA	CHD-C4C	4.07	1.48	1.39
33	D	406	LHG	O8-C23	4.07	1.45	1.33
33	d	406	LHG	O8-C23	4.07	1.45	1.33
28	b	621	LMG	O7-C10	4.07	1.45	1.34
28	D	409	LMG	O7-C10	4.07	1.45	1.34
28	d	409	LMG	O7-C10	4.07	1.45	1.34
25	B	605	CLA	C3C-C2C	4.07	1.45	1.36
25	C	510	CLA	C3D-C4D	-4.06	1.35	1.44
25	c	510	CLA	C3D-C4D	-4.06	1.35	1.44
28	D	409	LMG	O8-C28	4.06	1.45	1.33
25	B	611	CLA	CHC-C1C	4.06	1.46	1.38
25	b	611	CLA	CHC-C1C	4.06	1.46	1.38
28	B	621	LMG	O7-C10	4.06	1.45	1.34
28	d	409	LMG	O8-C28	4.06	1.45	1.33
34	c	516	DGD	O2G-C1B	4.06	1.45	1.34
25	b	605	CLA	C3C-C2C	4.06	1.45	1.36
28	C	519	LMG	O7-C10	4.04	1.45	1.34
28	c	519	LMG	O7-C10	4.04	1.45	1.34
25	B	612	CLA	CHB-C1B	4.04	1.48	1.39
25	b	612	CLA	CHB-C1B	4.04	1.48	1.39
25	C	514	CLA	CHD-C1D	4.04	1.46	1.38
33	d	407	LHG	O8-C23	4.04	1.45	1.33
25	B	616	CLA	CHD-C4C	4.04	1.48	1.39
25	b	616	CLA	CHD-C4C	4.04	1.48	1.39
33	D	407	LHG	O8-C23	4.03	1.45	1.33
25	B	609	CLA	C3C-C2C	4.03	1.45	1.36
25	b	609	CLA	C3C-C2C	4.03	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	104	DGD	O2G-C1B	4.03	1.45	1.34
34	h	104	DGD	O2G-C1B	4.03	1.45	1.34
25	c	514	CLA	CHD-C1D	4.03	1.46	1.38
34	H	104	DGD	O1G-C1A	4.03	1.45	1.33
34	h	104	DGD	O1G-C1A	4.03	1.45	1.33
34	C	518	DGD	O1G-C1A	4.03	1.45	1.33
34	c	518	DGD	O1G-C1A	4.03	1.45	1.33
25	B	607	CLA	CHD-C1D	4.02	1.46	1.38
25	b	607	CLA	CHD-C1D	4.02	1.46	1.38
25	b	604	CLA	CHC-C1C	4.01	1.46	1.38
34	c	518	DGD	O2G-C1B	4.01	1.45	1.34
25	B	611	CLA	CHD-C1D	4.01	1.46	1.38
25	B	603	CLA	CHD-C1D	4.01	1.46	1.38
25	b	603	CLA	CHD-C1D	4.01	1.46	1.38
25	c	505	CLA	CHD-C4C	4.01	1.48	1.39
34	C	516	DGD	O1G-C1A	4.00	1.45	1.33
34	c	516	DGD	O1G-C1A	4.00	1.45	1.33
25	B	616	CLA	C3C-C2C	4.00	1.45	1.36
25	C	505	CLA	CHD-C4C	4.00	1.48	1.39
25	b	616	CLA	C3C-C2C	4.00	1.45	1.36
25	B	613	CLA	CHD-C1D	4.00	1.46	1.38
25	b	613	CLA	CHD-C1D	4.00	1.46	1.38
25	C	510	CLA	CHD-C4C	4.00	1.48	1.39
25	c	510	CLA	CHD-C4C	4.00	1.48	1.39
25	b	602	CLA	CHD-C4C	4.00	1.48	1.39
25	B	615	CLA	C3C-C2C	4.00	1.45	1.36
25	B	604	CLA	CHC-C1C	3.99	1.46	1.38
34	C	518	DGD	O2G-C1B	3.99	1.45	1.34
25	C	513	CLA	C3D-C4D	-3.99	1.35	1.44
25	B	604	CLA	C3C-C2C	3.99	1.45	1.36
25	b	604	CLA	C3C-C2C	3.99	1.45	1.36
26	D	402	PHO	C1D-C2D	3.98	1.43	1.39
25	B	602	CLA	CHD-C4C	3.98	1.48	1.39
25	b	615	CLA	C3C-C2C	3.98	1.45	1.36
25	B	614	CLA	CHD-C1D	3.98	1.46	1.38
25	b	614	CLA	CHD-C1D	3.98	1.46	1.38
33	D	408	LHG	O8-C23	3.98	1.44	1.33
33	d	408	LHG	O8-C23	3.98	1.44	1.33
25	B	612	CLA	C3C-C2C	3.97	1.45	1.36
25	b	612	CLA	C3C-C2C	3.97	1.45	1.36
25	C	514	CLA	CHC-C4B	3.97	1.48	1.39
25	c	514	CLA	CHC-C4B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	CHD-C1D	3.96	1.46	1.38
25	c	513	CLA	C3D-C4D	-3.96	1.35	1.44
25	C	505	CLA	C3C-C2C	3.95	1.45	1.36
25	c	505	CLA	C3C-C2C	3.95	1.45	1.36
25	b	615	CLA	CHD-C1D	3.95	1.46	1.38
25	B	611	CLA	C1B-NB	-3.94	1.32	1.37
25	b	611	CLA	C1B-NB	-3.94	1.32	1.37
25	D	404	CLA	CHD-C4C	3.93	1.48	1.39
25	d	404	CLA	CHD-C4C	3.93	1.48	1.39
33	d	407	LHG	O7-C7	3.92	1.45	1.34
34	C	517	DGD	O2G-C1B	3.91	1.45	1.34
34	c	517	DGD	O2G-C1B	3.91	1.45	1.34
25	B	608	CLA	C1D-ND	-3.91	1.32	1.37
25	b	608	CLA	C1D-ND	-3.91	1.32	1.37
33	D	407	LHG	O7-C7	3.91	1.45	1.34
25	B	615	CLA	CHD-C1D	3.90	1.46	1.38
25	B	612	CLA	CHC-C4B	3.90	1.48	1.39
25	b	612	CLA	CHC-C4B	3.90	1.48	1.39
25	B	603	CLA	C1D-ND	-3.90	1.32	1.37
25	b	603	CLA	C1D-ND	-3.90	1.32	1.37
33	E	102	LHG	O7-C7	3.90	1.45	1.34
33	e	102	LHG	O7-C7	3.90	1.45	1.34
25	D	401	CLA	CHD-C4C	3.89	1.48	1.39
25	d	401	CLA	CHD-C4C	3.89	1.48	1.39
26	d	402	PHO	C1D-C2D	3.89	1.43	1.39
25	c	512	CLA	CHB-C1B	3.88	1.48	1.39
25	C	511	CLA	CHD-C4C	3.88	1.48	1.39
25	d	403	CLA	CHC-C4B	3.88	1.48	1.39
25	D	403	CLA	CHC-C4B	3.87	1.48	1.39
25	c	511	CLA	CHD-C4C	3.87	1.48	1.39
25	C	513	CLA	CHB-C1B	3.87	1.48	1.39
25	c	513	CLA	CHB-C1B	3.87	1.48	1.39
25	A	405	CLA	CHD-C1D	3.86	1.46	1.38
25	a	405	CLA	CHD-C1D	3.86	1.46	1.38
25	b	610	CLA	CHC-C4B	3.86	1.48	1.39
25	B	610	CLA	CHC-C4B	3.86	1.48	1.39
33	B	628	LHG	O7-C7	3.86	1.45	1.34
33	b	628	LHG	O7-C7	3.86	1.45	1.34
25	C	512	CLA	CHC-C4B	3.85	1.48	1.39
25	c	512	CLA	CHC-C4B	3.85	1.48	1.39
25	D	403	CLA	CHB-C1B	3.85	1.48	1.39
25	d	403	CLA	CHB-C1B	3.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	512	CLA	CHB-C1B	3.85	1.48	1.39
25	b	605	CLA	CHD-C1D	3.85	1.45	1.38
25	B	606	CLA	CHD-C4C	3.85	1.48	1.39
25	b	602	CLA	CHC-C4B	3.85	1.48	1.39
25	b	601	CLA	CHC-C4B	3.84	1.48	1.39
25	B	602	CLA	CHC-C4B	3.84	1.48	1.39
25	C	502	CLA	CHD-C4C	3.84	1.47	1.39
25	c	502	CLA	CHD-C4C	3.84	1.47	1.39
25	B	605	CLA	CHD-C1D	3.84	1.45	1.38
25	b	603	CLA	C1B-NB	-3.84	1.32	1.37
25	B	601	CLA	CHC-C4B	3.83	1.48	1.39
25	B	604	CLA	CHB-C1B	3.83	1.48	1.39
25	C	513	CLA	CHD-C1D	3.83	1.45	1.38
25	c	513	CLA	CHD-C1D	3.83	1.45	1.38
25	C	511	CLA	CHB-C1B	3.83	1.48	1.39
25	c	511	CLA	CHB-C1B	3.83	1.48	1.39
25	B	603	CLA	C1B-NB	-3.82	1.32	1.37
25	b	604	CLA	CHB-C1B	3.82	1.48	1.39
35	V	201	HEM	C4D-ND	-3.82	1.33	1.40
35	v	201	HEM	C4D-ND	-3.82	1.33	1.40
25	b	606	CLA	CHD-C4C	3.82	1.47	1.39
25	C	510	CLA	OBD-CAD	3.82	1.29	1.22
25	c	510	CLA	OBD-CAD	3.82	1.29	1.22
25	C	507	CLA	CHD-C4C	3.82	1.47	1.39
25	c	507	CLA	CHD-C4C	3.82	1.47	1.39
25	a	405	CLA	CHC-C4B	3.81	1.48	1.39
25	A	405	CLA	CHC-C4B	3.81	1.48	1.39
25	C	504	CLA	CHC-C4B	3.80	1.48	1.39
25	c	504	CLA	CHC-C4B	3.80	1.47	1.39
33	d	406	LHG	O7-C7	3.80	1.45	1.34
25	B	607	CLA	CHD-C4C	3.78	1.47	1.39
33	D	406	LHG	O7-C7	3.78	1.45	1.34
25	b	607	CLA	CHD-C4C	3.78	1.47	1.39
25	c	508	CLA	CHD-C4C	3.78	1.47	1.39
28	H	105	LMG	C37-C36	-3.78	1.33	1.51
25	C	508	CLA	CHD-C4C	3.77	1.47	1.39
25	C	513	CLA	C1D-ND	-3.77	1.32	1.37
28	h	105	LMG	C37-C36	-3.77	1.33	1.51
25	B	609	CLA	C1B-NB	-3.77	1.32	1.37
25	b	609	CLA	C1B-NB	-3.77	1.32	1.37
25	c	514	CLA	CHB-C1B	3.76	1.47	1.39
28	H	105	LMG	C40-C39	-3.76	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	h	105	LMG	C40-C39	-3.76	1.33	1.51
34	H	104	DGD	CAA-C9A	-3.76	1.33	1.51
34	h	104	DGD	CAA-C9A	-3.76	1.33	1.51
28	C	523	LMG	C22-C21	-3.76	1.33	1.51
28	c	523	LMG	C22-C21	-3.76	1.33	1.51
34	c	518	DGD	CDA-CCA	-3.76	1.33	1.51
25	C	506	CLA	CHC-C4B	3.75	1.47	1.39
25	B	613	CLA	CHD-C4C	3.75	1.47	1.39
25	b	613	CLA	CHD-C4C	3.75	1.47	1.39
34	C	518	DGD	CDA-CCA	-3.75	1.33	1.51
34	C	518	DGD	CAA-C9A	-3.75	1.33	1.51
34	c	518	DGD	CAA-C9A	-3.75	1.33	1.51
25	B	609	CLA	CHB-C1B	3.74	1.47	1.39
25	b	609	CLA	CHB-C1B	3.74	1.47	1.39
34	C	516	DGD	CAB-C9B	-3.74	1.33	1.51
34	c	516	DGD	CAB-C9B	-3.74	1.33	1.51
25	b	603	CLA	CHB-C1B	3.74	1.47	1.39
28	C	523	LMG	C37-C36	-3.74	1.33	1.51
28	c	523	LMG	C37-C36	-3.74	1.33	1.51
28	C	519	LMG	C22-C21	-3.74	1.33	1.51
28	c	519	LMG	C22-C21	-3.74	1.33	1.51
25	c	506	CLA	CHC-C4B	3.74	1.47	1.39
25	A	408	CLA	CHC-C4B	3.73	1.47	1.39
25	B	602	CLA	CHB-C1B	3.73	1.47	1.39
25	b	602	CLA	CHB-C1B	3.73	1.47	1.39
34	C	518	DGD	CDB-CCB	-3.73	1.33	1.51
34	c	518	DGD	CDB-CCB	-3.73	1.33	1.51
25	D	404	CLA	CHC-C4B	3.73	1.47	1.39
25	c	509	CLA	CHC-C4B	3.73	1.47	1.39
28	B	621	LMG	C40-C39	-3.73	1.33	1.51
28	b	621	LMG	C40-C39	-3.73	1.33	1.51
34	H	104	DGD	CAB-C9B	-3.73	1.33	1.51
34	h	104	DGD	CAB-C9B	-3.73	1.33	1.51
25	b	614	CLA	CHB-C1B	3.73	1.47	1.39
25	c	513	CLA	C1D-ND	-3.73	1.33	1.37
25	B	603	CLA	CHB-C1B	3.72	1.47	1.39
25	C	514	CLA	CHB-C1B	3.72	1.47	1.39
28	B	621	LMG	C37-C36	-3.72	1.33	1.51
28	b	621	LMG	C37-C36	-3.72	1.33	1.51
25	B	605	CLA	CHC-C4B	3.72	1.47	1.39
25	b	605	CLA	CHC-C4B	3.72	1.47	1.39
25	c	512	CLA	OBD-CAD	3.72	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	512	CLA	OBD-CAD	3.72	1.28	1.22
25	A	408	CLA	CHD-C4C	3.72	1.47	1.39
25	B	610	CLA	CHB-C1B	3.72	1.47	1.39
25	b	610	CLA	CHB-C1B	3.72	1.47	1.39
28	B	621	LMG	C19-C18	-3.71	1.33	1.51
28	b	621	LMG	C19-C18	-3.71	1.33	1.51
25	C	509	CLA	CHD-C4C	3.71	1.47	1.39
25	a	408	CLA	CHD-C4C	3.71	1.47	1.39
25	C	504	CLA	CHB-C1B	3.71	1.47	1.39
25	c	504	CLA	CHB-C1B	3.71	1.47	1.39
25	c	509	CLA	CHD-C4C	3.71	1.47	1.39
28	a	410	LMG	C22-C21	-3.71	1.33	1.51
34	C	517	DGD	CDA-CCA	-3.71	1.33	1.51
34	c	517	DGD	CDA-CCA	-3.71	1.33	1.51
25	B	614	CLA	CHB-C1B	3.71	1.47	1.39
28	b	621	LMG	C22-C21	-3.71	1.33	1.51
25	d	404	CLA	CHC-C4B	3.70	1.47	1.39
25	C	507	CLA	C1B-NB	-3.70	1.33	1.37
28	A	410	LMG	C22-C21	-3.70	1.33	1.51
34	H	104	DGD	CDA-CCA	-3.70	1.33	1.51
34	h	104	DGD	CDA-CCA	-3.70	1.33	1.51
25	C	507	CLA	CHC-C1C	3.70	1.45	1.38
25	c	507	CLA	CHC-C1C	3.70	1.45	1.38
25	a	408	CLA	CHC-C4B	3.70	1.47	1.39
25	C	509	CLA	CHC-C4B	3.70	1.47	1.39
34	C	516	DGD	CAA-C9A	-3.70	1.33	1.51
34	c	516	DGD	CAA-C9A	-3.70	1.33	1.51
34	H	104	DGD	CDB-CCB	-3.70	1.33	1.51
34	h	104	DGD	CDB-CCB	-3.70	1.33	1.51
25	c	512	CLA	CHD-C4C	3.69	1.47	1.39
25	C	512	CLA	CHD-C4C	3.69	1.47	1.39
28	B	621	LMG	C22-C21	-3.69	1.33	1.51
25	C	511	CLA	C1D-ND	-3.69	1.33	1.37
25	c	511	CLA	C1D-ND	-3.69	1.33	1.37
28	A	410	LMG	C40-C39	-3.69	1.33	1.51
28	a	410	LMG	C40-C39	-3.69	1.33	1.51
34	C	516	DGD	CDB-CCB	-3.69	1.33	1.51
34	c	516	DGD	CDB-CCB	-3.69	1.33	1.51
25	b	616	CLA	CHB-C1B	3.69	1.47	1.39
25	B	605	CLA	CHB-C1B	3.69	1.47	1.39
25	b	605	CLA	CHB-C1B	3.69	1.47	1.39
28	C	519	LMG	C19-C18	-3.69	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	410	LMG	C37-C36	-3.69	1.33	1.51
28	a	410	LMG	C37-C36	-3.69	1.33	1.51
28	C	523	LMG	C40-C39	-3.68	1.33	1.51
25	B	616	CLA	CHB-C1B	3.68	1.47	1.39
25	A	405	CLA	CHB-C1B	3.68	1.47	1.39
25	a	405	CLA	CHB-C1B	3.68	1.47	1.39
25	B	614	CLA	CHC-C4B	3.68	1.47	1.39
34	C	518	DGD	CAB-C9B	-3.68	1.33	1.51
34	c	518	DGD	CAB-C9B	-3.68	1.33	1.51
25	C	502	CLA	CHB-C1B	3.68	1.47	1.39
25	c	502	CLA	CHB-C1B	3.68	1.47	1.39
25	c	511	CLA	C1B-NB	-3.68	1.33	1.37
28	c	519	LMG	C19-C18	-3.68	1.33	1.51
25	B	601	CLA	CHB-C1B	3.68	1.47	1.39
34	C	516	DGD	CDA-CCA	-3.68	1.33	1.51
34	c	516	DGD	CDA-CCA	-3.68	1.33	1.51
25	B	616	CLA	CHC-C1C	3.67	1.45	1.38
25	b	616	CLA	CHC-C1C	3.67	1.45	1.38
25	b	601	CLA	CHB-C1B	3.67	1.47	1.39
25	b	614	CLA	CHC-C4B	3.67	1.47	1.39
28	C	519	LMG	C37-C36	-3.67	1.33	1.51
28	c	519	LMG	C37-C36	-3.67	1.33	1.51
25	A	406	CLA	OBD-CAD	3.67	1.28	1.22
25	a	406	CLA	OBD-CAD	3.67	1.28	1.22
25	C	503	CLA	CHB-C1B	3.67	1.47	1.39
25	c	503	CLA	CHB-C1B	3.67	1.47	1.39
34	c	517	DGD	CAA-C9A	-3.67	1.33	1.51
28	c	523	LMG	C40-C39	-3.67	1.33	1.51
34	C	517	DGD	CDB-CCB	-3.67	1.33	1.51
34	c	517	DGD	CDB-CCB	-3.67	1.33	1.51
25	B	604	CLA	CHD-C4C	3.67	1.47	1.39
25	B	615	CLA	CHB-C1B	3.66	1.47	1.39
25	b	615	CLA	CHB-C1B	3.66	1.47	1.39
25	c	507	CLA	C1B-NB	-3.66	1.33	1.37
28	D	409	LMG	C40-C39	-3.66	1.33	1.51
28	d	409	LMG	C40-C39	-3.66	1.33	1.51
34	C	517	DGD	CAA-C9A	-3.65	1.33	1.51
34	c	517	DGD	CAB-C9B	-3.65	1.33	1.51
28	A	410	LMG	C19-C18	-3.65	1.33	1.51
28	a	410	LMG	C19-C18	-3.65	1.33	1.51
25	b	604	CLA	CHD-C4C	3.65	1.47	1.39
25	B	606	CLA	CHC-C4B	3.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	606	CLA	CHC-C4B	3.65	1.47	1.39
25	C	511	CLA	C1B-NB	-3.65	1.33	1.37
25	C	508	CLA	C1D-ND	-3.64	1.33	1.37
25	c	508	CLA	C1D-ND	-3.64	1.33	1.37
28	D	409	LMG	C37-C36	-3.64	1.33	1.51
28	d	409	LMG	C37-C36	-3.64	1.33	1.51
34	C	517	DGD	CAB-C9B	-3.64	1.33	1.51
25	C	502	CLA	CHC-C4B	3.63	1.47	1.39
25	c	502	CLA	CHC-C4B	3.63	1.47	1.39
28	C	519	LMG	C40-C39	-3.63	1.33	1.51
28	c	519	LMG	C40-C39	-3.63	1.33	1.51
25	C	506	CLA	C1B-NB	-3.63	1.33	1.37
25	c	506	CLA	C1B-NB	-3.63	1.33	1.37
27	b	619	BCR	C11-C12	-3.62	1.25	1.34
25	B	601	CLA	OBD-CAD	3.62	1.28	1.22
25	b	601	CLA	OBD-CAD	3.62	1.28	1.22
25	C	513	CLA	OBD-CAD	3.62	1.28	1.22
25	c	513	CLA	OBD-CAD	3.62	1.28	1.22
25	C	506	CLA	CHD-C4C	3.62	1.47	1.39
25	c	506	CLA	CHD-C4C	3.62	1.47	1.39
25	C	504	CLA	CHD-C4C	3.61	1.47	1.39
25	b	603	CLA	MG-ND	-3.61	1.98	2.05
25	B	603	CLA	MG-ND	-3.61	1.98	2.05
25	c	504	CLA	CHD-C4C	3.61	1.47	1.39
25	C	507	CLA	CHB-C1B	3.60	1.47	1.39
25	c	507	CLA	CHB-C1B	3.60	1.47	1.39
27	B	619	BCR	C11-C12	-3.60	1.25	1.34
28	C	523	LMG	C19-C18	-3.60	1.33	1.51
25	a	408	CLA	OBD-CAD	3.60	1.28	1.22
28	c	523	LMG	C19-C18	-3.59	1.33	1.51
25	B	613	CLA	CHB-C1B	3.59	1.47	1.39
25	b	613	CLA	CHB-C1B	3.59	1.47	1.39
25	B	611	CLA	C1D-ND	-3.59	1.33	1.37
25	b	611	CLA	C1D-ND	-3.59	1.33	1.37
25	c	503	CLA	CHD-C4C	3.59	1.47	1.39
27	B	617	BCR	C11-C12	-3.59	1.25	1.34
27	b	617	BCR	C11-C12	-3.59	1.25	1.34
29	D	405	PL9	C7-C3	-3.59	1.46	1.51
29	d	405	PL9	C7-C3	-3.59	1.46	1.51
25	B	609	CLA	OBD-CAD	3.58	1.28	1.22
25	B	601	CLA	CHD-C4C	3.58	1.47	1.39
25	b	601	CLA	CHD-C4C	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	513	CLA	CHD-C4C	3.58	1.47	1.39
25	B	615	CLA	OBD-CAD	3.57	1.28	1.22
25	b	615	CLA	OBD-CAD	3.57	1.28	1.22
25	C	503	CLA	CHD-C4C	3.57	1.47	1.39
25	B	611	CLA	CHB-C1B	3.57	1.47	1.39
25	b	611	CLA	CHB-C1B	3.57	1.47	1.39
35	e	104	HEM	C1B-NB	-3.57	1.34	1.40
35	E	104	HEM	C4D-ND	-3.56	1.34	1.40
25	b	611	CLA	C3C-C2C	3.56	1.44	1.36
25	C	514	CLA	OBD-CAD	3.56	1.28	1.22
25	c	514	CLA	OBD-CAD	3.56	1.28	1.22
25	A	408	CLA	OBD-CAD	3.56	1.28	1.22
25	B	614	CLA	CHD-C4C	3.56	1.47	1.39
25	b	614	CLA	CHD-C4C	3.56	1.47	1.39
25	B	608	CLA	CHD-C4C	3.56	1.47	1.39
25	B	609	CLA	CHD-C4C	3.56	1.47	1.39
25	b	608	CLA	CHD-C4C	3.56	1.47	1.39
25	c	506	CLA	OBD-CAD	3.56	1.28	1.22
35	e	104	HEM	C4D-ND	-3.56	1.34	1.40
25	B	611	CLA	C3C-C2C	3.56	1.44	1.36
25	D	401	CLA	C1B-NB	-3.55	1.33	1.37
25	b	609	CLA	CHD-C4C	3.55	1.47	1.39
25	c	505	CLA	OBD-CAD	3.55	1.28	1.22
25	c	511	CLA	OBD-CAD	3.55	1.28	1.22
25	b	609	CLA	OBD-CAD	3.54	1.28	1.22
25	C	513	CLA	CHD-C4C	3.54	1.47	1.39
25	C	514	CLA	CHD-C4C	3.54	1.47	1.39
25	c	514	CLA	CHD-C4C	3.54	1.47	1.39
25	C	510	CLA	C1D-ND	-3.53	1.33	1.37
25	c	510	CLA	C1D-ND	-3.53	1.33	1.37
25	C	511	CLA	OBD-CAD	3.53	1.28	1.22
25	C	513	CLA	C3D-C2D	3.53	1.48	1.39
25	c	513	CLA	C3D-C2D	3.53	1.48	1.39
25	C	505	CLA	OBD-CAD	3.53	1.28	1.22
25	c	513	CLA	CHC-C4B	3.53	1.47	1.39
25	B	603	CLA	CHD-C4C	3.52	1.47	1.39
27	C	515	BCR	C11-C12	-3.52	1.25	1.34
27	c	515	BCR	C11-C12	-3.52	1.25	1.34
25	a	406	CLA	CHC-C4B	3.52	1.47	1.39
25	C	513	CLA	CHC-C4B	3.52	1.47	1.39
35	E	104	HEM	C1B-NB	-3.52	1.34	1.40
25	C	506	CLA	OBD-CAD	3.51	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	CHD-C4C	3.51	1.47	1.39
25	b	605	CLA	C1D-ND	-3.50	1.33	1.37
25	D	404	CLA	OBD-CAD	3.49	1.28	1.22
25	d	404	CLA	OBD-CAD	3.49	1.28	1.22
25	B	605	CLA	CHD-C4C	3.49	1.47	1.39
25	b	605	CLA	CHD-C4C	3.49	1.47	1.39
25	B	602	CLA	OBD-CAD	3.49	1.28	1.22
25	b	602	CLA	OBD-CAD	3.49	1.28	1.22
25	B	614	CLA	OBD-CAD	3.49	1.28	1.22
25	b	614	CLA	OBD-CAD	3.49	1.28	1.22
25	A	406	CLA	CHC-C4B	3.49	1.47	1.39
25	a	408	CLA	CHB-C1B	3.49	1.47	1.39
25	C	506	CLA	C1D-ND	-3.49	1.33	1.37
25	c	506	CLA	C1D-ND	-3.49	1.33	1.37
25	d	401	CLA	C1B-NB	-3.49	1.33	1.37
25	B	615	CLA	CHC-C4B	3.48	1.47	1.39
25	B	613	CLA	C1D-ND	-3.48	1.33	1.37
27	B	618	BCR	C11-C12	-3.48	1.25	1.34
25	B	605	CLA	C1D-ND	-3.48	1.33	1.37
25	b	615	CLA	CHD-C4C	3.47	1.47	1.39
25	b	615	CLA	CHC-C4B	3.47	1.47	1.39
27	b	618	BCR	C11-C12	-3.47	1.25	1.34
25	A	408	CLA	CHB-C1B	3.46	1.47	1.39
25	b	613	CLA	C1D-ND	-3.46	1.33	1.37
27	K	103	BCR	C11-C12	-3.45	1.25	1.34
25	B	605	CLA	OBD-CAD	3.45	1.28	1.22
25	b	608	CLA	CHB-C1B	3.45	1.47	1.39
25	B	606	CLA	CHB-C1B	3.44	1.47	1.39
25	b	606	CLA	CHB-C1B	3.44	1.47	1.39
25	B	615	CLA	CHD-C4C	3.44	1.47	1.39
25	B	608	CLA	CHB-C1B	3.44	1.47	1.39
25	a	405	CLA	C1B-NB	-3.44	1.33	1.37
25	A	405	CLA	C1B-NB	-3.43	1.33	1.37
25	B	607	CLA	OBD-CAD	3.43	1.28	1.22
25	b	605	CLA	OBD-CAD	3.43	1.28	1.22
25	b	607	CLA	OBD-CAD	3.43	1.28	1.22
27	k	103	BCR	C11-C12	-3.43	1.25	1.34
25	B	609	CLA	C1D-ND	-3.41	1.33	1.37
25	B	608	CLA	CHC-C4B	3.41	1.47	1.39
25	b	608	CLA	CHC-C4B	3.41	1.47	1.39
25	B	611	CLA	C1C-NC	-3.41	1.32	1.37
25	b	611	CLA	C1C-NC	-3.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	608	CLA	OBD-CAD	3.40	1.28	1.22
25	b	608	CLA	OBD-CAD	3.40	1.28	1.22
25	B	609	CLA	CHC-C4B	3.40	1.47	1.39
25	b	609	CLA	CHC-C4B	3.40	1.47	1.39
25	C	508	CLA	OBD-CAD	3.40	1.28	1.22
25	c	508	CLA	OBD-CAD	3.40	1.28	1.22
25	B	611	CLA	OBD-CAD	3.40	1.28	1.22
25	b	611	CLA	OBD-CAD	3.40	1.28	1.22
25	B	604	CLA	C1B-NB	-3.40	1.33	1.37
25	B	615	CLA	C1D-ND	-3.40	1.33	1.37
25	b	604	CLA	C1B-NB	-3.40	1.33	1.37
25	b	615	CLA	C1D-ND	-3.40	1.33	1.37
25	C	507	CLA	OBD-CAD	3.39	1.28	1.22
25	c	507	CLA	OBD-CAD	3.39	1.28	1.22
25	b	611	CLA	CHC-C4B	3.39	1.47	1.39
26	d	402	PHO	CMC-C2C	-3.38	1.45	1.50
25	B	612	CLA	CHD-C1D	3.38	1.45	1.38
25	b	612	CLA	CHD-C1D	3.38	1.45	1.38
25	B	610	CLA	C1B-NB	-3.38	1.33	1.37
25	b	610	CLA	C1B-NB	-3.38	1.33	1.37
25	B	613	CLA	CHC-C4B	3.38	1.47	1.39
25	b	609	CLA	C1D-ND	-3.38	1.33	1.37
25	C	510	CLA	CHC-C4B	3.37	1.47	1.39
29	D	405	PL9	C3-C4	-3.37	1.44	1.49
29	d	405	PL9	C3-C4	-3.37	1.44	1.49
25	B	611	CLA	CHC-C4B	3.37	1.47	1.39
25	A	406	CLA	CHB-C1B	3.37	1.47	1.39
25	a	406	CLA	CHB-C1B	3.37	1.47	1.39
25	C	511	CLA	CHC-C4B	3.37	1.47	1.39
25	c	511	CLA	CHC-C4B	3.37	1.47	1.39
25	B	610	CLA	CHD-C4C	3.37	1.46	1.39
25	b	610	CLA	CHD-C4C	3.37	1.46	1.39
25	b	614	CLA	C1D-ND	-3.36	1.33	1.37
25	B	606	CLA	OBD-CAD	3.36	1.28	1.22
25	b	606	CLA	OBD-CAD	3.36	1.28	1.22
25	C	509	CLA	C1B-NB	-3.36	1.33	1.37
25	C	508	CLA	CHB-C1B	3.36	1.47	1.39
25	c	508	CLA	CHB-C1B	3.36	1.47	1.39
25	B	603	CLA	CHC-C4B	3.36	1.47	1.39
25	b	603	CLA	CHC-C4B	3.36	1.47	1.39
25	b	613	CLA	CHC-C4B	3.36	1.47	1.39
25	C	508	CLA	MG-ND	-3.36	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	CHC-C4B	3.35	1.46	1.39
25	b	611	CLA	CHD-C4C	3.35	1.46	1.39
27	A	409	BCR	C11-C12	-3.35	1.25	1.34
27	a	409	BCR	C11-C12	-3.35	1.25	1.34
26	A	407	PHO	C4D-CHA	3.35	1.44	1.39
25	C	505	CLA	CHB-C1B	3.35	1.46	1.39
25	c	505	CLA	CHB-C1B	3.35	1.46	1.39
26	D	402	PHO	CMC-C2C	-3.35	1.45	1.50
26	a	407	PHO	C4D-CHA	3.35	1.44	1.39
25	A	405	CLA	C1D-ND	-3.34	1.33	1.37
25	a	405	CLA	C1D-ND	-3.34	1.33	1.37
25	c	509	CLA	C1B-NB	-3.34	1.33	1.37
25	C	506	CLA	CHB-C1B	3.34	1.46	1.39
25	c	506	CLA	CHB-C1B	3.34	1.46	1.39
25	B	614	CLA	C1D-ND	-3.34	1.33	1.37
25	b	616	CLA	C1D-ND	-3.34	1.33	1.37
25	c	508	CLA	MG-ND	-3.34	1.99	2.05
25	B	607	CLA	C1C-NC	-3.34	1.32	1.37
25	b	607	CLA	C1C-NC	-3.34	1.32	1.37
25	B	614	CLA	C1B-NB	-3.34	1.33	1.37
25	b	614	CLA	C1B-NB	-3.34	1.33	1.37
25	B	610	CLA	OBD-CAD	3.33	1.28	1.22
25	b	607	CLA	CHB-C1B	3.33	1.46	1.39
25	C	510	CLA	MG-NC	3.33	2.14	2.06
25	c	510	CLA	MG-NC	3.33	2.14	2.06
25	D	403	CLA	CHD-C4C	3.33	1.46	1.39
25	B	616	CLA	C1D-ND	-3.33	1.33	1.37
25	C	509	CLA	CHB-C1B	3.33	1.46	1.39
25	B	611	CLA	CHD-C4C	3.33	1.46	1.39
25	B	607	CLA	CHB-C1B	3.33	1.46	1.39
25	b	610	CLA	OBD-CAD	3.32	1.28	1.22
25	C	509	CLA	C3D-C2D	3.32	1.48	1.39
25	c	509	CLA	CHB-C1B	3.31	1.46	1.39
25	C	503	CLA	CHC-C4B	3.31	1.46	1.39
25	D	401	CLA	CHB-C1B	3.31	1.46	1.39
25	d	401	CLA	CHB-C1B	3.31	1.46	1.39
25	B	612	CLA	MG-NC	3.31	2.14	2.06
25	b	612	CLA	MG-NC	3.31	2.14	2.06
25	c	509	CLA	C3D-C2D	3.31	1.48	1.39
25	C	508	CLA	CHC-C4B	3.31	1.46	1.39
25	c	508	CLA	CHC-C4B	3.31	1.46	1.39
25	A	405	CLA	CHD-C4C	3.31	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Z	101	BCR	C11-C12	-3.30	1.26	1.34
27	z	101	BCR	C11-C12	-3.30	1.26	1.34
25	C	512	CLA	C1D-ND	-3.30	1.33	1.37
25	d	403	CLA	CHD-C4C	3.30	1.46	1.39
25	c	503	CLA	CHC-C4B	3.30	1.46	1.39
25	C	509	CLA	OBD-CAD	3.29	1.28	1.22
25	c	509	CLA	OBD-CAD	3.29	1.28	1.22
25	a	405	CLA	CHD-C4C	3.28	1.46	1.39
25	C	505	CLA	CHC-C4B	3.28	1.46	1.39
25	c	505	CLA	CHC-C4B	3.28	1.46	1.39
25	B	604	CLA	OBD-CAD	3.28	1.28	1.22
25	b	604	CLA	OBD-CAD	3.28	1.28	1.22
25	b	612	CLA	C1B-NB	-3.28	1.33	1.37
25	d	404	CLA	CHB-C1B	3.28	1.46	1.39
25	B	607	CLA	CHC-C4B	3.27	1.46	1.39
25	D	401	CLA	CHC-C4B	3.26	1.46	1.39
25	D	403	CLA	OBD-CAD	3.26	1.28	1.22
25	d	403	CLA	OBD-CAD	3.26	1.28	1.22
25	D	401	CLA	OBD-CAD	3.26	1.28	1.22
25	d	401	CLA	OBD-CAD	3.26	1.28	1.22
25	B	616	CLA	OBD-CAD	3.26	1.28	1.22
25	b	616	CLA	OBD-CAD	3.26	1.28	1.22
25	b	607	CLA	CHC-C4B	3.26	1.46	1.39
25	C	513	CLA	MG-NC	3.25	2.14	2.06
25	c	503	CLA	OBD-CAD	3.25	1.28	1.22
27	F	101	BCR	C11-C12	-3.25	1.26	1.34
27	f	101	BCR	C11-C12	-3.25	1.26	1.34
25	b	607	CLA	C1B-NB	-3.25	1.33	1.37
25	a	405	CLA	C3C-C2C	3.25	1.43	1.36
25	c	514	CLA	C1D-ND	-3.25	1.33	1.37
25	C	503	CLA	C1C-NC	-3.25	1.32	1.37
25	c	503	CLA	C1C-NC	-3.25	1.32	1.37
25	b	606	CLA	C1D-ND	-3.24	1.33	1.37
25	D	404	CLA	CHB-C1B	3.24	1.46	1.39
25	C	514	CLA	C1D-ND	-3.24	1.33	1.37
25	C	503	CLA	OBD-CAD	3.24	1.28	1.22
25	B	603	CLA	OBD-CAD	3.24	1.28	1.22
25	B	612	CLA	C1B-NB	-3.24	1.33	1.37
25	B	606	CLA	C1D-ND	-3.24	1.33	1.37
25	b	603	CLA	OBD-CAD	3.24	1.28	1.22
25	B	607	CLA	C1B-NB	-3.23	1.33	1.37
30	a	412	SQD	O48-C23	3.23	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	512	CLA	C1D-ND	-3.23	1.33	1.37
25	d	401	CLA	CHC-C4B	3.22	1.46	1.39
25	c	502	CLA	OBD-CAD	3.22	1.28	1.22
30	A	412	SQD	O48-C23	3.22	1.42	1.33
25	B	612	CLA	OBD-CAD	3.22	1.28	1.22
25	b	612	CLA	OBD-CAD	3.22	1.28	1.22
25	A	405	CLA	C3C-C2C	3.22	1.43	1.36
25	C	503	CLA	C1B-NB	-3.21	1.33	1.37
25	c	513	CLA	MG-NC	3.21	2.13	2.06
25	C	502	CLA	OBD-CAD	3.21	1.28	1.22
25	C	507	CLA	C1C-NC	-3.21	1.32	1.37
25	c	507	CLA	C1C-NC	-3.21	1.32	1.37
36	H	101	RRX	C8-C9	-3.21	1.39	1.46
36	h	101	RRX	C8-C9	-3.21	1.39	1.46
25	C	514	CLA	C3D-C2D	3.21	1.47	1.39
25	c	514	CLA	C3D-C2D	3.21	1.47	1.39
25	C	504	CLA	MG-NC	3.20	2.13	2.06
25	c	504	CLA	MG-NC	3.20	2.13	2.06
25	c	503	CLA	C1B-NB	-3.20	1.33	1.37
25	B	609	CLA	MG-NC	3.18	2.13	2.06
25	b	609	CLA	MG-NC	3.18	2.13	2.06
30	K	101	SQD	O48-C23	3.17	1.42	1.33
30	k	101	SQD	O48-C23	3.17	1.42	1.33
25	b	610	CLA	MG-NC	3.17	2.13	2.06
25	B	616	CLA	CHC-C4B	3.17	1.46	1.39
25	B	610	CLA	C1C-NC	-3.16	1.32	1.37
30	A	413	SQD	O48-C23	3.15	1.42	1.33
30	a	413	SQD	O48-C23	3.15	1.42	1.33
25	b	610	CLA	C1C-NC	-3.15	1.32	1.37
25	C	509	CLA	C1D-ND	-3.15	1.33	1.37
25	c	509	CLA	C1D-ND	-3.15	1.33	1.37
25	b	616	CLA	CHC-C4B	3.15	1.46	1.39
30	F	102	SQD	O48-C23	3.14	1.42	1.33
30	f	102	SQD	O48-C23	3.14	1.42	1.33
25	B	610	CLA	MG-NC	3.14	2.13	2.06
25	B	612	CLA	MG-ND	-3.13	1.99	2.05
25	b	612	CLA	MG-ND	-3.13	1.99	2.05
25	B	601	CLA	MG-NC	3.13	2.13	2.06
25	b	601	CLA	MG-NC	3.13	2.13	2.06
26	D	402	PHO	C4D-ND	-3.13	1.33	1.38
25	B	604	CLA	CHC-C4B	3.13	1.46	1.39
25	b	604	CLA	CHC-C4B	3.13	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	504	CLA	OBD-CAD	3.13	1.27	1.22
25	C	507	CLA	C3D-C2D	3.13	1.47	1.39
25	c	507	CLA	C3D-C2D	3.13	1.47	1.39
26	d	402	PHO	C4D-ND	-3.13	1.33	1.38
25	c	504	CLA	OBD-CAD	3.12	1.27	1.22
25	A	408	CLA	C1B-NB	-3.12	1.33	1.37
25	a	408	CLA	C1B-NB	-3.12	1.33	1.37
25	C	508	CLA	C4B-NB	-3.12	1.33	1.37
25	c	508	CLA	C4B-NB	-3.12	1.33	1.37
25	d	404	CLA	C3D-C2D	3.12	1.47	1.39
25	D	401	CLA	C1C-NC	-3.11	1.33	1.37
25	d	401	CLA	C1C-NC	-3.11	1.33	1.37
25	B	604	CLA	C1C-NC	-3.10	1.33	1.37
25	b	604	CLA	C1C-NC	-3.10	1.33	1.37
25	B	616	CLA	C3D-C2D	3.10	1.47	1.39
25	b	615	CLA	C3D-C2D	3.10	1.47	1.39
25	B	605	CLA	C1B-NB	-3.09	1.33	1.37
25	b	605	CLA	C1B-NB	-3.09	1.33	1.37
25	B	614	CLA	MG-NC	3.09	2.13	2.06
25	A	408	CLA	C1D-ND	-3.09	1.33	1.37
25	a	408	CLA	C1D-ND	-3.09	1.33	1.37
25	b	604	CLA	MG-ND	-3.09	1.99	2.05
25	b	614	CLA	MG-NC	3.09	2.13	2.06
25	B	610	CLA	C1D-ND	-3.09	1.33	1.37
25	b	610	CLA	C1D-ND	-3.09	1.33	1.37
25	D	404	CLA	C3D-C2D	3.09	1.47	1.39
27	K	102	BCR	C11-C12	-3.09	1.26	1.34
27	k	102	BCR	C11-C12	-3.09	1.26	1.34
25	C	513	CLA	C1B-NB	-3.09	1.33	1.37
25	c	513	CLA	C1B-NB	-3.09	1.33	1.37
25	B	609	CLA	C3D-C2D	3.09	1.47	1.39
25	B	604	CLA	C1D-ND	-3.08	1.33	1.37
25	b	604	CLA	C1D-ND	-3.08	1.33	1.37
25	b	616	CLA	C3D-C2D	3.08	1.47	1.39
25	B	615	CLA	MG-NC	3.08	2.13	2.06
25	b	615	CLA	MG-NC	3.08	2.13	2.06
25	C	505	CLA	C1B-NB	-3.08	1.33	1.37
25	c	505	CLA	C1B-NB	-3.08	1.33	1.37
30	H	103	SQD	O48-C23	3.07	1.42	1.33
25	D	401	CLA	C1D-ND	-3.07	1.33	1.37
25	d	401	CLA	C1D-ND	-3.07	1.33	1.37
30	h	103	SQD	O48-C23	3.07	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	615	CLA	C3D-C2D	3.06	1.47	1.39
25	C	503	CLA	C1D-ND	-3.06	1.33	1.37
25	c	503	CLA	C1D-ND	-3.06	1.33	1.37
25	b	609	CLA	C3D-C2D	3.06	1.47	1.39
25	a	408	CLA	C3D-C2D	3.06	1.47	1.39
25	B	604	CLA	MG-ND	-3.05	1.99	2.05
25	A	408	CLA	C3D-C2D	3.05	1.47	1.39
30	F	102	SQD	O47-C7	3.05	1.42	1.34
30	f	102	SQD	O47-C7	3.05	1.42	1.34
25	D	404	CLA	C1B-NB	-3.05	1.33	1.37
25	B	607	CLA	C1D-ND	-3.05	1.33	1.37
25	b	607	CLA	C1D-ND	-3.05	1.33	1.37
25	B	615	CLA	C1B-C2B	3.04	1.50	1.43
25	C	510	CLA	C3D-C2D	3.03	1.47	1.39
25	c	510	CLA	C3D-C2D	3.03	1.47	1.39
25	B	615	CLA	C1B-NB	-3.02	1.33	1.37
25	b	615	CLA	C1B-NB	-3.02	1.33	1.37
25	b	615	CLA	C1B-C2B	3.02	1.50	1.43
25	b	612	CLA	CHD-C4C	3.02	1.46	1.39
25	C	513	CLA	C4D-CHA	3.02	1.48	1.38
25	A	406	CLA	C1B-NB	-3.02	1.33	1.37
25	C	505	CLA	C3D-C2D	3.02	1.47	1.39
25	B	613	CLA	C3D-C2D	3.01	1.47	1.39
25	b	613	CLA	C3D-C2D	3.01	1.47	1.39
25	B	612	CLA	CHD-C4C	3.01	1.46	1.39
25	c	505	CLA	C3D-C2D	3.01	1.47	1.39
25	c	514	CLA	C1B-NB	-3.01	1.33	1.37
25	B	601	CLA	C1B-NB	-3.01	1.33	1.37
25	b	601	CLA	C1B-NB	-3.01	1.33	1.37
25	B	613	CLA	C4D-CHA	3.00	1.48	1.38
25	b	613	CLA	C4D-CHA	3.00	1.48	1.38
25	A	405	CLA	OBD-CAD	3.00	1.27	1.22
25	a	405	CLA	OBD-CAD	3.00	1.27	1.22
25	B	603	CLA	MG-NC	3.00	2.13	2.06
25	b	603	CLA	MG-NC	3.00	2.13	2.06
25	C	505	CLA	C1D-ND	-3.00	1.33	1.37
25	c	505	CLA	C1D-ND	-3.00	1.33	1.37
25	B	601	CLA	C1D-ND	-3.00	1.33	1.37
25	b	601	CLA	C1D-ND	-3.00	1.33	1.37
25	B	612	CLA	C4B-NB	-2.99	1.33	1.37
25	b	612	CLA	C4B-NB	-2.99	1.33	1.37
26	D	402	PHO	C4D-CHA	2.99	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	402	PHO	C4D-CHA	2.99	1.44	1.39
25	c	513	CLA	C4D-CHA	2.99	1.48	1.38
25	C	512	CLA	MG-NC	2.99	2.13	2.06
25	c	512	CLA	MG-NC	2.99	2.13	2.06
35	V	201	HEM	C4B-NB	-2.99	1.33	1.38
35	v	201	HEM	C4B-NB	-2.99	1.33	1.38
30	c	501	SQD	O48-C23	2.99	1.42	1.33
30	C	501	SQD	O48-C23	2.99	1.42	1.33
25	d	404	CLA	C1B-NB	-2.99	1.33	1.37
25	c	510	CLA	C1C-NC	-2.98	1.33	1.37
25	B	602	CLA	C3D-C2D	2.98	1.47	1.39
25	a	406	CLA	C1B-NB	-2.98	1.33	1.37
35	V	201	HEM	C1C-C2C	-2.98	1.39	1.45
25	b	606	CLA	C3D-C2D	2.98	1.47	1.39
25	c	508	CLA	C1C-NC	-2.98	1.33	1.37
25	B	605	CLA	C1B-C2B	2.98	1.50	1.43
25	b	605	CLA	C1B-C2B	2.98	1.50	1.43
25	C	514	CLA	C1B-NB	-2.98	1.34	1.37
25	A	408	CLA	MG-NC	2.98	2.13	2.06
25	C	503	CLA	MG-ND	-2.97	1.99	2.05
25	b	602	CLA	C3D-C2D	2.97	1.47	1.39
25	C	504	CLA	C4D-CHA	2.97	1.48	1.38
25	c	504	CLA	C4D-CHA	2.97	1.48	1.38
30	a	413	SQD	O47-C7	2.97	1.42	1.34
25	C	507	CLA	C1D-ND	-2.97	1.34	1.37
25	D	404	CLA	C1D-ND	-2.97	1.34	1.37
25	c	507	CLA	C1D-ND	-2.97	1.34	1.37
25	d	404	CLA	C1D-ND	-2.97	1.34	1.37
25	C	502	CLA	C3D-C2D	2.97	1.47	1.39
25	c	502	CLA	C3D-C2D	2.97	1.47	1.39
25	C	503	CLA	C3D-C2D	2.97	1.47	1.39
25	c	503	CLA	C3D-C2D	2.97	1.47	1.39
28	H	105	LMG	C19-C18	-2.96	1.33	1.51
28	h	105	LMG	C19-C18	-2.96	1.33	1.51
25	c	507	CLA	C4D-CHA	2.96	1.48	1.38
25	A	405	CLA	C1C-NC	-2.96	1.33	1.37
25	a	405	CLA	C1C-NC	-2.96	1.33	1.37
28	H	105	LMG	C43-C42	-2.96	1.33	1.51
28	h	105	LMG	C43-C42	-2.96	1.33	1.51
25	B	606	CLA	C3D-C2D	2.96	1.47	1.39
35	v	201	HEM	C1C-C2C	-2.96	1.39	1.45
25	B	610	CLA	C3D-C2D	2.96	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	610	CLA	C3D-C2D	2.96	1.47	1.39
25	c	503	CLA	MG-ND	-2.96	1.99	2.05
25	a	408	CLA	MG-NC	2.96	2.13	2.06
25	C	508	CLA	C1C-NC	-2.95	1.33	1.37
25	B	614	CLA	C1C-NC	-2.95	1.33	1.37
25	b	614	CLA	C1C-NC	-2.95	1.33	1.37
25	D	401	CLA	C3D-C2D	2.95	1.47	1.39
25	d	401	CLA	C3D-C2D	2.95	1.47	1.39
36	H	101	RRX	C23-C22	-2.95	1.39	1.46
36	h	101	RRX	C23-C22	-2.95	1.39	1.46
25	C	510	CLA	C1C-NC	-2.94	1.33	1.37
25	B	611	CLA	C3D-C2D	2.94	1.47	1.39
25	b	611	CLA	C3D-C2D	2.94	1.47	1.39
25	C	507	CLA	C4D-CHA	2.94	1.48	1.38
25	B	614	CLA	C4B-NB	-2.94	1.34	1.37
25	b	614	CLA	C4B-NB	-2.94	1.34	1.37
25	c	510	CLA	C1B-C2B	2.94	1.50	1.43
25	D	401	CLA	C4B-NB	-2.94	1.34	1.37
25	d	401	CLA	C4B-NB	-2.94	1.34	1.37
30	A	413	SQD	O47-C7	2.94	1.42	1.34
25	C	502	CLA	C1B-NB	-2.94	1.34	1.37
25	c	502	CLA	C1B-NB	-2.94	1.34	1.37
25	b	609	CLA	C4D-CHA	2.93	1.48	1.38
25	C	504	CLA	C1B-C2B	2.93	1.50	1.43
25	c	504	CLA	C1B-C2B	2.93	1.50	1.43
25	C	513	CLA	C1B-C2B	2.93	1.50	1.43
25	c	513	CLA	C1B-C2B	2.93	1.50	1.43
25	B	607	CLA	C3D-C2D	2.93	1.47	1.39
25	b	607	CLA	C3D-C2D	2.93	1.47	1.39
25	D	403	CLA	C1B-NB	-2.93	1.34	1.37
25	d	403	CLA	C1B-NB	-2.93	1.34	1.37
25	C	510	CLA	C1B-C2B	2.93	1.50	1.43
25	C	507	CLA	CHC-C4B	2.93	1.46	1.39
25	c	507	CLA	CHC-C4B	2.93	1.46	1.39
25	A	406	CLA	C4B-NB	-2.92	1.34	1.37
25	a	406	CLA	C4B-NB	-2.92	1.34	1.37
25	A	406	CLA	C1D-ND	-2.92	1.34	1.37
25	a	406	CLA	C1D-ND	-2.92	1.34	1.37
25	b	604	CLA	MG-NC	2.92	2.13	2.06
25	B	602	CLA	MG-NC	2.92	2.13	2.06
25	b	602	CLA	MG-NC	2.92	2.13	2.06
25	B	609	CLA	C4D-CHA	2.91	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	C4D-CHA	2.91	1.48	1.38
25	B	601	CLA	C3D-C2D	2.91	1.46	1.39
25	b	601	CLA	C3D-C2D	2.91	1.46	1.39
25	B	608	CLA	MG-NC	2.90	2.13	2.06
25	b	608	CLA	MG-NC	2.90	2.13	2.06
25	B	610	CLA	MG-ND	-2.90	2.00	2.05
25	C	507	CLA	MG-NC	2.90	2.13	2.06
25	c	507	CLA	MG-NC	2.90	2.13	2.06
25	C	514	CLA	MG-NC	2.90	2.13	2.06
25	c	514	CLA	MG-NC	2.90	2.13	2.06
26	A	407	PHO	C4D-ND	-2.90	1.34	1.38
26	a	407	PHO	C4D-ND	-2.90	1.34	1.38
25	C	510	CLA	C4D-CHA	2.90	1.48	1.38
30	H	103	SQD	O47-C7	2.90	1.42	1.34
30	h	103	SQD	O47-C7	2.90	1.42	1.34
25	D	403	CLA	MG-ND	-2.90	2.00	2.05
25	d	403	CLA	MG-ND	-2.90	2.00	2.05
25	C	511	CLA	MG-ND	-2.89	2.00	2.05
25	c	513	CLA	MG-ND	-2.89	2.00	2.05
25	B	604	CLA	MG-NC	2.89	2.13	2.06
25	C	513	CLA	MG-ND	-2.88	2.00	2.05
25	c	511	CLA	MG-ND	-2.88	2.00	2.05
25	c	508	CLA	C4D-CHA	2.88	1.48	1.38
25	C	504	CLA	C1B-NB	-2.88	1.34	1.37
25	c	504	CLA	C1B-NB	-2.88	1.34	1.37
25	C	502	CLA	C1B-C2B	2.87	1.49	1.43
25	c	502	CLA	C1B-C2B	2.87	1.49	1.43
25	b	616	CLA	C4D-CHA	2.87	1.48	1.38
25	b	607	CLA	C4D-CHA	2.87	1.48	1.38
25	C	502	CLA	MG-NC	2.87	2.13	2.06
25	c	502	CLA	MG-NC	2.87	2.13	2.06
25	c	511	CLA	MG-NC	2.87	2.13	2.06
25	B	601	CLA	C4D-CHA	2.87	1.48	1.38
25	C	508	CLA	C4D-CHA	2.87	1.48	1.38
25	b	601	CLA	C4D-CHA	2.87	1.48	1.38
25	b	610	CLA	MG-ND	-2.87	2.00	2.05
30	A	412	SQD	O47-C7	2.87	1.42	1.34
30	a	412	SQD	O47-C7	2.87	1.42	1.34
25	C	507	CLA	C4B-NB	-2.87	1.34	1.37
25	b	605	CLA	C1C-NC	-2.87	1.33	1.37
25	B	610	CLA	C4D-CHA	2.87	1.48	1.38
25	b	610	CLA	C4D-CHA	2.87	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	605	CLA	C1C-NC	-2.86	1.33	1.37
25	C	512	CLA	C1B-C2B	2.86	1.49	1.43
25	B	616	CLA	C4D-CHA	2.86	1.48	1.38
25	c	512	CLA	C1B-C2B	2.86	1.49	1.43
25	a	406	CLA	C3D-C2D	2.86	1.46	1.39
25	B	606	CLA	C1B-NB	-2.86	1.34	1.37
25	b	606	CLA	C1B-NB	-2.86	1.34	1.37
25	B	607	CLA	C4D-CHA	2.86	1.48	1.38
25	c	508	CLA	C3D-C2D	2.85	1.46	1.39
29	A	411	PL9	C3-C4	-2.85	1.45	1.49
25	C	511	CLA	MG-NC	2.85	2.13	2.06
25	B	608	CLA	C3D-C2D	2.85	1.46	1.39
25	C	507	CLA	MG-ND	-2.85	2.00	2.05
25	c	504	CLA	C1D-ND	-2.85	1.34	1.37
25	C	508	CLA	C3D-C2D	2.84	1.46	1.39
25	A	406	CLA	C3D-C2D	2.84	1.46	1.39
25	C	504	CLA	C1D-ND	-2.84	1.34	1.37
25	b	608	CLA	C3D-C2D	2.84	1.46	1.39
25	D	404	CLA	MG-NC	2.84	2.13	2.06
25	A	408	CLA	C4B-NB	-2.83	1.34	1.37
25	a	408	CLA	C4B-NB	-2.83	1.34	1.37
25	c	507	CLA	MG-ND	-2.83	2.00	2.05
25	D	403	CLA	C1B-C2B	2.83	1.49	1.43
25	d	403	CLA	C1B-C2B	2.83	1.49	1.43
25	C	506	CLA	MG-ND	-2.83	2.00	2.05
25	C	509	CLA	C1C-NC	-2.83	1.33	1.37
25	c	509	CLA	C1C-NC	-2.83	1.33	1.37
25	c	507	CLA	C4B-NB	-2.83	1.34	1.37
25	b	604	CLA	C4D-CHA	2.82	1.48	1.38
25	C	506	CLA	C1C-NC	-2.82	1.33	1.37
25	c	506	CLA	C1C-NC	-2.82	1.33	1.37
25	B	609	CLA	C1B-C2B	2.82	1.49	1.43
30	K	101	SQD	O47-C7	2.81	1.42	1.34
30	k	101	SQD	O47-C7	2.81	1.42	1.34
25	d	404	CLA	MG-NC	2.81	2.13	2.06
29	a	411	PL9	C3-C4	-2.81	1.45	1.49
25	B	613	CLA	C1B-NB	-2.81	1.34	1.37
25	b	613	CLA	C1B-NB	-2.81	1.34	1.37
25	C	502	CLA	C1D-ND	-2.81	1.34	1.37
25	c	502	CLA	C1D-ND	-2.81	1.34	1.37
25	C	512	CLA	C3D-C2D	2.80	1.46	1.39
25	c	512	CLA	C3D-C2D	2.80	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	MG-ND	-2.80	2.00	2.05
25	B	615	CLA	C4D-CHA	2.80	1.48	1.38
25	B	606	CLA	C4D-CHA	2.80	1.48	1.38
25	b	606	CLA	C4D-CHA	2.80	1.48	1.38
25	B	604	CLA	C4D-CHA	2.80	1.48	1.38
25	b	615	CLA	C4D-CHA	2.80	1.48	1.38
25	A	406	CLA	C1C-NC	-2.80	1.33	1.37
25	a	406	CLA	C1C-NC	-2.80	1.33	1.37
25	c	511	CLA	C4D-CHA	2.80	1.48	1.38
25	A	405	CLA	MG-ND	-2.80	2.00	2.05
25	b	609	CLA	C1B-C2B	2.79	1.49	1.43
25	A	408	CLA	C4D-CHA	2.79	1.48	1.38
25	a	408	CLA	C4D-CHA	2.79	1.48	1.38
25	B	614	CLA	MG-ND	-2.79	2.00	2.05
25	b	614	CLA	MG-ND	-2.79	2.00	2.05
25	a	405	CLA	MG-ND	-2.79	2.00	2.05
25	B	611	CLA	C4B-NB	-2.79	1.34	1.37
25	b	611	CLA	C4B-NB	-2.79	1.34	1.37
25	C	514	CLA	C4D-CHA	2.79	1.47	1.38
25	c	514	CLA	C4D-CHA	2.79	1.47	1.38
25	B	603	CLA	C1C-NC	-2.78	1.33	1.37
25	b	603	CLA	C1C-NC	-2.78	1.33	1.37
25	B	613	CLA	MG-ND	-2.78	2.00	2.05
25	b	613	CLA	MG-ND	-2.78	2.00	2.05
25	B	604	CLA	C1B-C2B	2.78	1.49	1.43
25	b	604	CLA	C1B-C2B	2.78	1.49	1.43
25	C	504	CLA	MG-ND	-2.78	2.00	2.05
25	c	504	CLA	MG-ND	-2.78	2.00	2.05
25	C	511	CLA	C4D-CHA	2.78	1.47	1.38
25	B	613	CLA	C1B-C2B	2.78	1.49	1.43
25	b	613	CLA	C1B-C2B	2.78	1.49	1.43
25	A	406	CLA	C4D-CHA	2.78	1.47	1.38
25	a	406	CLA	C4D-CHA	2.78	1.47	1.38
29	A	411	PL9	C53-C6	-2.77	1.45	1.50
25	B	616	CLA	C1B-C2B	2.77	1.49	1.43
25	b	616	CLA	C1B-C2B	2.77	1.49	1.43
29	a	411	PL9	C53-C6	-2.77	1.45	1.50
25	C	508	CLA	MG-NC	2.77	2.12	2.06
25	c	508	CLA	MG-NC	2.77	2.12	2.06
25	C	512	CLA	C1B-NB	-2.77	1.34	1.37
25	c	512	CLA	C1B-NB	-2.77	1.34	1.37
25	B	602	CLA	C4D-CHA	2.77	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	411	PL9	C7-C3	-2.77	1.47	1.51
29	a	411	PL9	C7-C3	-2.77	1.47	1.51
25	C	514	CLA	C1C-NC	-2.76	1.33	1.37
25	c	514	CLA	C1C-NC	-2.76	1.33	1.37
26	D	402	PHO	CMD-C2D	-2.76	1.46	1.51
26	d	402	PHO	CMD-C2D	-2.76	1.46	1.51
25	C	503	CLA	C4D-CHA	2.76	1.47	1.38
25	c	503	CLA	C4D-CHA	2.76	1.47	1.38
25	b	602	CLA	C4D-CHA	2.76	1.47	1.38
25	C	505	CLA	C4B-NB	-2.76	1.34	1.37
25	c	505	CLA	C4B-NB	-2.76	1.34	1.37
26	A	407	PHO	CMC-C2C	-2.76	1.46	1.50
26	a	407	PHO	CMC-C2C	-2.76	1.46	1.50
25	C	505	CLA	C1C-NC	-2.75	1.33	1.37
25	c	505	CLA	C1C-NC	-2.75	1.33	1.37
25	A	406	CLA	MG-NC	2.75	2.12	2.06
31	H	102	LMT	O2'-C2'	-2.75	1.36	1.43
31	h	102	LMT	O2'-C2'	-2.75	1.36	1.43
25	b	606	CLA	C1C-NC	-2.75	1.33	1.37
25	a	406	CLA	C1B-C2B	2.75	1.49	1.43
25	C	505	CLA	C4D-CHA	2.75	1.47	1.38
25	c	505	CLA	C4D-CHA	2.75	1.47	1.38
25	B	614	CLA	C1B-C2B	2.75	1.49	1.43
25	b	614	CLA	C1B-C2B	2.75	1.49	1.43
25	C	503	CLA	C4B-NB	-2.74	1.34	1.37
25	c	507	CLA	C4C-C3C	2.74	1.49	1.45
25	B	605	CLA	C4B-NB	-2.74	1.34	1.37
25	b	605	CLA	C4B-NB	-2.74	1.34	1.37
25	A	406	CLA	C1B-C2B	2.73	1.49	1.43
25	b	611	CLA	C4D-CHA	2.73	1.47	1.38
25	c	502	CLA	C4D-CHA	2.73	1.47	1.38
25	C	512	CLA	MG-ND	-2.72	2.00	2.05
25	c	512	CLA	MG-ND	-2.72	2.00	2.05
25	C	507	CLA	C4C-C3C	2.72	1.49	1.45
31	D	412	LMT	O3'-C3'	-2.72	1.36	1.43
31	d	412	LMT	O3'-C3'	-2.72	1.36	1.43
25	B	606	CLA	C1C-NC	-2.72	1.33	1.37
25	B	611	CLA	C4D-CHA	2.72	1.47	1.38
25	a	406	CLA	MG-NC	2.72	2.12	2.06
25	B	608	CLA	C4D-CHA	2.71	1.47	1.38
25	b	608	CLA	C4D-CHA	2.71	1.47	1.38
25	B	607	CLA	MG-ND	-2.71	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	C1C-NC	-2.71	1.33	1.37
25	b	613	CLA	C1C-NC	-2.71	1.33	1.37
25	B	613	CLA	MG-NC	2.71	2.12	2.06
25	b	613	CLA	MG-NC	2.71	2.12	2.06
25	C	502	CLA	C4D-CHA	2.71	1.47	1.38
25	c	503	CLA	C4B-NB	-2.70	1.34	1.37
25	b	607	CLA	MG-ND	-2.70	2.00	2.05
25	C	514	CLA	C1B-C2B	2.70	1.49	1.43
25	c	514	CLA	C1B-C2B	2.70	1.49	1.43
25	B	609	CLA	MG-ND	-2.70	2.00	2.05
25	b	609	CLA	MG-ND	-2.70	2.00	2.05
25	b	611	CLA	MG-ND	-2.70	2.00	2.05
25	d	403	CLA	C4B-NB	-2.70	1.34	1.37
25	C	502	CLA	C1C-NC	-2.70	1.33	1.37
25	c	502	CLA	C1C-NC	-2.70	1.33	1.37
25	D	404	CLA	C4D-CHA	2.69	1.47	1.38
25	d	404	CLA	C4D-CHA	2.69	1.47	1.38
25	C	509	CLA	MG-NC	2.69	2.12	2.06
25	c	509	CLA	MG-NC	2.69	2.12	2.06
25	B	611	CLA	MG-ND	-2.69	2.00	2.05
25	C	512	CLA	C4D-CHA	2.69	1.47	1.38
25	c	512	CLA	C4D-CHA	2.69	1.47	1.38
25	B	601	CLA	C1C-NC	-2.69	1.33	1.37
25	b	601	CLA	C1C-NC	-2.69	1.33	1.37
26	a	407	PHO	CMD-C2D	-2.69	1.46	1.51
29	d	405	PL9	C6-C1	-2.69	1.44	1.48
25	C	505	CLA	MG-ND	-2.68	2.00	2.05
25	c	505	CLA	MG-ND	-2.68	2.00	2.05
25	b	612	CLA	C3D-C2D	2.68	1.46	1.39
25	B	614	CLA	C4D-CHA	2.68	1.47	1.38
25	b	614	CLA	C4D-CHA	2.68	1.47	1.38
25	B	608	CLA	C4B-NB	-2.68	1.34	1.37
25	c	503	CLA	MG-NC	2.67	2.12	2.06
25	b	608	CLA	C4B-NB	-2.67	1.34	1.37
25	C	504	CLA	C3D-C2D	2.67	1.46	1.39
25	c	504	CLA	C3D-C2D	2.67	1.46	1.39
25	B	606	CLA	MG-ND	-2.67	2.00	2.05
25	b	606	CLA	MG-ND	-2.67	2.00	2.05
25	C	510	CLA	MG-ND	-2.67	2.00	2.05
25	B	609	CLA	C4B-NB	-2.67	1.34	1.37
25	b	609	CLA	C4B-NB	-2.67	1.34	1.37
29	D	405	PL9	C6-C1	-2.67	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	605	CLA	C3D-C2D	2.66	1.46	1.39
25	b	605	CLA	C3D-C2D	2.66	1.46	1.39
26	A	407	PHO	CMD-C2D	-2.66	1.46	1.51
25	A	408	CLA	C1B-C2B	2.66	1.49	1.43
25	a	408	CLA	C1B-C2B	2.66	1.49	1.43
25	B	603	CLA	C4D-CHA	2.66	1.47	1.38
25	B	601	CLA	MG-ND	-2.66	2.00	2.05
25	D	401	CLA	C4D-CHA	2.66	1.47	1.38
25	d	401	CLA	C4D-CHA	2.66	1.47	1.38
25	D	403	CLA	C4B-NB	-2.66	1.34	1.37
25	D	403	CLA	CHD-C1D	2.66	1.43	1.38
25	d	403	CLA	CHD-C1D	2.66	1.43	1.38
25	B	606	CLA	MG-NC	2.66	2.12	2.06
25	b	606	CLA	MG-NC	2.66	2.12	2.06
25	B	613	CLA	OBD-CAD	2.66	1.27	1.22
25	b	613	CLA	OBD-CAD	2.66	1.27	1.22
25	C	503	CLA	MG-NC	2.66	2.12	2.06
25	C	509	CLA	MG-ND	-2.65	2.00	2.05
25	c	510	CLA	MG-ND	-2.65	2.00	2.05
25	c	509	CLA	MG-ND	-2.65	2.00	2.05
25	D	403	CLA	C1C-NC	-2.65	1.33	1.37
25	C	506	CLA	MG-NC	2.64	2.12	2.06
25	B	612	CLA	C3D-C2D	2.64	1.46	1.39
25	b	603	CLA	C4D-CHA	2.64	1.47	1.38
25	C	502	CLA	C4B-NB	-2.64	1.34	1.37
25	c	502	CLA	C4B-NB	-2.64	1.34	1.37
25	B	615	CLA	C1C-NC	-2.64	1.33	1.37
25	B	616	CLA	MG-ND	-2.64	2.00	2.05
25	b	616	CLA	MG-ND	-2.64	2.00	2.05
25	b	615	CLA	C4B-NB	-2.63	1.34	1.37
25	b	611	CLA	MG-NC	2.63	2.12	2.06
25	D	404	CLA	C4B-NB	-2.63	1.34	1.37
25	d	404	CLA	C4B-NB	-2.63	1.34	1.37
25	C	514	CLA	C4B-NB	-2.63	1.34	1.37
25	c	514	CLA	C4B-NB	-2.63	1.34	1.37
25	c	506	CLA	C4D-CHA	2.63	1.47	1.38
25	C	509	CLA	C4D-CHA	2.63	1.47	1.38
25	c	509	CLA	C4D-CHA	2.63	1.47	1.38
25	b	601	CLA	MG-ND	-2.63	2.00	2.05
25	C	506	CLA	C4D-CHA	2.62	1.47	1.38
25	C	502	CLA	MG-ND	-2.62	2.00	2.05
31	M	102	LMT	O3'-C3'	-2.62	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	m	102	LMT	O3'-C3'	-2.62	1.36	1.43
25	C	503	CLA	C1B-C2B	2.62	1.49	1.43
31	D	411	LMT	O3'-C3'	-2.62	1.36	1.43
31	d	411	LMT	O3'-C3'	-2.62	1.36	1.43
35	E	104	HEM	C1C-C2C	-2.62	1.40	1.45
35	e	104	HEM	C1C-C2C	-2.62	1.40	1.45
25	B	612	CLA	C1B-C2B	2.62	1.49	1.43
25	b	612	CLA	C1B-C2B	2.62	1.49	1.43
31	i	103	LMT	O3'-C3'	-2.62	1.36	1.43
25	C	514	CLA	MG-ND	-2.61	2.00	2.05
25	c	514	CLA	MG-ND	-2.61	2.00	2.05
25	B	611	CLA	MG-NC	2.61	2.12	2.06
25	c	506	CLA	MG-NC	2.61	2.12	2.06
25	b	615	CLA	C1C-NC	-2.61	1.33	1.37
25	B	602	CLA	C1B-C2B	2.61	1.49	1.43
25	b	602	CLA	C1B-C2B	2.61	1.49	1.43
25	a	405	CLA	C4B-NB	-2.60	1.34	1.37
25	a	406	CLA	MG-ND	-2.60	2.00	2.05
31	I	103	LMT	O3'-C3'	-2.60	1.36	1.43
25	B	609	CLA	C1C-NC	-2.60	1.33	1.37
25	b	609	CLA	C1C-NC	-2.60	1.33	1.37
25	d	403	CLA	C1C-NC	-2.60	1.33	1.37
25	C	512	CLA	C1C-NC	-2.60	1.33	1.37
25	c	512	CLA	C1C-NC	-2.60	1.33	1.37
25	A	405	CLA	C1B-C2B	2.60	1.49	1.43
25	a	405	CLA	C1B-C2B	2.60	1.49	1.43
25	B	615	CLA	C4B-NB	-2.60	1.34	1.37
25	C	513	CLA	C4B-NB	-2.60	1.34	1.37
25	c	513	CLA	C4B-NB	-2.60	1.34	1.37
25	A	406	CLA	MG-ND	-2.59	2.00	2.05
25	B	604	CLA	C4B-NB	-2.59	1.34	1.37
25	b	604	CLA	C4B-NB	-2.59	1.34	1.37
25	b	608	CLA	MG-ND	-2.59	2.00	2.05
25	c	502	CLA	MG-ND	-2.59	2.00	2.05
25	B	606	CLA	C4B-NB	-2.59	1.34	1.37
25	b	602	CLA	C4B-NB	-2.59	1.34	1.37
25	b	606	CLA	C4B-NB	-2.59	1.34	1.37
30	c	501	SQD	O47-C7	2.59	1.41	1.34
25	B	608	CLA	MG-ND	-2.59	2.00	2.05
30	C	501	SQD	O47-C7	2.58	1.41	1.34
25	D	401	CLA	MG-ND	-2.58	2.00	2.05
25	d	401	CLA	MG-ND	-2.58	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	407	PHO	CMB-C2B	-2.58	1.46	1.51
26	a	407	PHO	CMB-C2B	-2.58	1.46	1.51
25	c	503	CLA	C1B-C2B	2.58	1.49	1.43
25	B	602	CLA	C1C-NC	-2.58	1.33	1.37
25	B	616	CLA	MG-NC	2.58	2.12	2.06
31	A	416	LMT	O3'-C3'	-2.57	1.36	1.43
31	X	102	LMT	O3'-C3'	-2.57	1.36	1.43
31	x	102	LMT	O3'-C3'	-2.57	1.36	1.43
31	X	101	LMT	O3'-C3'	-2.57	1.36	1.43
31	k	105	LMT	O3'-C3'	-2.57	1.36	1.43
25	B	607	CLA	C4B-NB	-2.57	1.34	1.37
25	b	602	CLA	C1C-NC	-2.57	1.33	1.37
25	A	405	CLA	C4B-NB	-2.56	1.34	1.37
31	B	623	LMT	O3'-C3'	-2.56	1.36	1.43
31	b	623	LMT	O3'-C3'	-2.56	1.36	1.43
25	b	607	CLA	C4B-NB	-2.56	1.34	1.37
25	C	508	CLA	C1B-C2B	2.56	1.49	1.43
25	c	508	CLA	C1B-C2B	2.56	1.49	1.43
31	K	105	LMT	O3'-C3'	-2.56	1.36	1.43
31	I	101	LMT	O3'-C3'	-2.56	1.36	1.43
31	i	101	LMT	O3'-C3'	-2.56	1.36	1.43
31	C	525	LMT	O3'-C3'	-2.56	1.36	1.43
31	c	525	LMT	O3'-C3'	-2.56	1.36	1.43
25	B	607	CLA	MG-NC	2.55	2.12	2.06
25	B	601	CLA	C1B-C2B	2.55	1.49	1.43
25	B	602	CLA	C4B-NB	-2.55	1.34	1.37
25	b	616	CLA	MG-NC	2.55	2.12	2.06
25	A	405	CLA	C4D-CHA	2.55	1.47	1.38
25	a	405	CLA	C4D-CHA	2.55	1.47	1.38
31	x	101	LMT	O3'-C3'	-2.55	1.36	1.43
25	A	408	CLA	C1C-NC	-2.55	1.33	1.37
25	a	408	CLA	C1C-NC	-2.55	1.33	1.37
31	b	629	LMT	O3'-C3'	-2.55	1.36	1.43
31	D	410	LMT	O3'-C3'	-2.55	1.36	1.43
31	J	101	LMT	O3'-C3'	-2.54	1.36	1.43
31	j	101	LMT	O3'-C3'	-2.54	1.36	1.43
25	D	403	CLA	MG-NC	2.54	2.12	2.06
31	F	103	LMT	O3'-C3'	-2.54	1.36	1.43
31	f	103	LMT	O3'-C3'	-2.54	1.36	1.43
25	C	505	CLA	MG-NC	2.54	2.12	2.06
25	c	505	CLA	MG-NC	2.54	2.12	2.06
31	a	416	LMT	O3'-C3'	-2.54	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	CLA	MG-NC	2.54	2.12	2.06
25	C	504	CLA	C1C-NC	-2.53	1.33	1.37
25	c	504	CLA	C1C-NC	-2.53	1.33	1.37
25	B	602	CLA	C1B-NB	-2.53	1.34	1.37
25	b	602	CLA	C1B-NB	-2.53	1.34	1.37
31	d	410	LMT	O3'-C3'	-2.53	1.36	1.43
35	V	201	HEM	C1D-ND	-2.53	1.33	1.38
35	v	201	HEM	C1D-ND	-2.53	1.33	1.38
25	C	505	CLA	C1B-C2B	2.53	1.49	1.43
25	C	511	CLA	C3D-C2D	2.53	1.45	1.39
25	c	511	CLA	C3D-C2D	2.53	1.45	1.39
31	B	629	LMT	O3'-C3'	-2.52	1.36	1.43
25	b	601	CLA	C1B-C2B	2.52	1.49	1.43
31	X	105	LMT	O3'-C3'	-2.52	1.36	1.43
31	x	105	LMT	O3'-C3'	-2.52	1.36	1.43
35	V	201	HEM	C4A-NA	-2.52	1.34	1.39
25	b	607	CLA	MG-NC	2.52	2.12	2.06
25	B	614	CLA	C3D-C2D	2.52	1.45	1.39
35	v	201	HEM	C4A-NA	-2.51	1.34	1.39
25	c	505	CLA	C1B-C2B	2.51	1.49	1.43
31	x	102	LMT	O2'-C2'	-2.51	1.36	1.43
25	b	614	CLA	C3D-C2D	2.51	1.45	1.39
25	D	404	CLA	C1B-C2B	2.51	1.49	1.43
35	E	104	HEM	FE-ND	-2.50	1.87	1.94
25	A	405	CLA	MG-NC	2.50	2.12	2.06
25	a	405	CLA	MG-NC	2.50	2.12	2.06
25	B	605	CLA	MG-NC	2.50	2.12	2.06
25	b	605	CLA	MG-NC	2.50	2.12	2.06
31	I	102	LMT	O3'-C3'	-2.50	1.36	1.43
31	i	102	LMT	O3'-C3'	-2.50	1.36	1.43
35	e	104	HEM	FE-ND	-2.50	1.87	1.94
31	B	624	LMT	O3'-C3'	-2.49	1.36	1.43
31	b	624	LMT	O3'-C3'	-2.49	1.36	1.43
31	X	102	LMT	O2'-C2'	-2.49	1.36	1.43
25	D	404	CLA	C1C-NC	-2.49	1.34	1.37
25	d	404	CLA	C1C-NC	-2.49	1.34	1.37
31	T	101	LMT	O3'-C3'	-2.49	1.36	1.43
31	t	101	LMT	O3'-C3'	-2.49	1.36	1.43
25	D	403	CLA	C3D-C2D	2.49	1.45	1.39
25	d	403	CLA	C3D-C2D	2.49	1.45	1.39
31	B	625	LMT	O2'-C2'	-2.49	1.36	1.43
31	b	625	LMT	O2'-C2'	-2.49	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	C4B-NB	-2.49	1.34	1.37
31	A	415	LMT	O3'-C3'	-2.49	1.36	1.43
31	a	415	LMT	O3'-C3'	-2.49	1.36	1.43
25	C	504	CLA	C4B-NB	-2.49	1.34	1.37
25	c	504	CLA	C4B-NB	-2.49	1.34	1.37
31	x	103	LMT	O3'-C3'	-2.49	1.36	1.43
25	B	604	CLA	C3D-C2D	2.48	1.45	1.39
25	b	604	CLA	C3D-C2D	2.48	1.45	1.39
31	I	104	LMT	O3'-C3'	-2.48	1.36	1.43
31	i	104	LMT	O3'-C3'	-2.48	1.36	1.43
31	X	103	LMT	O3'-C3'	-2.48	1.36	1.43
25	b	603	CLA	C4B-NB	-2.48	1.34	1.37
25	B	612	CLA	C1C-NC	-2.48	1.34	1.37
25	b	612	CLA	C1C-NC	-2.48	1.34	1.37
31	y	101	LMT	O3'-C3'	-2.48	1.36	1.43
25	d	401	CLA	MG-NC	2.48	2.12	2.06
25	B	601	CLA	C3B-C4B	2.47	1.49	1.42
25	b	601	CLA	C3B-C4B	2.47	1.49	1.42
25	D	401	CLA	C1B-C2B	2.47	1.48	1.43
31	T	101	LMT	O2'-C2'	-2.47	1.36	1.43
31	t	101	LMT	O2'-C2'	-2.47	1.36	1.43
25	D	401	CLA	MG-NC	2.47	2.12	2.06
25	d	404	CLA	C1B-C2B	2.47	1.48	1.43
31	Y	101	LMT	O3'-C3'	-2.46	1.36	1.43
25	B	610	CLA	C3B-C4B	2.46	1.49	1.42
25	C	512	CLA	C4B-NB	-2.46	1.34	1.37
25	c	512	CLA	C4B-NB	-2.46	1.34	1.37
31	C	524	LMT	O3'-C3'	-2.45	1.36	1.43
31	c	524	LMT	O3'-C3'	-2.45	1.36	1.43
25	d	404	CLA	C1D-C2D	2.45	1.50	1.45
31	B	626	LMT	O3'-C3'	-2.45	1.36	1.43
31	b	626	LMT	O3'-C3'	-2.45	1.36	1.43
25	d	401	CLA	C1B-C2B	2.45	1.48	1.43
25	B	605	CLA	C4D-CHA	2.44	1.46	1.38
25	B	612	CLA	C4D-CHA	2.44	1.46	1.38
25	b	605	CLA	C4D-CHA	2.44	1.46	1.38
25	b	612	CLA	C4D-CHA	2.44	1.46	1.38
25	D	404	CLA	C1D-C2D	2.44	1.50	1.45
25	b	610	CLA	C3B-C4B	2.44	1.49	1.42
25	C	510	CLA	C1D-C2D	2.43	1.50	1.45
25	c	510	CLA	C1D-C2D	2.43	1.50	1.45
31	D	411	LMT	O2'-C2'	-2.43	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	411	LMT	O2'-C2'	-2.43	1.36	1.43
31	b	623	LMT	O2B-C2B	-2.43	1.36	1.43
31	E	101	LMT	O3'-C3'	-2.42	1.37	1.43
31	e	101	LMT	O3'-C3'	-2.42	1.37	1.43
31	H	102	LMT	O3'-C3'	-2.42	1.37	1.43
31	h	102	LMT	O3'-C3'	-2.42	1.37	1.43
35	V	201	HEM	C1A-C2A	-2.42	1.39	1.44
35	v	201	HEM	C1A-C2A	-2.42	1.39	1.44
31	C	522	LMT	O2'-C2'	-2.42	1.37	1.43
25	b	610	CLA	C1B-C2B	2.41	1.48	1.43
31	B	625	LMT	O3'-C3'	-2.41	1.37	1.43
31	b	625	LMT	O3'-C3'	-2.41	1.37	1.43
25	B	616	CLA	C4B-NB	-2.41	1.34	1.37
25	b	616	CLA	C4B-NB	-2.41	1.34	1.37
31	X	101	LMT	O2'-C2'	-2.41	1.37	1.43
31	B	623	LMT	O2B-C2B	-2.41	1.37	1.43
31	x	101	LMT	O2'-C2'	-2.40	1.37	1.43
25	C	513	CLA	C1C-NC	-2.40	1.34	1.37
28	B	621	LMG	C25-C24	-2.40	1.33	1.50
28	b	621	LMG	C25-C24	-2.40	1.33	1.50
28	C	519	LMG	C25-C24	-2.40	1.33	1.50
31	c	522	LMT	O2'-C2'	-2.40	1.37	1.43
34	c	517	DGD	CGA-CFA	-2.39	1.33	1.50
34	c	517	DGD	CGB-CFB	-2.39	1.33	1.50
28	c	519	LMG	C25-C24	-2.39	1.33	1.50
34	C	517	DGD	CGB-CFB	-2.39	1.33	1.50
28	A	410	LMG	C25-C24	-2.39	1.33	1.50
28	a	410	LMG	C25-C24	-2.39	1.33	1.50
34	C	518	DGD	CGB-CFB	-2.39	1.33	1.50
34	c	518	DGD	CGB-CFB	-2.39	1.33	1.50
34	C	517	DGD	CGA-CFA	-2.39	1.33	1.50
25	C	506	CLA	C4B-NB	-2.39	1.34	1.37
25	c	506	CLA	C4B-NB	-2.39	1.34	1.37
25	B	606	CLA	C1B-C2B	2.38	1.48	1.43
25	b	606	CLA	C1B-C2B	2.38	1.48	1.43
25	B	610	CLA	C1B-C2B	2.38	1.48	1.43
28	a	410	LMG	C43-C42	-2.38	1.33	1.50
34	H	104	DGD	CGA-CFA	-2.38	1.33	1.50
25	B	603	CLA	C3D-C2D	2.38	1.45	1.39
25	b	603	CLA	C3D-C2D	2.38	1.45	1.39
34	h	104	DGD	CGA-CFA	-2.38	1.33	1.50
25	B	605	CLA	MG-ND	-2.38	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	605	CLA	MG-ND	-2.38	2.01	2.05
34	C	516	DGD	CGA-CFA	-2.38	1.33	1.50
34	c	516	DGD	CGA-CFA	-2.38	1.33	1.50
34	H	104	DGD	CGB-CFB	-2.37	1.33	1.50
34	h	104	DGD	CGB-CFB	-2.37	1.33	1.50
31	B	626	LMT	O2'-C2'	-2.37	1.37	1.43
31	b	626	LMT	O2'-C2'	-2.37	1.37	1.43
31	B	625	LMT	O3B-C3B	-2.37	1.37	1.43
31	b	625	LMT	O3B-C3B	-2.37	1.37	1.43
25	c	513	CLA	C1C-NC	-2.37	1.34	1.37
34	C	516	DGD	CGB-CFB	-2.37	1.33	1.50
34	c	516	DGD	CGB-CFB	-2.37	1.33	1.50
28	A	410	LMG	C43-C42	-2.37	1.33	1.50
34	C	518	DGD	CGA-CFA	-2.37	1.33	1.50
25	C	511	CLA	C1B-C2B	2.37	1.48	1.43
25	c	511	CLA	C1B-C2B	2.37	1.48	1.43
34	c	518	DGD	CGA-CFA	-2.36	1.33	1.50
25	B	603	CLA	C1B-C2B	2.36	1.48	1.43
25	b	603	CLA	C1B-C2B	2.36	1.48	1.43
31	F	103	LMT	O3B-C3B	-2.36	1.37	1.43
25	C	505	CLA	C1D-C2D	2.36	1.50	1.45
28	B	621	LMG	C43-C42	-2.36	1.33	1.50
28	b	621	LMG	C43-C42	-2.36	1.33	1.50
31	m	101	LMT	O3'-C3'	-2.35	1.37	1.43
31	f	103	LMT	O3B-C3B	-2.35	1.37	1.43
25	c	510	CLA	C4C-C3C	2.35	1.49	1.45
28	C	519	LMG	C43-C42	-2.35	1.33	1.50
28	c	519	LMG	C43-C42	-2.35	1.33	1.50
25	C	511	CLA	C1C-NC	-2.35	1.34	1.37
25	c	511	CLA	C1C-NC	-2.35	1.34	1.37
25	C	510	CLA	C1A-CHA	2.35	1.52	1.43
25	c	510	CLA	C1A-CHA	2.35	1.52	1.43
31	C	522	LMT	O3'-C3'	-2.34	1.37	1.43
25	c	509	CLA	C4B-NB	-2.34	1.34	1.37
26	A	407	PHO	CAC-C3C	-2.34	1.47	1.51
26	a	407	PHO	CAC-C3C	-2.34	1.47	1.51
25	c	505	CLA	C1D-C2D	2.34	1.50	1.45
28	D	409	LMG	C43-C42	-2.34	1.33	1.50
28	d	409	LMG	C43-C42	-2.34	1.33	1.50
25	B	608	CLA	C1C-NC	-2.34	1.34	1.37
25	b	608	CLA	C1C-NC	-2.34	1.34	1.37
31	i	103	LMT	O3B-C3B	-2.33	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	C4C-C3C	2.33	1.49	1.45
25	A	405	CLA	C3D-C2D	2.33	1.45	1.39
25	a	405	CLA	C3D-C2D	2.33	1.45	1.39
25	B	613	CLA	C1A-CHA	2.32	1.52	1.43
25	b	613	CLA	C1A-CHA	2.32	1.52	1.43
25	C	509	CLA	C4B-NB	-2.32	1.34	1.37
31	I	103	LMT	O3B-C3B	-2.32	1.37	1.43
31	M	102	LMT	O2'-C2'	-2.32	1.37	1.43
31	m	102	LMT	O2'-C2'	-2.32	1.37	1.43
31	M	101	LMT	O3'-C3'	-2.32	1.37	1.43
31	M	101	LMT	O2'-C2'	-2.32	1.37	1.43
25	C	506	CLA	C3B-C4B	2.32	1.49	1.42
25	c	506	CLA	C3B-C4B	2.32	1.49	1.42
31	M	101	LMT	O1'-C1'	-2.32	1.36	1.40
31	m	101	LMT	O1'-C1'	-2.32	1.36	1.40
25	B	615	CLA	C1A-CHA	2.32	1.52	1.43
25	b	615	CLA	C1A-CHA	2.32	1.52	1.43
25	D	401	CLA	C1D-C2D	2.31	1.49	1.45
25	d	401	CLA	C1D-C2D	2.31	1.49	1.45
25	c	504	CLA	C4C-C3C	2.31	1.49	1.45
25	B	610	CLA	C4B-NB	-2.31	1.34	1.37
25	b	610	CLA	C4B-NB	-2.31	1.34	1.37
25	D	404	CLA	MG-ND	-2.31	2.01	2.05
25	d	404	CLA	MG-ND	-2.31	2.01	2.05
29	D	405	PL9	C7-C8	-2.31	1.46	1.50
29	d	405	PL9	C7-C8	-2.31	1.46	1.50
31	c	522	LMT	O3'-C3'	-2.31	1.37	1.43
25	B	601	CLA	C4B-NB	-2.31	1.34	1.37
25	b	601	CLA	C4B-NB	-2.31	1.34	1.37
25	C	504	CLA	C4C-C3C	2.30	1.48	1.45
31	X	104	LMT	O3'-C3'	-2.30	1.37	1.43
31	m	101	LMT	O3B-C3B	-2.30	1.37	1.43
31	E	103	LMT	O3'-C3'	-2.30	1.37	1.43
31	e	103	LMT	O3'-C3'	-2.30	1.37	1.43
31	x	104	LMT	O3'-C3'	-2.30	1.37	1.43
31	B	623	LMT	O2'-C2'	-2.30	1.37	1.43
31	b	623	LMT	O2'-C2'	-2.30	1.37	1.43
31	M	101	LMT	O3B-C3B	-2.30	1.37	1.43
31	B	625	LMT	O1'-C1'	-2.30	1.36	1.40
31	b	625	LMT	O1'-C1'	-2.30	1.36	1.40
31	D	412	LMT	O2'-C2'	-2.29	1.37	1.43
31	b	629	LMT	O3B-C3B	-2.29	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	629	LMT	O2'-C2'	-2.29	1.37	1.43
31	D	412	LMT	O2B-C2B	-2.29	1.37	1.43
31	d	412	LMT	O2B-C2B	-2.29	1.37	1.43
31	d	412	LMT	O2'-C2'	-2.29	1.37	1.43
30	c	501	SQD	O47-C45	-2.29	1.41	1.46
31	m	101	LMT	O2'-C2'	-2.29	1.37	1.43
31	B	629	LMT	O3B-C3B	-2.29	1.37	1.43
35	e	104	HEM	C1D-ND	-2.28	1.34	1.38
31	B	625	LMT	O2B-C2B	-2.28	1.37	1.43
31	b	625	LMT	O2B-C2B	-2.28	1.37	1.43
31	E	101	LMT	O2'-C2'	-2.28	1.37	1.43
31	e	101	LMT	O2'-C2'	-2.28	1.37	1.43
31	M	101	LMT	O2B-C2B	-2.27	1.37	1.43
31	m	101	LMT	O2B-C2B	-2.27	1.37	1.43
31	b	629	LMT	O2'-C2'	-2.27	1.37	1.43
25	A	406	CLA	C1D-C2D	2.27	1.49	1.45
25	a	406	CLA	C1D-C2D	2.27	1.49	1.45
31	k	105	LMT	O2'-C2'	-2.27	1.37	1.43
25	B	606	CLA	C1D-C2D	2.27	1.49	1.45
25	b	606	CLA	C1D-C2D	2.27	1.49	1.45
31	A	415	LMT	O2B-C2B	-2.27	1.37	1.43
31	a	415	LMT	O2B-C2B	-2.27	1.37	1.43
30	C	501	SQD	O47-C45	-2.27	1.41	1.46
36	H	101	RRX	C12-C13	-2.26	1.41	1.46
36	h	101	RRX	C12-C13	-2.26	1.41	1.46
25	B	602	CLA	C1D-ND	-2.26	1.34	1.37
25	b	602	CLA	C1D-ND	-2.26	1.34	1.37
25	B	611	CLA	C1B-C2B	2.26	1.48	1.43
25	b	611	CLA	C1B-C2B	2.26	1.48	1.43
31	C	524	LMT	O2'-C2'	-2.26	1.37	1.43
31	c	524	LMT	O2'-C2'	-2.26	1.37	1.43
25	b	610	CLA	C4C-C3C	2.25	1.48	1.45
31	C	524	LMT	O2B-C2B	-2.25	1.37	1.43
31	c	524	LMT	O2B-C2B	-2.25	1.37	1.43
35	V	201	HEM	O2A-CGA	-2.25	1.23	1.30
25	C	502	CLA	C1D-C2D	2.25	1.49	1.45
25	c	502	CLA	C1D-C2D	2.25	1.49	1.45
31	i	103	LMT	O2B-C2B	-2.24	1.37	1.43
25	C	513	CLA	C1A-CHA	2.24	1.52	1.43
25	c	513	CLA	C1A-CHA	2.24	1.52	1.43
35	E	104	HEM	C1D-ND	-2.24	1.34	1.38
31	D	410	LMT	O2'-C2'	-2.24	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	105	LMT	O2'-C2'	-2.24	1.37	1.43
26	d	402	PHO	CMB-C2B	-2.23	1.47	1.51
31	I	103	LMT	O2B-C2B	-2.23	1.37	1.43
25	B	607	CLA	C1B-C2B	2.23	1.48	1.43
25	b	607	CLA	C1B-C2B	2.23	1.48	1.43
35	v	201	HEM	O2A-CGA	-2.23	1.23	1.30
25	B	615	CLA	MG-ND	-2.23	2.01	2.05
25	b	615	CLA	MG-ND	-2.23	2.01	2.05
25	B	616	CLA	C1B-NB	-2.23	1.34	1.37
25	b	616	CLA	C1B-NB	-2.23	1.34	1.37
31	A	415	LMT	O2'-C2'	-2.23	1.37	1.43
31	a	415	LMT	O2'-C2'	-2.23	1.37	1.43
31	I	103	LMT	O2'-C2'	-2.22	1.37	1.43
31	i	103	LMT	O2'-C2'	-2.22	1.37	1.43
25	b	607	CLA	C1A-CHA	2.22	1.52	1.43
25	B	607	CLA	C1A-CHA	2.22	1.52	1.43
25	B	610	CLA	C4C-C3C	2.22	1.48	1.45
36	H	101	RRX	C19-C18	-2.22	1.41	1.46
36	h	101	RRX	C19-C18	-2.22	1.41	1.46
25	B	602	CLA	C1D-C2D	2.22	1.49	1.45
25	b	602	CLA	C1D-C2D	2.22	1.49	1.45
31	d	410	LMT	O2'-C2'	-2.21	1.37	1.43
31	I	103	LMT	O1'-C1'	-2.21	1.36	1.40
31	i	103	LMT	O1'-C1'	-2.21	1.36	1.40
31	E	103	LMT	O3B-C3B	-2.21	1.37	1.43
30	c	501	SQD	O2-C2	-2.21	1.37	1.43
31	X	104	LMT	O2'-C2'	-2.20	1.37	1.43
31	x	104	LMT	O2'-C2'	-2.20	1.37	1.43
25	d	403	CLA	C4D-CHA	2.20	1.46	1.38
25	B	612	CLA	C1C-C2C	2.20	1.49	1.44
25	b	612	CLA	C1C-C2C	2.20	1.49	1.44
31	I	101	LMT	O2'-C2'	-2.20	1.37	1.43
25	C	509	CLA	C1D-C2D	2.20	1.49	1.45
25	c	509	CLA	C1D-C2D	2.20	1.49	1.45
29	D	405	PL9	C52-C5	-2.20	1.46	1.50
29	d	405	PL9	C52-C5	-2.20	1.46	1.50
25	C	509	CLA	C3B-C4B	2.19	1.49	1.42
25	c	509	CLA	C3B-C4B	2.19	1.49	1.42
25	D	403	CLA	C4D-CHA	2.19	1.45	1.38
36	h	101	RRX	C21-C22	2.19	1.40	1.35
25	C	508	CLA	C1B-NB	-2.19	1.35	1.37
25	c	508	CLA	C1B-NB	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I	104	LMT	O2'-C2'	-2.19	1.37	1.43
31	i	104	LMT	O2'-C2'	-2.19	1.37	1.43
26	D	402	PHO	CMB-C2B	-2.19	1.47	1.51
31	e	103	LMT	C3'-C2'	2.18	1.58	1.52
31	J	101	LMT	O2'-C2'	-2.18	1.37	1.43
31	j	101	LMT	O2'-C2'	-2.18	1.37	1.43
25	B	613	CLA	C4B-NB	-2.18	1.35	1.37
25	b	613	CLA	C4B-NB	-2.18	1.35	1.37
35	v	201	HEM	O2D-CGD	-2.18	1.23	1.30
31	X	104	LMT	O1'-C1'	-2.18	1.36	1.40
31	x	104	LMT	O1'-C1'	-2.18	1.36	1.40
25	B	605	CLA	C1D-C2D	2.18	1.49	1.45
25	b	605	CLA	C1D-C2D	2.18	1.49	1.45
36	H	101	RRX	C21-C22	2.18	1.40	1.35
30	C	501	SQD	O2-C2	-2.18	1.37	1.43
31	Y	101	LMT	O2'-C2'	-2.18	1.37	1.43
31	y	101	LMT	O2'-C2'	-2.18	1.37	1.43
31	B	624	LMT	O2'-C2'	-2.18	1.37	1.43
31	b	624	LMT	O2'-C2'	-2.18	1.37	1.43
25	c	504	CLA	C1A-CHA	2.17	1.52	1.43
31	E	103	LMT	C3'-C2'	2.17	1.58	1.52
31	e	103	LMT	O3B-C3B	-2.17	1.37	1.43
31	i	101	LMT	O2'-C2'	-2.17	1.37	1.43
35	V	201	HEM	O2D-CGD	-2.17	1.23	1.30
31	D	411	LMT	O3B-C3B	-2.16	1.37	1.43
25	C	507	CLA	C1B-C2B	2.16	1.48	1.43
25	c	507	CLA	C1B-C2B	2.16	1.48	1.43
25	B	613	CLA	C1D-C2D	2.16	1.49	1.45
25	b	613	CLA	C1D-C2D	2.16	1.49	1.45
25	A	408	CLA	MG-ND	-2.16	2.01	2.05
25	B	606	CLA	C4C-C3C	2.16	1.48	1.45
31	A	415	LMT	O3B-C3B	-2.16	1.37	1.43
31	a	415	LMT	O3B-C3B	-2.16	1.37	1.43
25	C	504	CLA	C1A-CHA	2.15	1.52	1.43
31	B	623	LMT	O3B-C3B	-2.15	1.37	1.43
31	b	623	LMT	O3B-C3B	-2.15	1.37	1.43
25	C	506	CLA	C3D-C2D	2.15	1.44	1.39
25	c	506	CLA	C3D-C2D	2.15	1.44	1.39
31	B	625	LMT	O4'-C4B	-2.15	1.37	1.43
31	b	625	LMT	O4'-C4B	-2.15	1.37	1.43
31	d	411	LMT	O3B-C3B	-2.15	1.37	1.43
31	f	103	LMT	O4'-C4B	-2.15	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	411	LMT	O4'-C4B	-2.15	1.37	1.43
35	V	201	HEM	C3C-C4C	-2.14	1.42	1.46
35	v	201	HEM	C3C-C4C	-2.14	1.42	1.46
25	C	506	CLA	C1B-C2B	2.14	1.48	1.43
25	c	506	CLA	C1B-C2B	2.14	1.48	1.43
31	D	412	LMT	O3B-C3B	-2.14	1.37	1.43
31	d	412	LMT	O3B-C3B	-2.14	1.37	1.43
31	K	105	LMT	C4B-C3B	2.13	1.57	1.52
31	d	411	LMT	O4'-C4B	-2.13	1.37	1.43
31	A	415	LMT	O4'-C4B	-2.13	1.37	1.43
31	a	415	LMT	O4'-C4B	-2.13	1.37	1.43
31	F	103	LMT	O4'-C4B	-2.13	1.37	1.43
25	B	601	CLA	C1A-CHA	2.13	1.51	1.43
25	b	601	CLA	C1A-CHA	2.13	1.51	1.43
25	B	608	CLA	C4C-C3C	2.13	1.48	1.45
25	b	608	CLA	C4C-C3C	2.13	1.48	1.45
25	b	606	CLA	C4C-C3C	2.12	1.48	1.45
31	k	105	LMT	C4B-C3B	2.12	1.57	1.52
25	C	512	CLA	C1D-C2D	2.12	1.49	1.45
25	A	408	CLA	C1D-C2D	2.12	1.49	1.45
25	a	408	CLA	MG-ND	-2.12	2.01	2.05
31	X	105	LMT	O2'-C2'	-2.12	1.37	1.43
31	x	105	LMT	O2'-C2'	-2.12	1.37	1.43
25	c	512	CLA	C1D-C2D	2.12	1.49	1.45
25	a	408	CLA	C1D-C2D	2.12	1.49	1.45
30	A	413	SQD	O2-C2	-2.11	1.37	1.43
30	a	413	SQD	O2-C2	-2.11	1.37	1.43
31	C	522	LMT	O1'-C1'	-2.11	1.36	1.40
31	c	522	LMT	O1'-C1'	-2.11	1.36	1.40
25	B	616	CLA	C1A-CHA	2.11	1.51	1.43
31	B	629	LMT	O2B-C2B	-2.11	1.37	1.43
35	V	201	HEM	FE-ND	-2.11	1.88	1.94
35	v	201	HEM	FE-ND	-2.11	1.88	1.94
25	d	401	CLA	C1A-CHA	2.11	1.51	1.43
25	b	616	CLA	C1A-CHA	2.11	1.51	1.43
31	A	416	LMT	O1'-C1'	-2.10	1.36	1.40
31	a	416	LMT	O1'-C1'	-2.10	1.36	1.40
25	D	401	CLA	C1A-CHA	2.10	1.51	1.43
30	F	102	SQD	O2-C2	-2.10	1.37	1.43
30	f	102	SQD	O2-C2	-2.10	1.37	1.43
29	A	411	PL9	C35-C34	-2.10	1.45	1.50
25	D	404	CLA	C4C-C3C	2.10	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	CLA	C4C-C3C	2.10	1.48	1.45
25	B	601	CLA	C4C-C3C	2.10	1.48	1.45
25	b	601	CLA	C4C-C3C	2.10	1.48	1.45
31	b	629	LMT	O2B-C2B	-2.09	1.37	1.43
25	c	506	CLA	C4C-C3C	2.09	1.48	1.45
36	h	101	RRX	C14-C13	2.09	1.40	1.35
31	K	105	LMT	O3B-C3B	-2.09	1.37	1.43
35	E	104	HEM	C4B-NB	-2.09	1.34	1.38
35	e	104	HEM	C4B-NB	-2.09	1.34	1.38
25	c	508	CLA	C1A-CHA	2.08	1.51	1.43
31	i	102	LMT	O2'-C2'	-2.08	1.37	1.43
29	a	411	PL9	C35-C34	-2.08	1.45	1.50
31	k	105	LMT	O3B-C3B	-2.08	1.37	1.43
30	h	103	SQD	O2-C2	-2.08	1.37	1.43
31	C	524	LMT	O3B-C3B	-2.08	1.37	1.43
31	c	524	LMT	O3B-C3B	-2.08	1.37	1.43
25	C	504	CLA	C1D-C2D	2.08	1.49	1.45
25	c	504	CLA	C1D-C2D	2.08	1.49	1.45
25	C	510	CLA	C4B-NB	-2.08	1.35	1.37
25	c	510	CLA	C4B-NB	-2.08	1.35	1.37
25	B	608	CLA	C1A-CHA	2.08	1.51	1.43
25	b	608	CLA	C1A-CHA	2.08	1.51	1.43
31	F	103	LMT	O2'-C2'	-2.08	1.37	1.43
31	f	103	LMT	O2'-C2'	-2.08	1.37	1.43
25	C	506	CLA	C4C-C3C	2.08	1.48	1.45
35	V	201	HEM	C1C-NC	-2.07	1.35	1.39
25	C	508	CLA	C1A-CHA	2.07	1.51	1.43
30	F	102	SQD	O4-C4	-2.07	1.37	1.43
30	f	102	SQD	O4-C4	-2.07	1.37	1.43
25	d	404	CLA	C3B-C4B	2.07	1.48	1.42
25	d	403	CLA	C3B-C2B	2.07	1.48	1.41
25	C	507	CLA	C1D-C2D	2.07	1.49	1.45
25	c	507	CLA	C1D-C2D	2.07	1.49	1.45
31	M	101	LMT	O4'-C4B	-2.07	1.37	1.43
31	m	101	LMT	O4'-C4B	-2.07	1.37	1.43
30	a	412	SQD	O2-C2	-2.07	1.37	1.43
31	D	412	LMT	O1'-C1'	-2.07	1.36	1.40
31	I	102	LMT	O1'-C1'	-2.07	1.36	1.40
31	d	412	LMT	O1'-C1'	-2.07	1.36	1.40
31	i	102	LMT	O1'-C1'	-2.07	1.36	1.40
35	v	201	HEM	C1C-NC	-2.06	1.35	1.39
25	A	408	CLA	C3B-C2B	2.06	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	408	CLA	C3B-C2B	2.06	1.48	1.41
31	K	105	LMT	O2B-C2B	-2.06	1.37	1.43
31	k	105	LMT	O2B-C2B	-2.06	1.37	1.43
25	A	405	CLA	C3B-C4B	2.06	1.48	1.42
25	a	405	CLA	C3B-C4B	2.06	1.48	1.42
25	D	403	CLA	C3B-C2B	2.06	1.48	1.41
25	C	514	CLA	C3B-C2B	2.06	1.48	1.41
25	c	514	CLA	C3B-C2B	2.06	1.48	1.41
31	E	103	LMT	O2'-C2'	-2.06	1.37	1.43
31	e	103	LMT	O2'-C2'	-2.06	1.37	1.43
36	H	101	RRX	C17-C18	2.06	1.40	1.35
33	D	406	LHG	O7-C5	-2.06	1.41	1.46
33	d	406	LHG	O7-C5	-2.06	1.41	1.46
31	I	102	LMT	O2'-C2'	-2.06	1.37	1.43
25	c	514	CLA	C3B-C4B	2.06	1.48	1.42
31	B	629	LMT	O4'-C4B	-2.06	1.37	1.43
31	b	629	LMT	O4'-C4B	-2.06	1.37	1.43
26	d	402	PHO	C3D-C4D	2.05	1.44	1.41
36	H	101	RRX	C14-C13	2.05	1.40	1.35
31	X	103	LMT	O2'-C2'	-2.05	1.37	1.43
31	x	103	LMT	O2'-C2'	-2.05	1.37	1.43
31	F	103	LMT	O2B-C2B	-2.05	1.37	1.43
31	f	103	LMT	O2B-C2B	-2.05	1.37	1.43
31	A	416	LMT	O2'-C2'	-2.05	1.37	1.43
31	a	416	LMT	O2'-C2'	-2.05	1.37	1.43
25	D	404	CLA	C3B-C4B	2.05	1.48	1.42
25	C	510	CLA	C1B-NB	-2.05	1.35	1.37
25	c	510	CLA	C1B-NB	-2.05	1.35	1.37
25	C	514	CLA	C3B-C4B	2.05	1.48	1.42
25	B	601	CLA	C1D-C2D	2.05	1.49	1.45
25	b	601	CLA	C1D-C2D	2.05	1.49	1.45
31	C	522	LMT	C4'-C5'	2.05	1.57	1.53
31	c	522	LMT	C4'-C5'	2.05	1.57	1.53
25	B	614	CLA	C1C-C2C	2.05	1.48	1.44
25	b	614	CLA	C1C-C2C	2.05	1.48	1.44
31	F	103	LMT	O1'-C1'	-2.05	1.36	1.40
31	f	103	LMT	O1'-C1'	-2.05	1.36	1.40
25	A	406	CLA	C4C-C3C	2.05	1.48	1.45
25	a	406	CLA	C4C-C3C	2.05	1.48	1.45
25	B	609	CLA	C4C-C3C	2.04	1.48	1.45
25	b	609	CLA	C4C-C3C	2.04	1.48	1.45
30	H	103	SQD	O2-C2	-2.04	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	402	PHO	CAC-C3C	-2.04	1.48	1.51
26	d	402	PHO	CAC-C3C	-2.04	1.48	1.51
25	C	512	CLA	C3B-C4B	2.04	1.48	1.42
25	c	512	CLA	C3B-C4B	2.04	1.48	1.42
36	h	101	RRX	C17-C18	2.04	1.40	1.35
31	D	411	LMT	O2B-C2B	-2.04	1.37	1.43
31	d	411	LMT	O2B-C2B	-2.04	1.37	1.43
31	J	101	LMT	O1'-C1'	-2.03	1.36	1.40
31	j	101	LMT	O1'-C1'	-2.03	1.36	1.40
30	A	412	SQD	O2-C2	-2.03	1.37	1.43
25	b	607	CLA	C4C-C3C	2.03	1.48	1.45
31	B	624	LMT	O1'-C1'	-2.03	1.36	1.40
31	b	624	LMT	O1'-C1'	-2.03	1.36	1.40
35	E	104	HEM	C3C-C4C	-2.03	1.42	1.46
35	e	104	HEM	C3C-C4C	-2.03	1.42	1.46
25	C	508	CLA	C1D-C2D	2.03	1.49	1.45
26	D	402	PHO	C3D-C4D	2.02	1.44	1.41
25	B	602	CLA	C4C-C3C	2.02	1.48	1.45
25	b	602	CLA	C4C-C3C	2.02	1.48	1.45
25	B	610	CLA	C1D-C2D	2.02	1.49	1.45
25	B	607	CLA	C4C-C3C	2.02	1.48	1.45
25	c	502	CLA	C4C-C3C	2.02	1.48	1.45
30	k	101	SQD	O2-C2	-2.02	1.38	1.43
25	B	606	CLA	C3B-C4B	2.02	1.48	1.42
25	b	606	CLA	C3B-C4B	2.02	1.48	1.42
25	C	511	CLA	C1D-C2D	2.02	1.49	1.45
25	c	511	CLA	C1D-C2D	2.02	1.49	1.45
36	H	101	RRX	C10-C9	2.02	1.40	1.35
36	h	101	RRX	C10-C9	2.02	1.40	1.35
25	C	502	CLA	C4C-C3C	2.02	1.48	1.45
25	C	512	CLA	C4C-C3C	2.02	1.48	1.45
25	c	512	CLA	C4C-C3C	2.02	1.48	1.45
26	A	407	PHO	C3D-C4D	2.01	1.44	1.41
26	a	407	PHO	C3D-C4D	2.01	1.44	1.41
30	K	101	SQD	O2-C2	-2.01	1.38	1.43
31	C	522	LMT	C3'-C2'	2.01	1.57	1.52
25	c	511	CLA	C1A-CHA	2.01	1.51	1.43
31	E	103	LMT	O2B-C2B	-2.01	1.38	1.43
31	e	103	LMT	O2B-C2B	-2.01	1.38	1.43
25	C	509	CLA	C1B-C2B	2.01	1.47	1.43
25	c	509	CLA	C1B-C2B	2.01	1.47	1.43
25	C	511	CLA	C1A-CHA	2.01	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	E	103	LMT	C4B-C5B	2.01	1.57	1.53
31	K	105	LMT	O4'-C4B	-2.00	1.38	1.43
31	k	105	LMT	O4'-C4B	-2.00	1.38	1.43
25	a	406	CLA	C1A-CHA	2.00	1.51	1.43
31	e	103	LMT	C4B-C5B	2.00	1.57	1.53
25	c	511	CLA	C4B-NB	-2.00	1.35	1.37

All (2764) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	k	102	BCR	C16-C17-C18	23.42	160.12	127.28
27	K	102	BCR	C16-C17-C18	23.40	160.10	127.28
27	K	102	BCR	C20-C21-C22	23.22	159.84	127.28
27	k	102	BCR	C20-C21-C22	23.20	159.81	127.28
27	C	515	BCR	C20-C21-C22	21.80	157.85	127.28
27	c	515	BCR	C20-C21-C22	21.80	157.85	127.28
27	B	617	BCR	C20-C21-C22	21.31	157.17	127.28
27	b	617	BCR	C20-C21-C22	21.31	157.17	127.28
27	F	101	BCR	C20-C21-C22	21.29	157.14	127.28
27	f	101	BCR	C20-C21-C22	21.29	157.13	127.28
27	Z	101	BCR	C20-C21-C22	21.22	157.03	127.28
27	z	101	BCR	C20-C21-C22	21.22	157.03	127.28
27	C	515	BCR	C16-C17-C18	21.03	156.77	127.28
27	c	515	BCR	C16-C17-C18	20.98	156.71	127.28
27	k	103	BCR	C20-C21-C22	20.94	156.64	127.28
27	K	103	BCR	C20-C21-C22	20.92	156.62	127.28
27	b	619	BCR	C20-C21-C22	20.85	156.53	127.28
27	B	619	BCR	C20-C21-C22	20.85	156.52	127.28
27	C	515	BCR	C15-C16-C17	20.68	165.84	123.52
27	c	515	BCR	C15-C16-C17	20.67	165.81	123.52
27	A	409	BCR	C20-C21-C22	20.62	156.19	127.28
27	a	409	BCR	C20-C21-C22	20.62	156.19	127.28
27	F	101	BCR	C15-C16-C17	20.53	165.54	123.52
27	f	101	BCR	C15-C16-C17	20.53	165.53	123.52
27	A	409	BCR	C15-C16-C17	20.53	165.53	123.52
27	a	409	BCR	C15-C16-C17	20.51	165.49	123.52
27	b	619	BCR	C15-C16-C17	20.48	165.42	123.52
27	B	619	BCR	C15-C16-C17	20.45	165.37	123.52
27	b	617	BCR	C15-C16-C17	20.45	165.36	123.52
27	B	617	BCR	C15-C16-C17	20.43	165.32	123.52
27	B	618	BCR	C15-C16-C17	20.13	164.71	123.52
27	b	618	BCR	C15-C16-C17	20.12	164.69	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	z	101	BCR	C16-C17-C18	20.12	155.50	127.28
27	B	619	BCR	C16-C17-C18	20.12	155.49	127.28
27	b	619	BCR	C16-C17-C18	20.12	155.49	127.28
27	Z	101	BCR	C16-C17-C18	20.11	155.49	127.28
27	K	103	BCR	C15-C16-C17	19.98	164.40	123.52
27	k	103	BCR	C15-C16-C17	19.96	164.37	123.52
27	B	618	BCR	C20-C21-C22	19.96	155.27	127.28
27	b	618	BCR	C20-C21-C22	19.94	155.25	127.28
27	B	618	BCR	C16-C17-C18	19.74	154.97	127.28
27	b	618	BCR	C16-C17-C18	19.74	154.97	127.28
27	z	101	BCR	C15-C16-C17	19.42	163.25	123.52
27	Z	101	BCR	C15-C16-C17	19.41	163.24	123.52
27	F	101	BCR	C16-C17-C18	19.30	154.35	127.28
27	f	101	BCR	C16-C17-C18	19.30	154.35	127.28
27	b	617	BCR	C16-C17-C18	19.02	153.95	127.28
27	B	617	BCR	C16-C17-C18	19.01	153.94	127.28
27	k	102	BCR	C15-C16-C17	18.95	162.30	123.52
27	K	102	BCR	C15-C16-C17	18.92	162.24	123.52
27	K	102	BCR	C10-C11-C12	18.89	177.93	123.20
27	k	102	BCR	C10-C11-C12	18.89	177.93	123.20
27	C	515	BCR	C10-C11-C12	18.87	177.88	123.20
27	c	515	BCR	C10-C11-C12	18.86	177.84	123.20
27	K	103	BCR	C10-C11-C12	18.85	177.82	123.20
27	k	103	BCR	C10-C11-C12	18.84	177.78	123.20
27	B	618	BCR	C10-C11-C12	18.63	177.19	123.20
27	b	618	BCR	C10-C11-C12	18.62	177.16	123.20
27	a	409	BCR	C16-C17-C18	18.62	153.39	127.28
27	K	103	BCR	C16-C17-C18	18.61	153.38	127.28
27	k	103	BCR	C16-C17-C18	18.61	153.38	127.28
27	A	409	BCR	C16-C17-C18	18.61	153.38	127.28
27	b	619	BCR	C10-C11-C12	18.59	177.08	123.20
27	B	619	BCR	C10-C11-C12	18.59	177.06	123.20
27	A	409	BCR	C10-C11-C12	18.34	176.33	123.20
27	a	409	BCR	C10-C11-C12	18.34	176.33	123.20
27	F	101	BCR	C10-C11-C12	18.26	176.12	123.20
27	f	101	BCR	C10-C11-C12	18.26	176.12	123.20
27	B	617	BCR	C10-C11-C12	18.07	175.56	123.20
27	b	617	BCR	C10-C11-C12	18.07	175.56	123.20
27	Z	101	BCR	C10-C11-C12	17.88	175.00	123.20
27	z	101	BCR	C10-C11-C12	17.88	175.00	123.20
27	B	618	BCR	C21-C20-C19	14.33	164.73	123.20
27	b	618	BCR	C21-C20-C19	14.32	164.69	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	103	BCR	C21-C20-C19	14.31	164.67	123.20
27	k	103	BCR	C21-C20-C19	14.31	164.66	123.20
27	B	619	BCR	C21-C20-C19	14.20	164.34	123.20
27	b	619	BCR	C21-C20-C19	14.20	164.34	123.20
27	B	617	BCR	C21-C20-C19	14.14	164.18	123.20
27	b	617	BCR	C21-C20-C19	14.14	164.18	123.20
27	f	101	BCR	C21-C20-C19	14.14	164.16	123.20
27	F	101	BCR	C21-C20-C19	14.14	164.16	123.20
27	k	102	BCR	C11-C10-C9	14.11	147.07	127.28
27	K	102	BCR	C11-C10-C9	14.11	147.06	127.28
27	z	101	BCR	C21-C20-C19	14.10	164.06	123.20
27	Z	101	BCR	C21-C20-C19	14.10	164.05	123.20
27	A	409	BCR	C21-C20-C19	14.09	164.03	123.20
27	a	409	BCR	C21-C20-C19	14.09	164.03	123.20
27	b	617	BCR	C11-C10-C9	14.01	146.93	127.28
27	B	617	BCR	C11-C10-C9	13.97	146.88	127.28
27	F	101	BCR	C11-C10-C9	13.75	146.57	127.28
27	f	101	BCR	C11-C10-C9	13.75	146.57	127.28
27	k	102	BCR	C16-C15-C14	13.56	151.26	123.52
27	K	102	BCR	C16-C15-C14	13.54	151.23	123.52
27	A	409	BCR	C11-C10-C9	13.35	146.01	127.28
27	a	409	BCR	C11-C10-C9	13.35	146.01	127.28
27	K	103	BCR	C16-C15-C14	13.35	150.83	123.52
27	Z	101	BCR	C16-C15-C14	13.34	150.81	123.52
27	z	101	BCR	C16-C15-C14	13.34	150.81	123.52
27	k	103	BCR	C16-C15-C14	13.33	150.80	123.52
27	c	515	BCR	C21-C20-C19	12.95	160.73	123.20
27	C	515	BCR	C21-C20-C19	12.95	160.72	123.20
27	K	102	BCR	C21-C20-C19	12.76	160.17	123.20
27	k	102	BCR	C21-C20-C19	12.76	160.17	123.20
27	b	618	BCR	C16-C15-C14	12.66	149.43	123.52
27	B	618	BCR	C16-C15-C14	12.66	149.42	123.52
27	K	103	BCR	C11-C10-C9	12.53	144.85	127.28
27	k	103	BCR	C11-C10-C9	12.53	144.85	127.28
27	A	409	BCR	C16-C15-C14	12.49	149.06	123.52
27	a	409	BCR	C16-C15-C14	12.47	149.04	123.52
27	f	101	BCR	C16-C15-C14	12.47	149.04	123.52
27	F	101	BCR	C16-C15-C14	12.47	149.04	123.52
27	B	619	BCR	C11-C10-C9	12.44	144.73	127.28
27	b	619	BCR	C11-C10-C9	12.44	144.73	127.28
27	b	617	BCR	C16-C15-C14	12.43	148.94	123.52
27	B	617	BCR	C16-C15-C14	12.40	148.90	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	618	BCR	C11-C10-C9	12.16	144.34	127.28
27	b	618	BCR	C11-C10-C9	12.16	144.34	127.28
27	C	515	BCR	C16-C15-C14	11.88	147.83	123.52
27	c	515	BCR	C16-C15-C14	11.88	147.83	123.52
27	C	515	BCR	C11-C10-C9	11.76	143.76	127.28
27	c	515	BCR	C11-C10-C9	11.73	143.73	127.28
27	b	619	BCR	C16-C15-C14	11.49	147.02	123.52
27	B	619	BCR	C16-C15-C14	11.47	146.99	123.52
27	f	101	BCR	C11-C12-C13	11.46	157.78	126.36
27	F	101	BCR	C11-C12-C13	11.45	157.77	126.36
27	b	619	BCR	C11-C12-C13	11.31	157.38	126.36
27	B	619	BCR	C11-C12-C13	11.31	157.37	126.36
27	B	617	BCR	C11-C12-C13	11.21	157.09	126.36
27	b	617	BCR	C11-C12-C13	11.21	157.09	126.36
27	a	409	BCR	C11-C12-C13	11.19	157.05	126.36
27	C	515	BCR	C11-C12-C13	11.19	157.04	126.36
27	c	515	BCR	C11-C12-C13	11.19	157.04	126.36
27	A	409	BCR	C11-C12-C13	11.18	157.03	126.36
27	B	618	BCR	C11-C12-C13	10.90	156.24	126.36
27	b	618	BCR	C11-C12-C13	10.89	156.22	126.36
27	z	101	BCR	C11-C10-C9	10.76	142.37	127.28
27	Z	101	BCR	C11-C10-C9	10.75	142.35	127.28
27	K	103	BCR	C11-C12-C13	10.67	155.62	126.36
27	k	103	BCR	C11-C12-C13	10.66	155.58	126.36
27	K	102	BCR	C11-C12-C13	10.46	155.04	126.36
27	k	102	BCR	C11-C12-C13	10.45	155.01	126.36
27	Z	101	BCR	C11-C12-C13	10.36	154.78	126.36
27	z	101	BCR	C11-C12-C13	10.36	154.78	126.36
25	A	405	CLA	CMD-C2D-C1D	9.18	140.89	124.73
25	a	405	CLA	CMD-C2D-C1D	9.17	140.87	124.73
25	C	506	CLA	CMD-C2D-C1D	8.78	140.20	124.73
25	c	506	CLA	CMD-C2D-C1D	8.78	140.19	124.73
25	c	504	CLA	CMD-C2D-C1D	8.72	140.08	124.73
25	C	504	CLA	CMD-C2D-C1D	8.69	140.04	124.73
25	c	511	CLA	CMD-C2D-C1D	8.68	140.02	124.73
25	C	511	CLA	CMD-C2D-C1D	8.67	140.00	124.73
25	B	605	CLA	CMD-C2D-C1D	8.55	139.78	124.73
25	b	605	CLA	CMD-C2D-C1D	8.55	139.78	124.73
25	a	406	CLA	CMD-C2D-C1D	8.46	139.63	124.73
25	A	406	CLA	CMD-C2D-C1D	8.44	139.59	124.73
25	c	510	CLA	CMD-C2D-C1D	8.29	139.33	124.73
25	C	508	CLA	CMD-C2D-C1D	8.29	139.32	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	510	CLA	CMD-C2D-C1D	8.29	139.32	124.73
25	c	508	CLA	CMD-C2D-C1D	8.28	139.31	124.73
25	B	602	CLA	CMD-C2D-C1D	8.26	139.27	124.73
25	b	602	CLA	CMD-C2D-C1D	8.26	139.27	124.73
25	b	606	CLA	CMD-C2D-C1D	8.13	139.04	124.73
25	B	606	CLA	CMD-C2D-C1D	8.11	139.01	124.73
25	C	512	CLA	CMD-C2D-C1D	8.09	138.97	124.73
25	c	512	CLA	CMD-C2D-C1D	8.09	138.97	124.73
35	V	201	HEM	CHC-C4B-NB	8.01	133.05	124.42
35	v	201	HEM	CHC-C4B-NB	8.01	133.05	124.42
25	c	502	CLA	CMD-C2D-C1D	7.99	138.80	124.73
25	C	502	CLA	CMD-C2D-C1D	7.98	138.79	124.73
25	B	613	CLA	CMD-C2D-C1D	7.97	138.76	124.73
25	b	613	CLA	CMD-C2D-C1D	7.97	138.76	124.73
25	c	505	CLA	CMD-C2D-C1D	7.91	138.66	124.73
25	C	505	CLA	CMD-C2D-C1D	7.90	138.64	124.73
25	B	604	CLA	CMD-C2D-C1D	7.89	138.63	124.73
25	b	604	CLA	CMD-C2D-C1D	7.88	138.61	124.73
25	B	614	CLA	CMD-C2D-C1D	7.85	138.56	124.73
25	b	614	CLA	CMD-C2D-C1D	7.85	138.56	124.73
25	B	607	CLA	C4A-NA-C1A	7.85	110.26	106.68
25	b	607	CLA	C4A-NA-C1A	7.77	110.22	106.68
27	c	515	BCR	C20-C19-C18	7.71	147.50	126.36
27	C	515	BCR	C20-C19-C18	7.70	147.49	126.36
25	d	404	CLA	CMD-C2D-C1D	7.70	138.29	124.73
25	D	404	CLA	CMD-C2D-C1D	7.69	138.27	124.73
25	b	610	CLA	CMD-C2D-C1D	7.69	138.27	124.73
25	B	610	CLA	CMD-C2D-C1D	7.68	138.25	124.73
25	b	601	CLA	CMD-C2D-C1D	7.67	138.24	124.73
25	B	601	CLA	CMD-C2D-C1D	7.66	138.21	124.73
25	B	603	CLA	CMD-C2D-C1D	7.64	138.19	124.73
25	b	603	CLA	CMD-C2D-C1D	7.64	138.19	124.73
25	b	607	CLA	CMD-C2D-C1D	7.59	138.09	124.73
25	B	607	CLA	CMD-C2D-C1D	7.59	138.09	124.73
25	d	401	CLA	CMD-C2D-C1D	7.58	138.08	124.73
25	D	401	CLA	CMD-C2D-C1D	7.58	138.07	124.73
25	b	616	CLA	C4A-NA-C1A	7.52	110.11	106.68
25	B	616	CLA	C4A-NA-C1A	7.50	110.10	106.68
25	C	506	CLA	O2D-CGD-CBD	7.50	124.35	111.23
25	c	506	CLA	O2D-CGD-CBD	7.50	124.35	111.23
25	c	507	CLA	C2C-C1C-NC	7.47	117.83	109.98
25	b	615	CLA	C4A-NA-C1A	7.45	110.08	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	407	PHO	C4D-CHA-CBD	-7.44	104.88	108.45
25	C	507	CLA	C2C-C1C-NC	7.43	117.79	109.98
25	D	403	CLA	C1D-ND-C4D	-7.41	101.11	106.31
25	d	403	CLA	C1D-ND-C4D	-7.41	101.11	106.31
25	b	615	CLA	CMD-C2D-C1D	7.40	137.77	124.73
26	a	407	PHO	C4D-CHA-CBD	-7.40	104.91	108.45
25	B	615	CLA	C4A-NA-C1A	7.40	110.05	106.68
25	B	615	CLA	CMD-C2D-C1D	7.38	137.72	124.73
25	C	507	CLA	CMD-C2D-C1D	7.37	137.71	124.73
25	c	507	CLA	CMD-C2D-C1D	7.37	137.71	124.73
25	D	403	CLA	C2D-C1D-ND	7.32	117.37	110.13
25	d	403	CLA	C2D-C1D-ND	7.32	117.37	110.13
25	B	616	CLA	CMD-C2D-C1D	7.27	137.53	124.73
25	b	616	CLA	CMD-C2D-C1D	7.25	137.50	124.73
25	A	408	CLA	CMD-C2D-C1D	7.23	137.46	124.73
25	a	408	CLA	CMD-C2D-C1D	7.21	137.43	124.73
26	d	402	PHO	C4D-CHA-CBD	-7.17	105.02	108.45
26	D	402	PHO	C4D-CHA-CBD	-7.09	105.05	108.45
25	b	613	CLA	C4A-NA-C1A	7.06	109.90	106.68
25	C	510	CLA	C4A-NA-C1A	7.02	109.88	106.68
25	B	613	CLA	C4A-NA-C1A	7.01	109.88	106.68
27	f	101	BCR	C20-C19-C18	6.99	145.53	126.36
27	F	101	BCR	C20-C19-C18	6.99	145.53	126.36
27	B	619	BCR	C20-C19-C18	6.96	145.45	126.36
27	b	619	BCR	C20-C19-C18	6.96	145.45	126.36
25	D	403	CLA	CMD-C2D-C1D	6.93	136.94	124.73
25	d	403	CLA	CMD-C2D-C1D	6.93	136.94	124.73
25	c	510	CLA	C4A-NA-C1A	6.92	109.83	106.68
25	c	503	CLA	CMD-C2D-C1D	6.91	136.89	124.73
25	C	503	CLA	CMD-C2D-C1D	6.90	136.88	124.73
27	z	101	BCR	C20-C19-C18	6.79	144.97	126.36
27	Z	101	BCR	C20-C19-C18	6.78	144.96	126.36
25	b	608	CLA	CMD-C2D-C1D	6.78	136.66	124.73
25	B	608	CLA	CMD-C2D-C1D	6.77	136.66	124.73
25	C	509	CLA	CMD-C2D-C1D	6.73	136.59	124.73
25	c	509	CLA	CMD-C2D-C1D	6.73	136.57	124.73
25	B	610	CLA	C2C-C1C-NC	6.71	117.03	109.98
25	D	401	CLA	C4A-NA-C1A	6.70	109.74	106.68
25	d	401	CLA	C4A-NA-C1A	6.70	109.74	106.68
25	B	604	CLA	C4A-NA-C1A	6.69	109.73	106.68
25	b	610	CLA	C2C-C1C-NC	6.69	117.00	109.98
25	b	612	CLA	C4A-NA-C1A	6.69	109.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	617	BCR	C20-C19-C18	6.68	144.69	126.36
27	b	617	BCR	C20-C19-C18	6.67	144.66	126.36
25	B	612	CLA	C4A-NA-C1A	6.65	109.71	106.68
25	b	604	CLA	C4A-NA-C1A	6.65	109.71	106.68
27	K	103	BCR	C20-C19-C18	6.65	144.59	126.36
25	c	513	CLA	C2C-C1C-NC	6.64	116.95	109.98
27	k	103	BCR	C20-C19-C18	6.64	144.56	126.36
25	c	510	CLA	C2C-C1C-NC	6.62	116.94	109.98
25	C	513	CLA	C2C-C1C-NC	6.61	116.92	109.98
25	c	512	CLA	C4A-NA-C1A	6.60	109.69	106.68
25	C	510	CLA	C2C-C1C-NC	6.59	116.91	109.98
25	C	512	CLA	C4A-NA-C1A	6.59	109.69	106.68
27	B	618	BCR	C20-C19-C18	6.58	144.40	126.36
27	b	618	BCR	C20-C19-C18	6.58	144.40	126.36
25	C	511	CLA	C1C-C2C-C3C	-6.57	100.07	106.98
25	c	511	CLA	C1C-C2C-C3C	-6.57	100.07	106.98
25	B	609	CLA	C2C-C1C-NC	6.53	116.84	109.98
25	b	609	CLA	C2C-C1C-NC	6.53	116.84	109.98
25	C	513	CLA	C4A-NA-C1A	6.51	109.65	106.68
25	c	513	CLA	C4A-NA-C1A	6.46	109.63	106.68
25	B	605	CLA	C1D-ND-C4D	-6.46	101.78	106.31
25	b	605	CLA	C1D-ND-C4D	-6.44	101.79	106.31
25	D	401	CLA	C2C-C1C-NC	6.42	116.73	109.98
25	d	401	CLA	C2C-C1C-NC	6.42	116.73	109.98
27	A	409	BCR	C20-C19-C18	6.41	143.93	126.36
27	a	409	BCR	C20-C19-C18	6.41	143.93	126.36
25	C	508	CLA	C3B-C2B-C1B	-6.41	99.62	107.17
25	c	508	CLA	C3B-C2B-C1B	-6.41	99.62	107.17
25	c	503	CLA	C4A-NA-C1A	6.38	109.59	106.68
25	B	601	CLA	C2C-C1C-NC	6.36	116.66	109.98
25	b	601	CLA	C2C-C1C-NC	6.36	116.66	109.98
25	B	603	CLA	C2C-C1C-NC	6.36	116.66	109.98
25	B	611	CLA	C4A-NA-C1A	6.36	109.58	106.68
25	b	611	CLA	C4A-NA-C1A	6.36	109.58	106.68
25	B	609	CLA	CMD-C2D-C1D	6.34	135.89	124.73
25	a	406	CLA	C4A-NA-C1A	6.34	109.57	106.68
25	B	604	CLA	C2C-C1C-NC	6.33	116.63	109.98
25	b	604	CLA	C2C-C1C-NC	6.33	116.63	109.98
25	A	406	CLA	C4A-NA-C1A	6.33	109.57	106.68
25	B	613	CLA	C3D-C2D-C1D	-6.33	97.19	105.83
25	b	613	CLA	C3D-C2D-C1D	-6.33	97.19	105.83
25	b	609	CLA	CMD-C2D-C1D	6.32	135.85	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	406	CLA	C2C-C1C-NC	6.31	116.61	109.98
25	b	603	CLA	C2C-C1C-NC	6.31	116.61	109.98
25	C	503	CLA	C4A-NA-C1A	6.30	109.55	106.68
25	b	611	CLA	CMD-C2D-C1D	6.29	135.81	124.73
25	B	608	CLA	C2C-C1C-NC	6.29	116.59	109.98
25	a	406	CLA	C2C-C1C-NC	6.29	116.59	109.98
25	b	608	CLA	C2C-C1C-NC	6.29	116.59	109.98
25	C	514	CLA	CMD-C2D-C1D	6.29	135.81	124.73
25	B	611	CLA	CMD-C2D-C1D	6.28	135.79	124.73
25	C	511	CLA	C2C-C1C-NC	6.28	116.58	109.98
25	c	511	CLA	C2C-C1C-NC	6.28	116.58	109.98
25	c	514	CLA	CMD-C2D-C1D	6.28	135.78	124.73
25	C	505	CLA	C4A-NA-C1A	6.28	109.54	106.68
25	c	505	CLA	C4A-NA-C1A	6.28	109.54	106.68
25	b	605	CLA	C2D-C1D-ND	6.27	116.33	110.13
25	B	605	CLA	C2D-C1D-ND	6.26	116.33	110.13
25	B	613	CLA	C2C-C1C-NC	6.24	116.53	109.98
25	b	613	CLA	C2C-C1C-NC	6.24	116.53	109.98
25	A	406	CLA	C1C-C2C-C3C	-6.24	100.42	106.98
25	a	406	CLA	C1C-C2C-C3C	-6.24	100.42	106.98
25	c	513	CLA	C2D-C1D-ND	6.23	116.29	110.13
25	C	513	CLA	C2D-C1D-ND	6.22	116.28	110.13
25	b	615	CLA	C2D-C1D-ND	6.22	116.28	110.13
25	B	615	CLA	C2D-C1D-ND	6.17	116.23	110.13
25	B	608	CLA	C1C-C2C-C3C	-6.11	100.55	106.98
25	b	608	CLA	C1C-C2C-C3C	-6.11	100.55	106.98
25	C	503	CLA	C2C-C1C-NC	6.10	116.39	109.98
25	c	503	CLA	C2C-C1C-NC	6.10	116.39	109.98
25	D	401	CLA	C1C-C2C-C3C	-6.08	100.58	106.98
25	d	401	CLA	C1C-C2C-C3C	-6.08	100.58	106.98
25	B	613	CLA	C1C-C2C-C3C	-6.08	100.59	106.98
25	b	613	CLA	C1C-C2C-C3C	-6.06	100.61	106.98
25	b	611	CLA	O2D-CGD-CBD	6.04	121.79	111.23
25	b	601	CLA	O2D-CGD-CBD	6.03	121.77	111.23
25	B	611	CLA	O2D-CGD-CBD	6.02	121.75	111.23
25	C	505	CLA	C2C-C1C-NC	6.02	116.30	109.98
25	c	505	CLA	C2C-C1C-NC	6.02	116.30	109.98
25	b	612	CLA	O2D-CGD-CBD	6.01	121.74	111.23
25	C	504	CLA	C2C-C1C-NC	6.01	116.30	109.98
25	c	504	CLA	C2C-C1C-NC	6.01	116.30	109.98
25	B	601	CLA	O2D-CGD-CBD	6.01	121.74	111.23
27	K	102	BCR	C20-C19-C18	6.01	142.84	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	k	102	BCR	C20-C19-C18	6.00	142.81	126.36
25	B	612	CLA	O2D-CGD-CBD	5.99	121.70	111.23
25	b	604	CLA	O2D-CGD-CBD	5.97	121.67	111.23
25	B	604	CLA	O2D-CGD-CBD	5.97	121.67	111.23
25	B	609	CLA	C4A-NA-C1A	5.96	109.40	106.68
25	c	508	CLA	C2C-C1C-NC	5.96	116.24	109.98
25	C	505	CLA	O2D-CGD-CBD	5.95	121.64	111.23
25	c	513	CLA	O2D-CGD-CBD	5.95	121.63	111.23
25	C	508	CLA	C2C-C1C-NC	5.94	116.22	109.98
25	C	513	CLA	O2D-CGD-CBD	5.94	121.61	111.23
25	c	505	CLA	O2D-CGD-CBD	5.94	121.61	111.23
25	D	403	CLA	C4A-NA-C1A	5.94	109.39	106.68
25	b	609	CLA	C4A-NA-C1A	5.92	109.38	106.68
25	d	403	CLA	C4A-NA-C1A	5.92	109.38	106.68
25	A	408	CLA	O2D-CGD-CBD	5.92	121.58	111.23
25	a	408	CLA	O2D-CGD-CBD	5.92	121.58	111.23
25	B	616	CLA	O2D-CGD-CBD	5.91	121.56	111.23
25	b	616	CLA	O2D-CGD-CBD	5.91	121.56	111.23
25	A	408	CLA	C2C-C1C-NC	5.89	116.17	109.98
25	a	408	CLA	C2C-C1C-NC	5.88	116.16	109.98
25	B	609	CLA	O2D-CGD-CBD	5.88	121.50	111.23
25	b	609	CLA	O2D-CGD-CBD	5.87	121.50	111.23
25	B	603	CLA	C4A-NA-C1A	5.85	109.35	106.68
25	b	603	CLA	C4A-NA-C1A	5.85	109.35	106.68
25	B	615	CLA	C2C-C1C-NC	5.82	116.09	109.98
25	B	609	CLA	C1C-C2C-C3C	-5.82	100.86	106.98
25	b	609	CLA	C1C-C2C-C3C	-5.82	100.86	106.98
25	B	614	CLA	C4A-NA-C1A	5.81	109.33	106.68
25	C	514	CLA	C3B-C2B-C1B	-5.81	100.33	107.17
25	c	514	CLA	C3B-C2B-C1B	-5.81	100.33	107.17
25	b	615	CLA	C2C-C1C-NC	5.80	116.08	109.98
25	C	510	CLA	C3D-C2D-C1D	-5.80	97.91	105.83
25	c	510	CLA	C3D-C2D-C1D	-5.80	97.91	105.83
25	d	404	CLA	C2C-C1C-NC	5.80	116.07	109.98
25	C	502	CLA	C2C-C1C-NC	5.80	116.07	109.98
25	c	502	CLA	C2C-C1C-NC	5.80	116.07	109.98
25	b	614	CLA	C4A-NA-C1A	5.79	109.32	106.68
25	b	612	CLA	C1D-ND-C4D	-5.78	102.25	106.31
25	C	503	CLA	O2D-CGD-CBD	5.78	121.33	111.23
25	C	513	CLA	C1C-C2C-C3C	-5.77	100.91	106.98
25	c	503	CLA	O2D-CGD-CBD	5.77	121.32	111.23
25	D	404	CLA	C2C-C1C-NC	5.77	116.04	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	C1C-C2C-C3C	-5.76	100.92	106.98
25	B	612	CLA	C1D-ND-C4D	-5.76	102.27	106.31
25	b	615	CLA	C3D-C2D-C1D	-5.76	97.97	105.83
25	c	510	CLA	O2A-CGA-O1A	-5.75	109.25	123.63
25	C	504	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
25	c	504	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
25	C	510	CLA	O2A-CGA-O1A	-5.73	109.28	123.63
27	K	103	BCR	C24-C23-C22	-5.73	117.76	126.23
25	B	615	CLA	C3D-C2D-C1D	-5.72	98.02	105.83
25	A	405	CLA	C4A-NA-C1A	5.72	109.29	106.68
25	a	405	CLA	C4A-NA-C1A	5.72	109.29	106.68
27	k	103	BCR	C24-C23-C22	-5.71	117.79	126.23
25	C	506	CLA	C2C-C1C-NC	5.71	115.98	109.98
25	c	506	CLA	C2C-C1C-NC	5.71	115.98	109.98
25	B	611	CLA	C2D-C1D-ND	5.71	115.77	110.13
25	b	611	CLA	C2D-C1D-ND	5.71	115.77	110.13
25	C	512	CLA	C2C-C1C-NC	5.70	115.97	109.98
25	c	512	CLA	C2C-C1C-NC	5.70	115.97	109.98
25	C	505	CLA	C1C-C2C-C3C	-5.70	100.98	106.98
25	c	505	CLA	C1C-C2C-C3C	-5.70	100.98	106.98
25	B	613	CLA	C2D-C1D-ND	5.70	115.77	110.13
25	B	605	CLA	C4A-NA-C1A	5.70	109.28	106.68
25	b	605	CLA	C4A-NA-C1A	5.70	109.28	106.68
25	c	508	CLA	C4A-NA-C1A	5.69	109.28	106.68
25	B	616	CLA	C2C-C1C-NC	5.69	115.96	109.98
25	b	613	CLA	C2D-C1D-ND	5.69	115.76	110.13
25	b	616	CLA	C2C-C1C-NC	5.69	115.96	109.98
25	b	612	CLA	C2D-C1D-ND	5.68	115.75	110.13
25	A	408	CLA	C1D-ND-C4D	-5.67	102.33	106.31
25	B	610	CLA	O2D-CGD-CBD	5.66	121.13	111.23
25	b	610	CLA	O2D-CGD-CBD	5.66	121.13	111.23
25	C	511	CLA	O2D-CGD-CBD	5.65	121.11	111.23
25	c	511	CLA	O2D-CGD-CBD	5.64	121.09	111.23
25	B	603	CLA	C1C-C2C-C3C	-5.63	101.06	106.98
25	B	601	CLA	C1C-C2C-C3C	-5.63	101.06	106.98
25	b	601	CLA	C1C-C2C-C3C	-5.63	101.06	106.98
25	B	612	CLA	C2D-C1D-ND	5.63	115.69	110.13
25	b	606	CLA	C2C-C1C-NC	5.62	115.89	109.98
25	C	502	CLA	O2D-CGD-CBD	5.62	121.05	111.23
25	B	605	CLA	C3D-C2D-C1D	-5.62	98.17	105.83
25	b	605	CLA	C3D-C2D-C1D	-5.62	98.17	105.83
25	B	606	CLA	O2D-CGD-CBD	5.61	121.03	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	508	CLA	C4A-NA-C1A	5.60	109.24	106.68
25	a	408	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
25	c	502	CLA	O2D-CGD-CBD	5.60	121.02	111.23
25	B	616	CLA	C3D-C2D-C1D	-5.60	98.19	105.83
25	b	601	CLA	C4A-NA-C1A	5.60	109.23	106.68
25	a	408	CLA	C1D-ND-C4D	-5.60	102.38	106.31
25	B	614	CLA	C2C-C1C-NC	5.60	115.86	109.98
25	b	614	CLA	C2C-C1C-NC	5.60	115.86	109.98
30	f	102	SQD	C1-O5-C5	5.59	124.64	113.72
25	b	616	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
25	A	408	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
25	a	408	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
25	C	507	CLA	C4A-NA-C1A	5.59	109.23	106.68
25	c	507	CLA	C4A-NA-C1A	5.59	109.23	106.68
25	b	606	CLA	O2D-CGD-CBD	5.59	121.00	111.23
25	B	606	CLA	C2C-C1C-NC	5.59	115.85	109.98
25	B	605	CLA	O2D-CGD-CBD	5.59	121.00	111.23
25	b	605	CLA	O2D-CGD-CBD	5.59	121.00	111.23
25	D	404	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
25	A	408	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
25	b	603	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
25	C	514	CLA	C4A-NA-C1A	5.58	109.23	106.68
30	F	102	SQD	C1-O5-C5	5.58	124.62	113.72
25	a	408	CLA	C4A-NA-C1A	5.58	109.22	106.68
30	a	413	SQD	C1-O5-C5	5.57	124.61	113.72
30	A	413	SQD	C1-O5-C5	5.57	124.61	113.72
25	d	404	CLA	C3B-C2B-C1B	-5.57	100.61	107.17
25	B	601	CLA	C4A-NA-C1A	5.56	109.22	106.68
25	A	408	CLA	C4A-NA-C1A	5.55	109.21	106.68
32	A	417	BCT	O2-C-O1	5.55	133.86	119.68
25	c	514	CLA	C4A-NA-C1A	5.54	109.21	106.68
32	a	417	BCT	O2-C-O1	5.54	133.84	119.68
25	B	610	CLA	C1C-C2C-C3C	-5.53	101.16	106.98
25	A	408	CLA	C2D-C1D-ND	5.53	115.60	110.13
25	B	604	CLA	C1C-C2C-C3C	-5.53	101.17	106.98
25	b	604	CLA	C1C-C2C-C3C	-5.53	101.17	106.98
25	C	502	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
25	c	507	CLA	C1C-C2C-C3C	-5.51	101.18	106.98
25	B	607	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
25	b	607	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
25	a	408	CLA	C2D-C1D-ND	5.51	115.58	110.13
25	b	610	CLA	C1C-C2C-C3C	-5.50	101.19	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	404	CLA	C4A-NA-C1A	5.50	109.19	106.68
25	C	507	CLA	C1C-C2C-C3C	-5.50	101.20	106.98
25	B	607	CLA	C2D-C1D-ND	5.49	115.56	110.13
25	b	607	CLA	C2D-C1D-ND	5.49	115.56	110.13
25	c	502	CLA	C1C-C2C-C3C	-5.49	101.21	106.98
25	D	403	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
25	d	403	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
25	C	514	CLA	O2A-CGA-O1A	-5.46	109.97	123.63
25	c	514	CLA	O2A-CGA-O1A	-5.46	109.97	123.63
25	d	404	CLA	C4A-NA-C1A	5.45	109.17	106.68
25	B	603	CLA	O2A-CGA-O1A	-5.45	109.99	123.63
25	b	603	CLA	O2A-CGA-O1A	-5.45	109.99	123.63
25	B	608	CLA	C4A-NA-C1A	5.45	109.16	106.68
25	b	608	CLA	C4A-NA-C1A	5.44	109.16	106.68
25	B	607	CLA	C2C-C1C-NC	5.44	115.69	109.98
25	C	504	CLA	C2D-C1D-ND	5.43	115.50	110.13
25	c	504	CLA	C2D-C1D-ND	5.43	115.50	110.13
25	B	602	CLA	C1D-ND-C4D	-5.43	102.50	106.31
25	b	602	CLA	C1D-ND-C4D	-5.43	102.50	106.31
25	C	512	CLA	C2D-C1D-ND	5.41	115.48	110.13
25	C	510	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
25	c	510	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
25	b	607	CLA	C2C-C1C-NC	5.41	115.66	109.98
25	B	605	CLA	C3B-C2B-C1B	-5.41	100.80	107.17
25	b	605	CLA	C3B-C2B-C1B	-5.41	100.80	107.17
25	c	512	CLA	C2D-C1D-ND	5.40	115.47	110.13
25	B	615	CLA	C1D-ND-C4D	-5.40	102.52	106.31
25	C	509	CLA	C2D-C1D-ND	5.40	115.47	110.13
25	c	509	CLA	C2D-C1D-ND	5.40	115.47	110.13
25	C	514	CLA	C2D-C1D-ND	5.40	115.47	110.13
25	C	508	CLA	O2D-CGD-CBD	5.39	120.66	111.23
25	c	508	CLA	O2D-CGD-CBD	5.39	120.65	111.23
25	C	504	CLA	C3B-C2B-C1B	-5.39	100.82	107.17
25	c	504	CLA	C3B-C2B-C1B	-5.39	100.82	107.17
25	b	615	CLA	C1D-ND-C4D	-5.39	102.53	106.31
25	b	605	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
35	E	104	HEM	CHC-C4B-NB	5.38	130.22	124.42
25	B	605	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
25	B	612	CLA	C2C-C1C-NC	5.38	115.63	109.98
25	b	612	CLA	C2C-C1C-NC	5.38	115.63	109.98
35	e	104	HEM	CHC-C4B-NB	5.38	130.21	124.42
25	B	609	CLA	O2A-CGA-O1A	-5.37	110.19	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	609	CLA	O2A-CGA-O1A	-5.37	110.19	123.63
25	B	616	CLA	C2D-C1D-ND	5.37	115.44	110.13
25	C	511	CLA	C4A-NA-C1A	5.36	109.13	106.68
25	b	616	CLA	C2D-C1D-ND	5.36	115.43	110.13
25	d	404	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
25	c	511	CLA	C4A-NA-C1A	5.36	109.12	106.68
25	B	601	CLA	C2D-C1D-ND	5.36	115.43	110.13
25	b	601	CLA	C2D-C1D-ND	5.36	115.43	110.13
25	c	514	CLA	C2D-C1D-ND	5.35	115.42	110.13
25	C	513	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
25	c	513	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
25	b	615	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
25	A	406	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
25	B	615	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
25	a	406	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
25	B	611	CLA	C2C-C1C-NC	5.33	115.58	109.98
25	b	611	CLA	C2C-C1C-NC	5.33	115.58	109.98
31	e	103	LMT	O5B-C5B-C4B	5.33	119.30	109.70
31	E	103	LMT	O5B-C5B-C4B	5.33	119.30	109.70
25	D	404	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
25	b	602	CLA	C3B-C2B-C1B	-5.32	100.89	107.17
25	B	614	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
25	b	614	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
25	B	602	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
25	B	611	CLA	C1D-ND-C4D	-5.30	102.59	106.31
25	b	611	CLA	C1D-ND-C4D	-5.30	102.59	106.31
25	C	508	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
25	C	509	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
25	B	602	CLA	O2D-CGD-CBD	5.28	120.47	111.23
25	b	602	CLA	O2D-CGD-CBD	5.28	120.47	111.23
25	C	514	CLA	C2C-C1C-NC	5.28	115.53	109.98
25	c	514	CLA	C2C-C1C-NC	5.28	115.53	109.98
25	c	508	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
25	c	512	CLA	C1D-ND-C4D	-5.27	102.62	106.31
35	V	201	HEM	C1B-NB-C4B	5.26	111.44	105.21
35	v	201	HEM	C1B-NB-C4B	5.26	111.44	105.21
25	c	509	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
25	D	401	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
25	d	401	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
25	B	601	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
25	b	601	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
25	B	616	CLA	C3B-C2B-C1B	-5.25	100.98	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	616	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
25	C	510	CLA	C2D-C1D-ND	5.25	115.32	110.13
25	c	510	CLA	C2D-C1D-ND	5.25	115.32	110.13
25	D	403	CLA	C3B-C2B-C1B	-5.25	100.99	107.17
25	d	403	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
25	C	512	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
25	B	602	CLA	C2C-C1C-NC	5.23	115.48	109.98
25	c	512	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
25	b	602	CLA	C2C-C1C-NC	5.23	115.47	109.98
25	C	507	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
25	c	507	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
25	C	508	CLA	O2A-CGA-O1A	-5.23	110.55	123.63
25	c	508	CLA	O2A-CGA-O1A	-5.23	110.55	123.63
25	C	512	CLA	C1D-ND-C4D	-5.23	102.64	106.31
25	D	404	CLA	C1D-ND-C4D	-5.22	102.65	106.31
25	d	404	CLA	C1D-ND-C4D	-5.22	102.65	106.31
25	C	512	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
25	B	612	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
25	b	612	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
25	c	512	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
25	c	505	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
25	b	602	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
25	C	507	CLA	O2D-CGD-CBD	5.20	120.32	111.23
25	B	602	CLA	C2D-C1D-ND	5.19	115.27	110.13
25	b	602	CLA	C2D-C1D-ND	5.19	115.27	110.13
25	C	505	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
25	B	602	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
25	C	512	CLA	O2A-CGA-O1A	-5.19	110.65	123.63
25	c	512	CLA	O2A-CGA-O1A	-5.19	110.65	123.63
25	b	606	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
25	C	502	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
25	c	502	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
25	B	606	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
25	b	606	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
25	c	507	CLA	O2D-CGD-CBD	5.17	120.27	111.23
25	C	513	CLA	O2A-CGA-O1A	-5.16	110.71	123.63
25	c	513	CLA	O2A-CGA-O1A	-5.16	110.72	123.63
25	B	606	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
25	B	614	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
25	b	614	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
25	C	509	CLA	C2C-C1C-NC	5.16	115.40	109.98
25	c	509	CLA	C2C-C1C-NC	5.16	115.40	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	505	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
25	D	403	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
25	d	403	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
25	C	503	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
25	c	503	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
25	a	406	CLA	O2A-CGA-O1A	-5.15	110.75	123.63
25	A	406	CLA	O2A-CGA-O1A	-5.14	110.77	123.63
25	B	615	CLA	O2A-CGA-O1A	-5.14	110.77	123.63
25	B	609	CLA	C2D-C1D-ND	5.14	115.21	110.13
25	b	615	CLA	O2A-CGA-O1A	-5.14	110.78	123.63
25	C	505	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
25	B	610	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
25	c	508	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
25	d	404	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
25	b	610	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
25	C	508	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
25	C	502	CLA	O2A-CGA-O1A	-5.13	110.81	123.63
25	c	502	CLA	O2A-CGA-O1A	-5.13	110.81	123.63
27	B	618	BCR	C24-C23-C22	-5.12	118.65	126.23
27	b	618	BCR	C24-C23-C22	-5.12	118.65	126.23
25	B	614	CLA	C1D-ND-C4D	-5.12	102.72	106.31
25	A	408	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
25	D	404	CLA	O2D-CGD-CBD	5.10	120.15	111.23
25	d	404	CLA	O2D-CGD-CBD	5.10	120.15	111.23
25	b	614	CLA	C1D-ND-C4D	-5.10	102.73	106.31
25	a	408	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
25	D	404	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
25	B	614	CLA	C2D-C1D-ND	5.10	115.17	110.13
25	C	506	CLA	C1C-C2C-C3C	-5.09	101.63	106.98
30	C	501	SQD	O6-C1-C2	5.09	116.00	108.27
25	B	611	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
25	b	611	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
25	C	502	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
25	c	502	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
25	b	614	CLA	C2D-C1D-ND	5.08	115.16	110.13
25	c	506	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
25	b	609	CLA	C2D-C1D-ND	5.08	115.15	110.13
30	c	501	SQD	O6-C1-C2	5.08	115.98	108.27
25	c	504	CLA	O2A-CGA-O1A	-5.08	110.93	123.63
25	C	504	CLA	C4A-NA-C1A	5.07	108.99	106.68
25	C	504	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
25	c	511	CLA	O2A-CGA-O1A	-5.06	110.97	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	504	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
25	C	513	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
25	c	513	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
25	B	607	CLA	O2A-CGA-O1A	-5.06	110.98	123.63
25	c	504	CLA	C1C-C2C-C3C	-5.05	101.66	106.98
25	B	611	CLA	O2A-CGA-O1A	-5.05	110.99	123.63
25	b	611	CLA	O2A-CGA-O1A	-5.05	110.99	123.63
25	c	504	CLA	C4A-NA-C1A	5.05	108.98	106.68
25	b	607	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
30	c	501	SQD	O9-S-C6	5.04	114.29	106.76
25	C	511	CLA	O2A-CGA-O1A	-5.04	111.01	123.63
25	C	512	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
25	c	512	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
25	d	404	CLA	C2D-C1D-ND	5.03	115.11	110.13
25	D	401	CLA	C2D-C1D-ND	5.03	115.11	110.13
25	d	401	CLA	C2D-C1D-ND	5.03	115.11	110.13
25	C	514	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
25	C	503	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
25	c	503	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
30	C	501	SQD	O9-S-C6	5.02	114.25	106.76
25	c	505	CLA	C2D-C1D-ND	5.02	115.09	110.13
25	B	603	CLA	O2D-CGD-CBD	5.02	120.00	111.23
25	b	603	CLA	O2D-CGD-CBD	5.02	120.00	111.23
25	c	509	CLA	O2A-CGA-O1A	-5.02	111.08	123.63
25	a	406	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
25	C	514	CLA	O2D-CGD-CBD	5.01	119.99	111.23
25	c	514	CLA	O2D-CGD-CBD	5.01	119.99	111.23
25	c	514	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
25	D	404	CLA	C2D-C1D-ND	5.00	115.08	110.13
25	b	606	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
25	C	509	CLA	O2A-CGA-O1A	-5.00	111.12	123.63
25	B	612	CLA	C1C-C2C-C3C	-5.00	101.72	106.98
25	b	612	CLA	C1C-C2C-C3C	-5.00	101.72	106.98
25	A	406	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
25	C	505	CLA	C2D-C1D-ND	4.99	115.07	110.13
25	A	405	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
25	a	405	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
25	A	405	CLA	C1D-ND-C4D	-4.99	102.81	106.31
25	a	405	CLA	C1D-ND-C4D	-4.99	102.81	106.31
25	A	405	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
25	a	405	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
25	B	606	CLA	C3D-C2D-C1D	-4.98	99.04	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	605	CLA	C2C-C1C-NC	4.97	115.20	109.98
25	B	602	CLA	C1C-C2C-C3C	-4.97	101.75	106.98
25	b	602	CLA	C1C-C2C-C3C	-4.97	101.75	106.98
25	b	606	CLA	O2A-CGA-O1A	-4.96	111.22	123.63
27	C	515	BCR	C24-C23-C22	-4.96	118.90	126.23
25	B	605	CLA	C2C-C1C-NC	4.96	115.19	109.98
25	D	404	CLA	O2A-CGA-O1A	-4.96	111.23	123.63
25	B	606	CLA	O2A-CGA-O1A	-4.95	111.24	123.63
25	C	502	CLA	C4A-NA-C1A	4.95	108.94	106.68
25	c	502	CLA	C4A-NA-C1A	4.95	108.94	106.68
25	d	404	CLA	O2A-CGA-O1A	-4.95	111.26	123.63
25	C	506	CLA	C1D-ND-C4D	-4.94	102.84	106.31
25	c	506	CLA	C1D-ND-C4D	-4.94	102.84	106.31
27	c	515	BCR	C24-C23-C22	-4.94	118.92	126.23
25	B	607	CLA	O2D-CGD-CBD	4.94	119.87	111.23
29	A	411	PL9	C7-C3-C4	4.94	120.98	116.91
25	b	607	CLA	O2D-CGD-CBD	4.93	119.85	111.23
25	B	609	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
25	c	509	CLA	C1D-ND-C4D	-4.92	102.86	106.31
25	C	507	CLA	C2D-C1D-ND	4.92	115.00	110.13
25	c	507	CLA	C2D-C1D-ND	4.92	115.00	110.13
25	c	505	CLA	O2A-CGA-O1A	-4.90	111.36	123.63
29	a	411	PL9	C7-C3-C4	4.90	120.95	116.91
25	B	602	CLA	C4A-NA-C1A	4.90	108.91	106.68
25	b	602	CLA	C4A-NA-C1A	4.89	108.91	106.68
25	C	505	CLA	O2A-CGA-O1A	-4.89	111.40	123.63
25	B	610	CLA	O2A-CGA-O1A	-4.89	111.40	123.63
25	b	610	CLA	O2A-CGA-O1A	-4.89	111.40	123.63
25	D	403	CLA	C2C-C1C-NC	4.89	115.12	109.98
25	D	401	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
25	d	403	CLA	C2C-C1C-NC	4.88	115.11	109.98
28	C	523	LMG	O7-C10-C11	4.88	122.04	111.48
25	B	607	CLA	C1D-ND-C4D	-4.88	102.89	106.31
25	b	607	CLA	C1D-ND-C4D	-4.88	102.89	106.31
28	c	523	LMG	O7-C10-C11	4.88	122.04	111.48
25	b	609	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
27	k	102	BCR	C7-C8-C9	-4.87	119.03	126.23
25	C	509	CLA	C1D-ND-C4D	-4.87	102.90	106.31
25	B	613	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
25	b	613	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
25	d	401	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
25	B	616	CLA	O2A-CGA-O1A	-4.86	111.47	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	406	CLA	O2D-CGD-CBD	4.86	119.72	111.23
25	a	406	CLA	O2D-CGD-CBD	4.85	119.71	111.23
27	K	102	BCR	C7-C8-C9	-4.85	119.06	126.23
25	C	503	CLA	C2D-C1D-ND	4.84	114.92	110.13
25	c	503	CLA	C2D-C1D-ND	4.84	114.92	110.13
25	b	616	CLA	O2A-CGA-O1A	-4.84	111.53	123.63
25	b	608	CLA	C1D-ND-C4D	-4.84	102.92	106.31
25	C	506	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
25	c	506	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
25	C	512	CLA	O2D-CGD-CBD	4.82	119.65	111.23
25	c	512	CLA	O2D-CGD-CBD	4.82	119.65	111.23
25	B	614	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
30	A	413	SQD	O5-C5-C4	4.80	118.36	109.70
30	a	413	SQD	O5-C5-C4	4.80	118.36	109.70
27	B	619	BCR	C24-C23-C22	-4.80	119.14	126.23
25	C	502	CLA	C2D-C1D-ND	4.80	114.88	110.13
25	c	502	CLA	C2D-C1D-ND	4.80	114.88	110.13
27	A	409	BCR	C24-C23-C22	-4.80	119.14	126.23
27	a	409	BCR	C24-C23-C22	-4.80	119.14	126.23
25	b	614	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
25	B	601	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
25	C	510	CLA	O2D-CGD-CBD	4.79	119.60	111.23
25	c	510	CLA	O2D-CGD-CBD	4.79	119.60	111.23
25	C	509	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
25	c	509	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
25	B	608	CLA	C1D-ND-C4D	-4.78	102.96	106.31
25	C	514	CLA	C1D-ND-C4D	-4.78	102.96	106.31
25	B	601	CLA	C1D-ND-C4D	-4.78	102.96	106.31
27	b	619	BCR	C24-C23-C22	-4.76	119.19	126.23
30	k	101	SQD	C4-C3-C2	4.76	119.19	110.83
25	A	405	CLA	C2D-C1D-ND	4.76	114.84	110.13
25	a	405	CLA	C2D-C1D-ND	4.76	114.84	110.13
30	K	101	SQD	C4-C3-C2	4.76	119.18	110.83
25	b	601	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
25	c	514	CLA	C1D-ND-C4D	-4.75	102.98	106.31
25	D	401	CLA	C1D-ND-C4D	-4.75	102.98	106.31
25	d	401	CLA	C1D-ND-C4D	-4.75	102.98	106.31
25	b	601	CLA	C1D-ND-C4D	-4.74	102.98	106.31
25	B	610	CLA	C2D-C1D-ND	4.74	114.81	110.13
25	b	608	CLA	O2D-CGD-CBD	4.74	119.51	111.23
25	b	610	CLA	C2D-C1D-ND	4.73	114.81	110.13
25	B	608	CLA	O2D-CGD-CBD	4.71	119.47	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	511	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
25	c	511	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
25	b	603	CLA	O2A-CGA-CBA	4.71	126.19	111.83
25	B	603	CLA	O2A-CGA-CBA	4.70	126.18	111.83
25	C	514	CLA	C1C-C2C-C3C	-4.70	102.03	106.98
25	c	514	CLA	C1C-C2C-C3C	-4.70	102.03	106.98
25	C	513	CLA	CMD-C2D-C1D	4.70	133.00	124.73
25	c	513	CLA	CMD-C2D-C1D	4.70	133.00	124.73
25	A	408	CLA	O2A-CGA-O1A	-4.69	111.90	123.63
25	a	408	CLA	O2A-CGA-O1A	-4.69	111.90	123.63
25	C	506	CLA	C4A-NA-C1A	4.69	108.82	106.68
25	c	506	CLA	C4A-NA-C1A	4.69	108.82	106.68
25	C	507	CLA	O2A-CGA-O1A	-4.68	111.93	123.63
25	B	615	CLA	C1C-C2C-C3C	-4.66	102.07	106.98
25	b	606	CLA	C2D-C1D-ND	4.66	114.74	110.13
27	Z	101	BCR	C7-C8-C9	-4.66	119.34	126.23
25	b	615	CLA	C1C-C2C-C3C	-4.66	102.08	106.98
27	Z	101	BCR	C24-C23-C22	-4.65	119.35	126.23
27	z	101	BCR	C24-C23-C22	-4.65	119.35	126.23
25	B	614	CLA	O2A-CGA-O1A	-4.65	111.99	123.63
25	A	405	CLA	O2A-CGA-O1A	-4.65	112.00	123.63
25	a	405	CLA	O2A-CGA-O1A	-4.65	112.00	123.63
25	b	614	CLA	O2A-CGA-O1A	-4.65	112.00	123.63
25	c	507	CLA	O2A-CGA-O1A	-4.65	112.00	123.63
25	B	601	CLA	O2A-CGA-O1A	-4.65	111.38	123.33
25	b	601	CLA	O2A-CGA-O1A	-4.65	111.38	123.33
27	z	101	BCR	C7-C8-C9	-4.65	119.36	126.23
25	B	606	CLA	C2D-C1D-ND	4.63	114.71	110.13
25	C	506	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
25	c	506	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
33	b	627	LHG	O7-C7-C8	4.62	121.47	111.48
33	B	627	LHG	O7-C7-C8	4.62	121.47	111.48
25	C	502	CLA	C1D-ND-C4D	-4.62	103.07	106.31
25	c	502	CLA	C1D-ND-C4D	-4.62	103.07	106.31
30	c	501	SQD	O9-S-O7	-4.61	98.82	113.82
30	C	501	SQD	O9-S-O7	-4.60	98.85	113.82
25	C	505	CLA	C1D-ND-C4D	-4.60	103.09	106.31
25	c	505	CLA	C1D-ND-C4D	-4.60	103.09	106.31
25	c	513	CLA	C1D-ND-C4D	-4.59	103.09	106.31
28	h	105	LMG	O7-C10-C11	4.59	121.41	111.48
25	C	504	CLA	O2D-CGD-CBD	4.58	119.25	111.23
25	c	504	CLA	O2D-CGD-CBD	4.58	119.25	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	511	CLA	C2D-C1D-ND	4.58	114.66	110.13
25	c	511	CLA	C2D-C1D-ND	4.58	114.66	110.13
25	C	513	CLA	C1D-ND-C4D	-4.58	103.10	106.31
28	H	105	LMG	O7-C10-C11	4.57	121.38	111.48
25	B	611	CLA	CAC-C3C-C4C	4.57	130.74	124.79
25	b	611	CLA	CAC-C3C-C4C	4.57	130.73	124.79
25	B	615	CLA	O2D-CGD-CBD	4.56	119.20	111.23
25	b	615	CLA	O2D-CGD-CBD	4.56	119.20	111.23
25	B	608	CLA	C2D-C1D-ND	4.56	114.64	110.13
25	b	608	CLA	C2D-C1D-ND	4.56	114.64	110.13
25	B	605	CLA	O2A-CGA-O1A	-4.56	112.23	123.63
25	b	605	CLA	O2A-CGA-O1A	-4.56	112.23	123.63
25	B	613	CLA	O2A-CGA-O1A	-4.55	112.24	123.63
25	b	613	CLA	O2A-CGA-O1A	-4.55	112.24	123.63
25	B	612	CLA	O2A-CGA-O1A	-4.55	112.25	123.63
25	b	612	CLA	O2A-CGA-O1A	-4.53	112.30	123.63
30	k	101	SQD	O5-C5-C4	4.53	117.70	109.55
30	K	101	SQD	O5-C5-C4	4.52	117.69	109.55
25	B	608	CLA	O2A-CGA-O1A	-4.52	112.33	123.63
25	C	504	CLA	C1D-ND-C4D	-4.52	103.14	106.31
25	c	504	CLA	C1D-ND-C4D	-4.52	103.14	106.31
25	b	608	CLA	O2A-CGA-O1A	-4.51	112.34	123.63
25	B	609	CLA	C1D-ND-C4D	-4.51	103.15	106.31
25	C	509	CLA	O2D-CGD-CBD	4.51	119.11	111.23
25	c	509	CLA	O2D-CGD-CBD	4.51	119.11	111.23
25	b	609	CLA	C1D-ND-C4D	-4.51	103.15	106.31
25	b	610	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
25	C	503	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
25	C	506	CLA	C4D-C3D-CAD	4.49	112.99	108.11
30	A	412	SQD	O7-S-C6	4.49	113.46	106.76
30	a	412	SQD	O7-S-C6	4.49	113.46	106.76
25	B	607	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
25	b	607	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
25	c	503	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
25	b	604	CLA	O2A-CGA-O1A	-4.48	112.43	123.63
25	d	401	CLA	O2D-CGD-CBD	4.46	119.03	111.23
25	B	610	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
25	B	604	CLA	O2A-CGA-O1A	-4.46	112.47	123.63
25	A	406	CLA	C2D-C1D-ND	4.46	114.54	110.13
25	a	406	CLA	C2D-C1D-ND	4.46	114.54	110.13
25	B	604	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
25	A	405	CLA	O2D-CGD-CBD	4.46	119.03	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	CLA	O2D-CGD-CBD	4.46	119.03	111.23
25	c	506	CLA	C4D-C3D-CAD	4.46	112.95	108.11
25	B	602	CLA	O2A-CGA-O1A	-4.46	112.48	123.63
25	D	401	CLA	O2D-CGD-CBD	4.45	119.02	111.23
25	b	602	CLA	O2A-CGA-O1A	-4.45	112.49	123.63
25	c	512	CLA	O2A-CGA-CBA	4.45	125.39	111.83
25	C	512	CLA	O2A-C1-C2	4.44	125.21	108.11
25	c	512	CLA	O2A-C1-C2	4.44	125.21	108.11
25	b	604	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
25	C	512	CLA	O2A-CGA-CBA	4.44	125.37	111.83
25	B	614	CLA	O2D-CGD-CBD	4.42	118.96	111.23
29	d	405	PL9	C7-C3-C4	4.42	120.55	116.91
27	F	101	BCR	C24-C23-C22	-4.42	119.70	126.23
27	f	101	BCR	C24-C23-C22	-4.42	119.70	126.23
25	C	503	CLA	O2A-C1-C2	4.42	125.11	108.11
29	D	405	PL9	C7-C3-C4	4.41	120.55	116.91
25	c	503	CLA	O2A-C1-C2	4.41	125.08	108.11
25	b	614	CLA	O2D-CGD-CBD	4.40	118.93	111.23
25	C	511	CLA	C1D-ND-C4D	-4.40	103.23	106.31
25	c	511	CLA	C1D-ND-C4D	-4.40	103.23	106.31
34	C	517	DGD	O2G-C1B-C2B	4.39	120.98	111.48
34	c	517	DGD	O2G-C1B-C2B	4.39	120.98	111.48
25	b	612	CLA	CMD-C2D-C1D	4.39	132.45	124.73
25	B	609	CLA	C3B-C2B-C1B	-4.38	102.01	107.17
25	B	607	CLA	C1C-C2C-C3C	-4.37	102.38	106.98
25	B	612	CLA	CMD-C2D-C1D	4.37	132.41	124.73
25	c	514	CLA	O2A-CGA-CBA	4.36	125.11	111.83
25	C	514	CLA	O2A-CGA-CBA	4.35	125.10	111.83
25	A	406	CLA	C1D-ND-C4D	-4.35	103.26	106.31
25	b	607	CLA	C1C-C2C-C3C	-4.34	102.41	106.98
25	C	513	CLA	O2A-CGA-CBA	4.34	125.07	111.83
25	C	508	CLA	C2D-C1D-ND	4.34	114.42	110.13
25	B	610	CLA	O2A-CGA-CBA	4.34	125.06	111.83
25	b	610	CLA	O2A-CGA-CBA	4.34	125.06	111.83
25	c	508	CLA	C2D-C1D-ND	4.33	114.42	110.13
27	k	103	BCR	C3-C4-C5	-4.33	106.33	114.06
25	c	513	CLA	O2A-CGA-CBA	4.33	125.04	111.83
25	b	609	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
27	f	101	BCR	C38-C26-C25	-4.33	119.76	124.48
30	H	103	SQD	O9-S-C6	4.33	113.22	106.76
30	h	103	SQD	O9-S-C6	4.33	113.22	106.76
27	K	103	BCR	C3-C4-C5	-4.32	106.35	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	518	DGD	O2G-C1B-C2B	4.32	120.82	111.48
25	B	606	CLA	C1D-ND-C4D	-4.31	103.29	106.31
25	a	406	CLA	C1D-ND-C4D	-4.31	103.29	106.31
25	C	509	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
25	c	509	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
34	C	518	DGD	O2G-C1B-C2B	4.31	120.80	111.48
25	B	609	CLA	O2A-CGA-CBA	4.30	124.95	111.83
25	b	609	CLA	O2A-CGA-CBA	4.30	124.95	111.83
25	b	606	CLA	C1D-ND-C4D	-4.30	103.29	106.31
25	B	616	CLA	O2A-CGA-CBA	4.30	124.94	111.83
27	F	101	BCR	C38-C26-C25	-4.29	119.80	124.48
30	A	412	SQD	C44-O6-C1	4.28	122.98	113.80
25	b	616	CLA	O2A-CGA-CBA	4.28	124.89	111.83
28	a	414	LMG	O7-C10-C11	4.28	120.74	111.48
30	a	412	SQD	C44-O6-C1	4.28	122.97	113.80
27	B	619	BCR	C7-C8-C9	-4.27	119.91	126.23
27	b	619	BCR	C7-C8-C9	-4.27	119.91	126.23
25	C	503	CLA	O2A-CGA-O1A	-4.27	112.94	123.63
35	e	104	HEM	CHD-C1D-ND	4.27	129.02	124.42
30	H	103	SQD	O9-S-O7	-4.27	99.95	113.82
30	h	103	SQD	O9-S-O7	-4.27	99.95	113.82
25	A	405	CLA	O2A-C1-C2	4.26	124.50	108.11
25	a	405	CLA	O2A-C1-C2	4.26	124.50	108.11
25	B	604	CLA	CMA-C3A-C4A	4.26	123.22	111.77
25	b	604	CLA	CMA-C3A-C4A	4.26	123.22	111.77
25	c	510	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
25	c	503	CLA	O2A-CGA-O1A	-4.26	112.98	123.63
35	E	104	HEM	CHD-C1D-ND	4.26	129.00	124.42
28	A	414	LMG	O7-C10-C11	4.26	120.69	111.48
26	A	407	PHO	C2B-C1B-NB	-4.25	106.36	109.43
25	b	608	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
25	B	612	CLA	CMC-C2C-C1C	4.24	131.66	125.03
25	b	612	CLA	CMC-C2C-C1C	4.24	131.66	125.03
25	C	510	CLA	C3B-C2B-C1B	-4.23	102.18	107.17
25	c	507	CLA	C1D-ND-C4D	-4.23	103.34	106.31
30	K	101	SQD	C3-C4-C5	4.23	116.24	109.81
25	a	408	CLA	CAA-C2A-C3A	-4.23	101.58	113.00
25	B	603	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
25	b	603	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
30	k	101	SQD	C3-C4-C5	4.22	116.22	109.81
25	A	408	CLA	CAA-C2A-C3A	-4.22	101.61	113.00
25	B	610	CLA	C4A-NA-C1A	4.21	108.60	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	V	201	HEM	CHD-C1D-ND	4.21	128.96	124.42
35	v	201	HEM	CHD-C1D-ND	4.21	128.96	124.42
25	B	608	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
26	a	407	PHO	C2B-C1B-NB	-4.20	106.39	109.43
25	D	403	CLA	O2A-CGA-O1A	-4.20	113.12	123.63
25	d	403	CLA	O2A-CGA-O1A	-4.20	113.12	123.63
27	z	101	BCR	C3-C4-C5	-4.20	106.57	114.06
30	A	412	SQD	O9-S-O7	-4.20	100.17	113.82
30	a	412	SQD	O9-S-O7	-4.20	100.17	113.82
25	b	616	CLA	C1D-ND-C4D	-4.19	103.37	106.31
27	k	102	BCR	C3-C4-C5	-4.19	106.59	114.06
25	C	507	CLA	C1D-ND-C4D	-4.19	103.38	106.31
25	b	610	CLA	C4A-NA-C1A	4.18	108.59	106.68
25	B	608	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
27	Z	101	BCR	C3-C4-C5	-4.18	106.60	114.06
27	K	102	BCR	C3-C4-C5	-4.18	106.60	114.06
25	B	616	CLA	C1D-ND-C4D	-4.18	103.38	106.31
25	b	608	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
25	c	514	CLA	C2B-C1B-NB	4.14	114.62	110.33
25	C	506	CLA	O2A-C1-C2	4.14	124.03	108.11
25	c	506	CLA	O2A-C1-C2	4.14	124.03	108.11
30	F	102	SQD	O9-S-O7	-4.13	100.39	113.82
25	B	610	CLA	C1D-ND-C4D	-4.13	103.42	106.31
30	f	102	SQD	O9-S-O7	-4.13	100.41	113.82
25	C	509	CLA	C2B-C1B-NB	4.12	114.60	110.33
25	c	509	CLA	C2B-C1B-NB	4.11	114.59	110.33
25	d	404	CLA	C2B-C1B-NB	4.11	114.59	110.33
25	C	514	CLA	C2B-C1B-NB	4.11	114.58	110.33
25	D	404	CLA	C2B-C1B-NB	4.10	114.58	110.33
25	b	610	CLA	C1D-ND-C4D	-4.10	103.44	106.31
25	C	505	CLA	O2A-C1-C2	4.10	123.88	108.11
25	C	507	CLA	O2A-C1-C2	4.10	123.87	108.11
25	c	507	CLA	O2A-C1-C2	4.10	123.87	108.11
25	B	613	CLA	O2D-CGD-CBD	4.10	118.39	111.23
25	b	613	CLA	O2D-CGD-CBD	4.10	118.39	111.23
25	c	505	CLA	O2A-C1-C2	4.09	123.87	108.11
25	D	401	CLA	O2A-CGA-O1A	-4.08	113.41	123.63
25	d	401	CLA	O2A-CGA-O1A	-4.08	113.41	123.63
25	A	405	CLA	O2A-CGA-CBA	4.07	124.24	111.83
25	a	405	CLA	O2A-CGA-CBA	4.07	124.24	111.83
26	d	402	PHO	CMB-C2B-C3B	4.06	132.80	124.68
25	C	503	CLA	C1D-ND-C4D	-4.06	103.47	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	503	CLA	C1D-ND-C4D	-4.06	103.47	106.31
26	D	402	PHO	CMB-C2B-C3B	4.04	132.76	124.68
25	c	509	CLA	O2A-C1-C2	4.03	123.63	108.11
25	C	509	CLA	O2A-C1-C2	4.03	123.62	108.11
25	b	612	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
25	C	511	CLA	O2A-CGA-CBA	4.02	124.09	111.83
30	K	101	SQD	C1-O5-C5	4.02	120.48	113.63
25	C	513	CLA	O2A-C1-C2	4.01	123.55	108.11
25	C	502	CLA	O2A-CGA-CBA	4.01	124.07	111.83
25	c	502	CLA	O2A-CGA-CBA	4.01	124.07	111.83
25	c	511	CLA	O2A-CGA-CBA	4.01	124.06	111.83
25	B	603	CLA	C2D-C1D-ND	4.00	114.09	110.13
25	b	603	CLA	C2D-C1D-ND	4.00	114.09	110.13
25	c	513	CLA	O2A-C1-C2	4.00	123.51	108.11
30	k	101	SQD	C1-O5-C5	4.00	120.45	113.63
25	B	612	CLA	C3D-C2D-C1D	-3.99	100.38	105.83
33	Z	102	LHG	O7-C7-C8	3.99	120.12	111.48
33	z	102	LHG	O7-C7-C8	3.99	120.11	111.48
25	B	604	CLA	C2D-C1D-ND	3.98	114.07	110.13
25	C	508	CLA	C2B-C1B-NB	3.98	114.46	110.33
25	c	508	CLA	C2B-C1B-NB	3.98	114.46	110.33
25	C	509	CLA	C4A-NA-C1A	3.98	108.50	106.68
25	b	604	CLA	C2D-C1D-ND	3.96	114.05	110.13
35	e	104	HEM	CHA-C4D-ND	3.96	129.26	124.37
25	A	405	CLA	C2C-C1C-NC	3.95	114.13	109.98
25	a	405	CLA	C2C-C1C-NC	3.95	114.13	109.98
25	B	607	CLA	O2A-CGA-CBA	3.95	123.88	111.83
25	B	605	CLA	CHD-C1D-ND	-3.95	119.24	124.80
25	b	607	CLA	O2A-CGA-CBA	3.95	123.87	111.83
25	b	605	CLA	CHD-C1D-ND	-3.95	119.25	124.80
35	E	104	HEM	CHA-C4D-ND	3.95	129.25	124.37
27	Z	101	BCR	C38-C26-C25	-3.94	120.18	124.48
27	z	101	BCR	C38-C26-C25	-3.94	120.18	124.48
25	B	613	CLA	C2B-C1B-NB	3.94	114.41	110.33
25	b	613	CLA	C2B-C1B-NB	3.94	114.41	110.33
25	B	611	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
25	b	611	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
25	B	602	CLA	CHD-C1D-ND	-3.94	119.26	124.80
25	b	602	CLA	CHD-C1D-ND	-3.94	119.26	124.80
28	b	621	LMG	O7-C10-C11	3.93	119.98	111.48
25	c	509	CLA	C4A-NA-C1A	3.93	108.47	106.68
25	c	502	CLA	O2D-CGD-O1D	-3.92	116.21	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	615	CLA	O2A-C1-C2	3.91	123.17	108.11
25	b	615	CLA	O2A-C1-C2	3.91	123.17	108.11
25	C	504	CLA	O2A-CGA-CBA	3.91	123.77	111.83
28	B	621	LMG	O7-C10-C11	3.91	119.95	111.48
25	c	504	CLA	O2A-CGA-CBA	3.91	123.75	111.83
30	A	413	SQD	O9-S-O7	-3.91	101.12	113.82
30	a	413	SQD	O9-S-O7	-3.91	101.12	113.82
25	A	406	CLA	C2B-C1B-NB	3.91	114.38	110.33
31	c	524	LMT	O5B-C5B-C4B	3.90	116.73	109.70
25	C	502	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
25	a	406	CLA	O2A-CGA-CBA	3.89	123.71	111.83
31	C	524	LMT	O5B-C5B-C4B	3.89	116.71	109.70
30	A	412	SQD	C4-C3-C2	3.89	117.66	110.83
25	A	406	CLA	O2A-CGA-CBA	3.89	123.69	111.83
25	C	512	CLA	C1-C2-C3	-3.89	119.83	126.20
25	c	512	CLA	C1-C2-C3	-3.88	119.84	126.20
25	D	401	CLA	C2B-C1B-NB	3.88	114.35	110.33
35	V	201	HEM	C3B-C4B-NB	-3.88	106.68	109.47
35	v	201	HEM	C3B-C4B-NB	-3.88	106.68	109.47
25	C	506	CLA	C2D-C1D-ND	3.87	113.96	110.13
25	c	506	CLA	C2D-C1D-ND	3.87	113.96	110.13
30	a	412	SQD	C4-C3-C2	3.87	117.63	110.83
25	a	406	CLA	C2B-C1B-NB	3.86	114.33	110.33
25	d	401	CLA	C2B-C1B-NB	3.86	114.33	110.33
25	C	506	CLA	O2A-CGA-CBA	3.86	123.60	111.83
25	c	506	CLA	O2A-CGA-CBA	3.86	123.60	111.83
25	c	505	CLA	C2B-C1B-NB	3.85	114.32	110.33
25	a	405	CLA	CAC-C3C-C4C	3.85	129.79	124.79
25	b	611	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
34	H	104	DGD	O2G-C1B-C2B	3.83	119.77	111.48
25	A	405	CLA	CAC-C3C-C4C	3.83	129.77	124.79
25	B	604	CLA	C3B-C2B-C1B	-3.83	102.66	107.17
25	b	604	CLA	C3B-C2B-C1B	-3.83	102.66	107.17
30	f	102	SQD	O9-S-C6	3.82	112.46	106.76
25	B	612	CLA	O2A-C1-C2	3.82	122.81	108.11
25	B	614	CLA	CMC-C2C-C1C	3.82	131.00	125.03
25	b	614	CLA	CMC-C2C-C1C	3.82	131.00	125.03
25	c	505	CLA	CHD-C1D-ND	-3.82	119.43	124.80
25	C	505	CLA	CHD-C1D-ND	-3.82	119.43	124.80
25	C	505	CLA	C2B-C1B-NB	3.81	114.28	110.33
34	h	104	DGD	O2G-C1B-C2B	3.81	119.73	111.48
25	b	612	CLA	O2A-C1-C2	3.81	122.77	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	611	CLA	C1C-C2C-C3C	-3.81	102.98	106.98
27	k	102	BCR	C24-C23-C22	-3.80	120.61	126.23
25	C	506	CLA	CMD-C2D-C3D	-3.80	118.98	127.69
30	F	102	SQD	O9-S-C6	3.79	112.42	106.76
25	c	506	CLA	CMD-C2D-C3D	-3.79	119.00	127.69
25	b	604	CLA	O2A-C1-C2	3.79	122.69	108.11
25	d	404	CLA	O2A-CGA-CBA	3.79	123.39	111.83
25	B	606	CLA	C2B-C1B-NB	3.79	114.25	110.33
25	b	606	CLA	C2B-C1B-NB	3.79	114.25	110.33
25	D	404	CLA	O2A-CGA-CBA	3.79	123.38	111.83
27	K	102	BCR	C24-C23-C22	-3.78	120.64	126.23
25	B	604	CLA	O2A-C1-C2	3.78	122.67	108.11
36	h	101	RRX	C16-C15-C14	3.78	131.26	123.52
25	B	607	CLA	C2B-C1B-NB	3.78	114.25	110.33
25	b	607	CLA	C2B-C1B-NB	3.78	114.25	110.33
25	D	403	CLA	CHD-C1D-ND	-3.78	119.49	124.80
25	d	403	CLA	CHD-C1D-ND	-3.78	119.49	124.80
36	H	101	RRX	C16-C15-C14	3.78	131.25	123.52
25	A	408	CLA	C2B-C1B-NB	3.77	114.23	110.33
25	a	408	CLA	C2B-C1B-NB	3.77	114.23	110.33
31	K	105	LMT	O5B-C5B-C4B	3.77	116.49	109.70
30	a	413	SQD	O7-S-C6	3.75	112.36	106.76
33	E	102	LHG	O7-C7-C8	3.75	119.59	111.48
33	e	102	LHG	O7-C7-C8	3.75	119.59	111.48
31	k	105	LMT	O5B-C5B-C4B	3.75	116.45	109.70
30	A	413	SQD	O7-S-C6	3.75	112.35	106.76
25	B	603	CLA	C4D-C3D-CAD	3.75	112.17	108.11
25	C	511	CLA	C1-C2-C3	-3.75	120.06	126.20
25	c	511	CLA	C1-C2-C3	-3.75	120.06	126.20
25	D	403	CLA	O2A-C1-C2	3.74	122.50	108.11
25	d	403	CLA	O2A-C1-C2	3.74	122.50	108.11
25	C	508	CLA	O2A-C1-C2	3.74	122.50	108.11
25	c	503	CLA	C1-C2-C3	-3.74	120.07	126.20
25	c	508	CLA	O2A-C1-C2	3.74	122.49	108.11
29	A	411	PL9	C7-C3-C2	-3.73	119.00	123.39
29	a	411	PL9	C7-C3-C2	-3.73	119.00	123.39
30	F	102	SQD	O5-C5-C4	3.73	116.42	109.70
30	f	102	SQD	O5-C5-C4	3.72	116.41	109.70
25	C	503	CLA	C1-C2-C3	-3.72	120.10	126.20
25	B	614	CLA	C4D-C3D-CAD	3.72	112.14	108.11
25	b	614	CLA	C4D-C3D-CAD	3.72	112.14	108.11
25	C	510	CLA	O2A-CGA-CBA	3.72	123.17	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	510	CLA	O2A-CGA-CBA	3.72	123.17	111.83
25	C	506	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
25	c	506	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
25	b	604	CLA	O2A-CGA-CBA	3.72	123.17	111.83
25	b	603	CLA	C4D-C3D-CAD	3.72	112.14	108.11
25	B	611	CLA	O2A-CGA-CBA	3.71	123.14	111.83
25	b	611	CLA	O2A-CGA-CBA	3.71	123.14	111.83
30	H	103	SQD	O47-C7-C8	3.70	119.50	111.48
30	h	103	SQD	O47-C7-C8	3.70	119.50	111.48
25	C	511	CLA	CHD-C1D-ND	-3.70	119.59	124.80
25	c	511	CLA	CHD-C1D-ND	-3.70	119.59	124.80
25	B	604	CLA	O2A-CGA-CBA	3.70	123.12	111.83
25	b	604	CLA	C4D-C3D-CAD	3.70	112.13	108.11
25	C	506	CLA	C2B-C1B-NB	3.70	114.16	110.33
25	c	506	CLA	C2B-C1B-NB	3.70	114.16	110.33
25	B	601	CLA	C2B-C1B-NB	3.70	114.16	110.33
25	b	603	CLA	C4-C3-C5	3.70	121.64	115.23
25	D	401	CLA	O2A-CGA-CBA	3.69	123.10	111.83
25	d	401	CLA	O2A-CGA-CBA	3.69	123.10	111.83
25	C	507	CLA	O2A-CGA-CBA	3.69	123.09	111.83
25	b	601	CLA	C2B-C1B-NB	3.69	114.15	110.33
25	B	612	CLA	C3C-C4C-NC	3.69	115.15	110.43
25	b	612	CLA	C3C-C4C-NC	3.69	115.15	110.43
25	d	403	CLA	O2D-CGD-CBD	3.68	117.67	111.23
25	c	507	CLA	O2A-CGA-CBA	3.68	123.06	111.83
25	B	603	CLA	C4-C3-C5	3.68	121.61	115.23
25	A	405	CLA	CAA-C2A-C3A	-3.68	103.06	113.00
25	B	612	CLA	O2A-CGA-CBA	3.68	123.05	111.83
25	b	606	CLA	CHD-C1D-ND	-3.68	119.63	124.80
25	B	604	CLA	C1D-ND-C4D	-3.68	103.73	106.31
25	b	604	CLA	C1D-ND-C4D	-3.68	103.73	106.31
25	B	604	CLA	C4D-C3D-CAD	3.67	112.10	108.11
25	b	612	CLA	O2A-CGA-CBA	3.67	123.03	111.83
25	A	408	CLA	O2A-CGA-CBA	3.67	123.03	111.83
25	a	408	CLA	O2A-CGA-CBA	3.67	123.03	111.83
25	B	613	CLA	C1D-ND-C4D	-3.67	103.74	106.31
28	D	409	LMG	O7-C10-C11	3.67	119.42	111.48
28	d	409	LMG	O7-C10-C11	3.67	119.42	111.48
33	D	408	LHG	O7-C7-C8	3.67	119.41	111.48
25	B	613	CLA	CHD-C1D-ND	-3.67	119.64	124.80
33	d	408	LHG	O7-C7-C8	3.67	119.41	111.48
25	B	610	CLA	O2A-C1-C2	3.67	122.22	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	403	CLA	O2D-CGD-CBD	3.66	117.64	111.23
25	b	610	CLA	O2A-C1-C2	3.66	122.21	108.11
25	a	405	CLA	CAA-C2A-C3A	-3.66	103.10	113.00
25	b	613	CLA	CHD-C1D-ND	-3.66	119.65	124.80
25	b	613	CLA	C1D-ND-C4D	-3.66	103.75	106.31
25	C	504	CLA	CMA-C3A-C4A	3.65	121.58	111.77
25	B	606	CLA	CHD-C1D-ND	-3.65	119.67	124.80
25	C	512	CLA	C2B-C1B-NB	3.64	114.11	110.33
25	c	512	CLA	C2B-C1B-NB	3.64	114.11	110.33
25	c	504	CLA	CMA-C3A-C4A	3.64	121.57	111.77
30	a	412	SQD	O5-C1-C2	3.64	117.85	110.37
28	A	410	LMG	O7-C10-C11	3.64	119.35	111.48
30	A	412	SQD	O5-C1-C2	3.63	117.84	110.37
25	B	613	CLA	O2A-CGA-CBA	3.63	122.91	111.83
25	b	613	CLA	O2A-CGA-CBA	3.63	122.91	111.83
25	b	603	CLA	C3B-C2B-C1B	-3.63	102.89	107.17
27	Z	101	BCR	C15-C14-C13	-3.63	122.18	127.28
25	B	602	CLA	C2B-C1B-NB	3.62	114.08	110.33
25	b	602	CLA	C2B-C1B-NB	3.62	114.08	110.33
28	a	410	LMG	O7-C10-C11	3.62	119.31	111.48
25	C	504	CLA	C2B-C1B-NB	3.62	114.08	110.33
25	c	504	CLA	C2B-C1B-NB	3.62	114.08	110.33
25	b	606	CLA	O2A-CGA-CBA	3.61	122.86	111.83
25	B	606	CLA	O2A-CGA-CBA	3.61	122.84	111.83
25	B	603	CLA	C3B-C2B-C1B	-3.61	102.92	107.17
29	d	405	PL9	C7-C3-C2	-3.61	119.14	123.39
30	K	101	SQD	O47-C7-C8	3.61	119.29	111.48
30	k	101	SQD	O47-C7-C8	3.61	119.29	111.48
27	k	103	BCR	C36-C18-C17	-3.60	116.98	122.82
25	c	509	CLA	O2A-CGA-CBA	3.60	122.81	111.83
29	D	405	PL9	C7-C3-C2	-3.60	119.14	123.39
27	z	101	BCR	C15-C14-C13	-3.60	122.23	127.28
25	B	608	CLA	O2A-CGA-CBA	3.60	122.81	111.83
25	C	506	CLA	C1-C2-C3	-3.59	120.31	126.20
25	c	506	CLA	C1-C2-C3	-3.59	120.31	126.20
25	c	512	CLA	CHD-C1D-ND	-3.59	119.75	124.80
25	d	404	CLA	CAA-C2A-C3A	-3.59	103.29	113.00
27	K	103	BCR	C36-C18-C17	-3.59	117.00	122.82
25	C	510	CLA	C1D-ND-C4D	-3.59	103.79	106.31
25	c	510	CLA	C1D-ND-C4D	-3.59	103.79	106.31
25	D	404	CLA	CAA-C2A-C3A	-3.59	103.30	113.00
25	C	509	CLA	O2A-CGA-CBA	3.59	122.78	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	616	CLA	C2B-C1B-NB	3.59	114.05	110.33
25	b	616	CLA	C2B-C1B-NB	3.59	114.05	110.33
25	A	405	CLA	CMC-C2C-C1C	3.59	130.64	125.03
25	a	405	CLA	CMC-C2C-C1C	3.59	130.64	125.03
25	b	608	CLA	O2A-CGA-CBA	3.58	122.77	111.83
33	D	406	LHG	O7-C7-C8	3.58	119.23	111.48
25	C	512	CLA	CHD-C1D-ND	-3.58	119.77	124.80
25	a	405	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
33	d	406	LHG	O7-C7-C8	3.57	119.20	111.48
28	C	519	LMG	O7-C10-C11	3.56	119.18	111.48
25	A	405	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
25	D	401	CLA	CAA-C2A-C3A	-3.56	103.39	113.00
25	c	509	CLA	CAA-C2A-C3A	-3.56	103.39	113.00
25	C	509	CLA	CAA-C2A-C3A	-3.55	103.39	113.00
25	C	502	CLA	C2B-C1B-NB	3.55	114.01	110.33
25	c	502	CLA	C2B-C1B-NB	3.55	114.01	110.33
25	B	603	CLA	C1D-ND-C4D	-3.55	103.82	106.31
25	d	401	CLA	CAA-C2A-C3A	-3.55	103.41	113.00
28	c	519	LMG	O7-C10-C11	3.54	119.14	111.48
30	f	102	SQD	O47-C7-C8	3.54	119.14	111.48
25	B	614	CLA	C2B-C1B-NB	3.54	114.00	110.33
25	b	614	CLA	C2B-C1B-NB	3.54	114.00	110.33
25	c	511	CLA	C3B-C2B-C1B	-3.54	103.00	107.17
28	a	410	LMG	O8-C28-C29	3.54	122.62	111.83
30	F	102	SQD	O47-C7-C8	3.53	119.13	111.48
27	K	103	BCR	C19-C18-C17	3.53	124.56	119.01
27	k	103	BCR	C19-C18-C17	3.53	124.56	119.01
25	b	611	CLA	O1D-CGD-CBD	-3.53	117.56	124.52
36	H	101	RRX	C15-C16-C17	3.53	130.74	123.52
27	k	102	BCR	C36-C18-C19	-3.53	112.70	118.09
36	h	101	RRX	C15-C16-C17	3.53	130.74	123.52
25	B	615	CLA	CHD-C1D-ND	-3.53	119.84	124.80
28	A	410	LMG	O8-C28-C29	3.52	122.58	111.83
27	K	102	BCR	C36-C18-C19	-3.52	112.70	118.09
25	b	608	CLA	O2A-C1-C2	3.52	121.67	108.11
33	D	407	LHG	O7-C7-C8	3.52	119.10	111.48
25	B	605	CLA	CMC-C2C-C1C	3.52	130.53	125.03
25	b	605	CLA	CMC-C2C-C1C	3.52	130.53	125.03
25	B	605	CLA	C2B-C1B-NB	3.52	113.97	110.33
25	b	605	CLA	C2B-C1B-NB	3.52	113.97	110.33
25	A	406	CLA	CHD-C1D-ND	-3.52	119.85	124.80
33	d	407	LHG	O7-C7-C8	3.52	119.09	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	608	CLA	O2A-C1-C2	3.52	121.64	108.11
25	D	403	CLA	C4D-C3D-CAD	3.52	111.92	108.11
25	B	611	CLA	O1D-CGD-CBD	-3.51	117.59	124.52
25	b	615	CLA	CHD-C1D-ND	-3.51	119.86	124.80
25	d	403	CLA	O2A-CGA-CBA	3.51	122.54	111.83
25	d	403	CLA	C4D-C3D-CAD	3.51	111.92	108.11
25	C	511	CLA	C3B-C2B-C1B	-3.51	103.03	107.17
25	b	615	CLA	C2B-C1B-NB	3.51	113.96	110.33
25	D	403	CLA	O2A-CGA-CBA	3.51	122.52	111.83
25	b	603	CLA	C1D-ND-C4D	-3.50	103.85	106.31
25	C	513	CLA	C1-C2-C3	-3.50	121.10	126.76
25	B	615	CLA	C2B-C1B-NB	3.50	113.95	110.33
31	E	103	LMT	C3'-C4'-C5'	-3.50	103.18	110.93
25	a	406	CLA	CHD-C1D-ND	-3.50	119.88	124.80
25	A	405	CLA	C2B-C1B-NB	3.50	113.95	110.33
25	C	514	CLA	O2A-C1-C2	3.49	121.55	108.11
25	c	514	CLA	O2A-C1-C2	3.49	121.55	108.11
25	B	602	CLA	O2A-CGA-CBA	3.49	122.48	111.83
25	b	602	CLA	O2A-CGA-CBA	3.49	122.47	111.83
25	C	503	CLA	O2A-CGA-CBA	3.49	122.47	111.83
25	c	503	CLA	O2A-CGA-CBA	3.49	122.47	111.83
25	A	405	CLA	C4D-C3D-CAD	3.48	111.89	108.11
25	a	405	CLA	C4D-C3D-CAD	3.48	111.89	108.11
25	c	513	CLA	C1-C2-C3	-3.48	121.13	126.76
31	e	103	LMT	C3'-C4'-C5'	-3.48	103.23	110.93
25	B	610	CLA	C2B-C1B-NB	3.47	113.93	110.33
25	a	405	CLA	C2B-C1B-NB	3.47	113.93	110.33
26	D	402	PHO	C2B-C1B-NB	-3.47	106.92	109.43
26	d	402	PHO	C2B-C1B-NB	-3.47	106.92	109.43
25	b	610	CLA	C2B-C1B-NB	3.47	113.92	110.33
30	A	412	SQD	O9-S-C6	3.47	111.93	106.76
30	a	412	SQD	O9-S-C6	3.47	111.93	106.76
25	c	505	CLA	O2A-CGA-CBA	3.46	122.39	111.83
36	h	101	RRX	C34-C9-C10	-3.46	117.22	122.82
25	D	404	CLA	O2A-C1-C2	3.45	121.40	108.11
25	d	404	CLA	O2A-C1-C2	3.45	121.40	108.11
25	B	611	CLA	O2A-C1-C2	3.45	121.39	108.11
27	a	409	BCR	C38-C26-C25	-3.45	120.72	124.48
36	H	101	RRX	C34-C9-C10	-3.45	117.22	122.82
25	C	505	CLA	O2A-CGA-CBA	3.45	122.36	111.83
25	b	611	CLA	O2A-C1-C2	3.45	121.37	108.11
25	D	401	CLA	CHD-C1D-ND	-3.45	119.95	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	CLA	CHD-C1D-ND	-3.44	119.96	124.80
25	B	613	CLA	O2A-C1-C2	3.44	121.36	108.11
30	A	413	SQD	C45-O47-C7	3.44	126.03	117.80
25	C	506	CLA	O1D-CGD-CBD	-3.44	117.73	124.52
25	c	506	CLA	O1D-CGD-CBD	-3.44	117.73	124.52
30	a	413	SQD	C45-O47-C7	3.44	126.03	117.80
25	d	401	CLA	CHD-C1D-ND	-3.44	119.96	124.80
25	b	613	CLA	O2A-C1-C2	3.44	121.34	108.11
25	D	404	CLA	C1-C2-C3	-3.43	120.57	126.20
25	d	403	CLA	C4-C3-C5	3.43	121.18	115.23
25	D	403	CLA	C3D-C4D-ND	3.43	115.56	109.99
25	d	403	CLA	C3D-C4D-ND	3.43	115.56	109.99
25	b	608	CLA	C2B-C1B-NB	3.43	113.88	110.33
27	c	515	BCR	C7-C8-C9	-3.42	121.17	126.23
27	A	409	BCR	C38-C26-C25	-3.42	120.75	124.48
27	B	617	BCR	C33-C5-C6	-3.42	120.75	124.48
27	b	617	BCR	C33-C5-C6	-3.42	120.75	124.48
25	C	502	CLA	CHD-C1D-ND	-3.42	119.99	124.80
25	c	502	CLA	CHD-C1D-ND	-3.42	119.99	124.80
35	e	104	HEM	CHB-C1B-NB	3.42	128.59	124.37
25	B	616	CLA	O2A-C1-C2	3.42	121.25	108.11
25	D	404	CLA	CHD-C1D-ND	-3.42	120.00	124.80
25	b	606	CLA	CAA-C2A-C3A	-3.41	103.77	113.00
25	D	403	CLA	C4-C3-C5	3.41	121.15	115.23
25	d	404	CLA	C1-C2-C3	-3.41	120.60	126.20
27	C	515	BCR	C7-C8-C9	-3.41	121.19	126.23
34	C	516	DGD	O2G-C1B-C2B	3.41	118.86	111.48
25	b	616	CLA	O2A-C1-C2	3.41	121.24	108.11
34	c	516	DGD	O2G-C1B-C2B	3.41	118.86	111.48
25	B	606	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
25	B	606	CLA	C4A-NA-C1A	3.41	108.23	106.68
31	T	101	LMT	O1'-C1'-C2'	3.41	113.45	108.27
31	t	101	LMT	O1'-C1'-C2'	3.41	113.45	108.27
35	E	104	HEM	CHB-C1B-NB	3.40	128.57	124.37
25	B	609	CLA	O2A-C1-C2	3.40	121.18	108.11
25	b	609	CLA	O2A-C1-C2	3.39	121.16	108.11
25	b	606	CLA	C4A-NA-C1A	3.39	108.23	106.68
25	B	608	CLA	C2B-C1B-NB	3.39	113.84	110.33
25	c	505	CLA	C1-O2A-CGA	3.39	124.86	116.65
27	A	409	BCR	C7-C8-C9	-3.39	121.22	126.23
27	a	409	BCR	C7-C8-C9	-3.39	121.22	126.23
25	B	602	CLA	CAA-C2A-C3A	-3.39	103.85	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	602	CLA	CAA-C2A-C3A	-3.39	103.85	113.00
25	C	505	CLA	C1-O2A-CGA	3.39	124.85	116.65
25	B	614	CLA	O2A-CGA-CBA	3.38	122.15	111.83
25	b	608	CLA	CMC-C2C-C1C	3.38	130.32	125.03
25	B	608	CLA	CMC-C2C-C1C	3.38	130.32	125.03
36	H	101	RRX	C37-C22-C21	-3.38	117.34	122.82
28	h	105	LMG	O8-C28-C29	3.37	122.12	111.83
25	b	614	CLA	O2A-CGA-CBA	3.37	122.12	111.83
28	H	105	LMG	O8-C28-C29	3.37	122.11	111.83
36	h	101	RRX	C37-C22-C21	-3.37	117.36	122.82
25	C	508	CLA	O2A-CGA-CBA	3.37	122.11	111.83
25	c	508	CLA	O2A-CGA-CBA	3.37	122.11	111.83
25	C	511	CLA	C4D-C3D-CAD	3.37	111.77	108.11
25	B	602	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
25	b	602	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
33	d	407	LHG	C5-O7-C7	-3.36	109.76	117.80
25	C	509	CLA	CHD-C1D-ND	-3.35	120.08	124.80
25	c	509	CLA	CHD-C1D-ND	-3.35	120.08	124.80
25	B	601	CLA	O2A-CGA-CBA	3.35	124.59	114.00
25	b	601	CLA	O2A-CGA-CBA	3.35	124.59	114.00
25	C	507	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
25	c	507	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
33	D	407	LHG	C5-O7-C7	-3.34	109.80	117.80
25	c	511	CLA	C4D-C3D-CAD	3.33	111.73	108.11
25	c	512	CLA	CMA-C3A-C4A	3.33	120.72	111.77
25	C	508	CLA	CMB-C2B-C1B	3.33	130.48	125.42
25	c	508	CLA	CMB-C2B-C1B	3.33	130.48	125.42
30	A	413	SQD	O9-S-C6	3.33	111.72	106.76
25	B	607	CLA	CHD-C1D-ND	-3.32	120.12	124.80
25	b	607	CLA	CHD-C1D-ND	-3.32	120.12	124.80
25	C	512	CLA	CMA-C3A-C4A	3.32	120.70	111.77
31	c	522	LMT	C4'-C3'-C2'	3.32	116.66	110.83
25	A	405	CLA	CMD-C2D-C3D	-3.32	120.08	127.69
25	C	513	CLA	C2B-C1B-NB	3.31	113.76	110.33
25	c	513	CLA	C2B-C1B-NB	3.31	113.76	110.33
27	B	617	BCR	C19-C18-C17	3.31	124.22	119.01
31	c	525	LMT	O5'-C5'-C4'	3.31	115.67	109.70
31	C	522	LMT	C4'-C3'-C2'	3.31	116.64	110.83
25	a	405	CLA	CMD-C2D-C3D	-3.31	120.10	127.69
35	V	201	HEM	CHB-C1B-NB	3.31	128.46	124.37
35	v	201	HEM	CHB-C1B-NB	3.31	128.46	124.37
30	a	413	SQD	O9-S-C6	3.30	111.69	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	504	CLA	O2A-C1-C2	3.30	120.82	108.11
25	c	504	CLA	O2A-C1-C2	3.30	120.82	108.11
27	b	617	BCR	C19-C18-C17	3.30	124.20	119.01
27	k	103	BCR	C15-C14-C13	-3.29	122.66	127.28
31	C	525	LMT	O5'-C5'-C4'	3.29	115.62	109.70
25	b	605	CLA	C4-C3-C5	3.28	120.92	115.23
30	C	501	SQD	C4-C3-C2	3.28	116.59	110.83
30	c	501	SQD	C4-C3-C2	3.28	116.59	110.83
25	B	608	CLA	CMB-C2B-C3B	3.27	134.25	126.55
25	b	608	CLA	CMB-C2B-C3B	3.27	134.25	126.55
30	F	102	SQD	O6-C1-C2	3.27	113.24	108.27
27	K	103	BCR	C15-C14-C13	-3.27	122.70	127.28
27	b	619	BCR	C40-C30-C25	3.27	115.36	110.24
25	B	605	CLA	C4-C3-C5	3.26	120.89	115.23
33	E	102	LHG	C5-O7-C7	-3.26	109.98	117.80
33	e	102	LHG	C5-O7-C7	-3.26	109.98	117.80
33	B	628	LHG	O7-C7-C8	3.26	118.53	111.48
31	i	102	LMT	C3'-C4'-C5'	-3.26	104.33	110.23
25	a	408	CLA	CHD-C1D-ND	-3.25	120.22	124.80
33	b	628	LHG	O7-C7-C8	3.25	118.51	111.48
27	B	619	BCR	C40-C30-C25	3.25	115.34	110.24
30	f	102	SQD	O6-C1-C2	3.25	113.20	108.27
25	C	512	CLA	C4D-C3D-CAD	3.25	111.63	108.11
25	c	512	CLA	C4D-C3D-CAD	3.25	111.63	108.11
31	I	102	LMT	C3'-C4'-C5'	-3.24	104.35	110.23
25	A	408	CLA	CHD-C1D-ND	-3.24	120.24	124.80
25	B	605	CLA	C3D-C4D-ND	3.24	115.25	109.99
25	b	605	CLA	C3D-C4D-ND	3.23	115.24	109.99
27	k	102	BCR	C33-C5-C6	-3.23	120.96	124.48
25	C	504	CLA	CHD-C1D-ND	-3.23	120.26	124.80
25	c	504	CLA	CHD-C1D-ND	-3.23	120.26	124.80
35	e	104	HEM	C1B-NB-C4B	3.23	109.03	105.21
25	C	502	CLA	CMA-C3A-C4A	3.22	120.44	111.77
25	c	502	CLA	CMA-C3A-C4A	3.22	120.44	111.77
27	B	617	BCR	C34-C9-C8	3.22	123.01	118.09
25	C	511	CLA	O2A-C1-C2	3.22	120.50	108.11
25	c	511	CLA	O2A-C1-C2	3.22	120.50	108.11
25	D	404	CLA	C3D-C4D-ND	3.22	115.22	109.99
25	d	404	CLA	C3D-C4D-ND	3.22	115.22	109.99
25	B	613	CLA	C1-C2-C3	-3.22	120.92	126.20
31	X	103	LMT	O5'-C5'-C4'	3.22	115.50	109.70
31	x	103	LMT	O5'-C5'-C4'	3.22	115.50	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	104	HEM	C1B-NB-C4B	3.22	109.02	105.21
25	b	613	CLA	C1-C2-C3	-3.22	120.92	126.20
25	b	603	CLA	CAA-C2A-C3A	-3.22	104.31	113.00
25	b	601	CLA	CMC-C2C-C1C	3.21	130.06	125.03
25	D	403	CLA	C2B-C1B-NB	3.21	113.66	110.33
25	d	403	CLA	C2B-C1B-NB	3.21	113.66	110.33
25	B	601	CLA	CMC-C2C-C1C	3.20	130.04	125.03
25	B	603	CLA	CAA-C2A-C3A	-3.20	104.35	113.00
27	b	617	BCR	C34-C9-C8	3.20	122.97	118.09
25	B	614	CLA	O2A-C1-C2	3.19	120.37	108.11
25	b	612	CLA	C4D-C3D-CAD	3.19	111.57	108.11
27	K	102	BCR	C33-C5-C6	-3.19	121.01	124.48
25	B	614	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
25	b	614	CLA	O2A-C1-C2	3.18	120.34	108.11
25	c	513	CLA	C3C-C4C-NC	3.18	114.50	110.43
25	b	614	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
25	d	403	CLA	CMC-C2C-C1C	3.18	130.00	125.03
25	c	513	CLA	CMC-C2C-C1C	3.17	129.99	125.03
25	D	403	CLA	CMC-C2C-C1C	3.17	129.99	125.03
25	c	503	CLA	C2B-C1B-NB	3.17	113.61	110.33
25	C	513	CLA	C3C-C4C-NC	3.16	114.48	110.43
27	a	409	BCR	C33-C5-C6	-3.16	121.03	124.48
30	K	101	SQD	O6-C1-C2	3.16	113.08	108.27
30	k	101	SQD	O6-C1-C2	3.16	113.08	108.27
25	c	508	CLA	C1-O2A-CGA	3.16	124.30	116.65
25	B	610	CLA	CAA-C2A-C3A	-3.16	104.46	113.00
25	b	610	CLA	CAA-C2A-C3A	-3.16	104.46	113.00
25	C	508	CLA	C1-O2A-CGA	3.16	124.30	116.65
25	C	513	CLA	CMC-C2C-C1C	3.16	129.97	125.03
25	B	612	CLA	C4D-C3D-CAD	3.15	111.53	108.11
25	b	616	CLA	CAC-C3C-C4C	3.15	128.89	124.79
25	b	608	CLA	C1-C2-C3	-3.15	121.04	126.20
27	A	409	BCR	C33-C5-C6	-3.14	121.05	124.48
25	B	608	CLA	C1-C2-C3	-3.14	121.05	126.20
25	B	616	CLA	C1C-C2C-C3C	-3.14	103.68	106.98
25	b	616	CLA	C1C-C2C-C3C	-3.14	103.68	106.98
25	B	616	CLA	CAC-C3C-C4C	3.14	128.87	124.79
25	A	408	CLA	CMC-C2C-C1C	3.14	129.94	125.03
25	B	604	CLA	C1-C2-C3	-3.13	121.06	126.20
25	B	607	CLA	O2A-C1-C2	3.13	120.16	108.11
25	b	607	CLA	O2A-C1-C2	3.13	120.16	108.11
27	F	101	BCR	C3-C4-C5	-3.13	108.47	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	408	CLA	CMC-C2C-C1C	3.13	129.93	125.03
25	C	511	CLA	CMC-C2C-C1C	3.13	129.93	125.03
25	c	511	CLA	CMC-C2C-C1C	3.13	129.93	125.03
25	B	601	CLA	CHD-C1D-ND	-3.13	120.40	124.80
25	b	601	CLA	CHD-C1D-ND	-3.13	120.40	124.80
25	C	506	CLA	CHD-C1D-ND	-3.13	120.40	124.80
25	c	506	CLA	CHD-C1D-ND	-3.13	120.40	124.80
27	F	101	BCR	C19-C18-C17	3.12	123.92	119.01
27	f	101	BCR	C19-C18-C17	3.12	123.92	119.01
25	b	604	CLA	C1-C2-C3	-3.12	121.08	126.20
25	b	615	CLA	C3C-C4C-NC	3.12	114.42	110.43
25	C	503	CLA	C2B-C1B-NB	3.12	113.56	110.33
27	f	101	BCR	C3-C4-C5	-3.12	108.50	114.06
25	c	511	CLA	CMD-C2D-C3D	-3.10	120.57	127.69
27	K	102	BCR	C15-C14-C13	-3.10	122.93	127.28
27	k	102	BCR	C15-C14-C13	-3.10	122.93	127.28
25	B	615	CLA	C3C-C4C-NC	3.09	114.39	110.43
25	C	511	CLA	CMD-C2D-C3D	-3.09	120.59	127.69
25	A	408	CLA	C3D-C4D-ND	3.09	115.02	109.99
25	b	616	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
26	A	407	PHO	C3B-C4B-NB	-3.09	105.45	107.46
25	B	616	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
25	A	405	CLA	CHD-C1D-ND	-3.09	120.45	124.80
25	a	405	CLA	CHD-C1D-ND	-3.09	120.45	124.80
25	a	406	CLA	O2A-C1-C2	3.09	120.00	108.11
25	b	610	CLA	C3C-C4C-NC	3.09	114.39	110.43
30	A	413	SQD	C44-O6-C1	3.09	120.41	113.80
30	a	413	SQD	C44-O6-C1	3.09	120.41	113.80
30	f	102	SQD	O7-S-C6	3.09	111.36	106.76
25	b	611	CLA	C1-C2-C3	-3.09	121.14	126.20
25	A	406	CLA	O2A-C1-C2	3.08	119.97	108.11
25	a	408	CLA	C3D-C4D-ND	3.08	114.99	109.99
30	F	102	SQD	O7-S-C6	3.08	111.35	106.76
25	C	510	CLA	CHD-C1D-ND	-3.08	120.47	124.80
25	c	510	CLA	CHD-C1D-ND	-3.08	120.47	124.80
27	Z	101	BCR	C19-C18-C17	3.08	123.85	119.01
27	z	101	BCR	C19-C18-C17	3.08	123.85	119.01
25	B	610	CLA	C3C-C4C-NC	3.07	114.36	110.43
28	H	105	LMG	C8-O7-C10	-3.07	110.44	117.80
28	h	105	LMG	C8-O7-C10	-3.07	110.45	117.80
25	c	507	CLA	CAA-C2A-C3A	-3.07	104.70	113.00
26	D	402	PHO	CBC-CAC-C3C	3.07	117.27	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	402	PHO	CBC-CAC-C3C	3.07	117.27	112.87
25	b	612	CLA	C3D-C4D-ND	3.07	114.98	109.99
25	C	507	CLA	CAA-C2A-C3A	-3.07	104.71	113.00
25	b	615	CLA	O2A-CGA-CBA	3.06	121.18	111.83
25	B	611	CLA	C1-C2-C3	-3.06	121.18	126.20
25	B	615	CLA	O2A-CGA-CBA	3.06	121.18	111.83
25	b	606	CLA	C4-C3-C5	3.06	120.54	115.23
25	B	612	CLA	C3D-C4D-ND	3.06	114.96	109.99
30	H	103	SQD	C44-O6-C1	3.06	120.36	113.80
27	b	617	BCR	C24-C23-C22	-3.06	121.71	126.23
25	C	505	CLA	CAC-C3C-C4C	3.06	128.76	124.79
26	a	407	PHO	C3B-C4B-NB	-3.05	105.47	107.46
27	b	618	BCR	C7-C8-C9	-3.05	121.72	126.23
25	c	505	CLA	CAC-C3C-C4C	3.05	128.76	124.79
25	B	606	CLA	C4-C3-C5	3.05	120.53	115.23
25	B	614	CLA	C1-O2A-CGA	3.05	124.03	116.65
27	B	617	BCR	C24-C23-C22	-3.05	121.72	126.23
25	c	509	CLA	C3D-C4D-ND	3.05	114.94	109.99
25	C	506	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
25	c	506	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
25	b	605	CLA	C4D-C3D-CAD	3.04	111.41	108.11
30	h	103	SQD	C44-O6-C1	3.04	120.31	113.80
25	B	603	CLA	O2A-C1-C2	3.04	119.81	108.11
25	b	603	CLA	O2A-C1-C2	3.04	119.81	108.11
25	b	614	CLA	C1-O2A-CGA	3.04	124.00	116.65
25	D	401	CLA	O2A-C1-C2	3.04	119.79	108.11
25	d	401	CLA	O2A-C1-C2	3.04	119.79	108.11
27	f	101	BCR	C38-C26-C27	3.03	120.07	113.60
25	b	604	CLA	C4-C3-C5	3.03	120.49	115.23
25	b	608	CLA	C3D-C4D-ND	3.03	114.91	109.99
25	c	502	CLA	O2A-C1-C2	3.03	119.77	108.11
31	D	410	LMT	O5'-C5'-C4'	3.03	115.16	109.70
31	d	410	LMT	O5'-C5'-C4'	3.03	115.16	109.70
27	C	515	BCR	C38-C26-C25	-3.03	121.18	124.48
25	B	604	CLA	C4-C3-C5	3.03	120.48	115.23
35	V	201	HEM	CHA-C4D-ND	3.03	128.11	124.37
35	v	201	HEM	CHA-C4D-ND	3.03	128.11	124.37
25	B	604	CLA	O1D-CGD-CBD	-3.03	118.55	124.52
27	B	618	BCR	C7-C8-C9	-3.02	121.76	126.23
25	C	502	CLA	O2A-C1-C2	3.02	119.74	108.11
25	C	502	CLA	OBD-CAD-C3D	-3.02	121.35	128.42
25	C	507	CLA	CAC-C3C-C4C	3.02	128.72	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	509	CLA	C3D-C4D-ND	3.02	114.90	109.99
25	c	502	CLA	OBD-CAD-C3D	-3.02	121.36	128.42
27	F	101	BCR	C38-C26-C27	3.02	120.03	113.60
25	C	506	CLA	C3D-C4D-ND	3.01	114.89	109.99
25	c	506	CLA	C3D-C4D-ND	3.01	114.89	109.99
25	b	616	CLA	C1-C2-C3	-3.01	121.26	126.20
25	B	605	CLA	C4D-C3D-CAD	3.01	111.38	108.11
25	c	514	CLA	CAA-C2A-C3A	-3.01	104.87	113.00
25	B	608	CLA	C3D-C4D-ND	3.01	114.88	109.99
25	b	604	CLA	O1D-CGD-CBD	-3.01	118.59	124.52
27	A	409	BCR	C19-C18-C17	3.00	123.73	119.01
27	a	409	BCR	C19-C18-C17	3.00	123.73	119.01
25	B	609	CLA	CMC-C2C-C1C	3.00	129.73	125.03
25	b	609	CLA	CMC-C2C-C1C	3.00	129.73	125.03
25	D	401	CLA	C1-C2-C3	-3.00	121.28	126.20
25	d	401	CLA	C1-C2-C3	-3.00	121.28	126.20
25	B	616	CLA	C1-C2-C3	-3.00	121.29	126.20
25	c	507	CLA	CAC-C3C-C4C	3.00	128.69	124.79
25	C	514	CLA	CAA-C2A-C3A	-3.00	104.91	113.00
25	C	508	CLA	C4-C3-C5	2.99	120.42	115.23
25	c	508	CLA	C4-C3-C5	2.99	120.42	115.23
27	c	515	BCR	C38-C26-C25	-2.99	121.22	124.48
25	C	509	CLA	CMB-C2B-C3B	2.99	133.58	126.55
25	c	509	CLA	CMB-C2B-C3B	2.99	133.58	126.55
25	c	507	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
30	A	413	SQD	O6-C1-C2	2.98	112.81	108.27
30	a	413	SQD	O6-C1-C2	2.98	112.81	108.27
28	A	414	LMG	O8-C28-C29	2.98	120.92	111.83
28	a	414	LMG	O8-C28-C29	2.98	120.92	111.83
31	C	522	LMT	O5'-C5'-C4'	2.98	115.06	109.70
31	c	522	LMT	O5'-C5'-C4'	2.98	115.06	109.70
25	C	507	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
25	C	510	CLA	CMC-C2C-C1C	2.97	129.68	125.03
25	c	510	CLA	CMC-C2C-C1C	2.97	129.68	125.03
25	c	510	CLA	CED-O2D-CGD	2.97	122.65	115.92
25	a	406	CLA	CMA-C3A-C4A	2.96	119.74	111.77
25	A	406	CLA	CMA-C3A-C4A	2.96	119.74	111.77
31	B	625	LMT	O1B-C4'-C3'	2.96	114.76	107.23
31	b	625	LMT	O1B-C4'-C3'	2.96	114.76	107.23
25	C	504	CLA	C3C-C4C-NC	2.96	114.22	110.43
25	c	504	CLA	C3C-C4C-NC	2.96	114.22	110.43
25	B	610	CLA	CHD-C1D-ND	-2.96	120.64	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	610	CLA	CHD-C1D-ND	-2.96	120.64	124.80
25	C	510	CLA	CED-O2D-CGD	2.95	122.62	115.92
25	B	615	CLA	CAC-C3C-C4C	2.95	128.63	124.79
25	b	615	CLA	CAC-C3C-C4C	2.95	128.63	124.79
25	C	503	CLA	CHD-C1D-ND	-2.95	120.65	124.80
25	B	601	CLA	C4D-C3D-CAD	2.95	111.31	108.11
25	A	408	CLA	C4-C3-C5	2.94	120.34	115.23
25	a	408	CLA	C4-C3-C5	2.94	120.34	115.23
25	B	602	CLA	C3D-C4D-ND	2.94	114.77	109.99
25	D	401	CLA	C3D-C4D-ND	2.94	114.77	109.99
25	d	401	CLA	C3D-C4D-ND	2.94	114.77	109.99
25	b	612	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
25	c	510	CLA	O2A-C1-C2	2.94	119.42	108.11
25	C	510	CLA	O2A-C1-C2	2.94	119.42	108.11
25	A	406	CLA	C4D-C3D-CAD	2.94	111.30	108.11
25	b	605	CLA	O2A-CGA-CBA	2.94	120.80	111.83
25	a	406	CLA	CBC-CAC-C3C	-2.94	104.46	112.42
25	b	602	CLA	C3D-C4D-ND	2.93	114.76	109.99
25	c	508	CLA	C4D-C3D-CAD	2.93	111.29	108.11
25	C	502	CLA	CMC-C2C-C1C	2.93	129.62	125.03
25	c	502	CLA	CMC-C2C-C1C	2.93	129.62	125.03
25	A	406	CLA	CBC-CAC-C3C	-2.93	104.47	112.42
31	x	101	LMT	C3'-C4'-C5'	-2.93	104.93	110.23
25	B	605	CLA	O2A-CGA-CBA	2.92	120.75	111.83
25	c	503	CLA	CHD-C1D-ND	-2.92	120.69	124.80
35	v	201	HEM	CHD-C1D-C2D	-2.92	120.42	125.03
28	C	523	LMG	O8-C28-C29	2.92	120.74	111.83
28	c	523	LMG	O8-C28-C29	2.92	120.74	111.83
27	k	103	BCR	C37-C22-C21	-2.92	118.08	122.82
25	C	508	CLA	C4D-C3D-CAD	2.92	111.27	108.11
31	m	102	LMT	C3'-C4'-C5'	-2.92	104.95	110.23
31	X	101	LMT	C3'-C4'-C5'	-2.91	104.95	110.23
35	V	201	HEM	CHD-C1D-C2D	-2.91	120.43	125.03
25	b	601	CLA	C4D-C3D-CAD	2.91	111.27	108.11
25	a	406	CLA	C4D-C3D-CAD	2.91	111.27	108.11
28	c	519	LMG	O8-C28-C29	2.91	120.71	111.83
28	C	519	LMG	O8-C28-C29	2.91	120.71	111.83
27	K	103	BCR	C37-C22-C21	-2.91	118.11	122.82
25	B	612	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
25	C	503	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
31	M	102	LMT	C3'-C4'-C5'	-2.90	104.97	110.23
25	c	514	CLA	CMB-C2B-C3B	2.90	133.37	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	101	RRX	C35-C13-C14	-2.90	118.12	122.82
25	c	503	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
25	C	514	CLA	CMB-C2B-C3B	2.89	133.35	126.55
30	A	412	SQD	O47-C7-C8	2.89	117.73	111.48
25	b	610	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
36	h	101	RRX	C35-C13-C14	-2.89	118.14	122.82
26	A	407	PHO	CMB-C2B-C3B	2.89	130.45	124.68
26	a	407	PHO	CMB-C2B-C3B	2.89	130.45	124.68
25	d	404	CLA	CMC-C2C-C1C	2.89	129.55	125.03
27	Z	101	BCR	C36-C18-C17	-2.89	118.14	122.82
25	B	610	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
25	c	502	CLA	C1-C2-C3	-2.88	121.47	126.20
30	a	412	SQD	O47-C7-C8	2.88	117.72	111.48
25	c	512	CLA	C3D-C4D-ND	2.88	114.67	109.99
25	B	601	CLA	C3C-C4C-NC	2.88	114.12	110.43
25	b	601	CLA	C3C-C4C-NC	2.88	114.12	110.43
25	B	615	CLA	CMC-C2C-C1C	2.88	129.53	125.03
25	b	615	CLA	CMC-C2C-C1C	2.88	129.53	125.03
25	C	507	CLA	CHD-C1D-ND	-2.88	120.75	124.80
25	c	507	CLA	CHD-C1D-ND	-2.88	120.75	124.80
34	C	517	DGD	O1G-C1A-C2A	2.88	120.61	111.83
30	H	103	SQD	O8-S-C6	2.88	111.53	105.97
30	h	103	SQD	O8-S-C6	2.88	111.53	105.97
25	C	502	CLA	C1-C2-C3	-2.88	121.49	126.20
27	z	101	BCR	C36-C18-C17	-2.87	118.17	122.82
25	C	508	CLA	CHD-C1D-ND	-2.87	120.77	124.80
25	c	508	CLA	CHD-C1D-ND	-2.87	120.77	124.80
25	B	613	CLA	CMC-C2C-C1C	2.87	129.52	125.03
25	b	613	CLA	CMC-C2C-C1C	2.87	129.52	125.03
34	c	517	DGD	O1G-C1A-C2A	2.87	120.58	111.83
25	d	403	CLA	CAA-C2A-C3A	-2.87	105.25	113.00
25	B	611	CLA	C3D-C4D-ND	2.87	114.64	109.99
25	b	611	CLA	C3D-C4D-ND	2.87	114.64	109.99
25	a	408	CLA	O2A-C1-C2	2.86	119.13	108.11
25	D	404	CLA	CMC-C2C-C1C	2.86	129.51	125.03
30	K	101	SQD	C44-O6-C1	2.86	119.94	113.80
30	k	101	SQD	C44-O6-C1	2.86	119.94	113.80
25	A	408	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
25	a	408	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
31	X	103	LMT	C3'-C4'-C5'	-2.86	105.04	110.23
31	x	103	LMT	C3'-C4'-C5'	-2.86	105.04	110.23
25	D	403	CLA	CAA-C2A-C3A	-2.86	105.27	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	512	CLA	C3D-C4D-ND	2.86	114.63	109.99
31	C	524	LMT	C3'-C4'-C5'	-2.86	104.60	110.93
25	B	616	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
30	A	412	SQD	C1-C2-C3	2.86	116.02	110.01
25	A	408	CLA	O2A-C1-C2	2.86	119.09	108.11
27	F	101	BCR	C40-C30-C25	-2.85	105.77	110.24
30	a	412	SQD	C1-C2-C3	2.85	116.01	110.01
25	A	408	CLA	CMA-C3A-C4A	2.85	119.44	111.77
28	H	105	LMG	C1-O6-C5	2.85	119.29	113.72
28	h	105	LMG	C1-O6-C5	2.85	119.29	113.72
30	F	102	SQD	C44-O6-C1	2.85	119.90	113.80
31	e	103	LMT	C4B-C3B-C2B	2.85	115.83	110.83
25	B	614	CLA	CHD-C1D-ND	-2.84	120.80	124.80
31	c	524	LMT	C3'-C4'-C5'	-2.84	104.63	110.93
25	B	608	CLA	CMA-C3A-C4A	2.84	119.42	111.77
25	b	608	CLA	CMA-C3A-C4A	2.84	119.42	111.77
25	b	616	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
25	C	508	CLA	C1D-ND-C4D	-2.84	104.32	106.31
25	c	508	CLA	C1D-ND-C4D	-2.84	104.32	106.31
25	b	614	CLA	C4-C3-C5	2.84	120.16	115.23
25	a	408	CLA	CMA-C3A-C4A	2.84	119.41	111.77
25	b	605	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
36	H	101	RRX	C36-C18-C17	-2.84	118.22	122.82
31	E	103	LMT	C4B-C3B-C2B	2.84	115.81	110.83
25	C	507	CLA	CMC-C2C-C3C	2.84	133.82	126.15
25	c	507	CLA	CMC-C2C-C3C	2.84	133.82	126.15
25	b	612	CLA	C1-C2-C3	-2.83	121.55	126.20
25	b	614	CLA	CHD-C1D-ND	-2.83	120.81	124.80
25	B	605	CLA	CAA-C2A-C3A	-2.83	105.34	113.00
27	b	618	BCR	C15-C14-C13	-2.83	123.31	127.28
30	f	102	SQD	C44-O6-C1	2.83	119.87	113.80
27	B	618	BCR	C15-C14-C13	-2.83	123.31	127.28
27	F	101	BCR	C36-C18-C17	-2.83	118.23	122.82
27	f	101	BCR	C36-C18-C17	-2.83	118.23	122.82
27	f	101	BCR	C40-C30-C25	-2.83	105.81	110.24
34	H	104	DGD	O1G-C1A-C2A	2.82	120.45	111.83
34	h	104	DGD	O1G-C1A-C2A	2.82	120.45	111.83
25	C	508	CLA	CBC-CAC-C3C	-2.82	104.77	112.42
25	c	508	CLA	CBC-CAC-C3C	-2.82	104.77	112.42
36	h	101	RRX	C36-C18-C17	-2.82	118.24	122.82
30	h	103	SQD	O48-C23-C24	2.82	120.44	111.83
25	B	614	CLA	C4-C3-C5	2.82	120.12	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	612	CLA	C1-C2-C3	-2.82	121.58	126.20
25	a	408	CLA	C1-O2A-CGA	2.82	123.47	116.65
28	C	523	LMG	C8-O7-C10	-2.81	111.07	117.80
30	h	103	SQD	C1-O5-C5	2.81	119.21	113.72
28	c	523	LMG	C8-O7-C10	-2.81	111.07	117.80
30	H	103	SQD	O48-C23-C24	2.81	120.40	111.83
25	B	616	CLA	CAA-C2A-C3A	-2.81	105.41	113.00
25	C	502	CLA	CAA-C2A-C3A	-2.81	105.42	113.00
25	c	502	CLA	CAA-C2A-C3A	-2.81	105.42	113.00
25	B	614	CLA	C3C-C4C-NC	2.80	114.02	110.43
25	C	512	CLA	C3C-C4C-NC	2.80	114.02	110.43
25	b	614	CLA	C3C-C4C-NC	2.80	114.02	110.43
25	c	512	CLA	C3C-C4C-NC	2.80	114.02	110.43
25	A	408	CLA	C1-O2A-CGA	2.80	123.44	116.65
25	B	607	CLA	CMA-C3A-C4A	2.80	119.31	111.77
25	b	607	CLA	CMA-C3A-C4A	2.80	119.31	111.77
25	C	514	CLA	CHD-C1D-ND	-2.80	120.86	124.80
30	H	103	SQD	C1-O5-C5	2.80	119.19	113.72
25	C	502	CLA	C4D-C3D-CAD	2.80	111.15	108.11
25	c	502	CLA	C4D-C3D-CAD	2.80	111.15	108.11
25	c	514	CLA	C3D-C4D-ND	2.80	114.53	109.99
25	B	611	CLA	C2B-C1B-NB	2.79	113.22	110.33
25	b	611	CLA	C2B-C1B-NB	2.79	113.22	110.33
25	b	616	CLA	CAA-C2A-C3A	-2.79	105.45	113.00
29	D	405	PL9	C7-C8-C9	-2.79	122.02	126.83
29	d	405	PL9	C7-C8-C9	-2.79	122.02	126.83
25	C	514	CLA	C3C-C4C-NC	2.79	114.00	110.43
25	c	514	CLA	C3C-C4C-NC	2.79	114.00	110.43
25	B	609	CLA	C2B-C1B-NB	2.79	113.22	110.33
31	e	103	LMT	O5'-C1'-C2'	2.79	116.10	110.37
25	B	601	CLA	CMA-C3A-C4A	2.79	119.27	111.77
27	K	102	BCR	C19-C18-C17	2.79	123.39	119.01
25	b	601	CLA	CMA-C3A-C4A	2.79	119.27	111.77
25	C	511	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
25	c	511	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
33	D	407	LHG	O8-C23-C24	2.78	120.32	111.83
25	C	514	CLA	C3D-C4D-ND	2.78	114.51	109.99
25	b	602	CLA	C1-O2A-CGA	2.78	123.39	116.65
25	B	616	CLA	C4D-C3D-CAD	2.78	111.13	108.11
25	c	514	CLA	CHD-C1D-ND	-2.78	120.89	124.80
25	C	505	CLA	C3D-C4D-ND	2.78	114.50	109.99
31	c	522	LMT	O5'-C1'-C2'	-2.78	104.66	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	607	CLA	C4D-C3D-CAD	2.78	111.12	108.11
25	B	602	CLA	C1-O2A-CGA	2.78	123.38	116.65
25	C	502	CLA	C3D-C4D-ND	2.78	114.50	109.99
25	c	502	CLA	C3D-C4D-ND	2.78	114.50	109.99
33	d	407	LHG	O8-C23-C24	2.78	120.30	111.83
27	K	103	BCR	C7-C8-C9	-2.78	122.13	126.23
27	k	103	BCR	C7-C8-C9	-2.78	122.13	126.23
25	C	514	CLA	CMC-C2C-C1C	2.78	129.37	125.03
25	c	514	CLA	CMC-C2C-C1C	2.78	129.37	125.03
25	B	614	CLA	C1-C2-C3	-2.78	121.65	126.20
25	b	614	CLA	C1-C2-C3	-2.78	121.65	126.20
31	E	103	LMT	O5'-C1'-C2'	2.77	116.07	110.37
30	A	413	SQD	O48-C23-C24	2.77	120.29	111.83
27	k	102	BCR	C19-C18-C17	2.77	123.37	119.01
25	C	505	CLA	C4D-C3D-CAD	2.77	111.11	108.11
25	b	609	CLA	C2B-C1B-NB	2.77	113.19	110.33
31	C	522	LMT	O5'-C1'-C2'	-2.76	104.69	110.37
25	b	616	CLA	OBD-CAD-C3D	-2.76	121.95	128.42
25	C	510	CLA	C2B-C1B-NB	2.76	113.19	110.33
30	a	413	SQD	O48-C23-C24	2.76	120.25	111.83
25	c	514	CLA	C4-C3-C5	2.76	120.02	115.23
25	B	616	CLA	OBD-CAD-C3D	-2.76	121.98	128.42
25	c	510	CLA	C2B-C1B-NB	2.75	113.18	110.33
25	c	505	CLA	C3D-C4D-ND	2.75	114.46	109.99
25	A	408	CLA	CMB-C2B-C3B	2.75	133.03	126.55
25	a	408	CLA	CMB-C2B-C3B	2.75	133.03	126.55
25	a	406	CLA	CMD-C2D-C3D	-2.75	121.38	127.69
25	b	616	CLA	C4D-C3D-CAD	2.75	111.09	108.11
36	H	101	RRX	C19-C18-C17	2.75	123.33	119.01
25	A	405	CLA	C3D-C4D-ND	2.75	114.45	109.99
25	a	405	CLA	C3D-C4D-ND	2.75	114.45	109.99
25	A	406	CLA	CMD-C2D-C3D	-2.74	121.40	127.69
34	C	516	DGD	O1G-C1A-C2A	2.74	120.19	111.83
34	c	516	DGD	O1G-C1A-C2A	2.74	120.19	111.83
25	C	505	CLA	CMC-C2C-C1C	2.74	129.32	125.03
25	c	505	CLA	CMC-C2C-C1C	2.74	129.32	125.03
25	C	514	CLA	C4-C3-C5	2.74	119.98	115.23
25	B	606	CLA	C1-O2A-CGA	2.74	123.28	116.65
33	B	628	LHG	O8-C23-C24	2.74	120.18	111.83
33	b	628	LHG	O8-C23-C24	2.74	120.18	111.83
25	b	607	CLA	C4D-C3D-CAD	2.74	111.08	108.11
25	B	606	CLA	C3D-C4D-ND	2.74	114.43	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	606	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
25	b	606	CLA	C1-O2A-CGA	2.73	123.27	116.65
25	b	606	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
36	h	101	RRX	C19-C18-C17	2.73	123.31	119.01
25	c	505	CLA	C4D-C3D-CAD	2.73	111.07	108.11
25	B	609	CLA	C3C-C4C-NC	2.73	113.93	110.43
25	C	508	CLA	C3C-C4C-NC	2.73	113.93	110.43
25	b	609	CLA	C3C-C4C-NC	2.73	113.93	110.43
25	c	508	CLA	C3C-C4C-NC	2.73	113.93	110.43
29	A	411	PL9	C22-C23-C24	-2.73	121.37	127.62
29	a	411	PL9	C22-C23-C24	-2.73	121.37	127.62
25	B	610	CLA	C4D-C3D-CAD	2.73	111.07	108.11
25	b	610	CLA	C4D-C3D-CAD	2.73	111.07	108.11
25	C	504	CLA	C4D-C3D-CAD	2.73	111.07	108.11
27	a	409	BCR	C36-C18-C17	-2.72	118.40	122.82
25	b	601	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
25	c	504	CLA	C4D-C3D-CAD	2.72	111.06	108.11
25	D	401	CLA	CMB-C2B-C3B	2.71	132.94	126.55
25	d	401	CLA	CMB-C2B-C3B	2.71	132.94	126.55
25	A	406	CLA	C3D-C4D-ND	2.71	114.40	109.99
25	b	606	CLA	C3D-C4D-ND	2.71	114.40	109.99
25	B	603	CLA	C3C-C4C-NC	2.71	113.90	110.43
25	B	601	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
27	A	409	BCR	C36-C18-C17	-2.70	118.44	122.82
25	b	603	CLA	C3C-C4C-NC	2.70	113.89	110.43
25	B	611	CLA	CHD-C1D-ND	-2.70	121.00	124.80
25	a	406	CLA	C3D-C4D-ND	2.70	114.37	109.99
25	B	608	CLA	C1-O2A-CGA	2.70	123.18	116.65
25	b	611	CLA	CHD-C1D-ND	-2.70	121.01	124.80
25	b	612	CLA	CHB-C4A-NA	2.70	128.29	124.40
25	b	608	CLA	C1-O2A-CGA	2.69	123.17	116.65
31	E	101	LMT	C1'-O5'-C5'	-2.69	108.46	113.72
25	D	403	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
25	d	403	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
25	B	612	CLA	CHB-C4A-NA	2.69	128.29	124.40
25	B	614	CLA	C3D-C4D-ND	2.69	114.36	109.99
25	b	614	CLA	C3D-C4D-ND	2.69	114.36	109.99
25	B	615	CLA	C4-C3-C5	2.69	119.90	115.23
25	b	615	CLA	C4-C3-C5	2.69	119.90	115.23
25	b	616	CLA	CHD-C1D-ND	-2.69	121.02	124.80
25	B	602	CLA	O2A-C1-C2	2.69	118.46	108.11
25	b	602	CLA	O2A-C1-C2	2.69	118.46	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	507	CLA	C1-C2-C3	-2.68	121.80	126.20
31	e	101	LMT	C1'-O5'-C5'	-2.68	108.48	113.72
25	B	608	CLA	CHD-C1D-ND	-2.68	121.03	124.80
25	b	608	CLA	CHD-C1D-ND	-2.68	121.03	124.80
31	k	105	LMT	C2'-C3'-C4'	2.68	115.77	109.68
35	E	104	HEM	CHD-C4C-NC	2.68	127.37	124.45
35	e	104	HEM	CHD-C4C-NC	2.68	127.37	124.45
25	b	615	CLA	C1-C2-C3	-2.67	121.82	126.20
31	K	105	LMT	C2'-C3'-C4'	2.67	115.74	109.68
25	B	616	CLA	CHD-C1D-ND	-2.67	121.05	124.80
25	D	401	CLA	C6-C5-C3	-2.66	106.98	113.47
25	d	401	CLA	C6-C5-C3	-2.66	106.98	113.47
25	B	604	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
25	b	604	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
25	B	615	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
25	b	615	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
25	c	505	CLA	C4-C3-C5	2.66	119.85	115.23
25	C	511	CLA	C3D-C4D-ND	2.66	114.31	109.99
25	c	511	CLA	C3D-C4D-ND	2.66	114.31	109.99
27	b	619	BCR	C35-C13-C12	2.66	122.15	118.09
25	C	505	CLA	C4-C3-C5	2.66	119.84	115.23
25	c	513	CLA	CHD-C1D-ND	-2.65	121.07	124.80
33	Z	102	LHG	O8-C23-C24	2.65	119.92	111.83
25	B	606	CLA	C4D-C3D-CAD	2.65	110.98	108.11
25	b	606	CLA	C4D-C3D-CAD	2.65	110.98	108.11
25	B	615	CLA	C1-C2-C3	-2.65	121.85	126.20
25	c	507	CLA	C1-C2-C3	-2.65	121.85	126.20
29	A	411	PL9	O2-C1-C6	2.65	124.69	120.48
25	c	505	CLA	O1D-CGD-CBD	-2.65	119.30	124.52
28	B	621	LMG	O8-C28-C29	2.65	119.91	111.83
29	a	411	PL9	O2-C1-C6	2.65	124.69	120.48
25	b	602	CLA	C4D-C3D-CAD	2.65	110.98	108.11
25	B	604	CLA	CMD-C2D-C3D	-2.65	121.62	127.69
25	b	604	CLA	CMD-C2D-C3D	-2.65	121.62	127.69
33	z	102	LHG	O8-C23-C24	2.65	119.90	111.83
25	C	513	CLA	CHD-C1D-ND	-2.64	121.08	124.80
25	B	602	CLA	C4D-C3D-CAD	2.64	110.98	108.11
28	b	621	LMG	O8-C28-C29	2.64	119.89	111.83
25	C	505	CLA	O1D-CGD-CBD	-2.64	119.31	124.52
31	e	103	LMT	C3B-C4B-C5B	2.64	115.02	110.23
27	B	619	BCR	C35-C13-C12	2.64	122.12	118.09
28	d	409	LMG	O8-C28-C29	2.64	119.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	401	CLA	CMC-C2C-C3C	2.63	133.27	126.15
31	E	103	LMT	C3B-C4B-C5B	2.63	115.00	110.23
25	B	607	CLA	C1-O2A-CGA	2.63	123.02	116.65
28	D	409	LMG	O8-C28-C29	2.63	119.84	111.83
27	Z	101	BCR	C2-C1-C6	2.62	114.25	110.44
25	d	401	CLA	CMC-C2C-C3C	2.62	133.24	126.15
25	D	403	CLA	CMB-C2B-C3B	2.62	132.72	126.55
25	b	607	CLA	CAC-C3C-C4C	2.62	128.20	124.79
25	B	613	CLA	CBC-CAC-C3C	-2.62	105.32	112.42
25	b	613	CLA	CBC-CAC-C3C	-2.62	105.32	112.42
25	d	403	CLA	CMB-C2B-C3B	2.62	132.71	126.55
25	b	614	CLA	CAC-C3C-C4C	2.62	128.20	124.79
25	B	614	CLA	CAC-C3C-C4C	2.62	128.20	124.79
25	c	513	CLA	O1D-CGD-CBD	-2.62	119.36	124.52
27	k	103	BCR	C2-C1-C6	2.62	114.24	110.44
25	C	514	CLA	C1-C2-C3	-2.62	121.91	126.20
25	c	514	CLA	C1-C2-C3	-2.62	121.91	126.20
25	b	607	CLA	C1-O2A-CGA	2.62	122.98	116.65
25	c	510	CLA	C3C-C4C-NC	2.61	113.78	110.43
25	B	607	CLA	C3D-C4D-ND	2.61	114.23	109.99
25	b	607	CLA	C3D-C4D-ND	2.61	114.23	109.99
25	C	510	CLA	C3C-C4C-NC	2.61	113.77	110.43
25	C	513	CLA	O1D-CGD-CBD	-2.61	119.38	124.52
25	b	609	CLA	C3D-C4D-ND	2.60	114.22	109.99
36	H	101	RRX	C12-C13-C14	2.60	123.10	119.01
25	C	507	CLA	CMB-C2B-C1B	2.60	129.38	125.42
25	c	507	CLA	CMB-C2B-C1B	2.60	129.38	125.42
25	B	609	CLA	C1-C2-C3	-2.60	121.93	126.20
25	b	609	CLA	C1-C2-C3	-2.60	121.93	126.20
27	z	101	BCR	C2-C1-C6	2.60	114.22	110.44
25	B	605	CLA	C1-O2A-CGA	2.60	122.94	116.65
25	b	605	CLA	C1-O2A-CGA	2.60	122.94	116.65
25	C	504	CLA	CAC-C3C-C4C	2.59	128.17	124.79
25	c	504	CLA	CAC-C3C-C4C	2.59	128.16	124.79
25	B	603	CLA	CMD-C2D-C3D	-2.59	121.74	127.69
25	b	603	CLA	CMD-C2D-C3D	-2.59	121.74	127.69
36	h	101	RRX	C12-C13-C14	2.59	123.09	119.01
26	A	407	PHO	O1D-CGD-CBD	2.59	128.66	124.72
27	K	103	BCR	C2-C1-C6	2.59	114.20	110.44
25	B	607	CLA	CAC-C3C-C4C	2.59	128.16	124.79
28	A	414	LMG	C8-O7-C10	-2.59	111.59	117.80
26	a	407	PHO	O1D-CGD-CBD	2.59	128.65	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	617	BCR	C36-C18-C17	-2.59	118.62	122.82
33	e	102	LHG	O8-C23-C24	2.59	119.72	111.83
25	b	609	CLA	O1D-CGD-CBD	-2.58	119.42	124.52
27	B	617	BCR	C36-C18-C17	-2.58	118.63	122.82
33	E	102	LHG	O8-C23-C24	2.58	119.70	111.83
30	K	101	SQD	C6-C5-C4	-2.58	108.37	113.08
25	B	606	CLA	CAC-C3C-C4C	2.58	128.14	124.79
30	C	501	SQD	O47-C7-O49	-2.58	117.68	123.70
25	B	609	CLA	C3D-C4D-ND	2.58	114.17	109.99
25	C	510	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
25	c	510	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
25	C	508	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
25	B	609	CLA	CHD-C1D-ND	-2.57	121.18	124.80
25	b	606	CLA	CAC-C3C-C4C	2.57	128.14	124.79
28	a	414	LMG	C8-O7-C10	-2.57	111.64	117.80
25	B	610	CLA	CMA-C3A-C4A	2.57	118.69	111.77
25	b	610	CLA	CMA-C3A-C4A	2.57	118.68	111.77
27	K	102	BCR	C30-C25-C26	-2.57	119.12	122.64
27	k	102	BCR	C30-C25-C26	-2.57	119.12	122.64
25	b	612	CLA	CMB-C2B-C3B	2.57	132.59	126.55
25	B	609	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
25	B	616	CLA	C3D-C4D-ND	2.57	114.16	109.99
25	B	616	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
25	c	507	CLA	C3D-C4D-ND	2.57	114.16	109.99
26	D	402	PHO	C2D-C1D-ND	-2.57	107.58	109.43
25	B	612	CLA	CMB-C2B-C3B	2.56	132.58	126.55
25	b	609	CLA	CHD-C1D-ND	-2.56	121.20	124.80
30	c	501	SQD	O47-C7-O49	-2.56	117.72	123.70
25	c	508	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
25	C	503	CLA	C3C-C4C-NC	2.56	113.71	110.43
25	c	503	CLA	C3C-C4C-NC	2.56	113.71	110.43
30	k	101	SQD	C6-C5-C4	-2.56	108.40	113.08
30	F	102	SQD	O5-C1-C2	2.56	115.62	110.37
25	b	616	CLA	C3D-C4D-ND	2.56	114.14	109.99
25	b	616	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
31	A	415	LMT	C1-O1'-C1'	2.55	118.04	113.68
25	C	507	CLA	C3D-C4D-ND	2.55	114.14	109.99
30	A	413	SQD	C3-C4-C5	2.55	114.85	110.23
30	a	413	SQD	C3-C4-C5	2.55	114.85	110.23
31	a	415	LMT	C1-O1'-C1'	2.55	118.03	113.68
25	C	502	CLA	C4-C3-C5	2.55	119.65	115.23
25	C	512	CLA	CAA-C2A-C3A	-2.55	106.12	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	CAA-C2A-C3A	-2.55	106.12	113.00
29	D	405	PL9	C22-C23-C24	-2.55	121.80	127.62
29	d	405	PL9	C22-C23-C24	-2.55	121.80	127.62
30	C	501	SQD	O8-S-C6	2.55	110.89	105.97
30	f	102	SQD	O5-C1-C2	2.54	115.60	110.37
25	B	610	CLA	C3D-C4D-ND	2.54	114.12	109.99
30	c	501	SQD	O8-S-C6	2.54	110.88	105.97
25	B	615	CLA	C3D-C4D-ND	2.54	114.11	109.99
25	c	502	CLA	C4-C3-C5	2.54	119.63	115.23
25	c	511	CLA	C2B-C1B-NB	2.54	112.96	110.33
25	b	615	CLA	C3D-C4D-ND	2.53	114.10	109.99
34	C	518	DGD	C2G-O2G-C1B	-2.53	111.73	117.80
25	A	408	CLA	C3C-C4C-NC	2.53	113.67	110.43
25	a	408	CLA	C3C-C4C-NC	2.53	113.67	110.43
27	B	618	BCR	C38-C26-C25	-2.53	121.72	124.48
27	b	618	BCR	C38-C26-C25	-2.53	121.72	124.48
31	B	623	LMT	O5'-C1'-O1'	-2.53	104.06	110.04
31	b	623	LMT	O5'-C1'-O1'	-2.53	104.06	110.04
34	c	518	DGD	C2G-O2G-C1B	-2.53	111.74	117.80
25	B	601	CLA	C3D-C4D-ND	2.53	114.10	109.99
25	b	610	CLA	C3D-C4D-ND	2.53	114.10	109.99
25	D	403	CLA	C3C-C4C-NC	2.53	113.67	110.43
27	B	618	BCR	C36-C18-C17	-2.52	118.73	122.82
27	b	618	BCR	C36-C18-C17	-2.52	118.73	122.82
25	B	603	CLA	CMA-C3A-C4A	2.52	118.56	111.77
25	B	612	CLA	C2B-C1B-NB	2.52	112.94	110.33
25	b	616	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
25	b	601	CLA	C3D-C4D-ND	2.52	114.08	109.99
25	c	503	CLA	CMA-C3A-C4A	2.52	118.54	111.77
25	A	405	CLA	CMB-C2B-C3B	2.52	132.47	126.55
25	b	603	CLA	CMA-C3A-C4A	2.52	118.54	111.77
31	K	105	LMT	C4B-C3B-C2B	2.52	115.25	110.83
31	k	105	LMT	C4B-C3B-C2B	2.52	115.25	110.83
33	D	406	LHG	O8-C23-C24	2.52	119.51	111.83
33	d	406	LHG	O8-C23-C24	2.52	119.51	111.83
26	d	402	PHO	C2D-C1D-ND	-2.52	107.61	109.43
25	C	511	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
25	c	511	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
25	c	504	CLA	CMD-C2D-C3D	-2.51	121.92	127.69
25	C	503	CLA	CMA-C3A-C4A	2.51	118.52	111.77
25	B	616	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
25	d	403	CLA	C3C-C4C-NC	2.51	113.64	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	103	BCR	C38-C26-C25	-2.51	121.75	124.48
27	k	103	BCR	C38-C26-C25	-2.51	121.75	124.48
25	a	405	CLA	CMB-C2B-C3B	2.51	132.45	126.55
25	C	511	CLA	C2B-C1B-NB	2.51	112.92	110.33
25	b	608	CLA	C4D-C3D-CAD	2.51	110.83	108.11
25	B	608	CLA	C4D-C3D-CAD	2.50	110.83	108.11
25	B	606	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
25	b	606	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
25	C	504	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
25	b	616	CLA	CMC-C2C-C3C	2.50	132.90	126.15
25	d	404	CLA	CAC-C3C-C4C	2.50	128.04	124.79
30	a	413	SQD	C4-C3-C2	2.50	115.21	110.83
25	D	404	CLA	CAC-C3C-C4C	2.49	128.04	124.79
30	H	103	SQD	O7-S-C6	2.49	110.48	106.76
30	h	103	SQD	O7-S-C6	2.49	110.48	106.76
35	V	201	HEM	CHD-C4C-NC	2.49	127.17	124.45
35	v	201	HEM	CHD-C4C-NC	2.49	127.17	124.45
25	C	513	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	c	513	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
25	B	602	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
35	e	104	HEM	CHD-C1D-C2D	-2.49	121.10	125.03
25	b	612	CLA	C2B-C1B-NB	2.49	112.91	110.33
25	B	609	CLA	CHA-C1A-NA	-2.49	120.76	126.39
25	b	609	CLA	CHA-C1A-NA	-2.49	120.76	126.39
25	B	614	CLA	CAA-C2A-C3A	-2.48	106.28	113.00
25	B	616	CLA	CMC-C2C-C3C	2.48	132.87	126.15
25	D	404	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
25	d	404	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
30	A	413	SQD	C4-C3-C2	2.48	115.19	110.83
25	b	602	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
27	C	515	BCR	C3-C4-C5	-2.48	109.63	114.06
27	c	515	BCR	C3-C4-C5	-2.48	109.63	114.06
35	E	104	HEM	CHA-C4D-C3D	-2.48	120.66	125.23
25	B	609	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
25	B	611	CLA	C4C-C3C-C2C	-2.48	103.29	106.89
27	K	103	BCR	C34-C9-C10	-2.48	118.80	122.82
27	k	103	BCR	C34-C9-C10	-2.48	118.80	122.82
25	B	604	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
25	b	604	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
35	e	104	HEM	CHA-C4D-C3D	-2.47	120.67	125.23
25	b	614	CLA	CAA-C2A-C3A	-2.47	106.32	113.00
27	A	409	BCR	C15-C14-C13	-2.47	123.81	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	511	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
27	b	619	BCR	C3-C4-C5	-2.47	109.65	114.06
25	c	511	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
27	a	409	BCR	C15-C14-C13	-2.47	123.81	127.28
35	E	104	HEM	CHD-C1D-C2D	-2.47	121.13	125.03
31	B	623	LMT	C2'-C3'-C4'	2.47	115.28	109.68
31	b	623	LMT	C2'-C3'-C4'	2.47	115.28	109.68
27	A	409	BCR	C37-C22-C21	-2.47	118.82	122.82
27	a	409	BCR	C37-C22-C21	-2.47	118.82	122.82
25	D	401	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
25	d	401	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
29	A	411	PL9	C42-C43-C44	-2.46	121.98	127.62
29	a	411	PL9	C42-C43-C44	-2.46	121.98	127.62
25	B	611	CLA	CMB-C2B-C3B	2.46	132.35	126.55
25	C	503	CLA	C3D-C4D-ND	2.46	113.99	109.99
25	c	503	CLA	C3D-C4D-ND	2.46	113.99	109.99
25	B	602	CLA	C4-C3-C5	2.46	119.50	115.23
25	b	602	CLA	C4-C3-C5	2.46	119.50	115.23
27	B	619	BCR	C3-C4-C5	-2.46	109.66	114.06
25	C	505	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
25	c	508	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
25	C	510	CLA	C4D-C3D-CAD	2.46	110.78	108.11
25	B	605	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
25	b	605	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
25	b	611	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
25	b	611	CLA	CMB-C2B-C3B	2.46	132.33	126.55
25	b	609	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
31	j	101	LMT	O5'-C5'-C4'	2.45	114.12	109.70
31	D	410	LMT	O1'-C1'-C2'	2.45	112.00	108.27
31	d	410	LMT	O1'-C1'-C2'	2.45	112.00	108.27
36	H	101	RRX	C23-C22-C21	2.45	122.87	119.01
25	B	601	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
25	b	601	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
30	k	101	SQD	O48-C23-C24	2.45	119.31	111.83
25	C	508	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
30	K	101	SQD	O48-C23-C24	2.45	119.29	111.83
25	C	509	CLA	C1-C2-C3	-2.44	122.19	126.20
25	c	509	CLA	C1-C2-C3	-2.44	122.19	126.20
25	c	510	CLA	C3B-C4B-NB	2.44	112.71	110.53
25	c	505	CLA	CAA-CBA-CGA	2.44	120.14	113.21
25	c	505	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
36	h	101	RRX	C23-C22-C21	2.44	122.85	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	J	101	LMT	O5'-C5'-C4'	2.44	114.10	109.70
25	d	401	CLA	CED-O2D-CGD	2.44	121.45	115.92
30	f	102	SQD	O48-C23-C24	2.44	119.27	111.83
25	C	505	CLA	CAA-CBA-CGA	2.44	120.12	113.21
30	F	102	SQD	O48-C23-C24	2.44	119.26	111.83
31	B	623	LMT	C3'-C4'-C5'	-2.43	105.53	110.93
25	c	510	CLA	C4D-C3D-CAD	2.43	110.75	108.11
27	k	103	BCR	C23-C22-C21	2.43	122.83	119.01
25	C	510	CLA	C3B-C4B-NB	2.43	112.70	110.53
25	c	506	CLA	CMB-C2B-C3B	2.43	132.27	126.55
25	B	613	CLA	C1-O2A-CGA	2.43	122.53	116.65
25	b	613	CLA	C1-O2A-CGA	2.43	122.53	116.65
25	C	506	CLA	CMB-C2B-C3B	2.43	132.26	126.55
25	D	401	CLA	CED-O2D-CGD	2.43	121.42	115.92
31	d	412	LMT	C3'-C4'-C5'	-2.43	105.55	110.93
31	b	623	LMT	C3'-C4'-C5'	-2.42	105.56	110.93
29	D	405	PL9	C27-C28-C29	-2.42	122.08	127.62
25	d	403	CLA	C1-C2-C3	-2.42	122.23	126.20
25	C	513	CLA	C3D-C4D-ND	2.42	113.92	109.99
30	A	413	SQD	O5-C1-C2	2.42	115.34	110.37
25	D	403	CLA	C1-C2-C3	-2.42	122.23	126.20
26	d	402	PHO	O2D-CGD-O1D	-2.42	119.14	123.85
27	k	102	BCR	C34-C9-C10	-2.42	118.90	122.82
25	c	513	CLA	C3D-C4D-ND	2.41	113.91	109.99
25	b	614	CLA	CMD-C2D-C3D	-2.41	122.15	127.69
30	a	413	SQD	O5-C1-C2	2.41	115.33	110.37
27	b	618	BCR	C37-C22-C21	-2.41	118.91	122.82
25	B	603	CLA	CMC-C2C-C1C	2.41	128.81	125.03
35	V	201	HEM	CHC-C4B-C3B	-2.41	120.25	125.07
35	v	201	HEM	CHC-C4B-C3B	-2.41	120.25	125.07
25	b	615	CLA	CHD-C4C-C3C	-2.41	121.26	124.77
27	K	103	BCR	C23-C22-C21	2.41	122.80	119.01
29	d	405	PL9	C27-C28-C29	-2.41	122.11	127.62
31	D	412	LMT	C3'-C4'-C5'	-2.41	105.59	110.93
25	b	603	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
27	B	618	BCR	C37-C22-C21	-2.41	118.92	122.82
29	a	411	PL9	C32-C33-C34	-2.41	122.11	127.62
25	B	614	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
25	b	610	CLA	C4B-CHC-C1C	2.41	131.91	126.25
25	C	514	CLA	CAC-C3C-C4C	2.41	127.92	124.79
25	B	604	CLA	C2B-C1B-NB	2.40	112.82	110.33
25	b	604	CLA	C2B-C1B-NB	2.40	112.82	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	614	CLA	CMB-C2B-C3B	2.40	132.21	126.55
27	k	103	BCR	C31-C1-C6	-2.40	106.47	110.24
27	K	102	BCR	C34-C9-C10	-2.40	118.93	122.82
25	b	603	CLA	CMC-C2C-C1C	2.40	128.78	125.03
29	A	411	PL9	C7-C8-C9	-2.40	122.70	126.83
29	a	411	PL9	C7-C8-C9	-2.40	122.70	126.83
25	B	614	CLA	CMB-C2B-C3B	2.40	132.19	126.55
25	C	504	CLA	CMC-C2C-C1C	2.40	128.78	125.03
25	c	504	CLA	CMC-C2C-C1C	2.40	128.78	125.03
31	J	101	LMT	O5'-C5'-C6'	2.40	112.39	106.44
25	B	605	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
25	b	605	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
31	Y	101	LMT	O1'-C1'-C2'	2.40	111.91	108.27
31	y	101	LMT	O1'-C1'-C2'	2.40	111.91	108.27
26	D	402	PHO	O2D-CGD-O1D	-2.40	119.18	123.85
25	D	401	CLA	C1-O2A-CGA	2.40	122.45	116.65
25	d	401	CLA	C1-O2A-CGA	2.40	122.45	116.65
25	c	514	CLA	CAC-C3C-C4C	2.40	127.91	124.79
25	B	605	CLA	O2A-C1-C2	2.39	117.32	108.11
25	b	605	CLA	O2A-C1-C2	2.39	117.32	108.11
25	B	610	CLA	C4B-CHC-C1C	2.39	131.88	126.25
25	B	603	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
25	C	508	CLA	OBD-CAD-C3D	-2.39	122.82	128.42
25	c	508	CLA	OBD-CAD-C3D	-2.39	122.82	128.42
25	b	616	CLA	C3C-C4C-NC	2.39	113.50	110.43
25	B	610	CLA	OBD-CAD-C3D	-2.39	122.82	128.42
25	B	615	CLA	C1-O2A-CGA	2.39	122.44	116.65
25	C	507	CLA	C1-O2A-CGA	2.39	122.43	116.65
33	B	627	LHG	O8-C23-C24	2.39	119.12	111.83
33	b	627	LHG	O8-C23-C24	2.39	119.12	111.83
25	B	605	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
25	b	605	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
31	F	103	LMT	C2'-C3'-C4'	2.39	115.10	109.68
31	f	103	LMT	C2'-C3'-C4'	2.39	115.10	109.68
25	b	615	CLA	C1-O2A-CGA	2.39	122.43	116.65
25	B	615	CLA	CHD-C4C-C3C	-2.38	121.30	124.77
29	A	411	PL9	C32-C33-C34	-2.38	122.17	127.62
31	j	101	LMT	O5'-C5'-C6'	2.38	112.34	106.44
25	C	503	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
25	c	503	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
25	c	507	CLA	C1-O2A-CGA	2.38	122.42	116.65
25	b	603	CLA	C2B-C1B-NB	2.38	112.80	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	505	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
25	c	505	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
27	K	103	BCR	C31-C1-C6	-2.38	106.51	110.24
27	B	619	BCR	C32-C1-C6	-2.38	106.51	110.24
27	b	619	BCR	C32-C1-C6	-2.38	106.51	110.24
30	A	412	SQD	C1-O5-C5	2.38	118.37	113.72
30	a	412	SQD	C1-O5-C5	2.38	118.37	113.72
25	b	610	CLA	OBD-CAD-C3D	-2.38	122.86	128.42
25	c	510	CLA	CAC-C3C-C4C	2.37	127.88	124.79
31	X	102	LMT	O5'-C5'-C4'	2.37	113.82	109.55
27	K	103	BCR	C34-C9-C8	2.37	121.71	118.09
27	k	103	BCR	C34-C9-C8	2.37	121.71	118.09
25	c	502	CLA	CMB-C2B-C3B	2.37	132.12	126.55
35	E	104	HEM	CBD-CAD-C3D	-2.37	105.99	112.53
35	e	104	HEM	CBD-CAD-C3D	-2.37	105.99	112.53
25	C	514	CLA	CMA-C3A-C4A	2.37	118.14	111.77
35	E	104	HEM	C3B-C4B-NB	-2.37	107.77	109.47
35	e	104	HEM	C3B-C4B-NB	-2.37	107.77	109.47
25	C	507	CLA	C3C-C4C-NC	2.37	113.46	110.43
25	b	610	CLA	C1-C2-C3	-2.37	122.32	126.20
29	D	405	PL9	C20-C19-C21	2.37	119.33	115.23
25	b	611	CLA	C3C-C4C-NC	2.37	113.46	110.43
25	B	611	CLA	C3C-C4C-NC	2.36	113.46	110.43
25	B	603	CLA	C2B-C1B-NB	2.36	112.78	110.33
25	c	512	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
29	d	405	PL9	C20-C19-C21	2.36	119.33	115.23
25	B	616	CLA	C3C-C4C-NC	2.36	113.46	110.43
25	C	509	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
25	c	509	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
29	d	405	PL9	O1-C4-C3	-2.36	118.24	120.73
27	b	619	BCR	C37-C22-C21	-2.36	118.99	122.82
25	a	406	CLA	C4-C3-C5	2.36	119.33	115.23
25	C	503	CLA	C1-O2A-CGA	2.36	122.36	116.65
25	c	503	CLA	C1-O2A-CGA	2.36	122.36	116.65
27	B	619	BCR	C37-C22-C21	-2.36	118.99	122.82
26	D	402	PHO	C3B-C4B-NB	-2.36	105.93	107.46
26	d	402	PHO	C3B-C4B-NB	-2.36	105.93	107.46
25	c	514	CLA	CMA-C3A-C4A	2.36	118.11	111.77
27	b	618	BCR	C19-C18-C17	2.36	122.72	119.01
25	C	502	CLA	CMB-C2B-C3B	2.36	132.09	126.55
34	C	517	DGD	O1G-C1A-O1A	-2.36	117.74	123.63
29	D	405	PL9	O1-C4-C3	-2.36	118.25	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	510	CLA	C4-C3-C5	2.35	119.31	115.23
25	c	510	CLA	C4-C3-C5	2.35	119.31	115.23
25	C	510	CLA	CAC-C3C-C4C	2.35	127.85	124.79
25	B	608	CLA	CBC-CAC-C3C	-2.35	106.04	112.42
25	b	608	CLA	CBC-CAC-C3C	-2.35	106.04	112.42
25	B	610	CLA	C1-C2-C3	-2.35	122.34	126.20
31	x	102	LMT	O5'-C5'-C4'	2.35	113.78	109.55
29	a	411	PL9	C20-C19-C21	2.35	119.31	115.23
25	C	512	CLA	CED-O2D-CGD	2.35	121.24	115.92
25	c	512	CLA	CED-O2D-CGD	2.35	121.24	115.92
25	c	507	CLA	C3C-C4C-NC	2.35	113.44	110.43
25	B	602	CLA	C1-C2-C3	-2.35	122.35	126.20
25	c	502	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
25	b	607	CLA	CAA-C2A-C3A	-2.35	106.66	113.00
31	H	102	LMT	C1'-O5'-C5'	-2.35	109.14	113.72
31	h	102	LMT	C1'-O5'-C5'	-2.35	109.14	113.72
25	b	604	CLA	C3D-C4D-ND	2.35	113.80	109.99
25	C	512	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
29	A	411	PL9	C20-C19-C21	2.35	119.30	115.23
25	b	602	CLA	C1-C2-C3	-2.34	122.36	126.20
25	c	505	CLA	CHC-C1C-C2C	-2.34	120.28	126.95
25	A	406	CLA	C4-C3-C5	2.34	119.30	115.23
25	C	505	CLA	C1-C2-C3	-2.34	122.36	126.20
25	B	607	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
25	C	505	CLA	CHC-C1C-C2C	-2.34	120.29	126.95
25	C	502	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
30	a	412	SQD	O48-C23-C24	2.34	118.98	111.83
25	B	604	CLA	CHD-C1D-ND	-2.34	121.51	124.80
27	B	618	BCR	C19-C18-C17	2.34	122.69	119.01
34	c	517	DGD	O1G-C1A-O1A	-2.34	117.77	123.63
25	B	606	CLA	C6-C5-C3	-2.34	107.77	113.47
25	b	606	CLA	C6-C5-C3	-2.34	107.77	113.47
27	F	101	BCR	C32-C1-C6	-2.34	106.57	110.24
27	f	101	BCR	C32-C1-C6	-2.34	106.57	110.24
25	B	608	CLA	C3C-C4C-NC	2.34	113.43	110.43
25	b	608	CLA	C3C-C4C-NC	2.34	113.43	110.43
25	c	512	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
25	B	603	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
27	a	409	BCR	C34-C9-C8	2.34	121.66	118.09
25	B	603	CLA	C3D-C4D-ND	2.34	113.79	109.99
25	C	508	CLA	CMC-C2C-C1C	2.34	128.69	125.03
25	b	604	CLA	CHD-C1D-ND	-2.34	121.51	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	613	CLA	C4-C3-C5	2.34	119.29	115.23
25	C	512	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
25	C	512	CLA	C4-C3-C5	2.34	119.28	115.23
25	c	512	CLA	C4-C3-C5	2.34	119.28	115.23
34	C	517	DGD	C2G-O2G-C1B	-2.34	112.20	117.80
34	c	517	DGD	C2G-O2G-C1B	-2.34	112.20	117.80
25	B	607	CLA	CHB-C4A-NA	2.33	127.77	124.40
25	c	508	CLA	CMC-C2C-C1C	2.33	128.68	125.03
30	A	412	SQD	O48-C23-C24	2.33	118.95	111.83
25	C	506	CLA	C3C-C4C-NC	2.33	113.42	110.43
25	b	615	CLA	C4D-C3D-CAD	2.33	110.64	108.11
25	c	506	CLA	C3C-C4C-NC	2.33	113.42	110.43
35	e	104	HEM	O2D-CGD-CBD	2.33	121.36	114.00
25	b	613	CLA	C4-C3-C5	2.33	119.27	115.23
30	c	501	SQD	O48-C23-C24	2.33	118.93	111.83
26	D	402	PHO	OBD-CAD-CBD	-2.33	122.41	125.82
26	d	402	PHO	OBD-CAD-CBD	-2.33	122.41	125.82
25	B	604	CLA	C3D-C4D-ND	2.33	113.77	109.99
25	C	511	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
35	E	104	HEM	O2D-CGD-CBD	2.33	121.35	114.00
30	C	501	SQD	O48-C23-C24	2.33	118.93	111.83
30	C	501	SQD	O47-C7-C8	2.32	116.51	111.48
25	B	613	CLA	C3B-C4B-NB	2.32	112.60	110.53
25	b	613	CLA	C3B-C4B-NB	2.32	112.60	110.53
25	b	607	CLA	CHB-C4A-NA	2.32	127.75	124.40
30	c	501	SQD	O47-C7-C8	2.32	116.50	111.48
25	A	406	CLA	C1-C2-C3	-2.32	122.40	126.20
25	C	509	CLA	CHB-C1B-C2B	-2.32	120.70	127.43
25	c	505	CLA	C1-C2-C3	-2.32	122.40	126.20
25	b	603	CLA	C3D-C4D-ND	2.32	113.75	109.99
25	c	511	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
25	b	603	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
25	B	611	CLA	C4D-C3D-CAD	2.32	110.62	108.11
25	b	611	CLA	C4D-C3D-CAD	2.32	110.62	108.11
25	C	509	CLA	C3C-C4C-NC	2.31	113.39	110.43
25	c	509	CLA	C3C-C4C-NC	2.31	113.39	110.43
27	A	409	BCR	C34-C9-C8	2.31	121.62	118.09
25	b	607	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
25	b	608	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
27	k	102	BCR	C37-C22-C21	-2.31	119.08	122.82
25	B	607	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
25	B	615	CLA	C4D-C3D-CAD	2.31	110.61	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	509	CLA	CED-O2D-CGD	2.30	121.14	115.92
25	c	509	CLA	CED-O2D-CGD	2.30	121.14	115.92
25	a	406	CLA	C1-C2-C3	-2.30	122.42	126.20
25	c	509	CLA	CHB-C1B-C2B	-2.30	120.74	127.43
31	c	525	LMT	C3'-C4'-C5'	-2.30	106.06	110.23
27	C	515	BCR	C35-C13-C12	2.30	121.60	118.09
27	c	515	BCR	C35-C13-C12	2.30	121.60	118.09
31	X	104	LMT	C1'-O5'-C5'	-2.30	109.23	113.72
31	x	104	LMT	C1'-O5'-C5'	-2.30	109.23	113.72
31	E	103	LMT	O1B-C4'-C3'	2.30	113.07	107.23
31	e	103	LMT	O1B-C4'-C3'	2.30	113.07	107.23
25	A	405	CLA	C3C-C4C-NC	2.30	113.37	110.43
25	B	603	CLA	CHD-C1D-ND	-2.30	121.57	124.80
25	b	603	CLA	CHD-C1D-ND	-2.30	121.57	124.80
25	B	606	CLA	CMC-C2C-C1C	2.30	128.62	125.03
25	b	606	CLA	CMC-C2C-C1C	2.30	128.62	125.03
25	B	611	CLA	CHC-C1C-C2C	-2.29	120.43	126.95
25	b	611	CLA	CHC-C1C-C2C	-2.29	120.43	126.95
31	C	525	LMT	C3'-C4'-C5'	-2.29	106.07	110.23
25	c	514	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
31	t	101	LMT	C1'-O5'-C5'	-2.29	109.25	113.72
27	F	101	BCR	C7-C8-C9	-2.29	122.85	126.23
35	V	201	HEM	CHA-C4D-C3D	-2.29	121.01	125.23
25	B	601	CLA	CAC-C3C-C4C	2.29	127.77	124.79
31	E	101	LMT	C4'-C3'-C2'	2.29	114.85	110.83
31	e	101	LMT	C4'-C3'-C2'	2.29	114.85	110.83
31	M	101	LMT	O1B-C4'-C3'	2.29	113.05	107.23
31	m	101	LMT	O1B-C4'-C3'	2.29	113.05	107.23
25	b	601	CLA	CAC-C3C-C4C	2.29	127.77	124.79
27	K	102	BCR	C37-C22-C21	-2.29	119.11	122.82
33	B	628	LHG	C5-O7-C7	-2.29	112.32	117.80
33	b	628	LHG	C5-O7-C7	-2.29	112.32	117.80
25	B	608	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
27	f	101	BCR	C7-C8-C9	-2.28	122.86	126.23
25	B	606	CLA	CMB-C2B-C3B	2.28	131.92	126.55
25	b	606	CLA	CMB-C2B-C3B	2.28	131.92	126.55
25	C	514	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
31	T	101	LMT	C1'-O5'-C5'	-2.28	109.27	113.72
35	v	201	HEM	CHA-C4D-C3D	-2.28	121.02	125.23
27	F	101	BCR	C34-C9-C10	-2.28	119.13	122.82
27	F	101	BCR	C2-C1-C6	2.27	113.74	110.44
27	f	101	BCR	C2-C1-C6	2.27	113.74	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	CLA	C3C-C4C-NC	2.27	113.34	110.43
26	D	402	PHO	C1-C2-C3	-2.27	122.47	126.20
25	D	401	CLA	CBC-CAC-C3C	-2.27	106.26	112.42
31	K	105	LMT	O1B-C1B-C2B	2.27	113.68	108.09
31	k	105	LMT	O1B-C1B-C2B	2.27	113.68	108.09
34	C	518	DGD	O1G-C1A-C2A	2.27	118.76	111.83
27	k	102	BCR	C2-C1-C6	2.27	113.74	110.44
27	B	619	BCR	C39-C30-C25	-2.27	106.68	110.24
27	b	619	BCR	C39-C30-C25	-2.27	106.68	110.24
27	C	515	BCR	C34-C9-C10	-2.27	119.14	122.82
27	b	618	BCR	C34-C9-C10	-2.27	119.14	122.82
27	f	101	BCR	C34-C9-C10	-2.27	119.14	122.82
27	C	515	BCR	C34-C9-C8	2.26	121.54	118.09
25	B	606	CLA	CED-O2D-CGD	2.26	121.05	115.92
27	c	515	BCR	C34-C9-C10	-2.26	119.15	122.82
25	C	503	CLA	CHC-C1C-C2C	-2.26	120.52	126.95
25	c	503	CLA	CHC-C1C-C2C	-2.26	120.52	126.95
25	b	601	CLA	CMB-C2B-C1B	2.26	128.86	125.42
27	z	101	BCR	C34-C9-C10	-2.26	119.15	122.82
34	c	518	DGD	O1G-C1A-C2A	2.26	118.73	111.83
25	C	507	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
25	c	507	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
25	d	401	CLA	CBC-CAC-C3C	-2.26	106.30	112.42
28	C	519	LMG	C8-O7-C10	-2.26	112.39	117.80
28	c	519	LMG	C8-O7-C10	-2.26	112.39	117.80
25	c	511	CLA	CMB-C2B-C3B	2.26	131.86	126.55
27	Z	101	BCR	C34-C9-C10	-2.26	119.16	122.82
27	c	515	BCR	C34-C9-C8	2.26	121.53	118.09
27	b	619	BCR	C33-C5-C6	-2.25	122.02	124.48
26	d	402	PHO	C1-C2-C3	-2.25	122.50	126.20
25	B	601	CLA	CMB-C2B-C1B	2.25	128.85	125.42
25	b	606	CLA	CED-O2D-CGD	2.25	121.03	115.92
25	B	609	CLA	CHB-C4A-NA	2.25	127.65	124.40
27	B	618	BCR	C34-C9-C10	-2.25	119.17	122.82
27	K	102	BCR	C2-C1-C6	2.25	113.70	110.44
25	B	611	CLA	C4B-C3B-C2B	-2.25	104.51	107.30
25	b	611	CLA	C4B-C3B-C2B	-2.25	104.51	107.30
27	B	618	BCR	C35-C13-C12	2.24	121.52	118.09
27	b	618	BCR	C35-C13-C12	2.24	121.52	118.09
28	h	105	LMG	O8-C28-O10	-2.24	118.01	123.63
31	h	102	LMT	C4'-C3'-C2'	2.24	114.77	110.83
25	C	511	CLA	CMB-C2B-C3B	2.24	131.82	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	619	BCR	C33-C5-C6	-2.24	122.04	124.48
33	Z	102	LHG	O4-P-O5	2.24	119.57	110.83
25	d	404	CLA	C3C-C4C-NC	2.24	113.30	110.43
28	H	105	LMG	O8-C28-O10	-2.24	118.02	123.63
31	H	102	LMT	C4'-C3'-C2'	2.24	114.76	110.83
25	b	609	CLA	CHB-C4A-NA	2.24	127.63	124.40
25	B	612	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
25	b	603	CLA	CAC-C3C-C4C	2.24	127.70	124.79
25	d	404	CLA	CMB-C2B-C1B	2.24	128.83	125.42
33	z	102	LHG	O4-P-O5	2.24	119.55	110.83
25	C	505	CLA	CMB-C2B-C3B	2.24	131.81	126.55
25	C	503	CLA	C4D-C3D-CAD	2.24	110.53	108.11
25	C	510	CLA	C3D-C4D-ND	2.23	113.62	109.99
25	c	510	CLA	C3D-C4D-ND	2.23	113.62	109.99
25	C	509	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
25	c	509	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
25	B	613	CLA	CHD-C4C-C3C	-2.23	121.52	124.77
25	b	613	CLA	CHD-C4C-C3C	-2.23	121.52	124.77
26	d	402	PHO	O1D-CGD-CBD	2.23	128.11	124.72
35	E	104	HEM	C1A-CHA-C4D	-2.23	121.00	126.25
25	b	615	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
25	c	505	CLA	CMB-C2B-C3B	2.23	131.80	126.55
25	D	404	CLA	CMB-C2B-C1B	2.23	128.81	125.42
35	E	104	HEM	CBA-CAA-C2A	-2.23	106.37	112.53
35	e	104	HEM	CBA-CAA-C2A	-2.23	106.37	112.53
29	a	411	PL9	O2-C1-C2	-2.23	116.76	121.83
25	b	610	CLA	C4-C3-C5	2.23	119.09	115.23
25	B	615	CLA	C4C-C3C-C2C	-2.23	103.65	106.89
25	B	613	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
25	b	613	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
25	B	604	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
25	b	604	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
25	A	408	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
25	a	408	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
25	B	607	CLA	C4-C3-C5	2.22	119.09	115.23
25	B	605	CLA	C3C-C4C-NC	2.22	113.28	110.43
25	b	605	CLA	C3C-C4C-NC	2.22	113.28	110.43
25	b	607	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
25	b	612	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
25	b	607	CLA	C4-C3-C5	2.22	119.08	115.23
27	K	103	BCR	C33-C5-C6	-2.22	122.06	124.48
27	k	103	BCR	C33-C5-C6	-2.22	122.06	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	CHA-C1A-NA	-2.22	121.36	126.39
25	a	406	CLA	CHC-C1C-C2C	-2.22	120.64	126.95
27	F	101	BCR	C37-C22-C21	-2.22	119.22	122.82
25	b	610	CLA	CMB-C2B-C3B	2.22	131.77	126.55
25	c	504	CLA	C4-C3-C5	2.22	119.08	115.23
25	B	612	CLA	C4-C3-C5	2.22	119.08	115.23
27	f	101	BCR	C37-C22-C21	-2.22	119.23	122.82
26	D	402	PHO	O1D-CGD-CBD	2.21	128.08	124.72
25	C	505	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
35	e	104	HEM	C1A-CHA-C4D	-2.21	121.04	126.25
31	A	415	LMT	C1'-O5'-C5'	-2.21	109.39	113.72
31	a	415	LMT	C1'-O5'-C5'	-2.21	109.39	113.72
25	B	603	CLA	CAC-C3C-C4C	2.21	127.67	124.79
25	c	505	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
25	C	504	CLA	CHA-C1A-NA	-2.21	121.38	126.39
25	B	610	CLA	C4-C3-C5	2.21	119.07	115.23
25	D	404	CLA	C3C-C4C-NC	2.21	113.26	110.43
25	A	406	CLA	CHC-C1C-C2C	-2.21	120.67	126.95
25	B	613	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
25	b	613	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
25	C	509	CLA	CHA-C1A-NA	-2.21	121.39	126.39
26	A	407	PHO	C2D-C1D-ND	-2.21	107.83	109.43
26	a	407	PHO	C2D-C1D-ND	-2.21	107.83	109.43
30	C	501	SQD	O7-S-C6	2.21	110.05	106.76
30	c	501	SQD	O7-S-C6	2.21	110.05	106.76
29	A	411	PL9	O2-C1-C2	-2.21	116.81	121.83
28	d	409	LMG	C7-O1-C1	-2.21	109.07	113.80
25	c	504	CLA	C1-O2A-CGA	2.20	121.99	116.65
34	c	517	DGD	O2G-C1B-O1B	-2.20	118.55	123.70
25	b	612	CLA	C4-C3-C5	2.20	119.05	115.23
25	c	509	CLA	CHA-C1A-NA	-2.20	121.40	126.39
25	b	612	CLA	CHD-C1D-C2D	-2.20	120.91	125.49
25	c	503	CLA	C4D-C3D-CAD	2.20	110.50	108.11
25	C	510	CLA	C6-C5-C3	-2.20	108.11	113.47
25	c	510	CLA	C6-C5-C3	-2.20	108.11	113.47
31	j	101	LMT	C1'-O5'-C5'	2.20	118.01	113.72
25	c	504	CLA	C4C-C3C-C2C	-2.20	103.69	106.89
31	I	101	LMT	C3'-C4'-C5'	-2.20	106.25	110.23
25	B	607	CLA	C4C-C3C-C2C	-2.20	103.69	106.89
25	C	504	CLA	C4-C3-C5	2.20	119.04	115.23
25	B	610	CLA	CMB-C2B-C3B	2.20	131.71	126.55
25	C	504	CLA	C4C-C3C-C2C	-2.20	103.70	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	409	LMG	C7-O1-C1	-2.20	109.09	113.80
25	C	507	CLA	CHA-C1A-NA	-2.20	121.42	126.39
25	c	507	CLA	CHA-C1A-NA	-2.20	121.42	126.39
34	C	517	DGD	O2G-C1B-O1B	-2.20	118.57	123.70
25	C	509	CLA	CMA-C3A-C4A	2.19	117.67	111.77
25	c	509	CLA	CMA-C3A-C4A	2.19	117.67	111.77
28	a	410	LMG	O8-C28-O10	-2.19	118.14	123.63
25	C	504	CLA	C1-O2A-CGA	2.19	121.96	116.65
25	B	604	CLA	C3B-C4B-NB	2.19	112.49	110.53
25	b	604	CLA	C3B-C4B-NB	2.19	112.49	110.53
31	i	101	LMT	C3'-C4'-C5'	-2.19	106.26	110.23
25	C	511	CLA	C4-C3-C5	2.19	119.03	115.23
31	J	101	LMT	C1'-O5'-C5'	2.19	117.99	113.72
25	b	601	CLA	C4B-CHC-C1C	2.19	131.39	126.25
25	B	612	CLA	CHD-C1D-C2D	-2.18	120.94	125.49
25	B	605	CLA	CMB-C2B-C3B	2.18	131.69	126.55
25	b	605	CLA	CMB-C2B-C3B	2.18	131.69	126.55
31	b	623	LMT	O6'-C6'-C5'	-2.18	103.91	111.33
28	A	410	LMG	O8-C28-O10	-2.18	118.17	123.63
25	B	603	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
25	C	503	CLA	C4C-C3C-C2C	-2.18	103.72	106.89
25	b	610	CLA	C4C-C3C-C2C	-2.18	103.72	106.89
25	c	503	CLA	C4C-C3C-C2C	-2.18	103.72	106.89
25	B	601	CLA	C4B-CHC-C1C	2.18	131.37	126.25
27	Z	101	BCR	C37-C22-C21	-2.18	119.29	122.82
27	z	101	BCR	C37-C22-C21	-2.18	119.29	122.82
25	c	511	CLA	C4-C3-C5	2.17	119.00	115.23
25	C	507	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
25	C	509	CLA	CHC-C1C-C2C	-2.17	120.77	126.95
25	c	509	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
25	C	514	CLA	C4C-C3C-C2C	-2.17	103.73	106.89
25	c	514	CLA	C4C-C3C-C2C	-2.17	103.73	106.89
27	B	619	BCR	C34-C9-C10	-2.17	119.30	122.82
27	b	619	BCR	C34-C9-C10	-2.17	119.30	122.82
25	B	615	CLA	OBD-CAD-C3D	-2.17	123.35	128.42
25	c	514	CLA	C4D-C3D-CAD	2.17	110.46	108.11
25	b	603	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
25	C	512	CLA	CMC-C2C-C1C	2.16	128.41	125.03
25	c	512	CLA	CMC-C2C-C1C	2.16	128.41	125.03
25	b	615	CLA	OBD-CAD-C3D	-2.16	123.37	128.42
31	B	623	LMT	O6'-C6'-C5'	-2.16	103.98	111.33
33	d	406	LHG	C5-O7-C7	-2.16	112.63	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	523	LMG	O7-C10-O9	-2.16	118.66	123.70
25	C	508	CLA	CHA-C1A-NA	-2.16	121.51	126.39
27	F	101	BCR	C34-C9-C8	2.16	121.38	118.09
28	H	105	LMG	O6-C1-O1	-2.16	104.95	110.04
28	h	105	LMG	O6-C1-O1	-2.16	104.95	110.04
31	K	105	LMT	O5'-C5'-C6'	2.15	111.78	106.44
25	b	611	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
25	B	611	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
25	c	510	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
31	k	105	LMT	O5'-C5'-C6'	2.15	111.77	106.44
25	d	404	CLA	CHB-C4A-NA	2.15	127.50	124.40
25	c	507	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
25	c	504	CLA	CMB-C2B-C3B	2.15	131.60	126.55
27	f	101	BCR	C34-C9-C8	2.15	121.37	118.09
25	C	504	CLA	CMB-C2B-C3B	2.15	131.60	126.55
33	D	406	LHG	C5-O7-C7	-2.15	112.66	117.80
25	B	610	CLA	C4C-C3C-C2C	-2.15	103.77	106.89
25	C	510	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
31	f	103	LMT	C3B-C4B-C5B	-2.15	106.34	110.23
25	b	610	CLA	CAC-C3C-C4C	2.15	127.58	124.79
25	C	514	CLA	C4D-C3D-CAD	2.15	110.44	108.11
28	C	523	LMG	O7-C10-O9	-2.14	118.69	123.70
27	K	102	BCR	C31-C1-C6	-2.14	106.88	110.24
27	k	102	BCR	C31-C1-C6	-2.14	106.88	110.24
25	B	607	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
25	B	612	CLA	C4C-C3C-C2C	-2.14	103.77	106.89
25	b	612	CLA	C4C-C3C-C2C	-2.14	103.77	106.89
27	z	101	BCR	C31-C1-C6	-2.14	106.89	110.24
27	B	617	BCR	C37-C22-C21	-2.14	119.35	122.82
31	M	101	LMT	O5B-C5B-C4B	2.14	113.56	109.70
27	K	103	BCR	C4-C5-C6	-2.14	119.81	122.70
27	b	617	BCR	C37-C22-C21	-2.14	119.35	122.82
31	m	101	LMT	O5B-C5B-C4B	2.14	113.55	109.70
25	a	405	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
25	b	604	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
25	d	403	CLA	CMA-C3A-C2A	-2.14	105.72	113.98
25	c	506	CLA	C1-O2A-CGA	2.14	121.82	116.65
25	a	405	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
25	C	507	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
25	b	607	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
29	d	405	PL9	C40-C39-C41	2.14	118.93	115.23
25	C	511	CLA	C11-C10-C8	-2.13	108.87	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	C11-C10-C8	-2.13	108.87	115.97
27	B	619	BCR	C12-C13-C14	-2.13	115.65	119.01
31	e	101	LMT	O1'-C1'-C2'	2.13	111.51	108.27
25	a	408	CLA	C4D-C3D-CAD	2.13	110.42	108.11
29	a	411	PL9	C12-C13-C14	-2.13	122.74	127.62
25	B	610	CLA	C6-C5-C3	-2.13	108.28	113.47
25	b	610	CLA	C6-C5-C3	-2.13	108.28	113.47
25	B	612	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
31	c	522	LMT	O1'-C1'-C2'	2.13	111.51	108.27
31	C	524	LMT	C4B-C3B-C2B	2.13	114.57	110.83
25	B	604	CLA	C3C-C4C-NC	2.13	113.16	110.43
25	b	604	CLA	C3C-C4C-NC	2.13	113.16	110.43
31	D	410	LMT	C1'-O5'-C5'	2.13	117.88	113.72
31	d	410	LMT	C1'-O5'-C5'	2.13	117.88	113.72
31	A	416	LMT	C1'-O5'-C5'	-2.13	109.56	113.72
25	D	403	CLA	CMA-C3A-C2A	-2.13	105.75	113.98
25	A	405	CLA	CAA-C2A-C1A	-2.13	105.00	111.97
25	A	408	CLA	C4D-C3D-CAD	2.13	110.42	108.11
25	d	404	CLA	C4D-C3D-CAD	2.13	110.42	108.11
28	h	105	LMG	O7-C10-O9	-2.13	118.73	123.70
25	c	507	CLA	C4C-C3C-C2C	-2.13	103.80	106.89
25	c	508	CLA	CHA-C1A-NA	-2.13	121.57	126.39
25	D	404	CLA	CHB-C4A-NA	2.13	127.47	124.40
25	A	406	CLA	CMC-C2C-C1C	2.13	128.36	125.03
35	V	201	HEM	O2A-CGA-O1A	-2.12	117.87	123.33
25	C	505	CLA	CHB-C4A-NA	2.12	127.46	124.40
25	c	505	CLA	CHB-C4A-NA	2.12	127.46	124.40
31	C	522	LMT	O1'-C1'-C2'	2.12	111.50	108.27
27	Z	101	BCR	C31-C1-C6	-2.12	106.92	110.24
27	b	619	BCR	C12-C13-C14	-2.12	115.67	119.01
25	C	508	CLA	CHB-C4A-NA	2.12	127.46	124.40
31	a	416	LMT	C1'-O5'-C5'	-2.12	109.58	113.72
29	D	405	PL9	C40-C39-C41	2.12	118.91	115.23
31	F	103	LMT	C3B-C4B-C5B	-2.12	106.39	110.23
25	c	512	CLA	CMB-C2B-C3B	2.12	131.54	126.55
29	A	411	PL9	C12-C13-C14	-2.12	122.77	127.62
25	c	510	CLA	CHC-C1C-NC	-2.12	121.12	124.31
30	a	412	SQD	O6-C1-C2	2.12	111.49	108.27
35	v	201	HEM	O2A-CGA-O1A	-2.12	117.88	123.33
25	B	609	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
28	H	105	LMG	O7-C10-O9	-2.12	118.75	123.70
25	C	506	CLA	C1-O2A-CGA	2.12	121.78	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	405	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
25	B	604	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
27	K	103	BCR	C33-C5-C4	2.12	118.11	113.60
25	b	613	CLA	C3C-C4C-NC	2.12	113.14	110.43
25	c	508	CLA	CHB-C4A-NA	2.11	127.45	124.40
25	b	612	CLA	CAA-C2A-C3A	-2.11	107.28	113.00
25	b	609	CLA	CHC-C1C-C2C	-2.11	120.94	126.95
25	a	406	CLA	CMC-C2C-C1C	2.11	128.34	125.03
30	A	412	SQD	O6-C1-C2	2.11	111.48	108.27
27	k	103	BCR	C4-C5-C6	-2.11	119.85	122.70
33	D	408	LHG	O8-C23-C24	2.11	118.27	111.83
33	d	408	LHG	O8-C23-C24	2.11	118.27	111.83
25	c	508	CLA	C3D-C4D-ND	2.11	113.42	109.99
25	B	610	CLA	CAC-C3C-C4C	2.11	127.53	124.79
31	c	524	LMT	C4B-C3B-C2B	2.11	114.53	110.83
31	E	101	LMT	O1'-C1'-C2'	2.11	111.48	108.27
25	B	616	CLA	C4-C3-C5	2.11	118.89	115.23
25	D	404	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
25	C	512	CLA	CMB-C2B-C3B	2.11	131.51	126.55
25	B	608	CLA	C4B-C3B-C2B	-2.11	104.68	107.30
25	D	401	CLA	C4-C3-C5	2.11	118.89	115.23
31	D	410	LMT	O5'-C5'-C6'	2.11	111.66	106.44
31	d	410	LMT	O5'-C5'-C6'	2.11	111.66	106.44
25	C	506	CLA	CHA-C4D-ND	2.11	136.89	132.55
25	B	613	CLA	C3C-C4C-NC	2.10	113.12	110.43
25	D	404	CLA	C4D-C3D-CAD	2.10	110.39	108.11
30	F	102	SQD	O8-S-C6	2.10	110.03	105.97
30	f	102	SQD	O8-S-C6	2.10	110.03	105.97
25	C	510	CLA	CHC-C1C-NC	-2.10	121.15	124.31
27	k	103	BCR	C33-C5-C4	2.10	118.07	113.60
27	B	618	BCR	C3-C4-C5	-2.10	110.31	114.06
25	C	508	CLA	C3D-C4D-ND	2.10	113.40	109.99
25	d	404	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
25	b	616	CLA	C4-C3-C5	2.10	118.87	115.23
25	b	604	CLA	C1-O2A-CGA	2.09	121.72	116.65
25	a	406	CLA	O2D-CGD-O1D	-2.09	119.77	123.85
25	c	504	CLA	C3D-C4D-ND	2.09	113.39	109.99
25	C	504	CLA	C3D-C4D-ND	2.09	113.39	109.99
25	b	610	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
27	a	409	BCR	C34-C9-C10	-2.09	119.43	122.82
25	d	401	CLA	C4-C3-C5	2.09	118.86	115.23
25	c	508	CLA	CHA-C4D-ND	2.09	136.86	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	412	SQD	O48-C23-O10	-2.09	118.41	123.63
30	A	412	SQD	O47-C7-O49	-2.09	118.83	123.70
30	a	412	SQD	O47-C7-O49	-2.09	118.83	123.70
25	C	506	CLA	CAC-C3C-C4C	2.09	127.50	124.79
25	C	511	CLA	CBC-CAC-C3C	-2.09	106.77	112.42
25	c	506	CLA	CAC-C3C-C4C	2.08	127.50	124.79
25	b	607	CLA	C3C-C4C-NC	2.08	113.10	110.43
33	D	407	LHG	O8-C23-O10	-2.08	118.42	123.63
35	V	201	HEM	CHA-C1A-NA	2.08	127.64	123.86
25	B	604	CLA	C1-O2A-CGA	2.08	121.69	116.65
25	c	506	CLA	CHA-C4D-ND	2.08	136.85	132.55
25	d	404	CLA	C4-C3-C5	2.08	118.84	115.23
25	b	615	CLA	CMB-C2B-C1B	2.08	128.59	125.42
25	B	610	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
25	b	608	CLA	C4-C3-C5	2.08	118.84	115.23
25	B	602	CLA	CMC-C2C-C1C	2.08	128.29	125.03
25	b	602	CLA	CMC-C2C-C1C	2.08	128.29	125.03
25	B	608	CLA	C4-C3-C5	2.08	118.84	115.23
27	b	618	BCR	C3-C4-C5	-2.08	110.34	114.06
31	X	103	LMT	O1'-C1'-C2'	2.08	111.43	108.27
31	x	103	LMT	O1'-C1'-C2'	2.08	111.43	108.27
25	D	404	CLA	C4-C3-C5	2.08	118.84	115.23
31	a	415	LMT	C3'-C4'-C5'	-2.08	106.32	110.93
25	A	406	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
30	A	412	SQD	O48-C23-O10	-2.08	118.43	123.63
25	c	511	CLA	CMA-C3A-C4A	2.08	117.36	111.77
25	B	615	CLA	CMB-C2B-C1B	2.08	128.58	125.42
25	b	608	CLA	C4B-C3B-C2B	-2.08	104.72	107.30
25	B	610	CLA	CMC-C2C-C1C	2.08	128.28	125.03
33	d	407	LHG	O8-C23-O10	-2.08	118.44	123.63
25	C	508	CLA	CHA-C4D-ND	2.07	136.83	132.55
35	v	201	HEM	CHA-C1A-NA	2.07	127.62	123.86
25	c	511	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
25	C	511	CLA	CMA-C3A-C4A	2.07	117.34	111.77
25	B	610	CLA	CHA-C1A-NA	-2.07	121.70	126.39
25	B	611	CLA	CMC-C2C-C1C	2.07	128.27	125.03
25	b	611	CLA	CMC-C2C-C1C	2.07	128.27	125.03
29	d	405	PL9	C32-C33-C34	-2.07	122.88	127.62
29	d	405	PL9	O2-C1-C6	2.07	123.77	120.48
25	B	606	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
25	C	502	CLA	CAC-C3C-C4C	2.07	127.48	124.79
25	b	610	CLA	CHA-C1A-NA	-2.07	121.71	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	103	BCR	C35-C13-C12	2.07	121.25	118.09
27	k	103	BCR	C35-C13-C12	2.07	121.25	118.09
25	b	615	CLA	C6-C5-C3	-2.07	108.43	113.47
25	B	604	CLA	CMC-C2C-C1C	2.07	128.26	125.03
25	b	604	CLA	CMC-C2C-C1C	2.07	128.26	125.03
25	C	503	CLA	CAC-C3C-C4C	2.07	127.48	124.79
31	A	415	LMT	C3'-C4'-C5'	-2.07	106.35	110.93
31	b	629	LMT	C3'-C4'-C5'	-2.06	106.35	110.93
34	h	104	DGD	O1G-C1A-O1A	-2.06	118.46	123.63
27	A	409	BCR	C34-C9-C10	-2.06	119.47	122.82
31	B	629	LMT	C3'-C4'-C5'	-2.06	106.36	110.93
25	b	603	CLA	CHA-C4D-ND	2.06	136.81	132.55
29	D	405	PL9	C32-C33-C34	-2.06	122.90	127.62
25	c	511	CLA	CHC-C1C-C2C	-2.06	121.09	126.95
25	B	603	CLA	CHA-C4D-ND	2.06	136.80	132.55
25	B	607	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
25	b	607	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
25	B	602	CLA	CMB-C2B-C1B	2.06	128.55	125.42
25	b	602	CLA	CMB-C2B-C1B	2.06	128.55	125.42
27	B	619	BCR	C19-C18-C17	2.06	122.24	119.01
27	b	619	BCR	C19-C18-C17	2.06	122.24	119.01
25	D	403	CLA	CHC-C1C-NC	-2.06	121.22	124.31
25	C	503	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
25	c	503	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
25	A	405	CLA	C4C-C3C-C2C	-2.06	103.90	106.89
25	c	503	CLA	OBD-CAD-C3D	-2.05	123.61	128.42
25	B	607	CLA	C3C-C4C-NC	2.05	113.06	110.43
25	b	606	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
25	D	401	CLA	CHB-C4A-NA	2.05	127.36	124.40
25	d	401	CLA	CHB-C4A-NA	2.05	127.36	124.40
25	C	511	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
25	b	604	CLA	CMB-C2B-C1B	2.05	128.54	125.42
26	a	407	PHO	O2D-CGD-O1D	-2.05	119.85	123.85
25	B	607	CLA	CED-O2D-CGD	2.05	120.57	115.92
25	B	615	CLA	C6-C5-C3	-2.05	108.47	113.47
25	c	506	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
25	c	503	CLA	CAC-C3C-C4C	2.05	127.46	124.79
25	d	403	CLA	CHC-C1C-NC	-2.05	121.22	124.31
25	b	609	CLA	C4D-C3D-CAD	2.05	110.33	108.11
29	d	405	PL9	O2-C1-C2	-2.05	117.17	121.83
25	C	506	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
25	A	406	CLA	O1D-CGD-CBD	-2.05	120.47	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	503	CLA	CMC-C2C-C3C	2.05	131.69	126.15
25	b	610	CLA	CMC-C2C-C1C	2.05	128.24	125.03
25	a	405	CLA	CHB-C4A-NA	2.05	127.36	124.40
25	c	508	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
25	C	503	CLA	OBD-CAD-C3D	-2.05	123.63	128.42
25	A	405	CLA	CHB-C4A-NA	2.05	127.35	124.40
32	A	417	BCT	O3-C-O1	-2.05	114.44	119.68
29	D	405	PL9	O2-C1-C2	-2.04	117.18	121.83
25	c	512	CLA	CAC-C3C-C4C	2.04	127.45	124.79
25	a	405	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
34	H	104	DGD	O1G-C1A-O1A	-2.04	118.52	123.63
27	b	618	BCR	C2-C1-C6	2.04	113.41	110.44
25	C	512	CLA	CAC-C3C-C4C	2.04	127.45	124.79
25	a	406	CLA	CMB-C2B-C3B	2.04	131.35	126.55
25	b	607	CLA	CED-O2D-CGD	2.04	120.55	115.92
25	B	612	CLA	CHC-C1C-NC	-2.04	121.24	124.31
25	B	602	CLA	CHB-C4A-NA	2.04	127.34	124.40
25	b	602	CLA	CHB-C4A-NA	2.04	127.34	124.40
25	b	602	CLA	C3C-C4C-NC	2.04	113.04	110.43
29	D	405	PL9	O2-C1-C6	2.04	123.72	120.48
25	C	508	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
25	C	502	CLA	C3C-C4C-NC	2.04	113.04	110.43
25	C	512	CLA	C4C-C3C-C2C	-2.04	103.93	106.89
25	c	512	CLA	C4C-C3C-C2C	-2.04	103.93	106.89
25	c	503	CLA	CMC-C2C-C3C	2.04	131.66	126.15
26	A	407	PHO	O2D-CGD-O1D	-2.04	119.89	123.85
25	B	604	CLA	CMB-C2B-C1B	2.04	128.52	125.42
31	I	103	LMT	C1'-O5'-C5'	-2.03	109.75	113.72
31	i	103	LMT	C1'-O5'-C5'	-2.03	109.75	113.72
32	a	417	BCT	O3-C-O1	-2.03	114.47	119.68
25	B	606	CLA	CHB-C1B-C2B	-2.03	121.52	127.43
25	b	606	CLA	CHB-C1B-C2B	-2.03	121.52	127.43
25	B	602	CLA	C3C-C4C-NC	2.03	113.03	110.43
25	A	405	CLA	CHA-C4D-ND	2.03	136.74	132.55
25	a	405	CLA	CHA-C4D-ND	2.03	136.74	132.55
25	a	406	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
29	A	411	PL9	C41-C39-C38	-2.03	116.61	121.17
30	a	412	SQD	O8-S-C6	2.03	109.89	105.97
25	c	511	CLA	C6-C7-C8	-2.03	109.22	115.97
25	B	610	CLA	CHC-C1C-C2C	-2.03	121.18	126.95
25	b	612	CLA	CHC-C1C-NC	-2.03	121.26	124.31
25	c	502	CLA	C3C-C4C-NC	2.03	113.03	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	502	CLA	C1-O2A-CGA	2.03	121.56	116.65
25	B	606	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
25	b	606	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
25	C	511	CLA	C6-C7-C8	-2.02	109.23	115.97
25	c	502	CLA	CAC-C3C-C4C	2.02	127.42	124.79
25	A	406	CLA	CMB-C2B-C3B	2.02	131.31	126.55
25	C	502	CLA	C1-O2A-CGA	2.02	121.55	116.65
27	A	409	BCR	C35-C13-C12	2.02	121.18	118.09
25	c	513	CLA	CMB-C2B-C3B	2.02	131.31	126.55
25	B	609	CLA	C4D-C3D-CAD	2.02	110.30	108.11
31	C	522	LMT	C1'-O5'-C5'	-2.02	109.77	113.72
31	c	522	LMT	C1'-O5'-C5'	-2.02	109.77	113.72
25	B	613	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
25	b	613	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
25	b	610	CLA	CHC-C1C-C2C	-2.02	121.21	126.95
25	C	506	CLA	C7-C6-C5	-2.02	107.88	113.26
27	B	618	BCR	C2-C1-C6	2.02	113.37	110.44
25	c	506	CLA	C7-C6-C5	-2.02	107.89	113.26
25	C	513	CLA	CMB-C2B-C3B	2.02	131.29	126.55
25	b	608	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
31	i	101	LMT	C1'-O5'-C5'	-2.01	109.78	113.72
29	a	411	PL9	C41-C39-C38	-2.01	116.64	121.17
30	A	412	SQD	O8-S-C6	2.01	109.86	105.97
25	B	608	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
27	B	617	BCR	C28-C27-C26	-2.01	110.47	114.06
25	C	504	CLA	CHA-C4D-ND	2.01	136.69	132.55
25	c	504	CLA	CHA-C4D-ND	2.01	136.69	132.55
27	B	619	BCR	C34-C9-C8	2.01	121.16	118.09
27	b	619	BCR	C34-C9-C8	2.01	121.16	118.09
31	J	101	LMT	O1'-C1'-C2'	2.01	111.32	108.27
31	j	101	LMT	O1'-C1'-C2'	2.01	111.32	108.27
25	B	605	CLA	C1-C2-C3	-2.01	122.91	126.20
27	a	409	BCR	C35-C13-C12	2.01	121.16	118.09
31	I	101	LMT	C1'-O5'-C5'	-2.01	109.80	113.72
25	C	506	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
25	c	506	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
25	C	504	CLA	CMA-C3A-C2A	2.01	121.74	113.98
25	b	601	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
27	b	617	BCR	C8-C7-C6	-2.00	121.65	127.00
25	c	504	CLA	CMA-C3A-C2A	2.00	121.72	113.98
25	B	613	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
25	b	613	CLA	CHC-C1C-C2C	-2.00	121.26	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	412	SQD	C45-O47-C7	2.00	122.58	117.80
30	a	412	SQD	C45-O47-C7	2.00	122.58	117.80

There are no chirality outliers.

All (2598) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	405	CLA	CBD-CGD-O2D-CED
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	606	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C4B-C3B-CAB-CBB
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C11-C10-C8-C9
25	B	616	CLA	C6-C7-C8-C9
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O1D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CBD-CGD-O2D-CED
25	C	505	CLA	C2-C3-C5-C6
25	C	505	CLA	C4-C3-C5-C6
25	C	507	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	C2B-C3B-CAB-CBB
25	C	508	CLA	C4B-C3B-CAB-CBB
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	C2-C1-O2A-CGA
25	C	512	CLA	CBD-CGD-O2D-CED
25	C	513	CLA	CBA-CGA-O2A-C1
25	C	513	CLA	O1A-CGA-O2A-C1
25	C	513	CLA	CBD-CGD-O2D-CED
25	D	401	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C2B-C3B-CAB-CBB
25	D	404	CLA	C4B-C3B-CAB-CBB
25	a	405	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	C3A-C2A-CAA-CBA
25	b	606	CLA	C2B-C3B-CAB-CBB
25	b	606	CLA	C4B-C3B-CAB-CBB
25	b	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	C11-C10-C8-C9
25	b	616	CLA	C6-C7-C8-C9
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O1D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CBD-CGD-O2D-CED
25	c	505	CLA	C2-C3-C5-C6
25	c	505	CLA	C4-C3-C5-C6
25	c	507	CLA	CBD-CGD-O2D-CED
25	c	508	CLA	C2B-C3B-CAB-CBB
25	c	508	CLA	C4B-C3B-CAB-CBB
25	c	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	510	CLA	C2-C1-O2A-CGA
25	c	512	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	CBD-CGD-O2D-CED
25	d	401	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	C2B-C3B-CAB-CBB
25	d	404	CLA	C4B-C3B-CAB-CBB
27	A	409	BCR	C7-C8-C9-C10
27	A	409	BCR	C11-C10-C9-C8
27	A	409	BCR	C11-C10-C9-C34
27	B	618	BCR	C7-C8-C9-C10
27	B	618	BCR	C7-C8-C9-C34
27	B	618	BCR	C11-C10-C9-C8
27	B	618	BCR	C11-C10-C9-C34
27	B	618	BCR	C10-C11-C12-C13
27	B	619	BCR	C7-C8-C9-C10
27	B	619	BCR	C7-C8-C9-C34
27	B	619	BCR	C11-C10-C9-C8
27	B	619	BCR	C11-C10-C9-C34
27	C	515	BCR	C7-C8-C9-C10
27	C	515	BCR	C7-C8-C9-C34
27	C	515	BCR	C11-C10-C9-C8
27	C	515	BCR	C11-C10-C9-C34
27	C	515	BCR	C10-C11-C12-C13
27	F	101	BCR	C11-C10-C9-C8
27	F	101	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
27	K	102	BCR	C5-C6-C7-C8
27	K	102	BCR	C7-C8-C9-C10
27	K	102	BCR	C7-C8-C9-C34
27	K	102	BCR	C11-C10-C9-C8
27	K	102	BCR	C11-C10-C9-C34
27	K	102	BCR	C10-C11-C12-C13
27	K	103	BCR	C11-C10-C9-C8
27	K	103	BCR	C11-C10-C9-C34
27	K	103	BCR	C10-C11-C12-C13
27	K	103	BCR	C17-C18-C19-C20
27	K	103	BCR	C36-C18-C19-C20
27	a	409	BCR	C7-C8-C9-C10
27	a	409	BCR	C11-C10-C9-C8
27	a	409	BCR	C11-C10-C9-C34
27	b	618	BCR	C7-C8-C9-C10
27	b	618	BCR	C7-C8-C9-C34
27	b	618	BCR	C11-C10-C9-C8
27	b	618	BCR	C11-C10-C9-C34
27	b	618	BCR	C10-C11-C12-C13
27	b	619	BCR	C7-C8-C9-C10
27	b	619	BCR	C7-C8-C9-C34
27	b	619	BCR	C11-C10-C9-C8
27	b	619	BCR	C11-C10-C9-C34
27	c	515	BCR	C7-C8-C9-C10
27	c	515	BCR	C7-C8-C9-C34
27	c	515	BCR	C11-C10-C9-C8
27	c	515	BCR	C11-C10-C9-C34
27	c	515	BCR	C10-C11-C12-C13
27	f	101	BCR	C11-C10-C9-C8
27	f	101	BCR	C11-C10-C9-C34
27	k	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C7-C8-C9-C10
27	k	102	BCR	C7-C8-C9-C34
27	k	102	BCR	C11-C10-C9-C8
27	k	102	BCR	C11-C10-C9-C34
27	k	102	BCR	C10-C11-C12-C13
27	k	103	BCR	C11-C10-C9-C8
27	k	103	BCR	C11-C10-C9-C34
27	k	103	BCR	C10-C11-C12-C13
27	k	103	BCR	C17-C18-C19-C20
27	k	103	BCR	C36-C18-C19-C20
29	A	411	PL9	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
29	A	411	PL9	C37-C38-C39-C40
29	A	411	PL9	C37-C38-C39-C41
29	A	411	PL9	C42-C43-C44-C45
29	A	411	PL9	C42-C43-C44-C46
29	D	405	PL9	C39-C41-C42-C43
29	D	405	PL9	C42-C43-C44-C45
29	D	405	PL9	C42-C43-C44-C46
29	a	411	PL9	C36-C37-C38-C39
29	a	411	PL9	C37-C38-C39-C40
29	a	411	PL9	C37-C38-C39-C41
29	a	411	PL9	C42-C43-C44-C45
29	a	411	PL9	C42-C43-C44-C46
29	d	405	PL9	C39-C41-C42-C43
29	d	405	PL9	C42-C43-C44-C45
29	d	405	PL9	C42-C43-C44-C46
30	A	412	SQD	C44-C45-O47-C7
30	A	412	SQD	O49-C7-O47-C45
30	A	412	SQD	C8-C7-O47-C45
30	A	412	SQD	C24-C23-O48-C46
30	A	412	SQD	C5-C6-S-O8
30	A	412	SQD	C5-C6-S-O9
30	A	413	SQD	C2-C1-O6-C44
30	A	413	SQD	O5-C5-C6-S
30	A	413	SQD	C5-C6-S-O7
30	A	413	SQD	C5-C6-S-O8
30	A	413	SQD	C5-C6-S-O9
30	B	620	SQD	O5-C1-O6-C44
30	B	620	SQD	O49-C7-O47-C45
30	B	620	SQD	O5-C5-C6-S
30	C	501	SQD	O47-C45-C46-O48
30	C	501	SQD	C5-C6-S-O7
30	C	501	SQD	C5-C6-S-O8
30	C	501	SQD	C5-C6-S-O9
30	F	102	SQD	C2-C1-O6-C44
30	F	102	SQD	O5-C5-C6-S
30	H	103	SQD	O5-C1-O6-C44
30	H	103	SQD	O49-C7-O47-C45
30	K	101	SQD	O5-C1-O6-C44
30	K	101	SQD	O47-C45-C46-O48
30	a	412	SQD	C44-C45-O47-C7
30	a	412	SQD	O49-C7-O47-C45
30	a	412	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
30	a	412	SQD	C24-C23-O48-C46
30	a	412	SQD	C5-C6-S-O8
30	a	412	SQD	C5-C6-S-O9
30	a	413	SQD	C2-C1-O6-C44
30	a	413	SQD	O5-C5-C6-S
30	a	413	SQD	C5-C6-S-O7
30	a	413	SQD	C5-C6-S-O8
30	a	413	SQD	C5-C6-S-O9
30	b	620	SQD	O5-C1-O6-C44
30	b	620	SQD	O49-C7-O47-C45
30	b	620	SQD	O5-C5-C6-S
30	c	501	SQD	O47-C45-C46-O48
30	c	501	SQD	C5-C6-S-O7
30	c	501	SQD	C5-C6-S-O8
30	c	501	SQD	C5-C6-S-O9
30	f	102	SQD	C2-C1-O6-C44
30	f	102	SQD	O5-C5-C6-S
30	h	103	SQD	O5-C1-O6-C44
30	h	103	SQD	O49-C7-O47-C45
30	k	101	SQD	O5-C1-O6-C44
30	k	101	SQD	O47-C45-C46-O48
31	A	415	LMT	O5'-C1'-O1'-C1
31	B	629	LMT	O5'-C1'-O1'-C1
31	C	522	LMT	C2-C1-O1'-C1'
31	C	524	LMT	C2-C1-O1'-C1'
31	D	410	LMT	C2'-C1'-O1'-C1
31	D	410	LMT	O5'-C1'-O1'-C1
31	F	103	LMT	C2'-C1'-O1'-C1
31	F	103	LMT	O5'-C1'-O1'-C1
31	F	103	LMT	C2-C1-O1'-C1'
31	I	101	LMT	C2'-C1'-O1'-C1
31	I	101	LMT	O5'-C1'-O1'-C1
31	K	105	LMT	C2-C1-O1'-C1'
31	M	101	LMT	C3'-C4'-O1B-C1B
31	X	102	LMT	C2'-C1'-O1'-C1
31	X	102	LMT	O5'-C1'-O1'-C1
31	X	104	LMT	O5'-C1'-O1'-C1
31	X	105	LMT	C2-C1-O1'-C1'
31	a	415	LMT	O5'-C1'-O1'-C1
31	b	629	LMT	O5'-C1'-O1'-C1
31	c	522	LMT	C2-C1-O1'-C1'
31	c	524	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
31	d	410	LMT	C2'-C1'-O1'-C1
31	d	410	LMT	O5'-C1'-O1'-C1
31	f	103	LMT	C2'-C1'-O1'-C1
31	f	103	LMT	O5'-C1'-O1'-C1
31	f	103	LMT	C2-C1-O1'-C1'
31	i	101	LMT	C2'-C1'-O1'-C1
31	i	101	LMT	O5'-C1'-O1'-C1
31	k	105	LMT	C2-C1-O1'-C1'
31	m	101	LMT	C3'-C4'-O1B-C1B
31	x	102	LMT	C2'-C1'-O1'-C1
31	x	102	LMT	O5'-C1'-O1'-C1
31	x	104	LMT	O5'-C1'-O1'-C1
31	x	105	LMT	C2-C1-O1'-C1'
33	B	627	LHG	C1-C2-C3-O3
33	B	627	LHG	C3-O3-P-O6
33	B	627	LHG	C4-O6-P-O3
33	B	627	LHG	C8-C7-O7-C5
33	B	628	LHG	O1-C1-C2-O2
33	B	628	LHG	O1-C1-C2-C3
33	B	628	LHG	C3-O3-P-O4
33	B	628	LHG	C4-O6-P-O3
33	D	406	LHG	O1-C1-C2-C3
33	D	406	LHG	C3-O3-P-O5
33	D	406	LHG	C3-O3-P-O6
33	D	407	LHG	O1-C1-C2-C3
33	D	407	LHG	C3-O3-P-O5
33	D	407	LHG	C4-O6-P-O3
33	D	408	LHG	O1-C1-C2-O2
33	D	408	LHG	O6-C4-C5-O7
33	E	102	LHG	C3-O3-P-O5
33	E	102	LHG	C4-O6-P-O3
33	Z	102	LHG	C4-O6-P-O3
33	Z	102	LHG	C4-O6-P-O4
33	b	627	LHG	C1-C2-C3-O3
33	b	627	LHG	C3-O3-P-O6
33	b	627	LHG	C4-O6-P-O3
33	b	627	LHG	C8-C7-O7-C5
33	b	628	LHG	O1-C1-C2-O2
33	b	628	LHG	O1-C1-C2-C3
33	b	628	LHG	C3-O3-P-O4
33	b	628	LHG	C4-O6-P-O3
33	d	406	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	d	406	LHG	C3-O3-P-O5
33	d	406	LHG	C3-O3-P-O6
33	d	407	LHG	O1-C1-C2-C3
33	d	407	LHG	C3-O3-P-O5
33	d	407	LHG	C4-O6-P-O3
33	d	408	LHG	O1-C1-C2-O2
33	d	408	LHG	O6-C4-C5-O7
33	e	102	LHG	C3-O3-P-O5
33	e	102	LHG	C4-O6-P-O3
33	z	102	LHG	C4-O6-P-O3
33	z	102	LHG	C4-O6-P-O4
35	E	104	HEM	C2C-C3C-CAC-CBC
35	E	104	HEM	C4C-C3C-CAC-CBC
35	e	104	HEM	C2C-C3C-CAC-CBC
35	e	104	HEM	C4C-C3C-CAC-CBC
36	H	101	RRX	C22-C23-C24-C25
36	H	101	RRX	C37-C22-C23-C24
36	H	101	RRX	C21-C22-C23-C24
36	H	101	RRX	C20-C21-C22-C23
36	H	101	RRX	C20-C21-C22-C37
36	H	101	RRX	C18-C19-C20-C21
36	H	101	RRX	C16-C17-C18-C19
36	H	101	RRX	C16-C17-C18-C36
36	h	101	RRX	C22-C23-C24-C25
36	h	101	RRX	C37-C22-C23-C24
36	h	101	RRX	C21-C22-C23-C24
36	h	101	RRX	C20-C21-C22-C23
36	h	101	RRX	C20-C21-C22-C37
36	h	101	RRX	C18-C19-C20-C21
36	h	101	RRX	C16-C17-C18-C19
36	h	101	RRX	C16-C17-C18-C36
31	B	625	LMT	C3'-C4'-O1B-C1B
31	b	625	LMT	C3'-C4'-O1B-C1B
25	A	405	CLA	O1D-CGD-O2D-CED
25	C	510	CLA	O1D-CGD-O2D-CED
25	a	405	CLA	O1D-CGD-O2D-CED
25	c	510	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	609	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	C	514	CLA	CBD-CGD-O2D-CED
25	D	404	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CBD-CGD-O2D-CED
25	c	510	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	c	514	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	CBD-CGD-O2D-CED
28	A	410	LMG	O10-C28-O8-C9
28	C	523	LMG	O10-C28-O8-C9
28	H	105	LMG	O10-C28-O8-C9
28	a	410	LMG	O10-C28-O8-C9
28	c	523	LMG	O10-C28-O8-C9
28	h	105	LMG	O10-C28-O8-C9
30	A	412	SQD	O10-C23-O48-C46
30	H	103	SQD	O10-C23-O48-C46
30	a	412	SQD	O10-C23-O48-C46
30	h	103	SQD	O10-C23-O48-C46
34	C	516	DGD	O1A-C1A-O1G-C1G
34	c	516	DGD	O1A-C1A-O1G-C1G
25	B	610	CLA	C15-C16-C17-C18
25	b	610	CLA	C15-C16-C17-C18
28	C	523	LMG	C29-C28-O8-C9
28	H	105	LMG	C29-C28-O8-C9
28	c	523	LMG	C29-C28-O8-C9
28	h	105	LMG	C29-C28-O8-C9
34	C	516	DGD	C2A-C1A-O1G-C1G
34	c	516	DGD	C2A-C1A-O1G-C1G
25	C	512	CLA	O1A-CGA-O2A-C1
25	D	404	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
25	d	404	CLA	O1A-CGA-O2A-C1
33	B	627	LHG	O10-C23-O8-C6
33	b	627	LHG	O10-C23-O8-C6
25	C	514	CLA	C13-C15-C16-C17
25	c	514	CLA	C13-C15-C16-C17
25	C	504	CLA	O1D-CGD-O2D-CED
25	C	512	CLA	O1D-CGD-O2D-CED
25	C	514	CLA	O1D-CGD-O2D-CED
25	c	504	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	c	514	CLA	O1D-CGD-O2D-CED
30	C	501	SQD	O49-C7-O47-C45
30	c	501	SQD	O49-C7-O47-C45
33	B	627	LHG	O9-C7-O7-C5
33	b	627	LHG	O9-C7-O7-C5
25	B	604	CLA	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	b	604	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	D	404	CLA	CBA-CGA-O2A-C1
25	d	404	CLA	CBA-CGA-O2A-C1
28	A	410	LMG	C29-C28-O8-C9
28	a	410	LMG	C29-C28-O8-C9
30	H	103	SQD	C24-C23-O48-C46
30	h	103	SQD	C24-C23-O48-C46
33	B	627	LHG	C24-C23-O8-C6
33	b	627	LHG	C24-C23-O8-C6
25	B	602	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	509	CLA	CBD-CGD-O2D-CED
25	b	602	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	509	CLA	CBD-CGD-O2D-CED
30	B	620	SQD	C8-C7-O47-C45
30	H	103	SQD	C8-C7-O47-C45
30	b	620	SQD	C8-C7-O47-C45
30	h	103	SQD	C8-C7-O47-C45
25	B	616	CLA	O1D-CGD-O2D-CED
25	C	507	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	O1D-CGD-O2D-CED
25	c	507	CLA	O1D-CGD-O2D-CED
31	X	101	LMT	O5'-C5'-C6'-O6'
31	x	101	LMT	O5'-C5'-C6'-O6'
25	B	603	CLA	C4-C3-C5-C6
25	B	604	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	C	508	CLA	C4-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	c	508	CLA	C4-C3-C5-C6
25	B	603	CLA	C2-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	C	508	CLA	C2-C3-C5-C6
25	b	603	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
25	c	508	CLA	C2-C3-C5-C6
29	A	411	PL9	C33-C34-C36-C37
29	a	411	PL9	C33-C34-C36-C37
25	B	609	CLA	O1D-CGD-O2D-CED
25	C	513	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
31	B	626	LMT	O5'-C5'-C6'-O6'
31	b	626	LMT	O5'-C5'-C6'-O6'
25	B	602	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
31	K	105	LMT	C3'-C4'-O1B-C1B
31	k	105	LMT	C3'-C4'-O1B-C1B
25	C	506	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
28	A	414	LMG	C29-C28-O8-C9
28	a	414	LMG	C29-C28-O8-C9
34	C	518	DGD	C2A-C1A-O1G-C1G
28	A	410	LMG	C17-C18-C19-C20
28	a	410	LMG	C17-C18-C19-C20
34	C	517	DGD	CBB-CCB-CDB-CEB
34	C	518	DGD	C8B-C9B-CAB-CBB
34	c	517	DGD	CBB-CCB-CDB-CEB
34	c	518	DGD	C8B-C9B-CAB-CBB
31	I	102	LMT	O5'-C5'-C6'-O6'
31	i	102	LMT	O5'-C5'-C6'-O6'
29	A	411	PL9	C12-C13-C14-C15
29	a	411	PL9	C12-C13-C14-C15
29	A	411	PL9	C12-C13-C14-C16
29	a	411	PL9	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
28	C	519	LMG	C20-C21-C22-C23
28	C	519	LMG	C38-C39-C40-C41
28	c	519	LMG	C20-C21-C22-C23
28	c	519	LMG	C38-C39-C40-C41
25	C	510	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
28	A	410	LMG	C20-C21-C22-C23
28	C	519	LMG	C17-C18-C19-C20
28	C	523	LMG	C17-C18-C19-C20
28	C	523	LMG	C38-C39-C40-C41
28	D	409	LMG	C35-C36-C37-C38
28	a	410	LMG	C20-C21-C22-C23
28	c	519	LMG	C17-C18-C19-C20
28	c	523	LMG	C17-C18-C19-C20
28	c	523	LMG	C38-C39-C40-C41
28	d	409	LMG	C35-C36-C37-C38
34	C	517	DGD	C8B-C9B-CAB-CBB
34	C	518	DGD	C8A-C9A-CAA-CBA
34	H	104	DGD	CBB-CCB-CDB-CEB
34	c	517	DGD	C8B-C9B-CAB-CBB
34	c	518	DGD	C8A-C9A-CAA-CBA
34	h	104	DGD	CBB-CCB-CDB-CEB
31	B	629	LMT	O5'-C5'-C6'-O6'
31	b	629	LMT	O5'-C5'-C6'-O6'
25	B	605	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
29	A	411	PL9	C47-C48-C49-C50
29	A	411	PL9	C47-C48-C49-C51
29	a	411	PL9	C47-C48-C49-C50
29	a	411	PL9	C47-C48-C49-C51
26	D	402	PHO	C3-C5-C6-C7
26	d	402	PHO	C3-C5-C6-C7
25	D	403	CLA	CBD-CGD-O2D-CED
25	d	403	CLA	CBD-CGD-O2D-CED
30	B	620	SQD	C34-C35-C36-C37
30	b	620	SQD	C34-C35-C36-C37
25	D	404	CLA	O1D-CGD-O2D-CED
25	d	404	CLA	O1D-CGD-O2D-CED
25	C	510	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
30	B	620	SQD	C24-C23-O48-C46
30	b	620	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
33	B	628	LHG	C24-C23-O8-C6
33	b	628	LHG	C24-C23-O8-C6
34	c	518	DGD	C2A-C1A-O1G-C1G
31	A	415	LMT	O5B-C5B-C6B-O6B
31	C	522	LMT	O5'-C5'-C6'-O6'
31	a	415	LMT	O5B-C5B-C6B-O6B
31	c	522	LMT	O5'-C5'-C6'-O6'
25	C	506	CLA	O1A-CGA-O2A-C1
25	c	506	CLA	O1A-CGA-O2A-C1
28	A	414	LMG	O10-C28-O8-C9
28	a	414	LMG	O10-C28-O8-C9
33	B	628	LHG	O10-C23-O8-C6
33	b	628	LHG	O10-C23-O8-C6
31	C	525	LMT	C4'-C5'-C6'-O6'
31	c	525	LMT	C4'-C5'-C6'-O6'
33	Z	102	LHG	C8-C7-O7-C5
33	z	102	LHG	C8-C7-O7-C5
34	C	518	DGD	O1A-C1A-O1G-C1G
34	c	518	DGD	O1A-C1A-O1G-C1G
31	X	101	LMT	C4'-C5'-C6'-O6'
31	x	101	LMT	C4'-C5'-C6'-O6'
31	B	624	LMT	C4'-C5'-C6'-O6'
31	B	625	LMT	C4B-C5B-C6B-O6B
31	B	626	LMT	C4'-C5'-C6'-O6'
31	E	103	LMT	C4'-C5'-C6'-O6'
31	I	102	LMT	C4'-C5'-C6'-O6'
31	I	104	LMT	C4'-C5'-C6'-O6'
31	b	624	LMT	C4'-C5'-C6'-O6'
31	b	625	LMT	C4B-C5B-C6B-O6B
31	b	626	LMT	C4'-C5'-C6'-O6'
31	e	103	LMT	C4'-C5'-C6'-O6'
31	i	102	LMT	C4'-C5'-C6'-O6'
31	i	104	LMT	C4'-C5'-C6'-O6'
25	C	511	CLA	O1D-CGD-O2D-CED
25	A	408	CLA	C4-C3-C5-C6
25	a	408	CLA	C4-C3-C5-C6
25	c	511	CLA	O1D-CGD-O2D-CED
29	A	411	PL9	C24-C26-C27-C28
29	A	411	PL9	C39-C41-C42-C43
29	a	411	PL9	C24-C26-C27-C28
29	a	411	PL9	C39-C41-C42-C43
28	C	523	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
28	c	523	LMG	O6-C5-C6-O5
31	K	105	LMT	O5B-C5B-C6B-O6B
31	k	105	LMT	O5B-C5B-C6B-O6B
30	B	620	SQD	O10-C23-O48-C46
30	b	620	SQD	O10-C23-O48-C46
26	A	407	PHO	C3-C5-C6-C7
26	a	407	PHO	C3-C5-C6-C7
28	C	523	LMG	O6-C1-O1-C7
28	c	523	LMG	O6-C1-O1-C7
30	A	413	SQD	O5-C1-O6-C44
30	F	102	SQD	O5-C1-O6-C44
30	a	413	SQD	O5-C1-O6-C44
30	f	102	SQD	O5-C1-O6-C44
31	C	522	LMT	O5'-C1'-O1'-C1
31	C	524	LMT	O5'-C1'-O1'-C1
31	D	412	LMT	O5'-C1'-O1'-C1
31	H	102	LMT	O5'-C1'-O1'-C1
31	I	104	LMT	O5'-C1'-O1'-C1
31	J	101	LMT	O5'-C1'-O1'-C1
31	M	101	LMT	O5'-C1'-O1'-C1
31	M	102	LMT	O5'-C1'-O1'-C1
31	X	105	LMT	O5'-C1'-O1'-C1
31	c	522	LMT	O5'-C1'-O1'-C1
31	c	524	LMT	O5'-C1'-O1'-C1
31	d	412	LMT	O5'-C1'-O1'-C1
31	h	102	LMT	O5'-C1'-O1'-C1
31	i	104	LMT	O5'-C1'-O1'-C1
31	j	101	LMT	O5'-C1'-O1'-C1
31	m	101	LMT	O5'-C1'-O1'-C1
31	m	102	LMT	O5'-C1'-O1'-C1
31	x	105	LMT	O5'-C1'-O1'-C1
25	B	611	CLA	CBD-CGD-O2D-CED
25	B	613	CLA	CBD-CGD-O2D-CED
25	b	611	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
31	E	103	LMT	C4B-C5B-C6B-O6B
31	e	103	LMT	C4B-C5B-C6B-O6B
31	I	103	LMT	O5'-C5'-C6'-O6'
31	K	105	LMT	O5'-C5'-C6'-O6'
31	i	103	LMT	O5'-C5'-C6'-O6'
31	k	105	LMT	O5'-C5'-C6'-O6'
31	K	105	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
31	k	105	LMT	C4B-C5B-C6B-O6B
25	B	615	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
31	J	101	LMT	C4'-C5'-C6'-O6'
31	j	101	LMT	C4'-C5'-C6'-O6'
33	Z	102	LHG	O9-C7-O7-C5
33	z	102	LHG	O9-C7-O7-C5
25	A	406	CLA	CBA-CGA-O2A-C1
25	B	605	CLA	CBA-CGA-O2A-C1
25	B	612	CLA	CBA-CGA-O2A-C1
25	B	616	CLA	CBA-CGA-O2A-C1
25	C	509	CLA	CBA-CGA-O2A-C1
25	a	406	CLA	CBA-CGA-O2A-C1
25	b	605	CLA	CBA-CGA-O2A-C1
25	b	612	CLA	CBA-CGA-O2A-C1
25	b	616	CLA	CBA-CGA-O2A-C1
25	c	509	CLA	CBA-CGA-O2A-C1
31	C	524	LMT	O5B-C5B-C6B-O6B
31	c	524	LMT	O5B-C5B-C6B-O6B
31	I	103	LMT	C4'-C5'-C6'-O6'
31	i	103	LMT	C4'-C5'-C6'-O6'
31	A	415	LMT	C4B-C5B-C6B-O6B
31	a	415	LMT	C4B-C5B-C6B-O6B
25	B	610	CLA	O1D-CGD-O2D-CED
25	C	505	CLA	C11-C12-C13-C14
25	C	510	CLA	C6-C7-C8-C9
25	C	510	CLA	C11-C12-C13-C14
25	C	514	CLA	C6-C7-C8-C9
25	c	505	CLA	C11-C12-C13-C14
25	c	510	CLA	C6-C7-C8-C9
25	c	510	CLA	C11-C12-C13-C14
25	c	514	CLA	C6-C7-C8-C9
31	b	629	LMT	C4'-C5'-C6'-O6'
25	B	606	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
25	b	610	CLA	O1D-CGD-O2D-CED
28	C	523	LMG	C2-C1-O1-C7
28	c	523	LMG	C2-C1-O1-C7
30	A	412	SQD	C2-C1-O6-C44
30	K	101	SQD	C2-C1-O6-C44
30	a	412	SQD	C2-C1-O6-C44
30	k	101	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
31	C	522	LMT	C2'-C1'-O1'-C1
31	C	524	LMT	C2'-C1'-O1'-C1
31	D	412	LMT	C2'-C1'-O1'-C1
31	H	102	LMT	C2'-C1'-O1'-C1
31	J	101	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	C2'-C1'-O1'-C1
31	X	105	LMT	C2'-C1'-O1'-C1
31	c	522	LMT	C2'-C1'-O1'-C1
31	c	524	LMT	C2'-C1'-O1'-C1
31	d	412	LMT	C2'-C1'-O1'-C1
31	h	102	LMT	C2'-C1'-O1'-C1
31	j	101	LMT	C2'-C1'-O1'-C1
31	m	102	LMT	C2'-C1'-O1'-C1
31	x	105	LMT	C2'-C1'-O1'-C1
33	E	102	LHG	O2-C2-C3-O3
33	e	102	LHG	O2-C2-C3-O3
31	H	102	LMT	O5'-C5'-C6'-O6'
31	h	102	LMT	O5'-C5'-C6'-O6'
31	B	629	LMT	C4'-C5'-C6'-O6'
31	K	105	LMT	C4'-C5'-C6'-O6'
31	k	105	LMT	C4'-C5'-C6'-O6'
27	A	409	BCR	C7-C8-C9-C34
27	a	409	BCR	C7-C8-C9-C34
36	H	101	RRX	C36-C18-C19-C20
36	h	101	RRX	C36-C18-C19-C20
31	B	624	LMT	O5'-C5'-C6'-O6'
31	B	625	LMT	O5B-C5B-C6B-O6B
31	E	103	LMT	O5'-C5'-C6'-O6'
31	b	624	LMT	O5'-C5'-C6'-O6'
31	b	625	LMT	O5B-C5B-C6B-O6B
31	e	103	LMT	O5'-C5'-C6'-O6'
36	H	101	RRX	C17-C18-C19-C20
36	h	101	RRX	C17-C18-C19-C20
25	B	607	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C2A-CAA-CBA-CGA
25	B	612	CLA	O1A-CGA-O2A-C1
25	B	616	CLA	O1A-CGA-O2A-C1
25	C	509	CLA	O1A-CGA-O2A-C1
25	b	612	CLA	O1A-CGA-O2A-C1
25	b	616	CLA	O1A-CGA-O2A-C1
25	c	509	CLA	O1A-CGA-O2A-C1
31	I	104	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	i	104	LMT	O5'-C5'-C6'-O6'
30	F	102	SQD	O49-C7-O47-C45
30	f	102	SQD	O49-C7-O47-C45
28	A	410	LMG	C8-C9-O8-C28
33	E	102	LHG	O7-C5-C6-O8
33	e	102	LHG	O7-C5-C6-O8
25	B	609	CLA	CBA-CGA-O2A-C1
25	b	609	CLA	CBA-CGA-O2A-C1
25	C	502	CLA	C15-C16-C17-C18
25	c	502	CLA	C15-C16-C17-C18
25	A	406	CLA	C2-C1-O2A-CGA
25	B	612	CLA	C2-C1-O2A-CGA
25	a	406	CLA	C2-C1-O2A-CGA
25	b	612	CLA	C2-C1-O2A-CGA
25	C	503	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	A	408	CLA	C5-C6-C7-C8
25	C	507	CLA	C13-C15-C16-C17
25	a	408	CLA	C5-C6-C7-C8
25	c	507	CLA	C13-C15-C16-C17
31	F	103	LMT	O5'-C5'-C6'-O6'
31	f	103	LMT	O5'-C5'-C6'-O6'
33	D	406	LHG	O1-C1-C2-O2
33	d	406	LHG	O1-C1-C2-O2
31	I	101	LMT	O5'-C5'-C6'-O6'
31	i	101	LMT	O5'-C5'-C6'-O6'
31	C	522	LMT	C4'-C5'-C6'-O6'
31	c	522	LMT	C4'-C5'-C6'-O6'
25	B	607	CLA	CBA-CGA-O2A-C1
25	b	607	CLA	CBA-CGA-O2A-C1
33	D	408	LHG	C10-C11-C12-C13
33	d	408	LHG	C10-C11-C12-C13
25	b	602	CLA	O1D-CGD-O2D-CED
25	d	403	CLA	O1D-CGD-O2D-CED
30	K	101	SQD	C7-C8-C9-C10
30	k	101	SQD	C7-C8-C9-C10
31	Y	101	LMT	O1'-C1-C2-C3
31	y	101	LMT	O1'-C1-C2-C3
25	B	602	CLA	O1D-CGD-O2D-CED
25	D	403	CLA	O1D-CGD-O2D-CED
29	A	411	PL9	C9-C11-C12-C13
29	a	411	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	D	403	CLA	C15-C16-C17-C18
25	d	403	CLA	C15-C16-C17-C18
28	a	410	LMG	C8-C9-O8-C28
31	H	102	LMT	O1'-C1-C2-C3
31	h	102	LMT	O1'-C1-C2-C3
28	D	409	LMG	O6-C5-C6-O5
28	d	409	LMG	O6-C5-C6-O5
33	D	408	LHG	C7-C8-C9-C10
33	E	102	LHG	C7-C8-C9-C10
33	Z	102	LHG	C7-C8-C9-C10
33	d	408	LHG	C7-C8-C9-C10
33	e	102	LHG	C7-C8-C9-C10
33	z	102	LHG	C7-C8-C9-C10
25	B	605	CLA	O1A-CGA-O2A-C1
25	B	609	CLA	O1A-CGA-O2A-C1
25	b	605	CLA	O1A-CGA-O2A-C1
25	b	609	CLA	O1A-CGA-O2A-C1
25	B	611	CLA	C15-C16-C17-C18
25	b	611	CLA	C15-C16-C17-C18
31	C	525	LMT	O5'-C5'-C6'-O6'
31	D	412	LMT	O5'-C5'-C6'-O6'
31	d	412	LMT	O5'-C5'-C6'-O6'
25	B	606	CLA	C2A-CAA-CBA-CGA
25	D	401	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	d	401	CLA	C2A-CAA-CBA-CGA
25	C	509	CLA	O1D-CGD-O2D-CED
25	c	509	CLA	O1D-CGD-O2D-CED
31	X	105	LMT	O1'-C1-C2-C3
31	x	105	LMT	O1'-C1-C2-C3
27	A	409	BCR	C10-C11-C12-C13
27	F	101	BCR	C10-C11-C12-C13
27	a	409	BCR	C10-C11-C12-C13
27	f	101	BCR	C10-C11-C12-C13
25	A	406	CLA	C15-C16-C17-C18
25	B	602	CLA	C15-C16-C17-C18
25	C	507	CLA	C15-C16-C17-C18
25	C	508	CLA	C15-C16-C17-C18
25	C	514	CLA	C10-C11-C12-C13
25	C	514	CLA	C15-C16-C17-C18
25	D	404	CLA	C13-C15-C16-C17
25	a	406	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	C15-C16-C17-C18
25	c	507	CLA	C15-C16-C17-C18
25	c	508	CLA	C15-C16-C17-C18
25	c	514	CLA	C10-C11-C12-C13
25	c	514	CLA	C15-C16-C17-C18
25	d	404	CLA	C13-C15-C16-C17
31	c	525	LMT	O5'-C5'-C6'-O6'
31	A	416	LMT	O1'-C1-C2-C3
31	a	416	LMT	O1'-C1-C2-C3
30	A	412	SQD	C23-C24-C25-C26
30	a	412	SQD	C23-C24-C25-C26
33	D	406	LHG	C23-C24-C25-C26
33	Z	102	LHG	C23-C24-C25-C26
33	d	406	LHG	C23-C24-C25-C26
33	z	102	LHG	C23-C24-C25-C26
25	A	408	CLA	C3-C5-C6-C7
25	a	408	CLA	C3-C5-C6-C7
31	D	412	LMT	C4'-C5'-C6'-O6'
31	d	412	LMT	C4'-C5'-C6'-O6'
25	B	611	CLA	C13-C15-C16-C17
25	B	614	CLA	C8-C10-C11-C12
25	D	401	CLA	C15-C16-C17-C18
25	b	611	CLA	C13-C15-C16-C17
25	b	614	CLA	C8-C10-C11-C12
25	d	401	CLA	C15-C16-C17-C18
33	B	627	LHG	O2-C2-C3-O3
33	b	627	LHG	O2-C2-C3-O3
25	C	505	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
25	A	406	CLA	O1A-CGA-O2A-C1
25	a	406	CLA	O1A-CGA-O2A-C1
28	H	105	LMG	C28-C29-C30-C31
28	h	105	LMG	C28-C29-C30-C31
33	B	627	LHG	C7-C8-C9-C10
33	D	408	LHG	C23-C24-C25-C26
33	b	627	LHG	C7-C8-C9-C10
33	d	408	LHG	C23-C24-C25-C26
25	B	608	CLA	C15-C16-C17-C18
25	C	511	CLA	C13-C15-C16-C17
25	b	608	CLA	C15-C16-C17-C18
25	c	511	CLA	C13-C15-C16-C17
31	T	101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	t	101	LMT	O1'-C1-C2-C3
31	I	103	LMT	O5B-C5B-C6B-O6B
31	i	103	LMT	O5B-C5B-C6B-O6B
25	B	613	CLA	C10-C11-C12-C13
25	C	505	CLA	C15-C16-C17-C18
25	b	613	CLA	C10-C11-C12-C13
25	c	505	CLA	C15-C16-C17-C18
25	B	607	CLA	O1A-CGA-O2A-C1
25	b	607	CLA	O1A-CGA-O2A-C1
31	F	103	LMT	O5B-C5B-C6B-O6B
31	f	103	LMT	O5B-C5B-C6B-O6B
25	B	609	CLA	C13-C15-C16-C17
25	C	512	CLA	C15-C16-C17-C18
25	b	609	CLA	C13-C15-C16-C17
25	c	512	CLA	C15-C16-C17-C18
33	D	406	LHG	C8-C7-O7-C5
33	d	406	LHG	C8-C7-O7-C5
33	E	102	LHG	C25-C26-C27-C28
33	e	102	LHG	C25-C26-C27-C28
33	D	406	LHG	O9-C7-O7-C5
33	d	406	LHG	O9-C7-O7-C5
31	D	410	LMT	C4'-C5'-C6'-O6'
31	d	410	LMT	C4'-C5'-C6'-O6'
25	C	514	CLA	CBA-CGA-O2A-C1
25	c	514	CLA	CBA-CGA-O2A-C1
25	A	405	CLA	C15-C16-C17-C18
25	B	611	CLA	C8-C10-C11-C12
25	C	504	CLA	C15-C16-C17-C18
25	D	404	CLA	C15-C16-C17-C18
25	a	405	CLA	C15-C16-C17-C18
25	b	611	CLA	C8-C10-C11-C12
25	c	504	CLA	C15-C16-C17-C18
25	d	404	CLA	C15-C16-C17-C18
25	C	503	CLA	C13-C15-C16-C17
25	C	508	CLA	C13-C15-C16-C17
25	a	406	CLA	C13-C15-C16-C17
25	c	503	CLA	C13-C15-C16-C17
31	B	629	LMT	O1'-C1-C2-C3
31	b	629	LMT	O1'-C1-C2-C3
31	D	410	LMT	O5'-C5'-C6'-O6'
31	d	410	LMT	O5'-C5'-C6'-O6'
25	A	406	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	C8-C10-C11-C12
25	C	512	CLA	C10-C11-C12-C13
25	b	604	CLA	C8-C10-C11-C12
25	c	508	CLA	C13-C15-C16-C17
25	c	512	CLA	C10-C11-C12-C13
25	C	514	CLA	C5-C6-C7-C8
25	c	514	CLA	C5-C6-C7-C8
25	B	616	CLA	C3-C5-C6-C7
25	b	616	CLA	C3-C5-C6-C7
30	C	501	SQD	C8-C7-O47-C45
30	c	501	SQD	C8-C7-O47-C45
31	B	623	LMT	C2'-C1'-O1'-C1
31	C	525	LMT	C2'-C1'-O1'-C1
31	M	101	LMT	C2'-C1'-O1'-C1
31	b	623	LMT	C2'-C1'-O1'-C1
31	c	525	LMT	C2'-C1'-O1'-C1
31	m	101	LMT	C2'-C1'-O1'-C1
25	C	507	CLA	CBA-CGA-O2A-C1
25	c	507	CLA	CBA-CGA-O2A-C1
25	A	405	CLA	C16-C17-C18-C20
25	a	405	CLA	C16-C17-C18-C20
27	B	617	BCR	C37-C22-C23-C24
27	Z	101	BCR	C37-C22-C23-C24
27	b	617	BCR	C37-C22-C23-C24
27	z	101	BCR	C37-C22-C23-C24
31	A	416	LMT	O5'-C5'-C6'-O6'
31	a	416	LMT	O5'-C5'-C6'-O6'
35	E	104	HEM	C3D-CAD-CBD-CGD
35	e	104	HEM	C3D-CAD-CBD-CGD
25	C	508	CLA	C2A-CAA-CBA-CGA
25	c	508	CLA	C2A-CAA-CBA-CGA
33	D	408	LHG	O1-C1-C2-C3
33	E	102	LHG	O1-C1-C2-C3
33	d	408	LHG	O1-C1-C2-C3
33	e	102	LHG	O1-C1-C2-C3
31	K	105	LMT	C1-C2-C3-C4
31	k	105	LMT	C1-C2-C3-C4
25	A	406	CLA	C16-C17-C18-C19
25	A	406	CLA	C16-C17-C18-C20
25	A	408	CLA	C11-C12-C13-C15
25	B	616	CLA	C11-C12-C13-C15
25	C	505	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	a	406	CLA	C16-C17-C18-C19
25	a	406	CLA	C16-C17-C18-C20
25	a	408	CLA	C11-C12-C13-C15
25	b	616	CLA	C11-C12-C13-C15
25	c	505	CLA	C16-C17-C18-C20
31	D	411	LMT	C1-C2-C3-C4
31	E	103	LMT	C1-C2-C3-C4
31	d	411	LMT	C1-C2-C3-C4
31	e	103	LMT	C1-C2-C3-C4
31	B	623	LMT	O5'-C1'-O1'-C1
31	b	623	LMT	O5'-C1'-O1'-C1
25	a	408	CLA	C2-C3-C5-C6
31	I	102	LMT	O1'-C1-C2-C3
31	i	102	LMT	O1'-C1-C2-C3
31	x	101	LMT	C1-C2-C3-C4
25	B	611	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	C2-C1-O2A-CGA
25	C	508	CLA	C2-C1-O2A-CGA
25	c	503	CLA	C2-C1-O2A-CGA
25	c	508	CLA	C2-C1-O2A-CGA
25	A	408	CLA	C11-C12-C13-C14
25	B	610	CLA	C16-C17-C18-C20
25	a	408	CLA	C11-C12-C13-C14
25	b	610	CLA	C16-C17-C18-C20
31	X	101	LMT	C1-C2-C3-C4
25	B	616	CLA	C10-C11-C12-C13
25	C	506	CLA	C5-C6-C7-C8
25	C	511	CLA	C8-C10-C11-C12
25	b	616	CLA	C10-C11-C12-C13
25	c	511	CLA	C8-C10-C11-C12
33	B	628	LHG	C5-C6-O8-C23
33	b	628	LHG	C5-C6-O8-C23
30	H	103	SQD	C15-C16-C17-C18
30	h	103	SQD	C15-C16-C17-C18
31	M	101	LMT	C11-C10-C9-C8
31	m	101	LMT	C11-C10-C9-C8
36	H	101	RRX	C14-C15-C16-C17
36	h	101	RRX	C14-C15-C16-C17
28	C	519	LMG	C34-C35-C36-C37
28	c	519	LMG	C34-C35-C36-C37
31	B	623	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	b	623	LMT	C5-C6-C7-C8
25	c	506	CLA	C5-C6-C7-C8
28	C	519	LMG	C39-C40-C41-C42
28	H	105	LMG	C13-C14-C15-C16
28	c	519	LMG	C39-C40-C41-C42
28	h	105	LMG	C13-C14-C15-C16
33	D	407	LHG	C13-C14-C15-C16
33	d	407	LHG	C13-C14-C15-C16
30	F	102	SQD	O10-C23-O48-C46
30	f	102	SQD	O10-C23-O48-C46
25	C	511	CLA	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1
28	C	519	LMG	C33-C34-C35-C36
28	H	105	LMG	C11-C12-C13-C14
28	c	519	LMG	C33-C34-C35-C36
28	h	105	LMG	C11-C12-C13-C14
30	K	101	SQD	C26-C27-C28-C29
30	k	101	SQD	C26-C27-C28-C29
31	I	102	LMT	C7-C8-C9-C10
31	i	102	LMT	C7-C8-C9-C10
33	D	408	LHG	C9-C10-C11-C12
33	E	102	LHG	C14-C15-C16-C17
33	Z	102	LHG	C29-C30-C31-C32
33	d	408	LHG	C9-C10-C11-C12
33	e	102	LHG	C14-C15-C16-C17
33	z	102	LHG	C29-C30-C31-C32
31	A	416	LMT	C2-C1-O1'-C1'
31	B	626	LMT	C2-C1-O1'-C1'
31	D	411	LMT	C2-C1-O1'-C1'
31	I	102	LMT	C2-C1-O1'-C1'
31	T	101	LMT	C2-C1-O1'-C1'
31	X	102	LMT	C2-C1-O1'-C1'
31	a	416	LMT	C2-C1-O1'-C1'
31	b	626	LMT	C2-C1-O1'-C1'
31	d	411	LMT	C2-C1-O1'-C1'
31	i	102	LMT	C2-C1-O1'-C1'
31	t	101	LMT	C2-C1-O1'-C1'
31	x	102	LMT	C2-C1-O1'-C1'
33	D	407	LHG	O1-C1-C2-O2
33	d	407	LHG	O1-C1-C2-O2
30	A	413	SQD	C9-C10-C11-C12
30	C	501	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	c	501	SQD	C25-C26-C27-C28
31	K	105	LMT	C3-C4-C5-C6
31	i	104	LMT	C2-C3-C4-C5
31	k	105	LMT	C3-C4-C5-C6
30	F	102	SQD	C7-C8-C9-C10
30	f	102	SQD	C7-C8-C9-C10
30	a	413	SQD	C9-C10-C11-C12
31	I	104	LMT	C2-C3-C4-C5
31	J	101	LMT	C7-C8-C9-C10
31	T	101	LMT	C11-C10-C9-C8
31	j	101	LMT	C7-C8-C9-C10
31	t	101	LMT	C11-C10-C9-C8
31	M	102	LMT	O5'-C5'-C6'-O6'
31	m	102	LMT	O5'-C5'-C6'-O6'
25	B	610	CLA	C16-C17-C18-C19
25	B	616	CLA	C11-C12-C13-C14
25	C	505	CLA	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C19
25	b	616	CLA	C11-C12-C13-C14
25	c	505	CLA	C16-C17-C18-C19
25	B	613	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
30	A	412	SQD	C11-C10-C9-C8
30	a	412	SQD	C11-C10-C9-C8
31	C	525	LMT	C5-C6-C7-C8
31	J	101	LMT	C4-C5-C6-C7
31	X	103	LMT	C5-C6-C7-C8
31	c	525	LMT	C5-C6-C7-C8
31	j	101	LMT	C4-C5-C6-C7
31	x	103	LMT	C5-C6-C7-C8
34	C	516	DGD	CAA-CBA-CCA-CDA
34	c	516	DGD	CAA-CBA-CCA-CDA
25	C	509	CLA	C8-C10-C11-C12
25	c	509	CLA	C8-C10-C11-C12
33	B	628	LHG	C27-C28-C29-C30
33	b	628	LHG	C27-C28-C29-C30
30	K	101	SQD	C24-C23-O48-C46
30	k	101	SQD	C24-C23-O48-C46
31	X	104	LMT	C1-C2-C3-C4
31	M	101	LMT	O5'-C5'-C6'-O6'
31	m	101	LMT	O5'-C5'-C6'-O6'
31	X	102	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	x	102	LMT	C5-C6-C7-C8
25	C	505	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
33	B	627	LHG	C18-C19-C20-C21
33	D	407	LHG	C24-C25-C26-C27
33	b	627	LHG	C18-C19-C20-C21
33	d	407	LHG	C24-C25-C26-C27
34	H	104	DGD	C4A-C5A-C6A-C7A
34	h	104	DGD	C4A-C5A-C6A-C7A
25	A	408	CLA	C2-C3-C5-C6
31	C	524	LMT	C1-C2-C3-C4
31	M	101	LMT	C1-C2-C3-C4
31	c	524	LMT	C1-C2-C3-C4
31	m	101	LMT	C1-C2-C3-C4
31	x	104	LMT	C1-C2-C3-C4
34	C	518	DGD	C9B-CAB-CBB-CCB
34	c	518	DGD	C9B-CAB-CBB-CCB
25	B	603	CLA	C5-C6-C7-C8
25	b	603	CLA	C5-C6-C7-C8
28	C	523	LMG	C4-C5-C6-O5
28	A	414	LMG	C28-C29-C30-C31
28	a	414	LMG	C28-C29-C30-C31
25	C	514	CLA	O1A-CGA-O2A-C1
25	c	514	CLA	O1A-CGA-O2A-C1
30	B	620	SQD	C32-C33-C34-C35
30	b	620	SQD	C32-C33-C34-C35
34	H	104	DGD	CCB-CDB-CEB-CFB
34	h	104	DGD	CCB-CDB-CEB-CFB
28	c	523	LMG	C4-C5-C6-O5
31	I	104	LMT	C6-C7-C8-C9
31	i	104	LMT	C6-C7-C8-C9
28	A	410	LMG	C32-C33-C34-C35
28	a	410	LMG	C32-C33-C34-C35
31	F	103	LMT	C11-C10-C9-C8
31	H	102	LMT	C6-C7-C8-C9
31	I	104	LMT	C5-C6-C7-C8
31	f	103	LMT	C11-C10-C9-C8
31	h	102	LMT	C6-C7-C8-C9
31	i	104	LMT	C5-C6-C7-C8
28	B	621	LMG	C33-C34-C35-C36
28	b	621	LMG	C33-C34-C35-C36
33	B	628	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	D	406	LHG	C28-C29-C30-C31
33	D	408	LHG	C33-C34-C35-C36
33	Z	102	LHG	C30-C31-C32-C33
33	b	628	LHG	C13-C14-C15-C16
33	d	406	LHG	C28-C29-C30-C31
33	d	408	LHG	C33-C34-C35-C36
33	z	102	LHG	C30-C31-C32-C33
25	C	507	CLA	O1A-CGA-O2A-C1
25	c	507	CLA	O1A-CGA-O2A-C1
28	D	409	LMG	C32-C33-C34-C35
28	d	409	LMG	C32-C33-C34-C35
34	C	518	DGD	C7A-C8A-C9A-CAA
34	c	518	DGD	C7A-C8A-C9A-CAA
25	B	615	CLA	O1D-CGD-O2D-CED
25	b	615	CLA	O1D-CGD-O2D-CED
28	D	409	LMG	C34-C35-C36-C37
31	Y	101	LMT	C1-C2-C3-C4
31	y	101	LMT	C1-C2-C3-C4
28	d	409	LMG	C34-C35-C36-C37
30	B	620	SQD	C31-C32-C33-C34
30	C	501	SQD	C17-C18-C19-C20
30	F	102	SQD	C9-C10-C11-C12
30	b	620	SQD	C31-C32-C33-C34
30	c	501	SQD	C17-C18-C19-C20
30	f	102	SQD	C9-C10-C11-C12
31	b	629	LMT	C4-C5-C6-C7
27	B	617	BCR	C1-C6-C7-C8
27	B	617	BCR	C5-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C26
27	K	102	BCR	C1-C6-C7-C8
27	b	617	BCR	C1-C6-C7-C8
27	b	617	BCR	C5-C6-C7-C8
27	b	619	BCR	C23-C24-C25-C26
27	k	102	BCR	C1-C6-C7-C8
31	B	629	LMT	C4-C5-C6-C7
31	E	103	LMT	C2-C3-C4-C5
31	K	105	LMT	C2-C3-C4-C5
31	X	102	LMT	C6-C7-C8-C9
31	e	103	LMT	C2-C3-C4-C5
31	k	105	LMT	C2-C3-C4-C5
31	x	102	LMT	C6-C7-C8-C9
28	H	105	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
28	h	105	LMG	C11-C10-O7-C8
33	D	408	LHG	C32-C33-C34-C35
33	d	408	LHG	C32-C33-C34-C35
31	B	629	LMT	C6-C7-C8-C9
25	C	511	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
31	b	629	LMT	C6-C7-C8-C9
31	j	101	LMT	C6-C7-C8-C9
30	A	413	SQD	O49-C7-O47-C45
30	a	413	SQD	O49-C7-O47-C45
31	J	101	LMT	C6-C7-C8-C9
33	D	407	LHG	C26-C27-C28-C29
33	d	407	LHG	C26-C27-C28-C29
27	B	619	BCR	C10-C11-C12-C13
27	Z	101	BCR	C10-C11-C12-C13
27	z	101	BCR	C10-C11-C12-C13
36	H	101	RRX	C10-C11-C12-C13
36	h	101	RRX	C10-C11-C12-C13
30	K	101	SQD	C12-C13-C14-C15
30	k	101	SQD	C12-C13-C14-C15
31	X	102	LMT	C4-C5-C6-C7
31	x	102	LMT	C4-C5-C6-C7
31	B	623	LMT	C3-C4-C5-C6
31	b	623	LMT	C3-C4-C5-C6
34	H	104	DGD	C7B-C8B-C9B-CAB
34	h	104	DGD	C7B-C8B-C9B-CAB
31	C	525	LMT	O5'-C1'-O1'-C1
31	c	525	LMT	O5'-C1'-O1'-C1
34	C	516	DGD	O6E-C1E-O5D-C6D
34	C	517	DGD	O6E-C1E-O5D-C6D
34	c	516	DGD	O6E-C1E-O5D-C6D
34	c	517	DGD	O6E-C1E-O5D-C6D
31	I	101	LMT	C11-C10-C9-C8
31	Y	101	LMT	C5-C6-C7-C8
31	i	101	LMT	C11-C10-C9-C8
31	y	101	LMT	C5-C6-C7-C8
33	D	406	LHG	C13-C14-C15-C16
33	d	406	LHG	C13-C14-C15-C16
31	C	525	LMT	O1'-C1-C2-C3
31	c	525	LMT	O1'-C1-C2-C3
31	B	624	LMT	C2'-C1'-O1'-C1
31	D	411	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	X	104	LMT	C2'-C1'-O1'-C1
31	b	624	LMT	C2'-C1'-O1'-C1
31	d	411	LMT	C2'-C1'-O1'-C1
31	x	104	LMT	C2'-C1'-O1'-C1
34	C	517	DGD	C2E-C1E-O5D-C6D
34	c	517	DGD	C2E-C1E-O5D-C6D
31	C	522	LMT	C4-C5-C6-C7
31	c	522	LMT	C4-C5-C6-C7
33	B	627	LHG	C15-C16-C17-C18
33	b	627	LHG	C15-C16-C17-C18
27	K	102	BCR	C9-C10-C11-C12
27	k	102	BCR	C9-C10-C11-C12
28	C	523	LMG	C11-C10-O7-C8
28	c	523	LMG	C11-C10-O7-C8
30	F	102	SQD	C8-C7-O47-C45
30	f	102	SQD	C8-C7-O47-C45
33	E	102	LHG	C8-C7-O7-C5
33	e	102	LHG	C8-C7-O7-C5
28	A	410	LMG	C28-C29-C30-C31
28	a	410	LMG	C28-C29-C30-C31
31	B	623	LMT	C7-C8-C9-C10
31	b	623	LMT	C7-C8-C9-C10
34	C	517	DGD	CAA-CBA-CCA-CDA
34	c	517	DGD	CAA-CBA-CCA-CDA
28	C	523	LMG	O9-C10-O7-C8
28	c	523	LMG	O9-C10-O7-C8
31	C	524	LMT	O1'-C1-C2-C3
31	c	524	LMT	O1'-C1-C2-C3
30	A	413	SQD	C14-C15-C16-C17
30	a	413	SQD	C14-C15-C16-C17
33	Z	102	LHG	C10-C11-C12-C13
33	z	102	LHG	C10-C11-C12-C13
34	C	518	DGD	C3A-C4A-C5A-C6A
34	c	518	DGD	C3A-C4A-C5A-C6A
30	B	620	SQD	C9-C10-C11-C12
31	X	103	LMT	C4-C5-C6-C7
33	B	628	LHG	C11-C10-C9-C8
33	D	407	LHG	C33-C34-C35-C36
33	Z	102	LHG	C26-C27-C28-C29
33	b	628	LHG	C11-C10-C9-C8
33	d	407	LHG	C33-C34-C35-C36
33	z	102	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	b	620	SQD	C9-C10-C11-C12
31	x	103	LMT	C4-C5-C6-C7
28	B	621	LMG	C10-C11-C12-C13
28	b	621	LMG	C10-C11-C12-C13
30	C	501	SQD	C7-C8-C9-C10
30	c	501	SQD	C7-C8-C9-C10
27	Z	101	BCR	C7-C8-C9-C10
27	z	101	BCR	C7-C8-C9-C10
28	A	410	LMG	C12-C13-C14-C15
28	a	410	LMG	C12-C13-C14-C15
31	X	102	LMT	O1'-C1-C2-C3
31	x	102	LMT	O1'-C1-C2-C3
28	D	409	LMG	C37-C38-C39-C40
28	d	409	LMG	C37-C38-C39-C40
31	M	101	LMT	C4-C5-C6-C7
31	m	101	LMT	C4-C5-C6-C7
28	D	409	LMG	C36-C37-C38-C39
28	d	409	LMG	C36-C37-C38-C39
31	D	410	LMT	C3-C4-C5-C6
31	d	410	LMT	C3-C4-C5-C6
31	B	625	LMT	O1'-C1-C2-C3
31	b	625	LMT	O1'-C1-C2-C3
28	B	621	LMG	C16-C17-C18-C19
31	B	626	LMT	C2-C3-C4-C5
31	b	626	LMT	C2-C3-C4-C5
25	C	509	CLA	C13-C15-C16-C17
25	C	510	CLA	C10-C11-C12-C13
25	c	510	CLA	C10-C11-C12-C13
28	b	621	LMG	C16-C17-C18-C19
33	D	406	LHG	C16-C17-C18-C19
33	d	406	LHG	C16-C17-C18-C19
31	K	105	LMT	C5'-C4'-O1B-C1B
31	k	105	LMT	C5'-C4'-O1B-C1B
25	c	509	CLA	C13-C15-C16-C17
31	E	101	LMT	O1'-C1-C2-C3
31	e	101	LMT	O1'-C1-C2-C3
28	H	105	LMG	C30-C31-C32-C33
28	h	105	LMG	C30-C31-C32-C33
30	A	413	SQD	C26-C27-C28-C29
30	a	413	SQD	C26-C27-C28-C29
31	I	104	LMT	C3-C4-C5-C6
31	Y	101	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	i	104	LMT	C3-C4-C5-C6
33	D	408	LHG	C28-C29-C30-C31
33	d	408	LHG	C28-C29-C30-C31
31	C	525	LMT	C1-C2-C3-C4
31	c	525	LMT	C1-C2-C3-C4
30	A	413	SQD	C12-C13-C14-C15
30	a	413	SQD	C12-C13-C14-C15
31	y	101	LMT	C4-C5-C6-C7
34	C	516	DGD	C4B-C5B-C6B-C7B
34	c	516	DGD	C4B-C5B-C6B-C7B
30	C	501	SQD	C14-C15-C16-C17
30	C	501	SQD	C29-C30-C31-C32
30	c	501	SQD	C14-C15-C16-C17
30	c	501	SQD	C29-C30-C31-C32
31	B	625	LMT	C2-C3-C4-C5
31	B	626	LMT	C11-C10-C9-C8
31	F	103	LMT	C3-C4-C5-C6
31	b	625	LMT	C2-C3-C4-C5
31	b	626	LMT	C11-C10-C9-C8
31	f	103	LMT	C3-C4-C5-C6
33	D	407	LHG	C11-C12-C13-C14
33	d	407	LHG	C11-C12-C13-C14
25	B	604	CLA	C5-C6-C7-C8
25	b	604	CLA	C5-C6-C7-C8
34	C	516	DGD	O6E-C5E-C6E-O5E
34	c	516	DGD	O6E-C5E-C6E-O5E
31	D	411	LMT	C2-C3-C4-C5
31	d	411	LMT	C2-C3-C4-C5
31	X	104	LMT	O1'-C1-C2-C3
31	x	104	LMT	O1'-C1-C2-C3
28	C	523	LMG	C13-C14-C15-C16
28	c	523	LMG	C13-C14-C15-C16
30	H	103	SQD	C14-C15-C16-C17
30	h	103	SQD	C14-C15-C16-C17
31	i	102	LMT	C2-C3-C4-C5
25	B	615	CLA	C2-C1-O2A-CGA
25	C	514	CLA	C2-C1-O2A-CGA
25	b	615	CLA	C2-C1-O2A-CGA
25	c	514	CLA	C2-C1-O2A-CGA
26	A	407	PHO	C16-C17-C18-C20
26	a	407	PHO	C16-C17-C18-C20
25	B	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	b	603	CLA	C15-C16-C17-C18
31	A	416	LMT	C4'-C5'-C6'-O6'
31	a	416	LMT	C4'-C5'-C6'-O6'
31	I	102	LMT	C2-C3-C4-C5
30	C	501	SQD	C11-C10-C9-C8
30	a	413	SQD	C28-C29-C30-C31
31	B	623	LMT	C6-C7-C8-C9
31	b	623	LMT	C6-C7-C8-C9
34	C	518	DGD	C5B-C6B-C7B-C8B
34	c	518	DGD	C5B-C6B-C7B-C8B
25	B	601	CLA	C2A-CAA-CBA-CGA
25	C	502	CLA	C2A-CAA-CBA-CGA
25	b	601	CLA	C2A-CAA-CBA-CGA
25	c	502	CLA	C2A-CAA-CBA-CGA
28	A	410	LMG	C21-C22-C23-C24
28	a	410	LMG	C21-C22-C23-C24
30	A	412	SQD	C12-C13-C14-C15
30	A	413	SQD	C28-C29-C30-C31
30	a	412	SQD	C12-C13-C14-C15
30	c	501	SQD	C11-C10-C9-C8
28	D	409	LMG	C31-C32-C33-C34
28	d	409	LMG	C31-C32-C33-C34
25	B	609	CLA	C15-C16-C17-C18
25	b	609	CLA	C15-C16-C17-C18
30	A	412	SQD	C27-C28-C29-C30
30	A	413	SQD	C11-C10-C9-C8
30	a	412	SQD	C27-C28-C29-C30
30	a	413	SQD	C11-C10-C9-C8
31	D	411	LMT	O1'-C1-C2-C3
31	d	411	LMT	O1'-C1-C2-C3
33	D	407	LHG	C34-C35-C36-C37
25	A	408	CLA	C1A-C2A-CAA-CBA
25	B	603	CLA	C1A-C2A-CAA-CBA
25	B	605	CLA	C1A-C2A-CAA-CBA
25	B	606	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C1A-C2A-CAA-CBA
25	C	502	CLA	C1A-C2A-CAA-CBA
25	C	507	CLA	C1A-C2A-CAA-CBA
25	C	509	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	C	514	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	a	408	CLA	C1A-C2A-CAA-CBA
25	b	603	CLA	C1A-C2A-CAA-CBA
25	b	605	CLA	C1A-C2A-CAA-CBA
25	b	606	CLA	C1A-C2A-CAA-CBA
25	b	609	CLA	C1A-C2A-CAA-CBA
25	c	502	CLA	C1A-C2A-CAA-CBA
25	c	507	CLA	C1A-C2A-CAA-CBA
25	c	509	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	514	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	C1A-C2A-CAA-CBA
25	C	502	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	CBA-CGA-O2A-C1
31	C	524	LMT	C4-C5-C6-C7
31	c	524	LMT	C4-C5-C6-C7
33	d	407	LHG	C34-C35-C36-C37
30	B	620	SQD	C26-C27-C28-C29
30	F	102	SQD	C11-C10-C9-C8
30	b	620	SQD	C26-C27-C28-C29
30	f	102	SQD	C11-C10-C9-C8
33	B	627	LHG	O6-C4-C5-C6
33	b	627	LHG	O6-C4-C5-C6
28	H	105	LMG	O9-C10-O7-C8
28	h	105	LMG	O9-C10-O7-C8
33	E	102	LHG	O9-C7-O7-C5
33	e	102	LHG	O9-C7-O7-C5
31	A	415	LMT	C4-C5-C6-C7
31	a	415	LMT	C4-C5-C6-C7
25	B	608	CLA	C11-C12-C13-C15
25	B	616	CLA	C6-C7-C8-C10
25	B	616	CLA	C11-C10-C8-C7
25	C	510	CLA	C6-C7-C8-C10
25	b	608	CLA	C11-C12-C13-C15
25	b	616	CLA	C6-C7-C8-C10
25	b	616	CLA	C11-C10-C8-C7
25	c	510	CLA	C6-C7-C8-C10
28	H	105	LMG	C8-C9-O8-C28
28	h	105	LMG	C8-C9-O8-C28
25	B	607	CLA	C13-C15-C16-C17
25	B	612	CLA	C10-C11-C12-C13
25	B	616	CLA	C8-C10-C11-C12
25	b	607	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	b	612	CLA	C10-C11-C12-C13
25	b	616	CLA	C8-C10-C11-C12
30	A	412	SQD	C7-C8-C9-C10
30	a	412	SQD	C7-C8-C9-C10
29	D	405	PL9	C13-C14-C16-C17
29	d	405	PL9	C13-C14-C16-C17
33	Z	102	LHG	C31-C32-C33-C34
33	z	102	LHG	C31-C32-C33-C34
25	C	512	CLA	C13-C15-C16-C17
25	c	512	CLA	C13-C15-C16-C17
34	C	517	DGD	C2B-C1B-O2G-C2G
34	c	517	DGD	C2B-C1B-O2G-C2G
25	B	610	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA
25	B	603	CLA	C6-C7-C8-C9
25	B	608	CLA	C11-C12-C13-C14
25	C	514	CLA	C14-C13-C15-C16
25	b	603	CLA	C6-C7-C8-C9
25	b	608	CLA	C11-C12-C13-C14
25	c	514	CLA	C14-C13-C15-C16
31	A	416	LMT	C7-C8-C9-C10
31	a	416	LMT	C7-C8-C9-C10
31	T	101	LMT	C3-C4-C5-C6
31	t	101	LMT	C3-C4-C5-C6
33	E	102	LHG	C15-C16-C17-C18
33	Z	102	LHG	C11-C10-C9-C8
33	e	102	LHG	C15-C16-C17-C18
33	z	102	LHG	C11-C10-C9-C8
30	F	102	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
33	D	407	LHG	C35-C36-C37-C38
33	d	407	LHG	C35-C36-C37-C38
33	b	627	LHG	C26-C27-C28-C29
31	A	415	LMT	C2'-C1'-O1'-C1
31	a	415	LMT	C2'-C1'-O1'-C1
33	B	627	LHG	C26-C27-C28-C29
31	T	101	LMT	O5'-C5'-C6'-O6'
31	t	101	LMT	O5'-C5'-C6'-O6'
30	A	412	SQD	O6-C44-C45-C46
30	C	501	SQD	C44-C45-C46-O48
30	a	412	SQD	O6-C44-C45-C46
30	c	501	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
33	D	407	LHG	C4-C5-C6-O8
33	E	102	LHG	C4-C5-C6-O8
33	d	407	LHG	C4-C5-C6-O8
33	e	102	LHG	C4-C5-C6-O8
34	c	518	DGD	CDA-CEA-CFA-CGA
31	D	411	LMT	C11-C10-C9-C8
31	d	411	LMT	C11-C10-C9-C8
34	C	518	DGD	CDA-CEA-CFA-CGA
25	C	511	CLA	C15-C16-C17-C18
25	c	511	CLA	C15-C16-C17-C18
30	H	103	SQD	C25-C26-C27-C28
30	h	103	SQD	C25-C26-C27-C28
33	E	102	LHG	C16-C17-C18-C19
33	e	102	LHG	C16-C17-C18-C19
33	d	406	LHG	C24-C23-O8-C6
28	A	414	LMG	O6-C5-C6-O5
28	a	414	LMG	O6-C5-C6-O5
31	B	623	LMT	O5B-C5B-C6B-O6B
31	E	103	LMT	O5B-C5B-C6B-O6B
31	b	623	LMT	O5B-C5B-C6B-O6B
33	D	408	LHG	C11-C12-C13-C14
33	b	627	LHG	C13-C14-C15-C16
33	d	408	LHG	C11-C12-C13-C14
31	K	105	LMT	C6-C7-C8-C9
31	k	105	LMT	C6-C7-C8-C9
33	B	627	LHG	C13-C14-C15-C16
31	e	103	LMT	O5B-C5B-C6B-O6B
30	B	620	SQD	C24-C25-C26-C27
30	b	620	SQD	C24-C25-C26-C27
28	B	621	LMG	C28-C29-C30-C31
28	b	621	LMG	C28-C29-C30-C31
25	C	502	CLA	O1A-CGA-O2A-C1
25	c	502	CLA	O1A-CGA-O2A-C1
31	B	624	LMT	C7-C8-C9-C10
31	b	624	LMT	C7-C8-C9-C10
25	C	506	CLA	C4-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
26	D	402	PHO	CBD-CGD-O2D-CED
25	C	506	CLA	C2-C3-C5-C6
25	c	506	CLA	C2-C3-C5-C6
33	D	406	LHG	C24-C23-O8-C6
27	Z	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
27	z	101	BCR	C7-C8-C9-C34
31	A	415	LMT	O1'-C1-C2-C3
31	a	415	LMT	O1'-C1-C2-C3
25	B	615	CLA	C10-C11-C12-C13
25	b	615	CLA	C10-C11-C12-C13
26	d	402	PHO	CBD-CGD-O2D-CED
33	Z	102	LHG	C4-O6-P-O5
33	z	102	LHG	C4-O6-P-O5
31	X	104	LMT	O5'-C5'-C6'-O6'
31	x	104	LMT	O5'-C5'-C6'-O6'
30	k	101	SQD	C27-C28-C29-C30
30	K	101	SQD	C27-C28-C29-C30
31	Y	101	LMT	C3-C4-C5-C6
31	y	101	LMT	C3-C4-C5-C6
25	B	611	CLA	CBA-CGA-O2A-C1
25	b	611	CLA	CBA-CGA-O2A-C1
28	C	519	LMG	C22-C23-C24-C25
28	c	519	LMG	C22-C23-C24-C25
30	A	413	SQD	C44-C45-O47-C7
30	C	501	SQD	C44-C45-O47-C7
30	a	413	SQD	C44-C45-O47-C7
30	c	501	SQD	C44-C45-O47-C7
31	C	524	LMT	C3-C4-C5-C6
34	C	516	DGD	O6D-C5D-C6D-O5D
34	c	516	DGD	O6D-C5D-C6D-O5D
27	b	619	BCR	C10-C11-C12-C13
31	Y	101	LMT	C2-C3-C4-C5
31	y	101	LMT	C2-C3-C4-C5
31	c	524	LMT	C3-C4-C5-C6
33	D	406	LHG	C26-C27-C28-C29
33	D	407	LHG	O6-C4-C5-O7
33	d	407	LHG	O6-C4-C5-O7
25	A	408	CLA	C10-C11-C12-C13
25	B	604	CLA	C13-C15-C16-C17
25	a	408	CLA	C10-C11-C12-C13
25	b	604	CLA	C13-C15-C16-C17
31	D	412	LMT	C6-C7-C8-C9
31	d	412	LMT	C6-C7-C8-C9
33	d	406	LHG	C26-C27-C28-C29
30	K	101	SQD	C10-C11-C12-C13
30	k	101	SQD	C10-C11-C12-C13
33	E	102	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	e	102	LHG	C13-C14-C15-C16
34	c	518	DGD	C4A-C5A-C6A-C7A
34	C	518	DGD	C4A-C5A-C6A-C7A
25	C	514	CLA	C4-C3-C5-C6
25	c	514	CLA	C4-C3-C5-C6
31	I	104	LMT	O1'-C1-C2-C3
31	i	104	LMT	O1'-C1-C2-C3
31	Y	101	LMT	C6-C7-C8-C9
31	y	101	LMT	C6-C7-C8-C9
25	B	615	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
28	A	410	LMG	C37-C38-C39-C40
33	Z	102	LHG	C11-C12-C13-C14
33	z	102	LHG	C11-C12-C13-C14
28	a	410	LMG	C37-C38-C39-C40
30	H	103	SQD	C11-C12-C13-C14
30	h	103	SQD	C11-C12-C13-C14
30	A	413	SQD	O47-C45-C46-O48
30	F	102	SQD	O6-C44-C45-O47
30	a	413	SQD	O47-C45-C46-O48
30	f	102	SQD	O6-C44-C45-O47
33	B	628	LHG	O7-C5-C6-O8
33	b	628	LHG	O7-C5-C6-O8
31	i	101	LMT	C7-C8-C9-C10
33	D	406	LHG	C25-C26-C27-C28
33	d	406	LHG	C25-C26-C27-C28
30	H	103	SQD	C35-C36-C37-C38
31	C	524	LMT	C9-C10-C11-C12
31	c	524	LMT	C9-C10-C11-C12
31	I	101	LMT	C7-C8-C9-C10
30	h	103	SQD	C35-C36-C37-C38
34	H	104	DGD	O2G-C1B-C2B-C3B
34	h	104	DGD	O2G-C1B-C2B-C3B
25	C	504	CLA	C2A-CAA-CBA-CGA
25	c	504	CLA	C2A-CAA-CBA-CGA
30	B	620	SQD	C35-C36-C37-C38
30	b	620	SQD	C35-C36-C37-C38
33	B	627	LHG	C35-C36-C37-C38
33	b	627	LHG	C35-C36-C37-C38
34	H	104	DGD	CDA-CEA-CFA-CGA
34	h	104	DGD	CDA-CEA-CFA-CGA
31	D	411	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	d	411	LMT	C6-C7-C8-C9
31	M	101	LMT	C9-C10-C11-C12
31	m	101	LMT	C9-C10-C11-C12
31	D	411	LMT	C4'-C5'-C6'-O6'
31	d	411	LMT	C4'-C5'-C6'-O6'
28	C	519	LMG	O6-C5-C6-O5
28	c	519	LMG	O6-C5-C6-O5
30	K	101	SQD	C24-C25-C26-C27
30	k	101	SQD	C24-C25-C26-C27
33	B	627	LHG	C11-C12-C13-C14
33	b	627	LHG	C11-C12-C13-C14
25	B	616	CLA	C4-C3-C5-C6
25	b	616	CLA	C4-C3-C5-C6
26	A	407	PHO	C4-C3-C5-C6
26	a	407	PHO	C4-C3-C5-C6
31	I	104	LMT	C7-C8-C9-C10
31	i	104	LMT	C7-C8-C9-C10
33	B	627	LHG	C34-C35-C36-C37
33	b	627	LHG	C34-C35-C36-C37
25	C	514	CLA	C8-C10-C11-C12
25	c	514	CLA	C8-C10-C11-C12
31	B	624	LMT	C2-C1-O1'-C1'
31	b	624	LMT	C2-C1-O1'-C1'
25	A	408	CLA	C6-C7-C8-C9
25	B	616	CLA	C11-C10-C8-C9
25	a	408	CLA	C6-C7-C8-C9
25	b	616	CLA	C11-C10-C8-C9
33	E	102	LHG	C12-C13-C14-C15
33	B	627	LHG	C5-C4-O6-P
33	b	627	LHG	C5-C4-O6-P
25	B	602	CLA	C4B-C3B-CAB-CBB
25	C	507	CLA	C4B-C3B-CAB-CBB
25	b	602	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	C4B-C3B-CAB-CBB
33	e	102	LHG	C12-C13-C14-C15
31	D	412	LMT	C11-C10-C9-C8
31	d	412	LMT	C11-C10-C9-C8
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
33	E	102	LHG	C9-C10-C11-C12
33	e	102	LHG	C9-C10-C11-C12
33	E	102	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
33	e	102	LHG	C18-C19-C20-C21
25	A	405	CLA	C3-C5-C6-C7
25	a	405	CLA	C3-C5-C6-C7
33	B	628	LHG	O6-C4-C5-C6
33	D	407	LHG	O6-C4-C5-C6
33	b	628	LHG	O6-C4-C5-C6
33	d	407	LHG	O6-C4-C5-C6
33	B	627	LHG	C25-C26-C27-C28
33	b	627	LHG	C25-C26-C27-C28
30	K	101	SQD	C14-C15-C16-C17
30	k	101	SQD	C14-C15-C16-C17
31	H	102	LMT	C4'-C5'-C6'-O6'
31	h	102	LMT	C4'-C5'-C6'-O6'
25	B	603	CLA	C6-C7-C8-C10
25	C	512	CLA	C6-C7-C8-C10
25	C	514	CLA	C12-C13-C15-C16
25	D	404	CLA	C11-C12-C13-C15
25	b	603	CLA	C6-C7-C8-C10
25	c	512	CLA	C6-C7-C8-C10
25	c	514	CLA	C12-C13-C15-C16
25	d	404	CLA	C11-C12-C13-C15
33	B	627	LHG	C23-C24-C25-C26
33	b	627	LHG	C23-C24-C25-C26
28	C	519	LMG	C40-C41-C42-C43
28	c	519	LMG	C40-C41-C42-C43
33	D	406	LHG	C11-C12-C13-C14
33	d	406	LHG	C11-C12-C13-C14
30	A	413	SQD	C11-C12-C13-C14
25	A	406	CLA	C3A-C2A-CAA-CBA
25	B	607	CLA	C3A-C2A-CAA-CBA
25	B	608	CLA	C3A-C2A-CAA-CBA
25	B	609	CLA	C3A-C2A-CAA-CBA
25	B	609	CLA	C4-C3-C5-C6
25	a	406	CLA	C3A-C2A-CAA-CBA
25	b	607	CLA	C3A-C2A-CAA-CBA
25	b	608	CLA	C3A-C2A-CAA-CBA
25	b	609	CLA	C3A-C2A-CAA-CBA
25	b	609	CLA	C4-C3-C5-C6
30	a	413	SQD	C11-C12-C13-C14
25	C	510	CLA	C13-C15-C16-C17
25	c	510	CLA	C13-C15-C16-C17
34	C	516	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
34	c	516	DGD	C4D-C5D-C6D-O5D
33	d	407	LHG	C11-C10-C9-C8
27	C	515	BCR	C9-C10-C11-C12
27	c	515	BCR	C9-C10-C11-C12
25	A	405	CLA	C16-C17-C18-C19
25	a	405	CLA	C16-C17-C18-C19
33	D	408	LHG	C13-C14-C15-C16
33	d	408	LHG	C13-C14-C15-C16
31	X	104	LMT	C2-C3-C4-C5
33	D	407	LHG	C11-C10-C9-C8
33	b	627	LHG	C30-C31-C32-C33
31	A	415	LMT	O5'-C5'-C6'-O6'
31	a	415	LMT	O5'-C5'-C6'-O6'
31	x	104	LMT	C2-C3-C4-C5
33	B	627	LHG	C30-C31-C32-C33
30	b	620	SQD	C10-C11-C12-C13
33	B	627	LHG	C4-C5-C6-O8
33	B	628	LHG	C4-C5-C6-O8
33	b	627	LHG	C4-C5-C6-O8
33	b	628	LHG	C4-C5-C6-O8
30	B	620	SQD	C10-C11-C12-C13
30	B	620	SQD	C19-C20-C21-C22
33	D	407	LHG	C7-C8-C9-C10
33	d	407	LHG	C7-C8-C9-C10
30	b	620	SQD	C19-C20-C21-C22
25	D	403	CLA	C13-C15-C16-C17
25	d	403	CLA	C13-C15-C16-C17
30	A	412	SQD	C14-C15-C16-C17
30	a	412	SQD	C14-C15-C16-C17
31	J	101	LMT	C1-C2-C3-C4
31	j	101	LMT	C1-C2-C3-C4
31	B	625	LMT	C7-C8-C9-C10
31	b	625	LMT	C7-C8-C9-C10
30	H	103	SQD	C34-C35-C36-C37
30	h	103	SQD	C34-C35-C36-C37
25	B	616	CLA	C2-C3-C5-C6
25	b	616	CLA	C2-C3-C5-C6
26	A	407	PHO	C2-C3-C5-C6
26	a	407	PHO	C2-C3-C5-C6
25	B	611	CLA	O1A-CGA-O2A-C1
25	b	611	CLA	O1A-CGA-O2A-C1
30	H	103	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	h	103	SQD	C16-C17-C18-C19
33	B	627	LHG	O6-C4-C5-O7
33	b	627	LHG	O6-C4-C5-O7
31	a	415	LMT	C4'-C5'-C6'-O6'
27	B	619	BCR	C1-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C30
27	C	515	BCR	C23-C24-C25-C30
27	F	101	BCR	C1-C6-C7-C8
27	Z	101	BCR	C23-C24-C25-C30
27	b	619	BCR	C1-C6-C7-C8
27	b	619	BCR	C23-C24-C25-C30
27	c	515	BCR	C23-C24-C25-C30
27	f	101	BCR	C1-C6-C7-C8
27	z	101	BCR	C23-C24-C25-C30
31	A	415	LMT	C4'-C5'-C6'-O6'
28	A	414	LMG	C29-C30-C31-C32
28	a	414	LMG	C29-C30-C31-C32
30	b	620	SQD	C27-C28-C29-C30
28	B	621	LMG	C13-C14-C15-C16
28	b	621	LMG	C13-C14-C15-C16
30	A	412	SQD	C30-C31-C32-C33
30	B	620	SQD	C27-C28-C29-C30
30	a	412	SQD	C30-C31-C32-C33
31	I	103	LMT	C11-C10-C9-C8
33	D	408	LHG	C34-C35-C36-C37
31	X	101	LMT	O1'-C1-C2-C3
31	x	101	LMT	O1'-C1-C2-C3
30	H	103	SQD	C17-C18-C19-C20
30	h	103	SQD	C17-C18-C19-C20
31	i	103	LMT	C11-C10-C9-C8
30	F	102	SQD	O47-C45-C46-O48
30	f	102	SQD	O47-C45-C46-O48
33	B	627	LHG	O7-C5-C6-O8
33	D	406	LHG	O7-C5-C6-O8
33	b	627	LHG	O7-C5-C6-O8
33	d	406	LHG	O7-C5-C6-O8
33	d	408	LHG	C34-C35-C36-C37
34	C	518	DGD	C9A-CAA-CBA-CCA
34	c	518	DGD	C9A-CAA-CBA-CCA
31	J	101	LMT	O5'-C5'-C6'-O6'
31	j	101	LMT	O5'-C5'-C6'-O6'
25	b	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	X	105	LMT	C4-C5-C6-C7
31	x	105	LMT	C4-C5-C6-C7
34	C	517	DGD	O1B-C1B-O2G-C2G
34	c	517	DGD	O1B-C1B-O2G-C2G
25	B	609	CLA	C2-C3-C5-C6
25	b	609	CLA	C2-C3-C5-C6
31	M	101	LMT	C3-C4-C5-C6
31	m	101	LMT	C3-C4-C5-C6
26	A	407	PHO	C16-C17-C18-C19
26	a	407	PHO	C16-C17-C18-C19
28	A	410	LMG	C33-C34-C35-C36
28	a	410	LMG	C33-C34-C35-C36
30	A	413	SQD	C23-C24-C25-C26
30	a	413	SQD	C23-C24-C25-C26
25	B	603	CLA	O1D-CGD-O2D-CED
25	b	603	CLA	O1D-CGD-O2D-CED
31	B	623	LMT	C1-C2-C3-C4
31	b	623	LMT	C1-C2-C3-C4
25	B	613	CLA	C3-C5-C6-C7
25	C	512	CLA	C6-C7-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	C	512	CLA	C14-C13-C15-C16
25	D	403	CLA	C11-C12-C13-C14
25	c	512	CLA	C6-C7-C8-C9
25	c	512	CLA	C11-C10-C8-C9
25	c	512	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C14
31	i	103	LMT	C6-C7-C8-C9
33	Z	102	LHG	C34-C35-C36-C37
33	z	102	LHG	C34-C35-C36-C37
31	I	103	LMT	C6-C7-C8-C9
33	d	408	LHG	C29-C30-C31-C32
31	T	101	LMT	C9-C10-C11-C12
31	t	101	LMT	C9-C10-C11-C12
31	B	623	LMT	C2-C3-C4-C5
31	b	623	LMT	C2-C3-C4-C5
33	D	408	LHG	C29-C30-C31-C32
31	D	411	LMT	C9-C10-C11-C12
31	d	411	LMT	C9-C10-C11-C12
28	H	105	LMG	C29-C30-C31-C32
28	h	105	LMG	C29-C30-C31-C32
33	D	408	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
33	d	408	LHG	C24-C23-O8-C6
27	K	103	BCR	C9-C10-C11-C12
27	k	103	BCR	C9-C10-C11-C12
28	A	414	LMG	C14-C15-C16-C17
28	a	414	LMG	C14-C15-C16-C17
29	D	405	PL9	C28-C29-C31-C32
29	d	405	PL9	C28-C29-C31-C32
30	C	501	SQD	C9-C10-C11-C12
30	c	501	SQD	C9-C10-C11-C12
33	d	407	LHG	C25-C26-C27-C28
33	d	408	LHG	C26-C27-C28-C29
25	B	602	CLA	C8-C10-C11-C12
25	B	605	CLA	C5-C6-C7-C8
25	b	602	CLA	C8-C10-C11-C12
28	D	409	LMG	C29-C30-C31-C32
28	d	409	LMG	C29-C30-C31-C32
33	D	407	LHG	C25-C26-C27-C28
33	D	408	LHG	C26-C27-C28-C29
33	d	406	LHG	O10-C23-O8-C6
33	Z	102	LHG	C35-C36-C37-C38
33	z	102	LHG	C35-C36-C37-C38
25	B	613	CLA	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1
25	b	605	CLA	C5-C6-C7-C8
33	D	408	LHG	O6-C4-C5-C6
33	d	408	LHG	O6-C4-C5-C6
31	I	101	LMT	C1-C2-C3-C4
31	i	101	LMT	C1-C2-C3-C4
33	D	406	LHG	O10-C23-O8-C6
25	B	605	CLA	C8-C10-C11-C12
25	b	605	CLA	C8-C10-C11-C12
27	B	619	BCR	C37-C22-C23-C24
27	b	619	BCR	C37-C22-C23-C24
25	A	408	CLA	C11-C10-C8-C7
25	B	602	CLA	C11-C10-C8-C7
25	B	604	CLA	C6-C7-C8-C10
25	B	605	CLA	C11-C10-C8-C7
25	C	512	CLA	C12-C13-C15-C16
25	C	514	CLA	C6-C7-C8-C10
25	D	403	CLA	C11-C12-C13-C15
25	a	408	CLA	C11-C10-C8-C7
25	b	602	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C6-C7-C8-C10
25	b	605	CLA	C11-C10-C8-C7
25	c	512	CLA	C12-C13-C15-C16
25	c	514	CLA	C6-C7-C8-C10
25	d	403	CLA	C11-C12-C13-C15
30	H	103	SQD	C12-C13-C14-C15
30	k	101	SQD	C11-C10-C9-C8
31	H	102	LMT	C5-C6-C7-C8
31	h	102	LMT	C5-C6-C7-C8
33	B	628	LHG	C31-C32-C33-C34
33	b	628	LHG	C31-C32-C33-C34
28	D	409	LMG	C14-C15-C16-C17
30	K	101	SQD	C11-C10-C9-C8
30	h	103	SQD	C12-C13-C14-C15
33	B	627	LHG	C24-C25-C26-C27
33	b	627	LHG	C24-C25-C26-C27
34	c	518	DGD	CCA-CDA-CEA-CFA
28	d	409	LMG	C14-C15-C16-C17
27	B	617	BCR	C21-C22-C23-C24
27	Z	101	BCR	C21-C22-C23-C24
27	b	617	BCR	C21-C22-C23-C24
27	z	101	BCR	C21-C22-C23-C24
34	C	518	DGD	CCA-CDA-CEA-CFA
28	H	105	LMG	C8-C7-O1-C1
28	h	105	LMG	C8-C7-O1-C1
34	C	517	DGD	C2G-C3G-O3G-C1D
34	C	517	DGD	C5D-C6D-O5D-C1E
34	c	517	DGD	C2G-C3G-O3G-C1D
34	c	517	DGD	C5D-C6D-O5D-C1E
30	K	101	SQD	C23-C24-C25-C26
30	k	101	SQD	C23-C24-C25-C26
28	c	519	LMG	C37-C38-C39-C40
33	D	407	LHG	C27-C28-C29-C30
33	d	407	LHG	C27-C28-C29-C30
30	K	101	SQD	O47-C7-C8-C9
30	k	101	SQD	O47-C7-C8-C9
28	C	519	LMG	C37-C38-C39-C40
30	A	413	SQD	C31-C32-C33-C34
30	a	413	SQD	C31-C32-C33-C34
30	B	620	SQD	C46-C45-O47-C7
30	F	102	SQD	C44-C45-O47-C7
30	b	620	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
30	f	102	SQD	C44-C45-O47-C7
34	C	518	DGD	CAA-CBA-CCA-CDA
34	c	518	DGD	CAA-CBA-CCA-CDA
33	b	628	LHG	C28-C29-C30-C31
33	B	628	LHG	C28-C29-C30-C31
25	B	613	CLA	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
25	B	615	CLA	C5-C6-C7-C8
25	b	615	CLA	C5-C6-C7-C8
31	T	101	LMT	C4-C5-C6-C7
31	t	101	LMT	C4-C5-C6-C7
33	B	628	LHG	O6-C4-C5-O7
33	Z	102	LHG	O6-C4-C5-O7
33	b	628	LHG	O6-C4-C5-O7
33	z	102	LHG	O6-C4-C5-O7
31	E	101	LMT	C3-C4-C5-C6
31	e	101	LMT	C3-C4-C5-C6
31	B	624	LMT	O5'-C1'-O1'-C1
31	b	624	LMT	O5'-C1'-O1'-C1
25	A	408	CLA	O1D-CGD-O2D-CED
25	a	408	CLA	O1D-CGD-O2D-CED
30	K	101	SQD	C44-C45-C46-O48
30	k	101	SQD	C44-C45-C46-O48
25	B	615	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
31	B	625	LMT	C6-C7-C8-C9
31	b	625	LMT	C6-C7-C8-C9
33	D	406	LHG	C30-C31-C32-C33
33	d	406	LHG	C30-C31-C32-C33
25	B	604	CLA	C6-C7-C8-C9
25	B	605	CLA	C11-C10-C8-C9
25	B	611	CLA	C11-C12-C13-C14
25	D	404	CLA	C11-C12-C13-C14
25	b	604	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	611	CLA	C11-C12-C13-C14
25	d	404	CLA	C11-C12-C13-C14
31	A	415	LMT	C11-C10-C9-C8
31	a	415	LMT	C11-C10-C9-C8
33	B	627	LHG	C12-C13-C14-C15
33	b	627	LHG	C12-C13-C14-C15
28	c	519	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	B	610	CLA	C2-C1-O2A-CGA
25	b	610	CLA	C2-C1-O2A-CGA
34	C	516	DGD	C2E-C1E-O5D-C6D
34	c	516	DGD	C2E-C1E-O5D-C6D
25	B	613	CLA	C16-C17-C18-C20
25	b	613	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C19
25	B	612	CLA	C13-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
28	C	519	LMG	C29-C30-C31-C32
33	E	102	LHG	C1-C2-C3-O3
33	e	102	LHG	C1-C2-C3-O3
33	D	408	LHG	C11-C10-C9-C8
25	D	403	CLA	C16-C17-C18-C19
33	d	408	LHG	C11-C10-C9-C8
31	I	101	LMT	C6-C7-C8-C9
31	i	101	LMT	C6-C7-C8-C9
25	A	408	CLA	CBD-CGD-O2D-CED
25	a	408	CLA	CBD-CGD-O2D-CED
31	D	411	LMT	C7-C8-C9-C10
31	d	411	LMT	C7-C8-C9-C10
33	D	406	LHG	C15-C16-C17-C18
33	d	406	LHG	C15-C16-C17-C18
31	B	623	LMT	C2-C1-O1'-C1'
31	J	101	LMT	C2-C1-O1'-C1'
31	b	623	LMT	C2-C1-O1'-C1'
31	j	101	LMT	C2-C1-O1'-C1'
31	D	412	LMT	O1'-C1-C2-C3
31	d	412	LMT	O1'-C1-C2-C3
25	C	506	CLA	C4B-C3B-CAB-CBB
25	c	506	CLA	C4B-C3B-CAB-CBB
26	D	402	PHO	O1D-CGD-O2D-CED
26	d	402	PHO	O1D-CGD-O2D-CED
31	M	101	LMT	C7-C8-C9-C10
31	m	101	LMT	C7-C8-C9-C10
29	D	405	PL9	C15-C14-C16-C17
29	d	405	PL9	C15-C14-C16-C17
27	F	101	BCR	C19-C20-C21-C22
27	f	101	BCR	C19-C20-C21-C22
31	T	101	LMT	C2-C3-C4-C5
31	c	522	LMT	C2-C3-C4-C5
31	t	101	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	C	522	LMT	C2-C3-C4-C5
33	D	407	LHG	C28-C29-C30-C31
33	d	407	LHG	C28-C29-C30-C31
33	E	102	LHG	O6-C4-C5-C6
33	Z	102	LHG	O6-C4-C5-C6
33	e	102	LHG	O6-C4-C5-C6
33	z	102	LHG	O6-C4-C5-C6
30	a	412	SQD	C9-C10-C11-C12
30	A	412	SQD	C9-C10-C11-C12
30	A	412	SQD	C5-C6-S-O7
30	a	412	SQD	C5-C6-S-O7
25	A	406	CLA	C11-C10-C8-C7
25	B	602	CLA	C6-C7-C8-C10
25	B	603	CLA	C11-C10-C8-C7
25	B	607	CLA	C12-C13-C15-C16
25	B	612	CLA	C11-C10-C8-C7
25	B	615	CLA	C12-C13-C15-C16
25	a	406	CLA	C11-C10-C8-C7
25	b	602	CLA	C6-C7-C8-C10
25	b	603	CLA	C11-C10-C8-C7
25	b	607	CLA	C12-C13-C15-C16
25	b	612	CLA	C11-C10-C8-C7
25	b	615	CLA	C12-C13-C15-C16
31	e	103	LMT	C5-C6-C7-C8
25	B	603	CLA	C16-C17-C18-C19
25	C	512	CLA	C16-C17-C18-C20
25	b	603	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C20
31	E	103	LMT	C5-C6-C7-C8
34	h	104	DGD	CCA-CDA-CEA-CFA
28	d	409	LMG	C4-C5-C6-O5
34	H	104	DGD	CCA-CDA-CEA-CFA
33	d	408	LHG	O10-C23-O8-C6
28	D	409	LMG	C4-C5-C6-O5
33	D	408	LHG	O10-C23-O8-C6
33	E	102	LHG	O6-C4-C5-O7
33	e	102	LHG	O6-C4-C5-O7
30	c	501	SQD	C10-C11-C12-C13
25	B	602	CLA	C6-C7-C8-C9
25	B	602	CLA	C11-C10-C8-C9
25	B	612	CLA	C11-C10-C8-C9
25	b	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	C11-C10-C8-C9
25	b	612	CLA	C11-C10-C8-C9
30	C	501	SQD	C10-C11-C12-C13
25	B	614	CLA	C13-C15-C16-C17
25	b	614	CLA	C13-C15-C16-C17
27	B	618	BCR	C9-C10-C11-C12
27	C	515	BCR	C19-C20-C21-C22
27	K	102	BCR	C19-C20-C21-C22
27	k	102	BCR	C19-C20-C21-C22
30	H	103	SQD	O5-C5-C6-S
30	h	103	SQD	O5-C5-C6-S
30	A	412	SQD	O6-C44-C45-O47
30	a	412	SQD	O6-C44-C45-O47
33	D	407	LHG	O7-C5-C6-O8
33	Z	102	LHG	O7-C5-C6-O8
33	d	407	LHG	O7-C5-C6-O8
33	z	102	LHG	O7-C5-C6-O8
31	D	410	LMT	C2-C3-C4-C5
31	d	410	LMT	C2-C3-C4-C5
33	d	408	LHG	C25-C26-C27-C28
31	I	101	LMT	C9-C10-C11-C12
31	i	101	LMT	C9-C10-C11-C12
25	C	512	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C19
33	D	408	LHG	C25-C26-C27-C28
28	H	105	LMG	O1-C7-C8-C9
28	h	105	LMG	O1-C7-C8-C9
30	F	102	SQD	C44-C45-C46-O48
30	f	102	SQD	C44-C45-C46-O48
33	Z	102	LHG	C4-C5-C6-O8
33	z	102	LHG	C4-C5-C6-O8
30	B	620	SQD	C15-C16-C17-C18
30	b	620	SQD	C15-C16-C17-C18
25	B	603	CLA	CAD-CBD-CGD-O2D
25	B	604	CLA	CAD-CBD-CGD-O2D
25	B	605	CLA	CAD-CBD-CGD-O2D
25	B	607	CLA	CAD-CBD-CGD-O2D
25	B	609	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O2D
25	C	507	CLA	CAD-CBD-CGD-O2D
25	b	603	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	b	605	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	b	609	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O2D
25	c	507	CLA	CAD-CBD-CGD-O2D
31	e	101	LMT	O5'-C1'-O1'-C1
25	B	611	CLA	C3-C5-C6-C7
25	b	611	CLA	C3-C5-C6-C7
31	X	101	LMT	C7-C8-C9-C10
31	x	101	LMT	C7-C8-C9-C10
25	B	603	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	607	CLA	CAD-CBD-CGD-O1D
25	B	609	CLA	CAD-CBD-CGD-O1D
25	B	610	CLA	CHA-CBD-CGD-O1D
25	B	610	CLA	CHA-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CAD-CBD-CGD-O1D
25	b	603	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	b	609	CLA	CAD-CBD-CGD-O1D
25	b	610	CLA	CHA-CBD-CGD-O1D
25	b	610	CLA	CHA-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	c	507	CLA	CAD-CBD-CGD-O1D
27	b	618	BCR	C9-C10-C11-C12
27	c	515	BCR	C19-C20-C21-C22
33	B	627	LHG	C3-O3-P-O5
33	B	627	LHG	C4-O6-P-O5
33	B	628	LHG	C3-O3-P-O6
33	B	628	LHG	C4-O6-P-O5
33	D	407	LHG	C4-O6-P-O5
33	D	408	LHG	C4-O6-P-O5
33	E	102	LHG	C4-O6-P-O4
33	E	102	LHG	C4-O6-P-O5
33	b	627	LHG	C3-O3-P-O5
33	b	627	LHG	C4-O6-P-O5
33	b	628	LHG	C3-O3-P-O6
33	b	628	LHG	C4-O6-P-O5
33	d	407	LHG	C4-O6-P-O5
33	d	408	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
33	e	102	LHG	C4-O6-P-O4
33	e	102	LHG	C4-O6-P-O5
31	B	629	LMT	C7-C8-C9-C10
31	b	629	LMT	C7-C8-C9-C10
25	C	506	CLA	C2B-C3B-CAB-CBB
25	c	506	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C3-C5-C6-C7
25	c	512	CLA	C3-C5-C6-C7
31	F	103	LMT	C4'-C5'-C6'-O6'
31	f	103	LMT	C4'-C5'-C6'-O6'
28	C	523	LMG	O7-C10-C11-C12
28	c	523	LMG	O7-C10-C11-C12
33	B	628	LHG	C34-C35-C36-C37
28	C	523	LMG	C33-C34-C35-C36
28	c	523	LMG	C33-C34-C35-C36
28	d	409	LMG	C33-C34-C35-C36
30	c	501	SQD	C11-C12-C13-C14
33	b	628	LHG	C34-C35-C36-C37
28	D	409	LMG	C33-C34-C35-C36
30	C	501	SQD	C11-C12-C13-C14
25	B	608	CLA	C13-C15-C16-C17
34	c	516	DGD	C2B-C3B-C4B-C5B
27	K	102	BCR	C18-C19-C20-C21
27	k	102	BCR	C18-C19-C20-C21
25	b	608	CLA	C13-C15-C16-C17
25	C	514	CLA	C2-C3-C5-C6
25	c	514	CLA	C2-C3-C5-C6
30	B	620	SQD	C7-C8-C9-C10
30	b	620	SQD	C7-C8-C9-C10
33	D	407	LHG	C23-C24-C25-C26
33	d	407	LHG	C23-C24-C25-C26
34	C	516	DGD	C2B-C3B-C4B-C5B
25	C	507	CLA	C16-C17-C18-C19
25	C	507	CLA	C16-C17-C18-C20
25	c	507	CLA	C16-C17-C18-C19
25	c	507	CLA	C16-C17-C18-C20
31	A	415	LMT	C6-C7-C8-C9
31	I	101	LMT	C5-C6-C7-C8
31	a	415	LMT	C6-C7-C8-C9
31	i	101	LMT	C5-C6-C7-C8
25	B	615	CLA	C11-C12-C13-C14
25	C	507	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	615	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C15
25	C	507	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C15
25	c	507	CLA	C12-C13-C15-C16
31	D	410	LMT	C4-C5-C6-C7
31	d	410	LMT	C4-C5-C6-C7
28	C	523	LMG	C36-C37-C38-C39
28	c	523	LMG	C36-C37-C38-C39
31	E	101	LMT	O5'-C1'-O1'-C1
31	X	101	LMT	O5'-C1'-O1'-C1
31	x	101	LMT	O5'-C1'-O1'-C1
25	B	613	CLA	C16-C17-C18-C19
25	b	613	CLA	C16-C17-C18-C19
30	C	501	SQD	C2-C1-O6-C44
30	c	501	SQD	C2-C1-O6-C44
28	b	621	LMG	C15-C16-C17-C18
28	B	621	LMG	C15-C16-C17-C18
34	C	516	DGD	O2G-C1B-C2B-C3B
34	c	516	DGD	O2G-C1B-C2B-C3B
27	K	102	BCR	C13-C14-C15-C16
27	k	102	BCR	C13-C14-C15-C16
28	D	409	LMG	C13-C14-C15-C16
28	d	409	LMG	C13-C14-C15-C16
33	Z	102	LHG	C25-C26-C27-C28
33	z	102	LHG	C25-C26-C27-C28
30	A	413	SQD	O47-C7-C8-C9
30	a	413	SQD	O47-C7-C8-C9
25	C	506	CLA	C2A-CAA-CBA-CGA
25	c	506	CLA	C2A-CAA-CBA-CGA
33	E	102	LHG	C19-C20-C21-C22
33	e	102	LHG	C19-C20-C21-C22
33	E	102	LHG	C26-C27-C28-C29
33	e	102	LHG	C26-C27-C28-C29
25	B	616	CLA	C2-C1-O2A-CGA
25	b	616	CLA	C2-C1-O2A-CGA
29	A	411	PL9	C45-C44-C46-C47
29	a	411	PL9	C45-C44-C46-C47
31	B	623	LMT	C9-C10-C11-C12
31	b	623	LMT	C9-C10-C11-C12
33	D	408	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
33	d	408	LHG	C19-C20-C21-C22
30	A	413	SQD	C45-C44-O6-C1
30	F	102	SQD	C45-C44-O6-C1
30	a	413	SQD	C45-C44-O6-C1
30	f	102	SQD	C45-C44-O6-C1
34	C	516	DGD	C5D-C6D-O5D-C1E
34	c	516	DGD	C5D-C6D-O5D-C1E
28	C	519	LMG	C15-C16-C17-C18
28	c	519	LMG	C15-C16-C17-C18
25	B	603	CLA	C2A-CAA-CBA-CGA
25	b	603	CLA	C2A-CAA-CBA-CGA
27	F	101	BCR	C13-C14-C15-C16
27	f	101	BCR	C13-C14-C15-C16
34	H	104	DGD	O1B-C1B-C2B-C3B
34	h	104	DGD	O1B-C1B-C2B-C3B
31	B	625	LMT	C2-C1-O1'-C1'
31	C	525	LMT	C2-C1-O1'-C1'
31	D	410	LMT	C2-C1-O1'-C1'
31	b	625	LMT	C2-C1-O1'-C1'
31	c	525	LMT	C2-C1-O1'-C1'
31	d	410	LMT	C2-C1-O1'-C1'
31	m	102	LMT	C9-C10-C11-C12
31	X	102	LMT	C1-C2-C3-C4
31	x	102	LMT	C1-C2-C3-C4
25	B	603	CLA	C11-C10-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	b	603	CLA	C11-C10-C8-C9
25	b	615	CLA	C14-C13-C15-C16
25	B	603	CLA	CBA-CGA-O2A-C1
34	C	517	DGD	C2A-C1A-O1G-C1G
34	c	517	DGD	C2A-C1A-O1G-C1G
33	D	408	LHG	C2-C3-O3-P
33	E	102	LHG	C2-C3-O3-P
33	d	408	LHG	C2-C3-O3-P
33	e	102	LHG	C2-C3-O3-P
31	M	102	LMT	C9-C10-C11-C12
31	T	101	LMT	C1-C2-C3-C4
31	t	101	LMT	C1-C2-C3-C4
25	b	614	CLA	C5-C6-C7-C8
35	E	104	HEM	C2A-CAA-CBA-CGA
35	e	104	HEM	C2A-CAA-CBA-CGA
33	Z	102	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
33	z	102	LHG	C24-C23-O8-C6
31	B	625	LMT	C4'-C5'-C6'-O6'
25	B	614	CLA	C5-C6-C7-C8
34	C	517	DGD	O1A-C1A-O1G-C1G
34	c	517	DGD	O1A-C1A-O1G-C1G
28	H	105	LMG	C2-C1-O1-C7
28	h	105	LMG	C2-C1-O1-C7
25	a	406	CLA	C3-C5-C6-C7
31	b	625	LMT	C4'-C5'-C6'-O6'
30	K	101	SQD	C29-C30-C31-C32
30	k	101	SQD	C29-C30-C31-C32
25	b	603	CLA	CBA-CGA-O2A-C1
28	A	410	LMG	C31-C32-C33-C34
28	a	410	LMG	C31-C32-C33-C34
28	C	519	LMG	C19-C20-C21-C22
28	c	519	LMG	C19-C20-C21-C22
25	B	602	CLA	C11-C12-C13-C15
25	b	602	CLA	C11-C12-C13-C15
25	A	406	CLA	C3-C5-C6-C7
30	C	501	SQD	C28-C29-C30-C31
30	c	501	SQD	C28-C29-C30-C31
31	T	101	LMT	C5-C6-C7-C8
31	t	101	LMT	C5-C6-C7-C8
25	A	405	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
25	D	401	CLA	C2C-C3C-CAC-CBC
25	d	401	CLA	C2C-C3C-CAC-CBC
28	A	410	LMG	O7-C8-C9-O8
28	a	410	LMG	O7-C8-C9-O8
30	k	101	SQD	C28-C29-C30-C31
25	D	404	CLA	C4-C3-C5-C6
25	d	404	CLA	C4-C3-C5-C6
30	K	101	SQD	C28-C29-C30-C31
27	K	102	BCR	C20-C21-C22-C37
27	k	102	BCR	C20-C21-C22-C37
31	T	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
25	B	604	CLA	C10-C11-C12-C13
25	b	604	CLA	C10-C11-C12-C13
33	B	627	LHG	C28-C29-C30-C31
27	Z	101	BCR	C11-C12-C13-C35
27	z	101	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
30	A	412	SQD	C28-C29-C30-C31
30	a	412	SQD	C28-C29-C30-C31
33	D	408	LHG	C31-C32-C33-C34
33	b	627	LHG	C28-C29-C30-C31
33	d	408	LHG	C31-C32-C33-C34
34	c	517	DGD	C9A-CAA-CBA-CCA
34	C	517	DGD	C9A-CAA-CBA-CCA
31	F	103	LMT	C4B-C5B-C6B-O6B
31	f	103	LMT	C4B-C5B-C6B-O6B
25	C	503	CLA	C2A-CAA-CBA-CGA
25	c	503	CLA	C2A-CAA-CBA-CGA
30	B	620	SQD	C29-C30-C31-C32
30	b	620	SQD	C29-C30-C31-C32
33	D	406	LHG	C31-C32-C33-C34
29	A	411	PL9	C19-C21-C22-C23
29	a	411	PL9	C19-C21-C22-C23
33	D	406	LHG	C4-C5-C6-O8
33	d	406	LHG	C4-C5-C6-O8
26	A	407	PHO	C15-C16-C17-C18
26	a	407	PHO	C15-C16-C17-C18
33	d	406	LHG	C31-C32-C33-C34
35	V	201	HEM	CAD-CBD-CGD-O1D
35	v	201	HEM	CAD-CBD-CGD-O1D
25	A	406	CLA	C11-C10-C8-C9
25	B	609	CLA	C6-C7-C8-C9
25	C	503	CLA	C11-C12-C13-C14
25	a	406	CLA	C11-C10-C8-C9
25	b	609	CLA	C6-C7-C8-C9
25	c	503	CLA	C11-C12-C13-C14
30	C	501	SQD	C16-C17-C18-C19
30	c	501	SQD	C16-C17-C18-C19
35	V	201	HEM	CAD-CBD-CGD-O2D
35	v	201	HEM	CAD-CBD-CGD-O2D
30	K	101	SQD	C25-C26-C27-C28
28	H	105	LMG	C32-C33-C34-C35
28	h	105	LMG	C32-C33-C34-C35
30	k	101	SQD	C25-C26-C27-C28
33	D	406	LHG	C11-C10-C9-C8
25	C	502	CLA	C4-C3-C5-C6
25	c	502	CLA	C4-C3-C5-C6
33	d	406	LHG	C11-C10-C9-C8
31	B	625	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	i	101	LMT	C4'-C5'-C6'-O6'
31	J	101	LMT	C3-C4-C5-C6
31	b	625	LMT	O5'-C5'-C6'-O6'
31	j	101	LMT	C3-C4-C5-C6
25	c	511	CLA	C5-C6-C7-C8
25	B	608	CLA	C1A-C2A-CAA-CBA
25	b	608	CLA	C1A-C2A-CAA-CBA
27	K	102	BCR	C20-C21-C22-C23
27	k	102	BCR	C20-C21-C22-C23
31	I	103	LMT	C7-C8-C9-C10
31	i	103	LMT	C7-C8-C9-C10
25	A	405	CLA	O1A-CGA-O2A-C1
25	a	405	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	C5-C6-C7-C8
25	B	602	CLA	C2B-C3B-CAB-CBB
25	b	602	CLA	C2B-C3B-CAB-CBB
27	A	409	BCR	C1-C6-C7-C8
27	A	409	BCR	C23-C24-C25-C30
27	B	617	BCR	C23-C24-C25-C30
27	B	619	BCR	C5-C6-C7-C8
27	C	515	BCR	C23-C24-C25-C26
27	F	101	BCR	C5-C6-C7-C8
27	F	101	BCR	C23-C24-C25-C30
27	K	102	BCR	C23-C24-C25-C26
27	K	102	BCR	C23-C24-C25-C30
27	Z	101	BCR	C23-C24-C25-C26
27	a	409	BCR	C1-C6-C7-C8
27	a	409	BCR	C23-C24-C25-C30
27	b	617	BCR	C23-C24-C25-C30
27	b	619	BCR	C5-C6-C7-C8
27	c	515	BCR	C23-C24-C25-C26
27	f	101	BCR	C5-C6-C7-C8
27	f	101	BCR	C23-C24-C25-C30
27	k	102	BCR	C23-C24-C25-C26
27	k	102	BCR	C23-C24-C25-C30
27	z	101	BCR	C23-C24-C25-C26
31	I	101	LMT	C4'-C5'-C6'-O6'
31	I	103	LMT	C4B-C5B-C6B-O6B
31	i	103	LMT	C4B-C5B-C6B-O6B
31	B	629	LMT	C5-C6-C7-C8
31	b	629	LMT	C5-C6-C7-C8
34	C	518	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
34	c	518	DGD	C2A-C3A-C4A-C5A
33	B	628	LHG	O9-C7-O7-C5
33	b	628	LHG	O9-C7-O7-C5
25	B	606	CLA	C11-C10-C8-C7
25	B	615	CLA	C6-C7-C8-C10
25	C	503	CLA	C11-C12-C13-C15
25	b	606	CLA	C11-C10-C8-C7
25	b	615	CLA	C6-C7-C8-C10
25	c	503	CLA	C11-C12-C13-C15
28	C	519	LMG	C21-C22-C23-C24
28	c	519	LMG	C21-C22-C23-C24
28	B	621	LMG	C32-C33-C34-C35
28	b	621	LMG	C32-C33-C34-C35
30	A	413	SQD	C30-C31-C32-C33
29	A	411	PL9	C4-C3-C7-C8
29	D	405	PL9	C4-C3-C7-C8
29	a	411	PL9	C4-C3-C7-C8
29	d	405	PL9	C4-C3-C7-C8
30	a	413	SQD	C30-C31-C32-C33
35	E	104	HEM	CAA-CBA-CGA-O1A
35	e	104	HEM	CAA-CBA-CGA-O1A
30	c	501	SQD	C31-C32-C33-C34
31	F	103	LMT	C7-C8-C9-C10
34	C	518	DGD	CAB-CBB-CCB-CDB
34	c	518	DGD	CAB-CBB-CCB-CDB
25	C	506	CLA	C6-C7-C8-C10
25	c	506	CLA	C6-C7-C8-C10
30	C	501	SQD	C31-C32-C33-C34
31	f	103	LMT	C7-C8-C9-C10
28	c	519	LMG	O10-C28-O8-C9
29	A	411	PL9	C23-C24-C26-C27
29	a	411	PL9	C23-C24-C26-C27
31	I	102	LMT	C11-C10-C9-C8
28	C	519	LMG	O10-C28-O8-C9
25	C	502	CLA	C2-C1-O2A-CGA
25	C	513	CLA	C2-C1-O2A-CGA
25	c	502	CLA	C2-C1-O2A-CGA
25	c	513	CLA	C2-C1-O2A-CGA
31	i	102	LMT	C11-C10-C9-C8
30	a	412	SQD	C18-C19-C20-C21
30	A	412	SQD	C18-C19-C20-C21
34	C	517	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
34	c	517	DGD	C5B-C6B-C7B-C8B
25	C	508	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	O1A-CGA-O2A-C1
28	A	410	LMG	C16-C17-C18-C19
28	a	410	LMG	C16-C17-C18-C19
25	B	607	CLA	C15-C16-C17-C18
31	J	101	LMT	C11-C10-C9-C8
31	j	101	LMT	C11-C10-C9-C8
33	B	628	LHG	C17-C18-C19-C20
25	C	509	CLA	C4-C3-C5-C6
25	C	511	CLA	C4-C3-C5-C6
25	c	509	CLA	C4-C3-C5-C6
25	c	511	CLA	C4-C3-C5-C6
29	A	411	PL9	C25-C24-C26-C27
29	a	411	PL9	C25-C24-C26-C27
25	b	607	CLA	C15-C16-C17-C18
33	b	628	LHG	C17-C18-C19-C20
25	B	603	CLA	O1A-CGA-O2A-C1
25	b	603	CLA	O1A-CGA-O2A-C1
31	E	103	LMT	O1'-C1-C2-C3
31	e	103	LMT	O1'-C1-C2-C3
34	C	517	DGD	CAB-CBB-CCB-CDB
31	i	102	LMT	C6-C7-C8-C9
34	c	517	DGD	CAB-CBB-CCB-CDB
33	B	628	LHG	C8-C7-O7-C5
31	I	102	LMT	C6-C7-C8-C9
30	A	413	SQD	C44-C45-C46-O48
30	a	413	SQD	C44-C45-C46-O48
34	C	516	DGD	C1G-C2G-C3G-O3G
34	H	104	DGD	O1G-C1G-C2G-C3G
34	c	516	DGD	C1G-C2G-C3G-O3G
34	h	104	DGD	O1G-C1G-C2G-C3G
33	Z	102	LHG	O10-C23-O8-C6
33	z	102	LHG	O10-C23-O8-C6
25	C	512	CLA	C5-C6-C7-C8
25	c	512	CLA	C5-C6-C7-C8
30	H	103	SQD	C10-C11-C12-C13
30	h	103	SQD	C10-C11-C12-C13
33	b	628	LHG	C8-C7-O7-C5
31	C	524	LMT	C11-C10-C9-C8
31	c	524	LMT	C11-C10-C9-C8
33	D	406	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	d	406	LHG	C27-C28-C29-C30
25	B	607	CLA	C4B-C3B-CAB-CBB
25	b	607	CLA	C4B-C3B-CAB-CBB
25	C	512	CLA	C8-C10-C11-C12
25	c	512	CLA	C8-C10-C11-C12
31	b	624	LMT	C5-C6-C7-C8
26	D	402	PHO	CHA-CBD-CGD-O1D
26	d	402	PHO	CHA-CBD-CGD-O1D
36	H	101	RRX	C11-C10-C9-C34
36	h	101	RRX	C11-C10-C9-C34
31	B	624	LMT	C5-C6-C7-C8
25	B	603	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	CBD-CGD-O2D-CED
30	A	412	SQD	C24-C25-C26-C27
30	a	412	SQD	C24-C25-C26-C27
34	H	104	DGD	C9A-CAA-CBA-CCA
34	h	104	DGD	C9A-CAA-CBA-CCA
28	H	105	LMG	O6-C1-O1-C7
28	h	105	LMG	O6-C1-O1-C7
35	E	104	HEM	CAA-CBA-CGA-O2A
35	e	104	HEM	CAA-CBA-CGA-O2A
25	B	614	CLA	C15-C16-C17-C18
25	b	614	CLA	C15-C16-C17-C18
25	B	607	CLA	C14-C13-C15-C16
25	b	607	CLA	C14-C13-C15-C16
30	c	501	SQD	C26-C27-C28-C29
33	B	627	LHG	C29-C30-C31-C32
33	b	627	LHG	C29-C30-C31-C32
25	c	502	CLA	O1D-CGD-O2D-CED
28	D	409	LMG	C8-C7-O1-C1
28	d	409	LMG	C8-C7-O1-C1
30	C	501	SQD	C26-C27-C28-C29
31	E	101	LMT	C1-C2-C3-C4
31	e	101	LMT	C1-C2-C3-C4
34	c	517	DGD	C2A-C3A-C4A-C5A
34	C	517	DGD	C2A-C3A-C4A-C5A
25	D	401	CLA	C3A-C2A-CAA-CBA
25	d	401	CLA	C3A-C2A-CAA-CBA
28	A	410	LMG	C15-C16-C17-C18
28	a	410	LMG	C15-C16-C17-C18
30	K	101	SQD	O48-C23-C24-C25
30	k	101	SQD	O48-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	D	404	CLA	C2-C3-C5-C6
25	d	404	CLA	C2-C3-C5-C6
25	C	502	CLA	O1D-CGD-O2D-CED
29	D	405	PL9	C7-C8-C9-C10
29	d	405	PL9	C7-C8-C9-C10
34	C	517	DGD	C6B-C7B-C8B-C9B
25	C	507	CLA	C3-C5-C6-C7
25	c	507	CLA	C3-C5-C6-C7
34	c	517	DGD	C6B-C7B-C8B-C9B
30	b	620	SQD	C30-C31-C32-C33
30	B	620	SQD	C30-C31-C32-C33
31	x	102	LMT	C2-C3-C4-C5
31	b	629	LMT	C11-C10-C9-C8
31	B	629	LMT	C11-C10-C9-C8
31	X	102	LMT	C2-C3-C4-C5
25	B	608	CLA	C16-C17-C18-C19
25	b	608	CLA	C16-C17-C18-C19
28	C	519	LMG	C29-C28-O8-C9
28	c	519	LMG	C29-C28-O8-C9
30	F	102	SQD	O6-C44-C45-C46
30	f	102	SQD	O6-C44-C45-C46
28	h	105	LMG	C33-C34-C35-C36
28	H	105	LMG	C33-C34-C35-C36
25	A	408	CLA	C2A-CAA-CBA-CGA
25	a	408	CLA	C2A-CAA-CBA-CGA
36	H	101	RRX	C9-C10-C11-C12
36	h	101	RRX	C9-C10-C11-C12
28	A	410	LMG	C39-C40-C41-C42
28	a	410	LMG	C39-C40-C41-C42
31	b	624	LMT	C4-C5-C6-C7
31	B	624	LMT	C4-C5-C6-C7
33	E	102	LHG	C17-C18-C19-C20
25	B	602	CLA	C16-C17-C18-C19
25	B	614	CLA	C16-C17-C18-C20
25	C	509	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C20
25	c	509	CLA	C16-C17-C18-C20
31	K	105	LMT	C11-C10-C9-C8
31	k	105	LMT	C11-C10-C9-C8
33	B	628	LHG	C15-C16-C17-C18
33	b	628	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	A	410	LMG	O7-C10-C11-C12
33	e	102	LHG	C17-C18-C19-C20
27	B	619	BCR	C21-C22-C23-C24
27	b	619	BCR	C21-C22-C23-C24
28	a	410	LMG	O7-C10-C11-C12
25	B	614	CLA	C11-C10-C8-C7
25	C	505	CLA	C11-C12-C13-C15
25	D	401	CLA	C11-C10-C8-C7
25	D	401	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C12-C13-C15
25	d	401	CLA	C12-C13-C15-C16
25	C	507	CLA	C2B-C3B-CAB-CBB
25	c	507	CLA	C2B-C3B-CAB-CBB
27	A	409	BCR	C5-C6-C7-C8
27	A	409	BCR	C23-C24-C25-C26
27	B	617	BCR	C23-C24-C25-C26
27	F	101	BCR	C23-C24-C25-C26
27	K	103	BCR	C23-C24-C25-C26
27	K	103	BCR	C23-C24-C25-C30
27	a	409	BCR	C5-C6-C7-C8
27	a	409	BCR	C23-C24-C25-C26
27	b	617	BCR	C23-C24-C25-C26
27	f	101	BCR	C23-C24-C25-C26
27	k	103	BCR	C23-C24-C25-C26
27	k	103	BCR	C23-C24-C25-C30
25	B	602	CLA	C2-C1-O2A-CGA
25	b	602	CLA	C2-C1-O2A-CGA
33	E	102	LHG	O8-C23-C24-C25
33	e	102	LHG	O8-C23-C24-C25
28	C	523	LMG	O8-C28-C29-C30
28	c	523	LMG	O8-C28-C29-C30
31	H	102	LMT	C3-C4-C5-C6
25	B	614	CLA	CAA-CBA-CGA-O2A
25	C	506	CLA	CAA-CBA-CGA-O2A
25	b	614	CLA	CAA-CBA-CGA-O2A
25	c	506	CLA	CAA-CBA-CGA-O2A
31	h	102	LMT	C3-C4-C5-C6
25	c	505	CLA	C8-C10-C11-C12
30	A	412	SQD	C4-C5-C6-S
30	B	620	SQD	C4-C5-C6-S
30	a	412	SQD	C4-C5-C6-S

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Mol	Chain	Res	Type	Atoms
30	b	620	SQD	C4-C5-C6-S
25	C	505	CLA	C8-C10-C11-C12
25	C	502	CLA	C2-C3-C5-C6
25	c	502	CLA	C2-C3-C5-C6
33	D	406	LHG	C17-C18-C19-C20
33	d	406	LHG	C17-C18-C19-C20
34	H	104	DGD	CAB-CBB-CCB-CDB
25	B	609	CLA	C2A-CAA-CBA-CGA
25	b	609	CLA	C2A-CAA-CBA-CGA
34	h	104	DGD	CAB-CBB-CCB-CDB
30	C	501	SQD	O47-C7-C8-C9
30	c	501	SQD	O47-C7-C8-C9
31	h	102	LMT	C1-C2-C3-C4
30	K	101	SQD	O10-C23-C24-C25
30	k	101	SQD	O10-C23-C24-C25
31	B	629	LMT	C2-C1-O1'-C1'
31	E	101	LMT	C2-C1-O1'-C1'
31	X	104	LMT	C2-C1-O1'-C1'
31	b	629	LMT	C2-C1-O1'-C1'
31	e	101	LMT	C2-C1-O1'-C1'
31	x	104	LMT	C2-C1-O1'-C1'
33	E	102	LHG	O1-C1-C2-O2
33	e	102	LHG	O1-C1-C2-O2
28	c	523	LMG	C32-C33-C34-C35
25	C	511	CLA	CAA-CBA-CGA-O2A
25	c	511	CLA	CAA-CBA-CGA-O2A
33	D	407	LHG	O8-C23-C24-C25
33	d	407	LHG	O8-C23-C24-C25
28	H	105	LMG	C12-C13-C14-C15
28	h	105	LMG	C12-C13-C14-C15
31	f	103	LMT	C5-C6-C7-C8
31	H	102	LMT	C1-C2-C3-C4
28	A	410	LMG	C7-C8-C9-O8
28	a	410	LMG	C7-C8-C9-O8
28	C	523	LMG	C32-C33-C34-C35
31	F	103	LMT	C5-C6-C7-C8
31	E	103	LMT	C5'-C4'-O1B-C1B
25	B	606	CLA	C4-C3-C5-C6
25	b	606	CLA	C4-C3-C5-C6
34	C	517	DGD	O6D-C1D-O3G-C3G
34	c	517	DGD	O6D-C1D-O3G-C3G
25	B	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	b	612	CLA	CAA-CBA-CGA-O2A
30	c	501	SQD	O48-C23-C24-C25
33	b	628	LHG	C10-C11-C12-C13
36	H	101	RRX	C15-C16-C17-C18
36	h	101	RRX	C15-C16-C17-C18
31	e	103	LMT	C5'-C4'-O1B-C1B
30	A	412	SQD	C26-C27-C28-C29
30	a	412	SQD	C26-C27-C28-C29
33	B	628	LHG	C10-C11-C12-C13
33	D	406	LHG	C19-C20-C21-C22
33	d	406	LHG	C19-C20-C21-C22
28	C	519	LMG	C32-C33-C34-C35
28	c	519	LMG	C32-C33-C34-C35
30	C	501	SQD	O48-C23-C24-C25
31	i	101	LMT	C4-C5-C6-C7
31	I	101	LMT	C4-C5-C6-C7
25	d	401	CLA	C3-C5-C6-C7
25	C	504	CLA	C2-C1-O2A-CGA
25	C	512	CLA	C2-C1-O2A-CGA
25	c	504	CLA	C2-C1-O2A-CGA
25	c	512	CLA	C2-C1-O2A-CGA
25	C	510	CLA	C11-C12-C13-C15
25	c	510	CLA	C11-C12-C13-C15
25	d	401	CLA	C11-C10-C8-C7
25	B	612	CLA	C16-C17-C18-C19
25	b	612	CLA	C16-C17-C18-C19
28	A	410	LMG	C36-C37-C38-C39
33	D	407	LHG	C32-C33-C34-C35
33	d	407	LHG	C32-C33-C34-C35
28	a	410	LMG	C36-C37-C38-C39
30	C	501	SQD	C19-C20-C21-C22
30	c	501	SQD	C19-C20-C21-C22
25	D	401	CLA	C3-C5-C6-C7
31	B	624	LMT	C3-C4-C5-C6
31	b	624	LMT	C3-C4-C5-C6
25	A	405	CLA	C2A-CAA-CBA-CGA
25	a	405	CLA	C2A-CAA-CBA-CGA
25	c	508	CLA	C8-C10-C11-C12
29	D	405	PL9	C44-C46-C47-C48
29	d	405	PL9	C44-C46-C47-C48
25	C	508	CLA	C8-C10-C11-C12
25	d	403	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	c	501	SQD	C34-C35-C36-C37
25	B	602	CLA	C3A-C2A-CAA-CBA
25	b	602	CLA	C3A-C2A-CAA-CBA
26	A	407	PHO	C3A-C2A-CAA-CBA
26	a	407	PHO	C3A-C2A-CAA-CBA
30	C	501	SQD	C34-C35-C36-C37
25	C	513	CLA	CAA-CBA-CGA-O2A
25	c	513	CLA	CAA-CBA-CGA-O2A
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
25	D	403	CLA	C10-C11-C12-C13
25	A	408	CLA	C11-C10-C8-C9
25	B	606	CLA	C11-C10-C8-C9
25	D	401	CLA	C14-C13-C15-C16
25	a	408	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	d	401	CLA	C11-C10-C8-C9
25	d	401	CLA	C14-C13-C15-C16
28	D	409	LMG	O7-C10-C11-C12
28	d	409	LMG	O7-C10-C11-C12
30	K	101	SQD	C11-C12-C13-C14
30	k	101	SQD	C11-C12-C13-C14
33	E	102	LHG	O10-C23-C24-C25
33	e	102	LHG	O10-C23-C24-C25
30	A	412	SQD	O5-C5-C6-S
30	a	412	SQD	O5-C5-C6-S
31	X	105	LMT	C1-C2-C3-C4
31	x	105	LMT	C1-C2-C3-C4
28	A	410	LMG	O9-C10-C11-C12
28	a	410	LMG	O9-C10-C11-C12
30	c	501	SQD	C24-C25-C26-C27
25	B	602	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C20
25	c	502	CLA	CBD-CGD-O2D-CED
30	C	501	SQD	C24-C25-C26-C27
25	C	506	CLA	CAA-CBA-CGA-O1A
25	c	506	CLA	CAA-CBA-CGA-O1A
28	C	523	LMG	O10-C28-C29-C30
33	D	407	LHG	O10-C23-C24-C25
33	d	407	LHG	O10-C23-C24-C25
30	B	620	SQD	O48-C23-C24-C25
30	b	620	SQD	O48-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
34	C	516	DGD	C6A-C7A-C8A-C9A
34	c	516	DGD	C6A-C7A-C8A-C9A
25	C	502	CLA	CBD-CGD-O2D-CED
31	K	105	LMT	O5B-C1B-O1B-C4'
31	k	105	LMT	O5B-C1B-O1B-C4'
31	b	625	LMT	C4-C5-C6-C7
25	B	614	CLA	CAA-CBA-CGA-O1A
25	b	614	CLA	CAA-CBA-CGA-O1A
28	c	523	LMG	O10-C28-C29-C30
31	B	625	LMT	C4-C5-C6-C7
25	d	403	CLA	CAA-CBA-CGA-O2A
35	E	104	HEM	C2B-C3B-CAB-CBB
35	e	104	HEM	C2B-C3B-CAB-CBB
25	C	513	CLA	CAA-CBA-CGA-O1A
25	c	513	CLA	CAA-CBA-CGA-O1A
33	z	102	LHG	C24-C25-C26-C27
25	B	610	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	D	403	CLA	CAA-CBA-CGA-O2A
30	A	412	SQD	O49-C7-C8-C9
30	a	412	SQD	O49-C7-C8-C9
28	A	410	LMG	C29-C30-C31-C32
28	a	410	LMG	C29-C30-C31-C32
33	Z	102	LHG	C24-C25-C26-C27
25	B	604	CLA	C2-C1-O2A-CGA
25	b	604	CLA	C2-C1-O2A-CGA
25	C	511	CLA	CAA-CBA-CGA-O1A
25	c	511	CLA	CAA-CBA-CGA-O1A
30	c	501	SQD	O10-C23-C24-C25
25	b	608	CLA	CAA-CBA-CGA-O2A
31	X	103	LMT	C1-C2-C3-C4
31	x	103	LMT	C1-C2-C3-C4
34	C	518	DGD	C5A-C6A-C7A-C8A
30	C	501	SQD	O10-C23-C24-C25
25	C	505	CLA	C10-C11-C12-C13
25	c	505	CLA	C10-C11-C12-C13
28	a	410	LMG	C11-C12-C13-C14
34	c	518	DGD	C5A-C6A-C7A-C8A
25	B	608	CLA	CAA-CBA-CGA-O2A
28	A	410	LMG	C11-C12-C13-C14
30	B	620	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
30	b	620	SQD	O10-C23-C24-C25

There are no ring outliers.

178 monomers are involved in 523 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	d	408	LHG	6	0
30	b	620	SQD	2	0
25	b	614	CLA	5	0
29	D	405	PL9	2	0
25	c	514	CLA	3	0
25	c	504	CLA	6	0
27	b	618	BCR	1	0
25	b	608	CLA	5	0
31	e	101	LMT	1	0
25	c	502	CLA	4	0
31	X	103	LMT	2	0
33	z	102	LHG	1	0
31	M	102	LMT	2	0
25	d	401	CLA	4	0
25	b	616	CLA	4	0
25	c	506	CLA	5	0
27	C	515	BCR	4	0
31	E	103	LMT	3	0
25	c	512	CLA	7	0
33	B	627	LHG	8	0
25	C	506	CLA	5	0
27	B	618	BCR	1	0
25	B	613	CLA	4	0
25	b	607	CLA	6	0
28	D	409	LMG	1	0
25	C	512	CLA	9	0
31	y	101	LMT	2	0
30	A	413	SQD	1	0
25	C	508	CLA	4	0
25	C	505	CLA	4	0
33	B	628	LHG	4	0
30	B	620	SQD	2	0
31	E	101	LMT	1	0
25	B	604	CLA	4	0
33	Z	102	LHG	1	0
27	F	101	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	612	CLA	4	0
28	A	414	LMG	2	0
31	h	102	LMT	2	0
25	B	605	CLA	6	0
31	B	624	LMT	1	0
25	B	614	CLA	6	0
25	A	408	CLA	7	0
25	b	605	CLA	5	0
25	b	601	CLA	2	0
33	D	406	LHG	2	0
31	X	102	LMT	3	0
26	a	407	PHO	6	0
31	H	102	LMT	1	0
27	k	103	BCR	4	0
31	e	103	LMT	3	0
25	C	513	CLA	1	0
30	k	101	SQD	4	0
31	I	101	LMT	1	0
31	x	103	LMT	2	0
30	a	413	SQD	1	0
31	t	101	LMT	1	0
27	b	619	BCR	1	0
27	B	617	BCR	4	0
35	v	201	HEM	3	0
31	d	410	LMT	3	0
27	K	102	BCR	5	0
25	c	507	CLA	3	0
31	I	102	LMT	2	0
36	H	101	RRX	2	0
28	A	410	LMG	3	0
31	M	101	LMT	6	0
27	c	515	BCR	4	0
31	m	102	LMT	2	0
25	d	403	CLA	7	0
25	c	508	CLA	5	0
28	a	410	LMG	3	0
31	I	103	LMT	2	0
28	B	621	LMG	1	0
25	B	610	CLA	2	0
33	d	407	LHG	7	0
25	d	404	CLA	4	0
31	Y	101	LMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	z	101	BCR	3	0
31	d	412	LMT	1	0
31	x	102	LMT	3	0
25	B	608	CLA	6	0
25	c	511	CLA	6	0
30	K	101	SQD	4	0
25	b	609	CLA	7	0
34	H	104	DGD	4	0
34	c	516	DGD	6	0
34	c	518	DGD	5	0
30	C	501	SQD	4	0
26	A	407	PHO	5	0
31	i	101	LMT	1	0
34	c	517	DGD	5	0
27	a	409	BCR	4	0
25	B	615	CLA	3	0
25	b	602	CLA	2	0
27	b	617	BCR	4	0
31	b	623	LMT	3	0
31	K	105	LMT	8	0
33	e	102	LHG	2	0
34	C	516	DGD	7	0
30	h	103	SQD	2	0
25	b	606	CLA	1	0
31	C	525	LMT	1	0
31	f	103	LMT	2	0
25	c	503	CLA	4	0
33	b	628	LHG	4	0
26	d	402	PHO	1	0
25	b	604	CLA	5	0
27	B	619	BCR	2	0
33	E	102	LHG	2	0
30	c	501	SQD	4	0
25	B	609	CLA	8	0
25	C	507	CLA	4	0
25	B	612	CLA	4	0
25	b	603	CLA	2	0
25	b	613	CLA	4	0
31	b	624	LMT	1	0
27	Z	101	BCR	2	0
25	B	607	CLA	6	0
25	B	603	CLA	2	0

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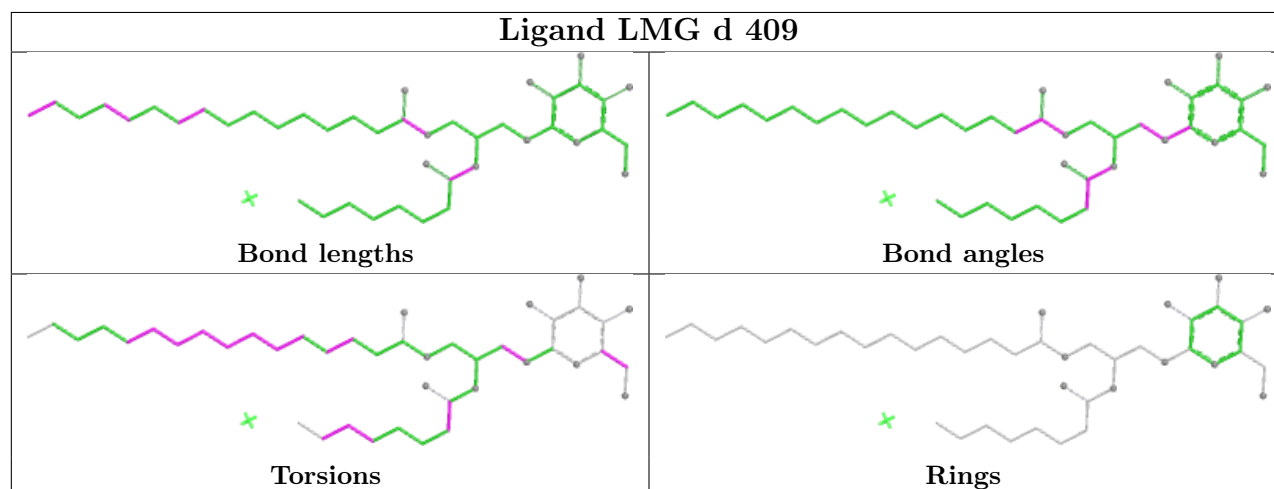
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	519	LMG	7	0
27	f	101	BCR	4	0
31	m	101	LMT	7	0
30	a	412	SQD	3	0
25	b	611	CLA	3	0
25	c	505	CLA	3	0
25	c	513	CLA	1	0
29	a	411	PL9	8	0
25	B	602	CLA	2	0
31	B	623	LMT	4	0
31	k	105	LMT	8	0
35	V	201	HEM	3	0
25	C	502	CLA	3	0
31	F	103	LMT	2	0
25	c	509	CLA	7	0
29	A	411	PL9	8	0
31	c	525	LMT	1	0
27	A	409	BCR	4	0
25	C	511	CLA	6	0
33	D	407	LHG	7	0
25	B	606	CLA	1	0
25	C	504	CLA	7	0
27	k	102	BCR	5	0
33	d	406	LHG	2	0
34	h	104	DGD	4	0
35	E	104	HEM	7	0
25	D	403	CLA	6	0
33	b	627	LHG	7	0
25	D	404	CLA	2	0
25	B	601	CLA	2	0
34	C	518	DGD	6	0
25	a	405	CLA	4	0
33	D	408	LHG	5	0
25	C	514	CLA	1	0
31	i	103	LMT	2	0
25	b	615	CLA	4	0
35	e	104	HEM	7	0
25	C	503	CLA	4	0
28	b	621	LMG	1	0
29	d	405	PL9	2	0
30	H	103	SQD	3	0
27	K	103	BCR	4	0

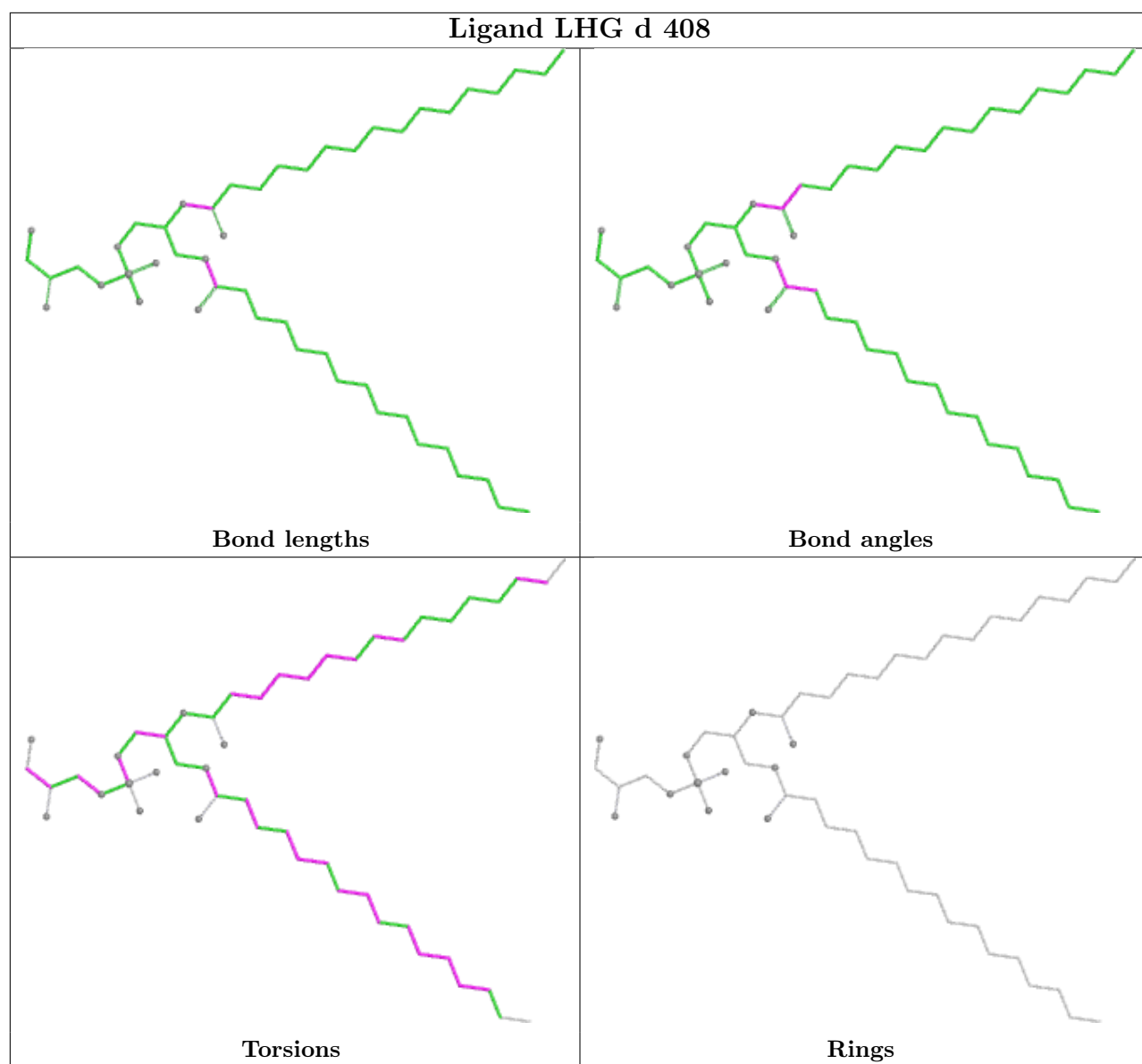
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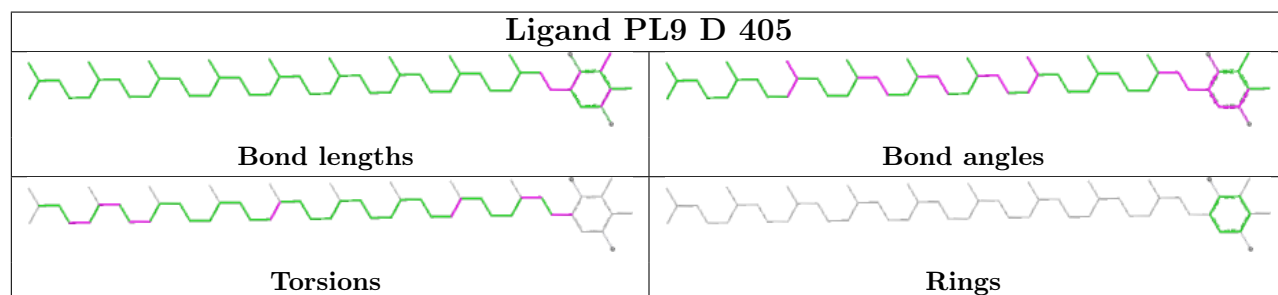
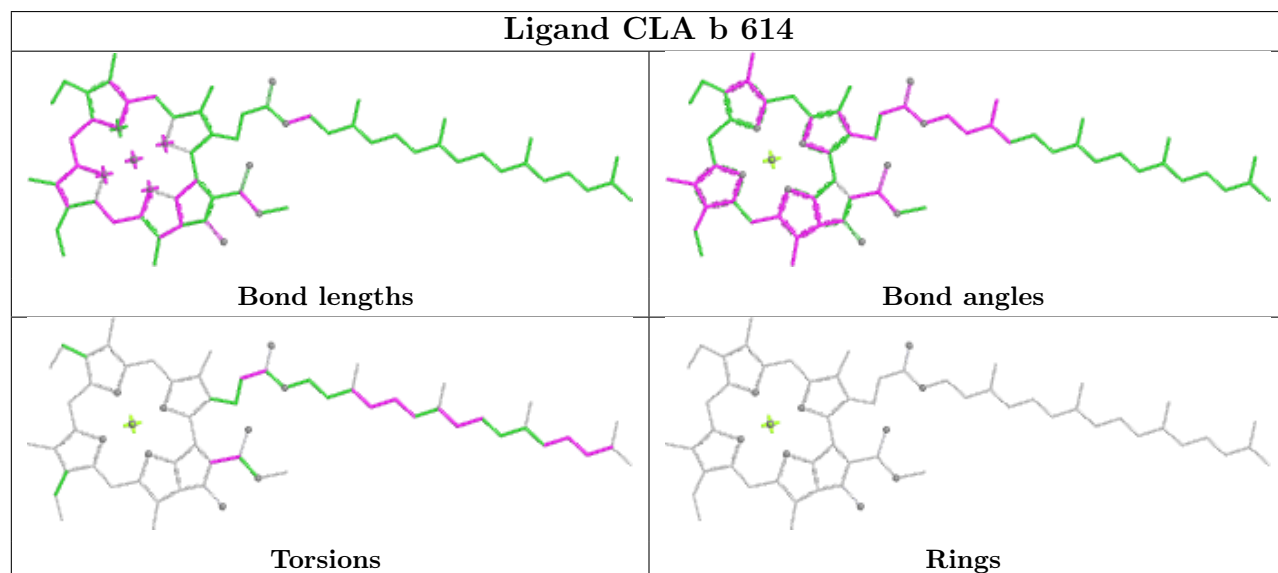
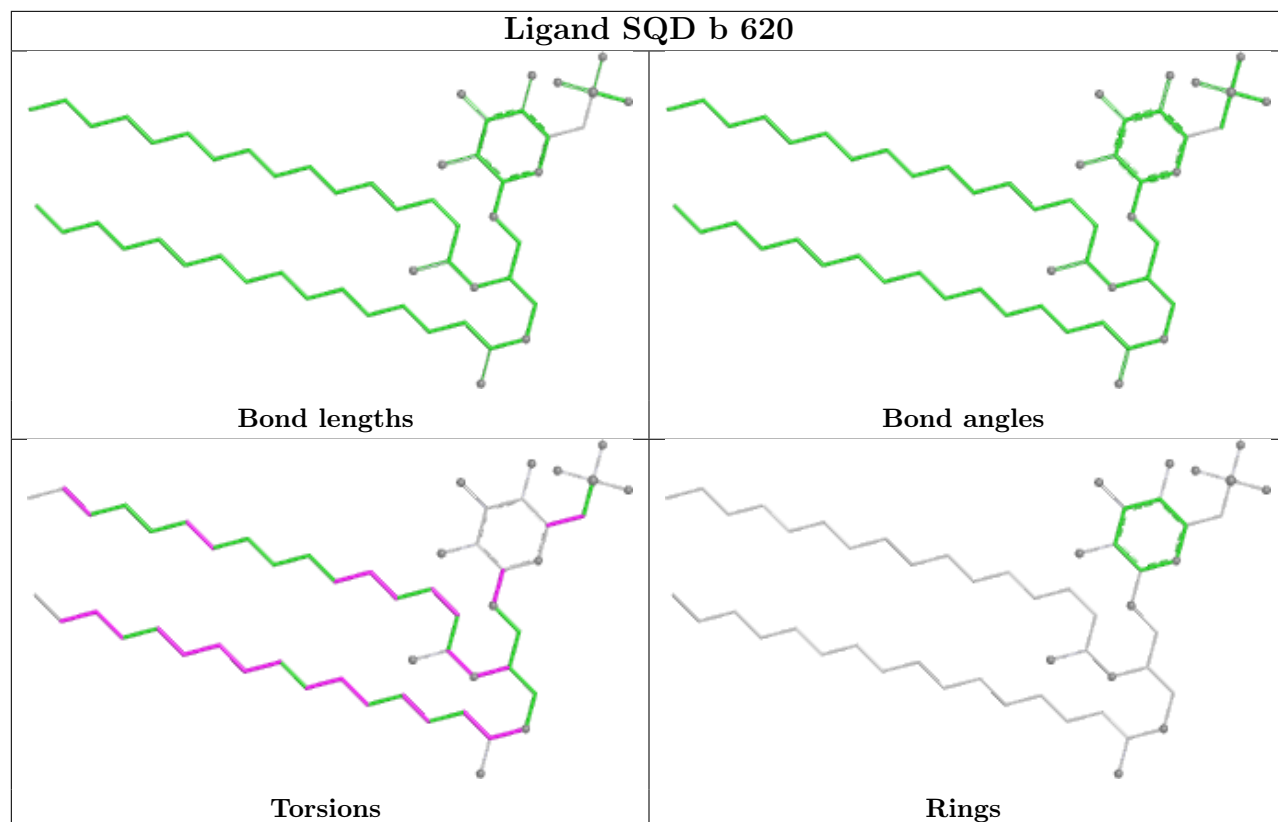
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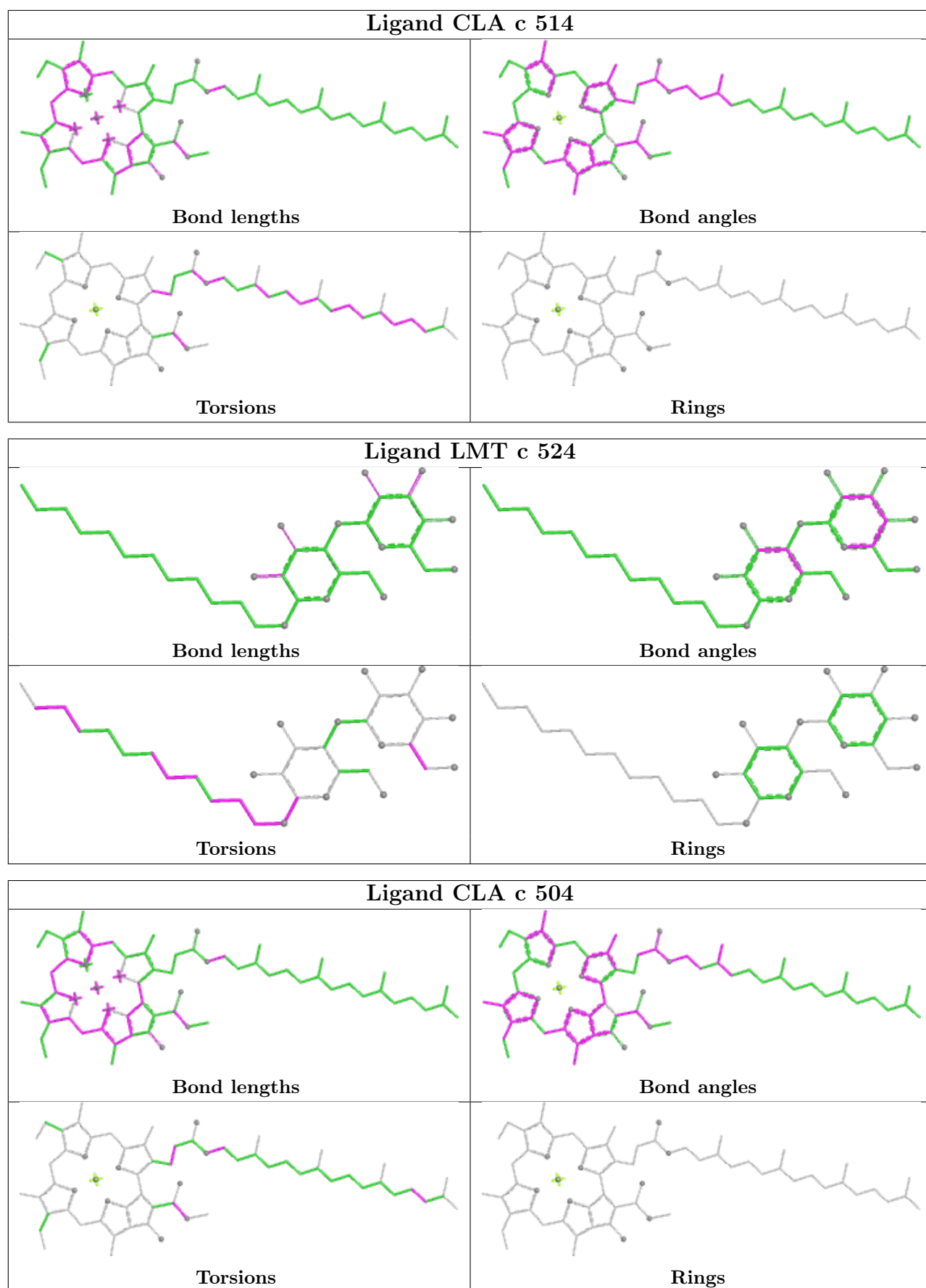
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	408	CLA	6	0
25	B	616	CLA	4	0
25	C	509	CLA	7	0
25	D	401	CLA	5	0
26	D	402	PHO	1	0
36	h	101	RRX	2	0
31	D	412	LMT	1	0
31	D	410	LMT	3	0
25	A	405	CLA	6	0
28	c	519	LMG	6	0
30	A	412	SQD	4	0
25	B	611	CLA	3	0
34	C	517	DGD	6	0
31	T	101	LMT	1	0
28	a	414	LMG	3	0
25	b	610	CLA	1	0

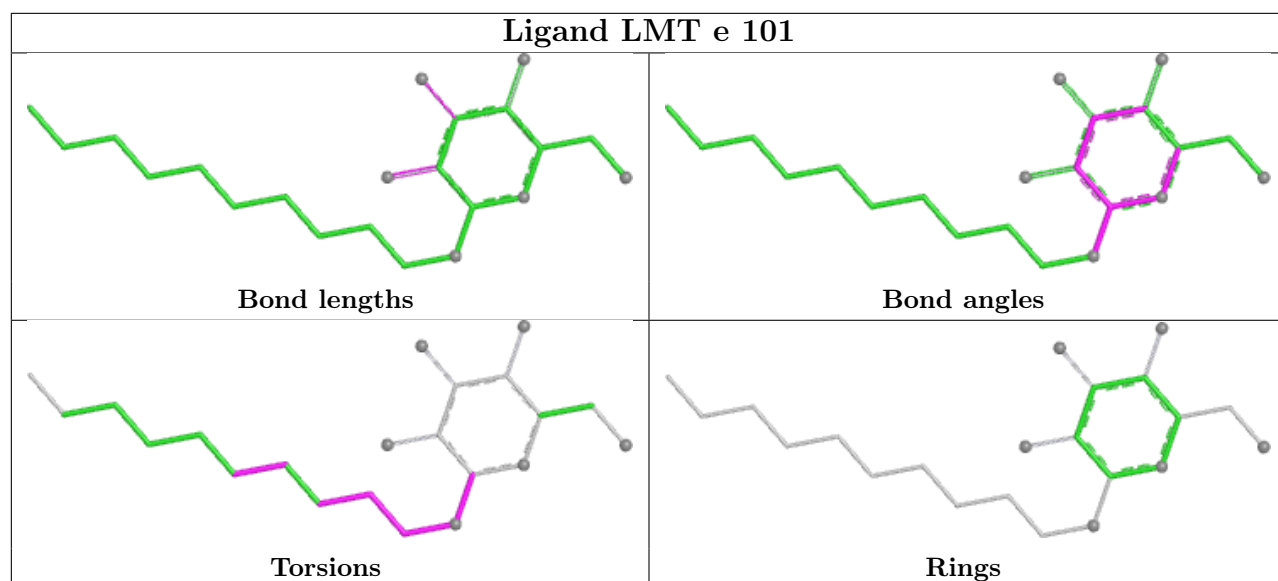
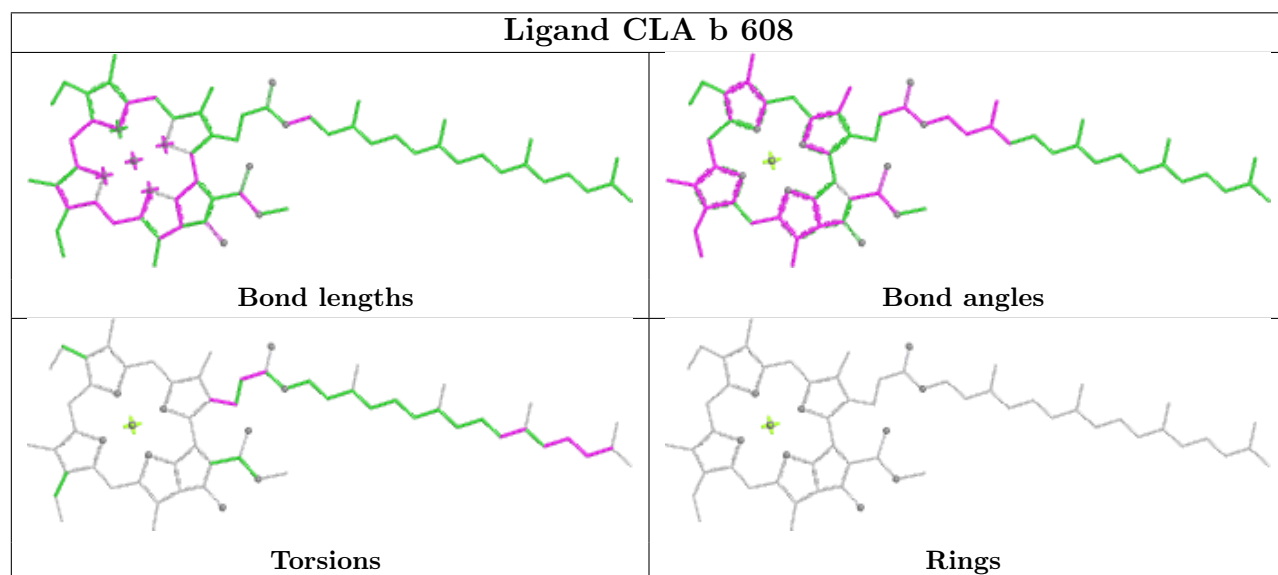
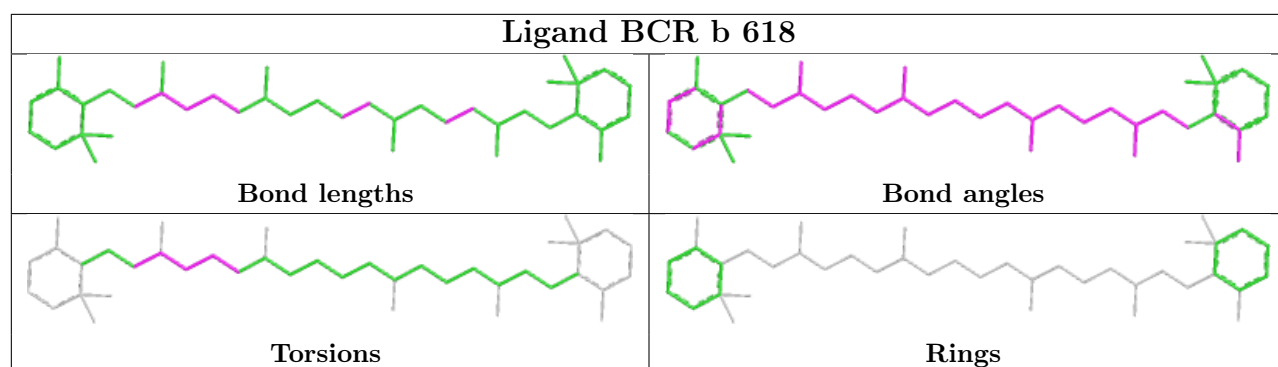
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

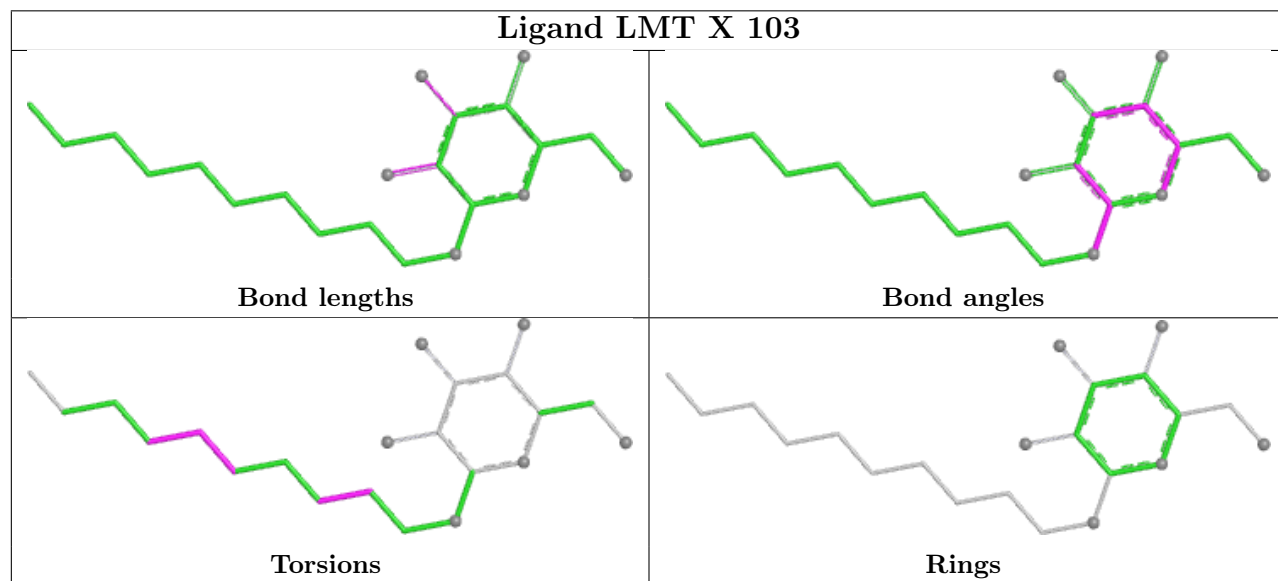
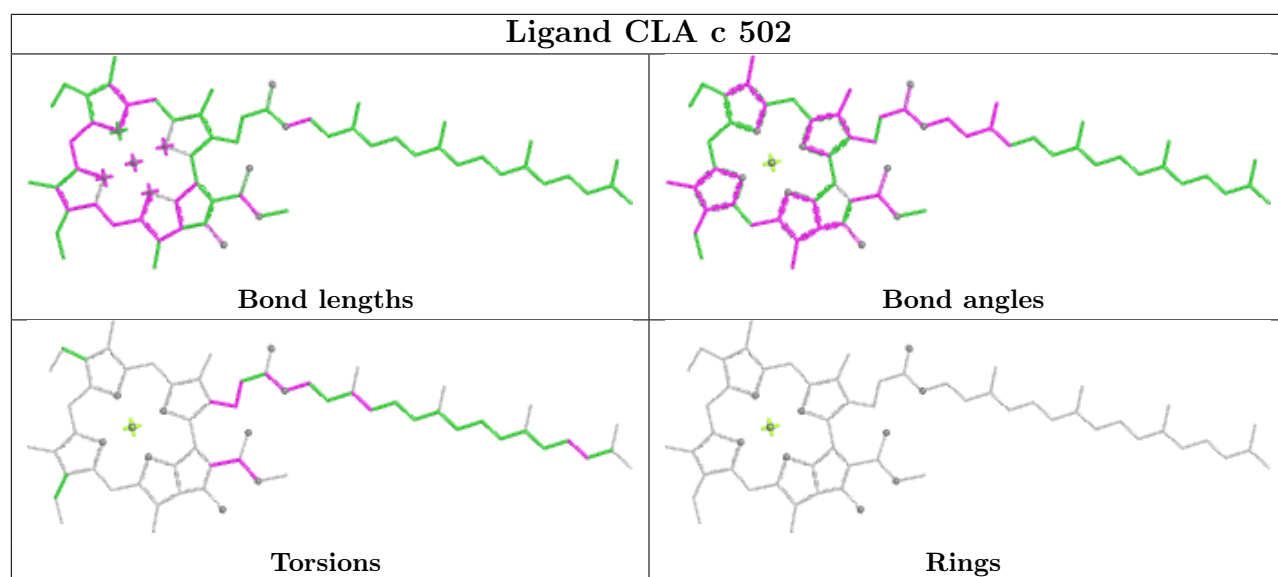


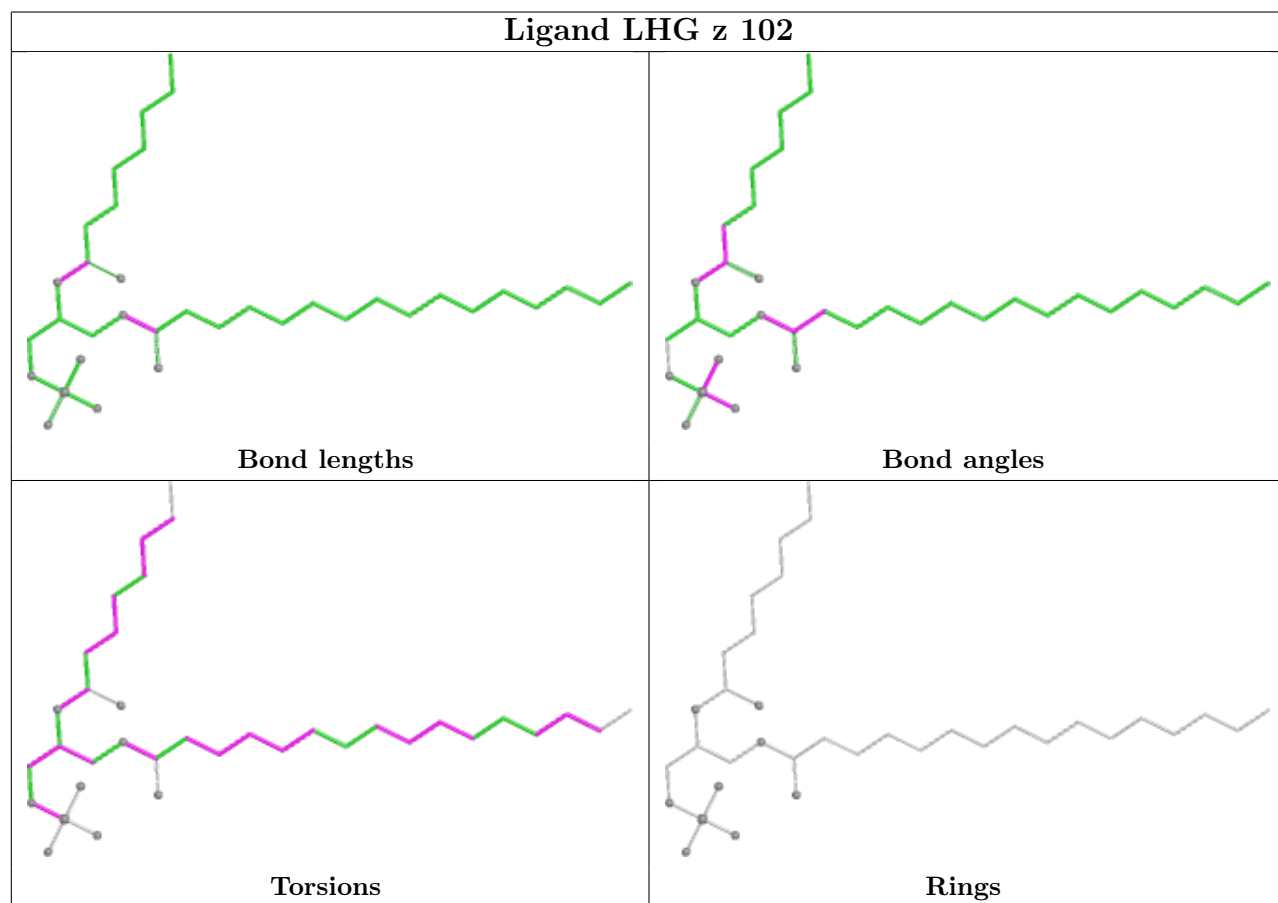
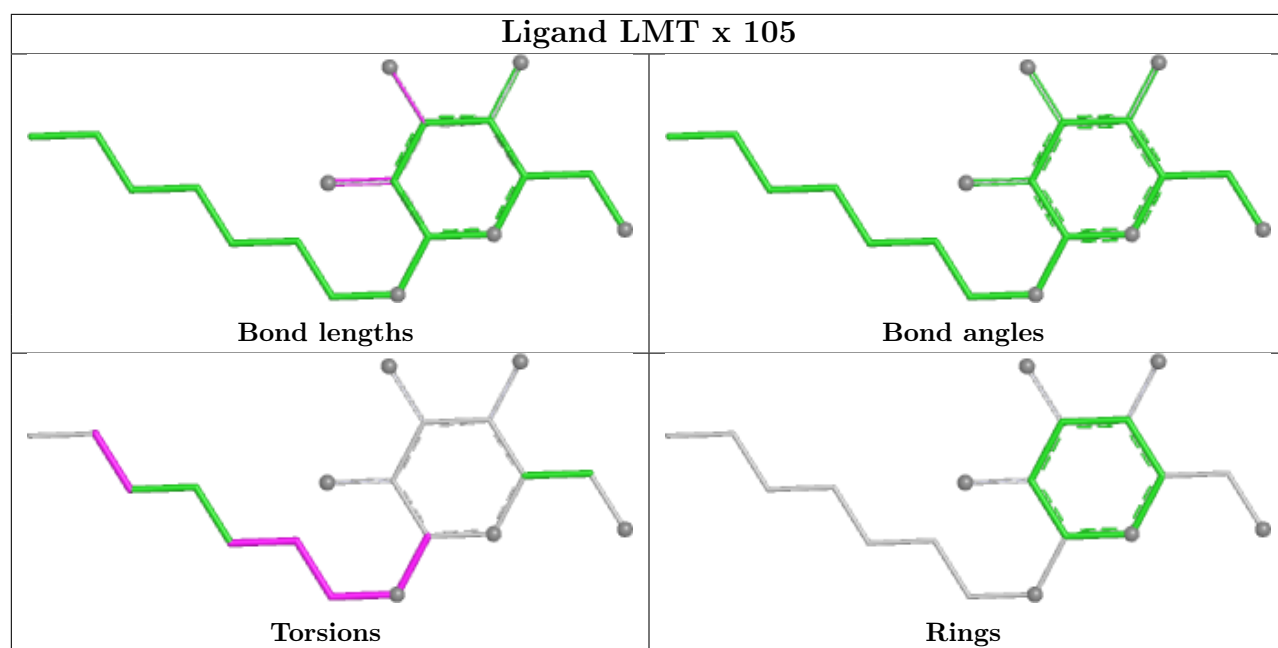


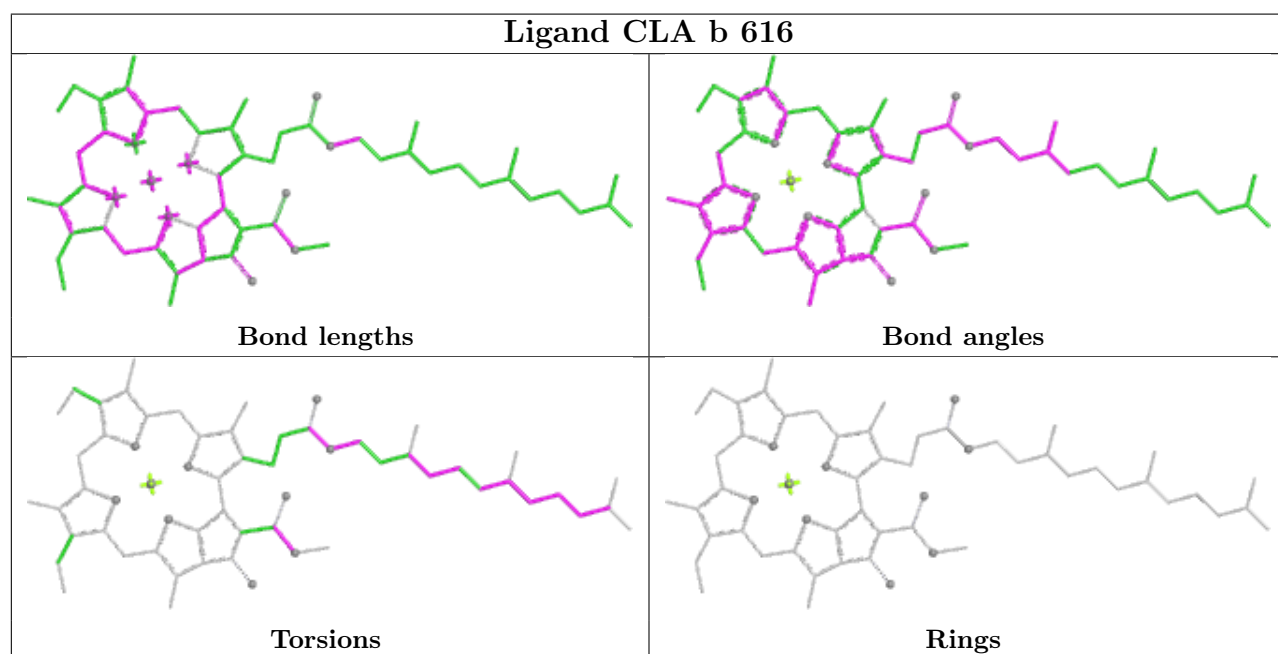
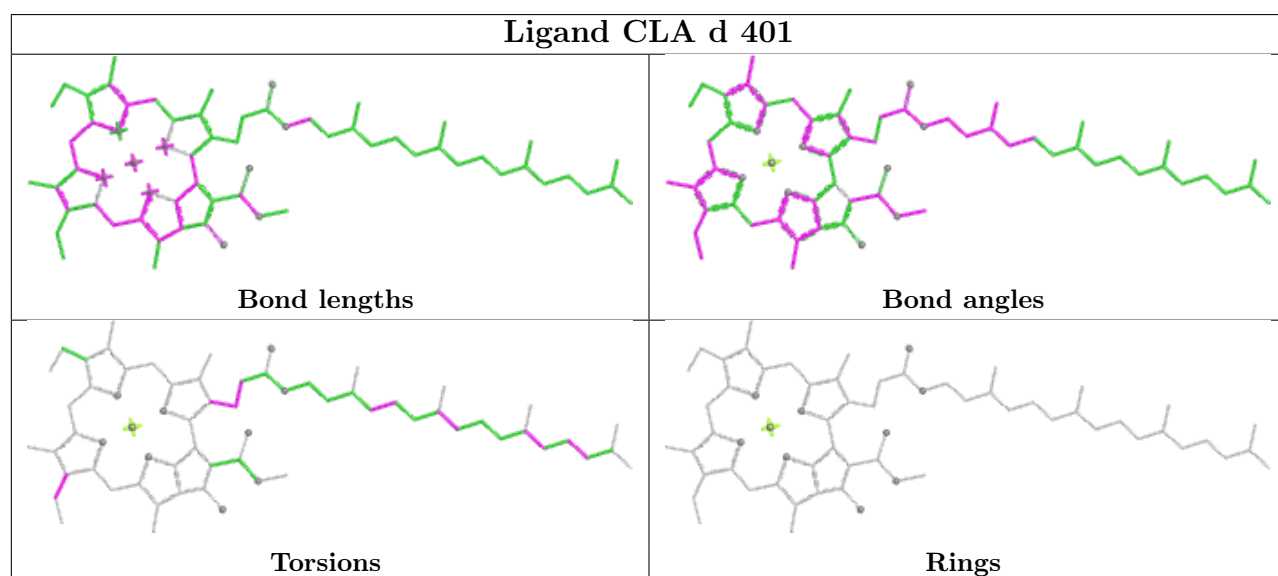
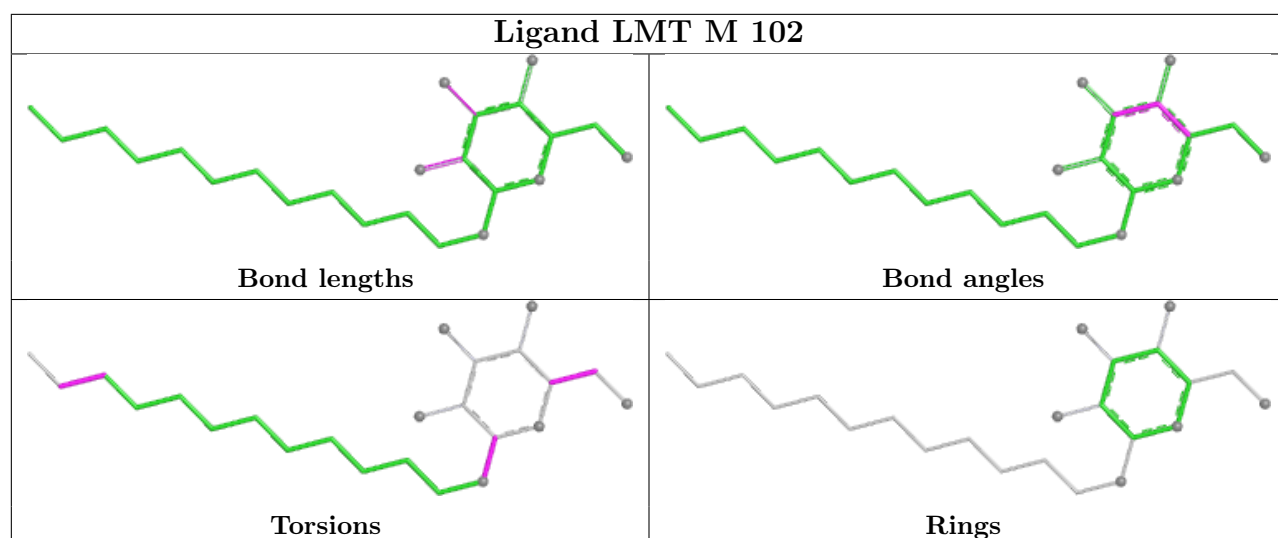


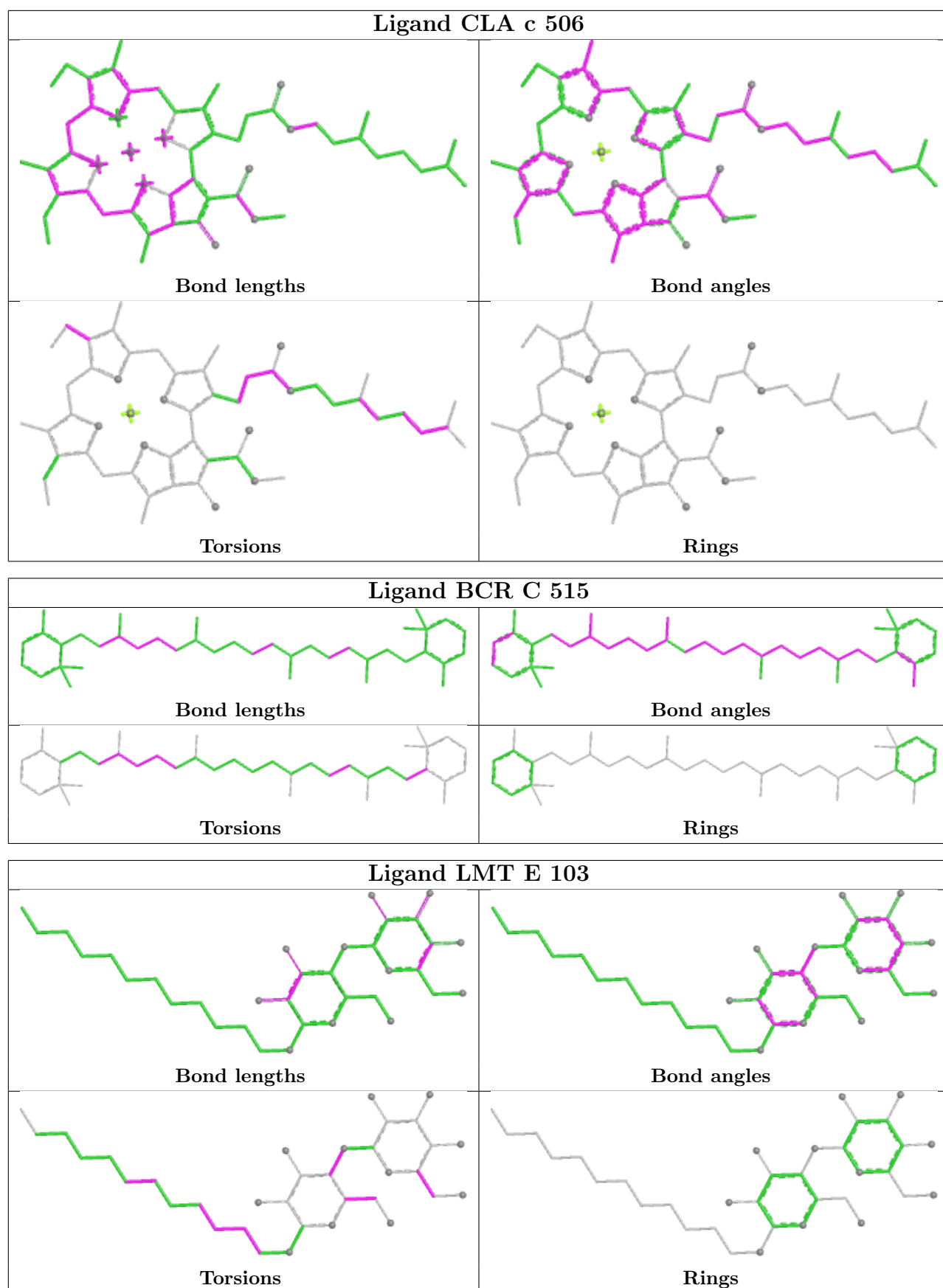


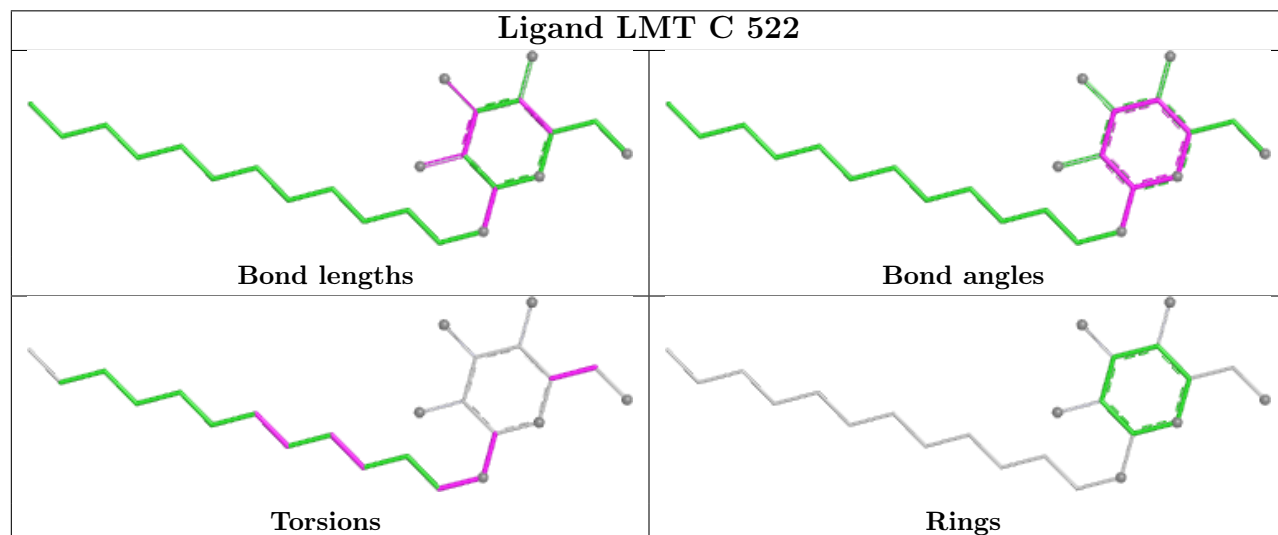
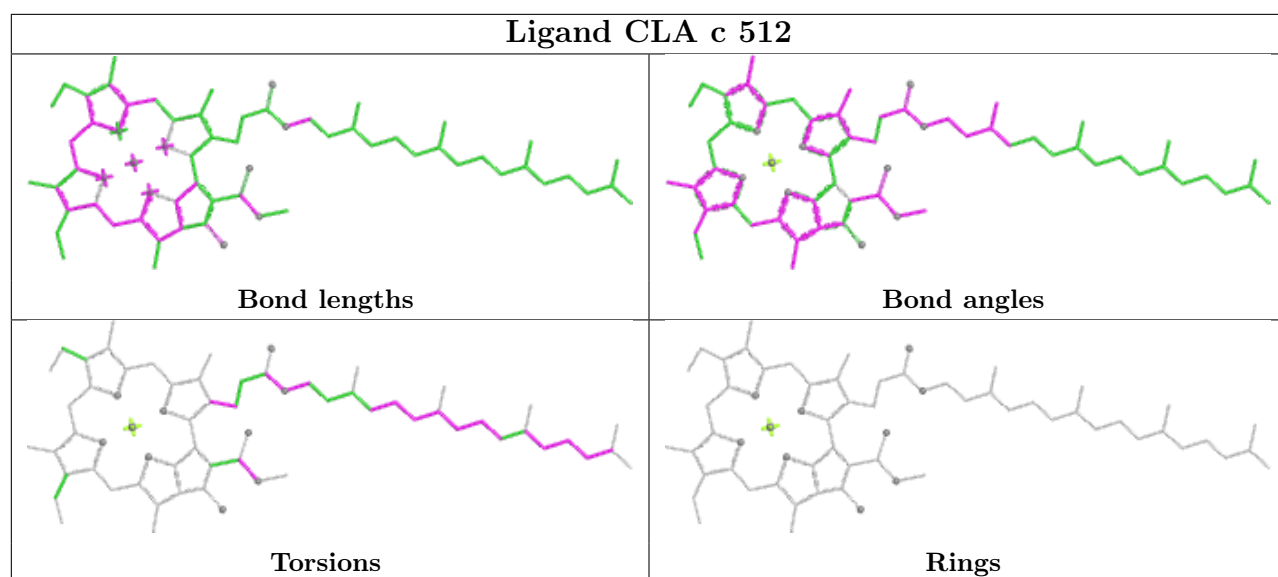


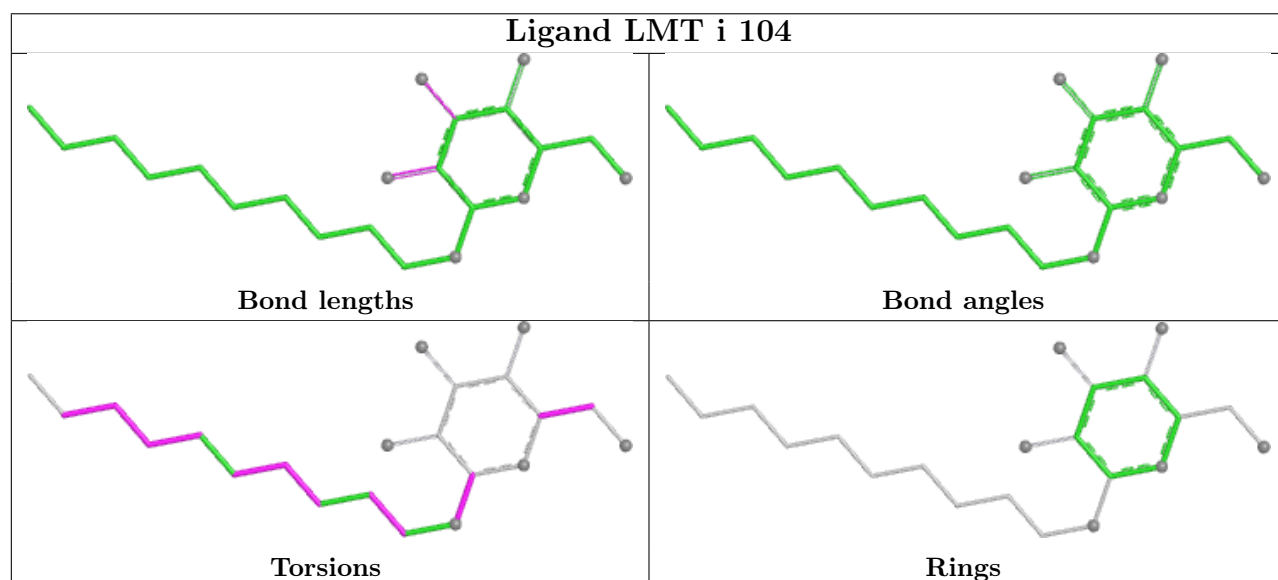
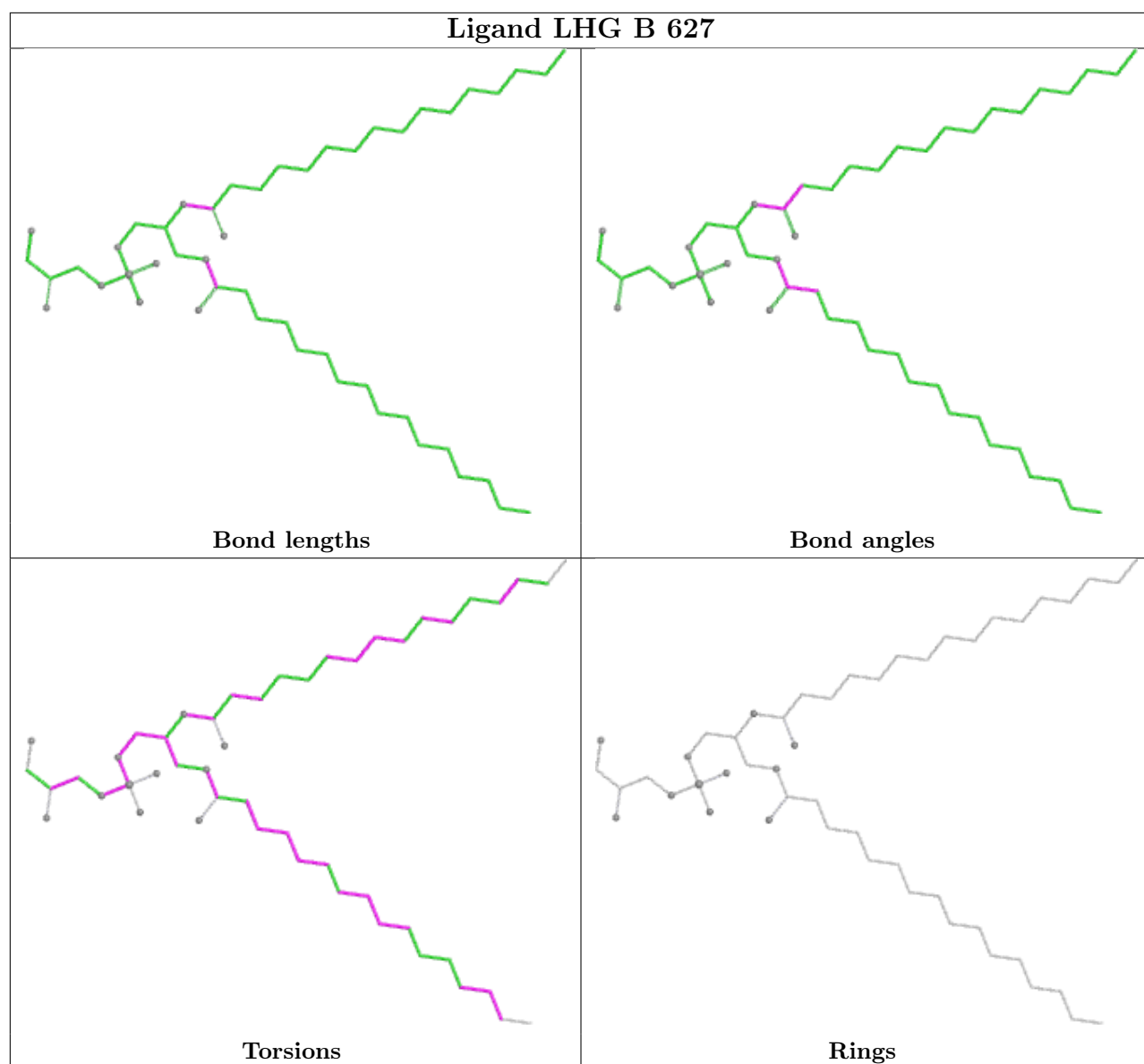


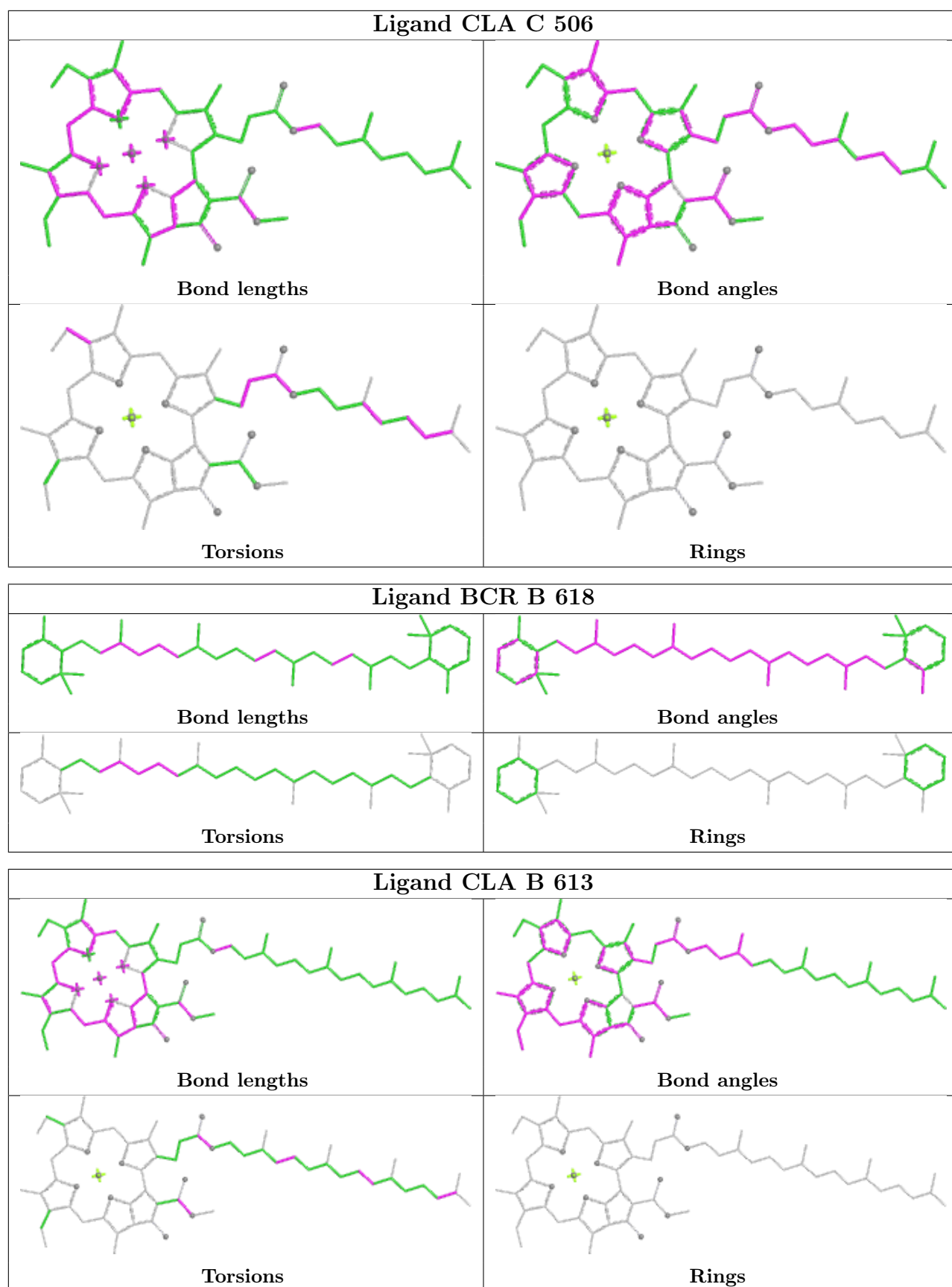




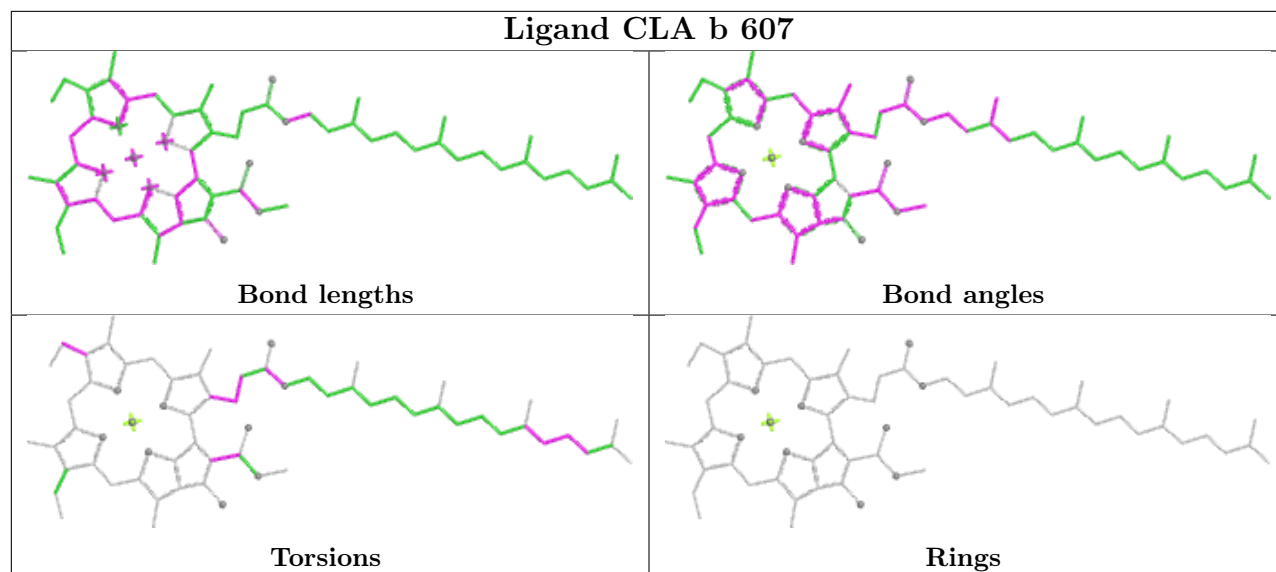




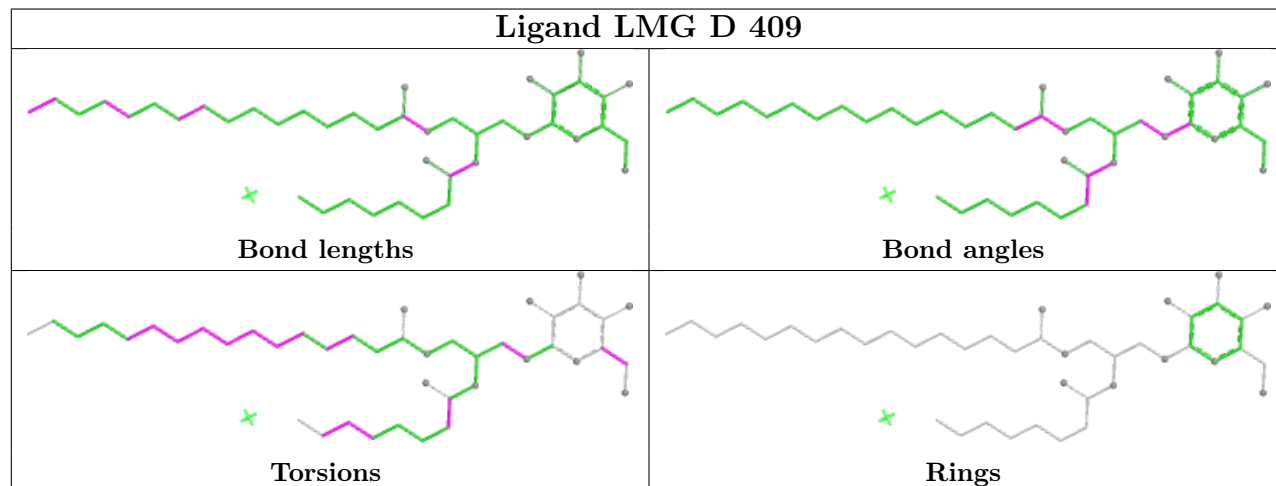




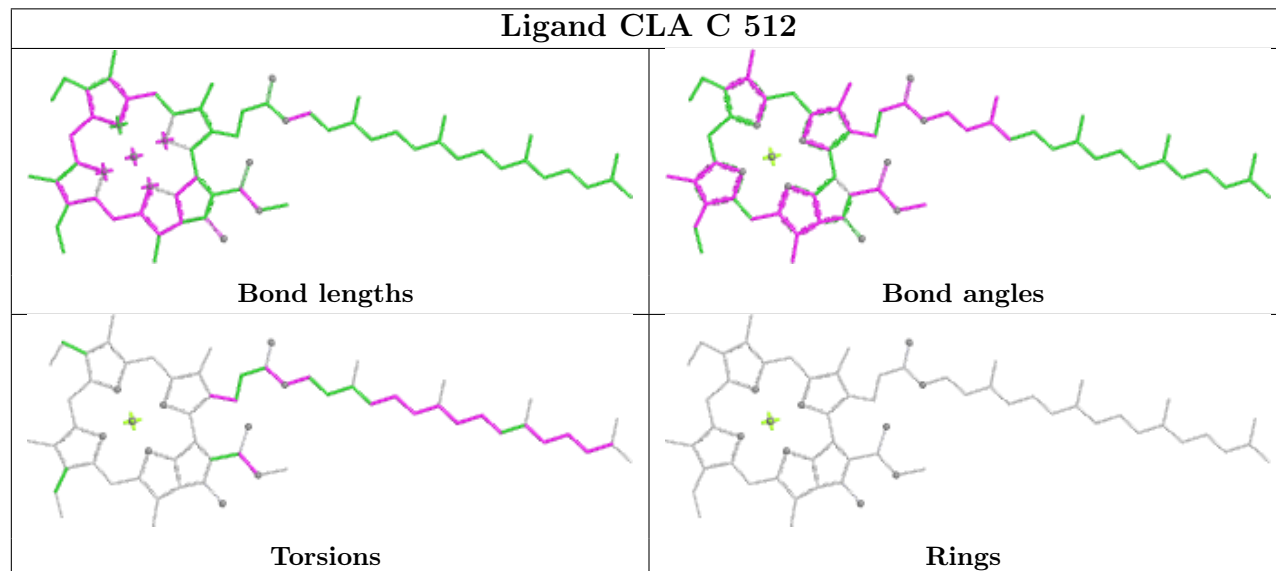
Ligand CLA b 607

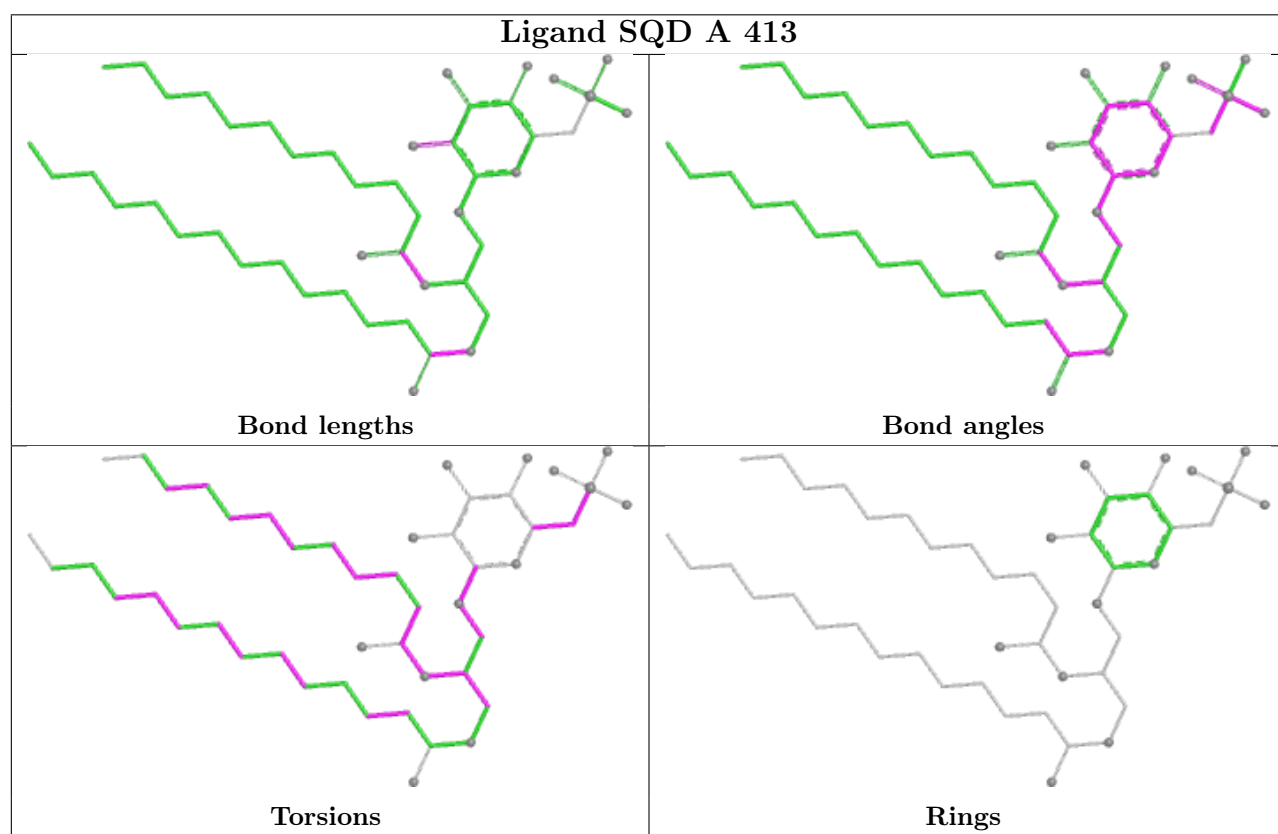
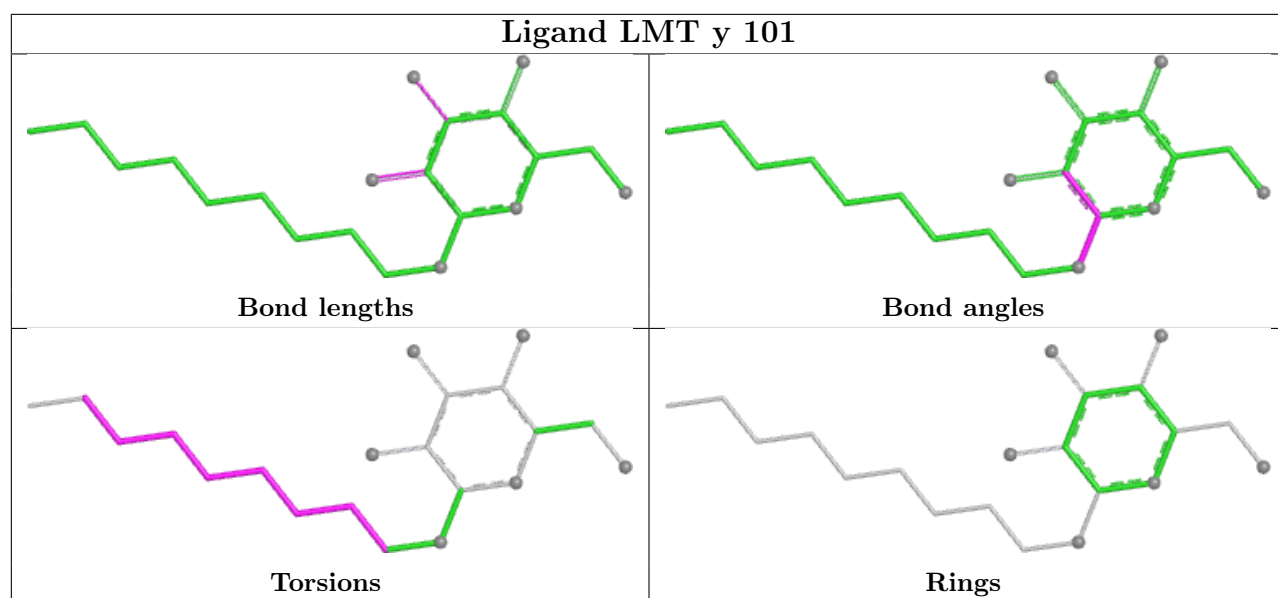


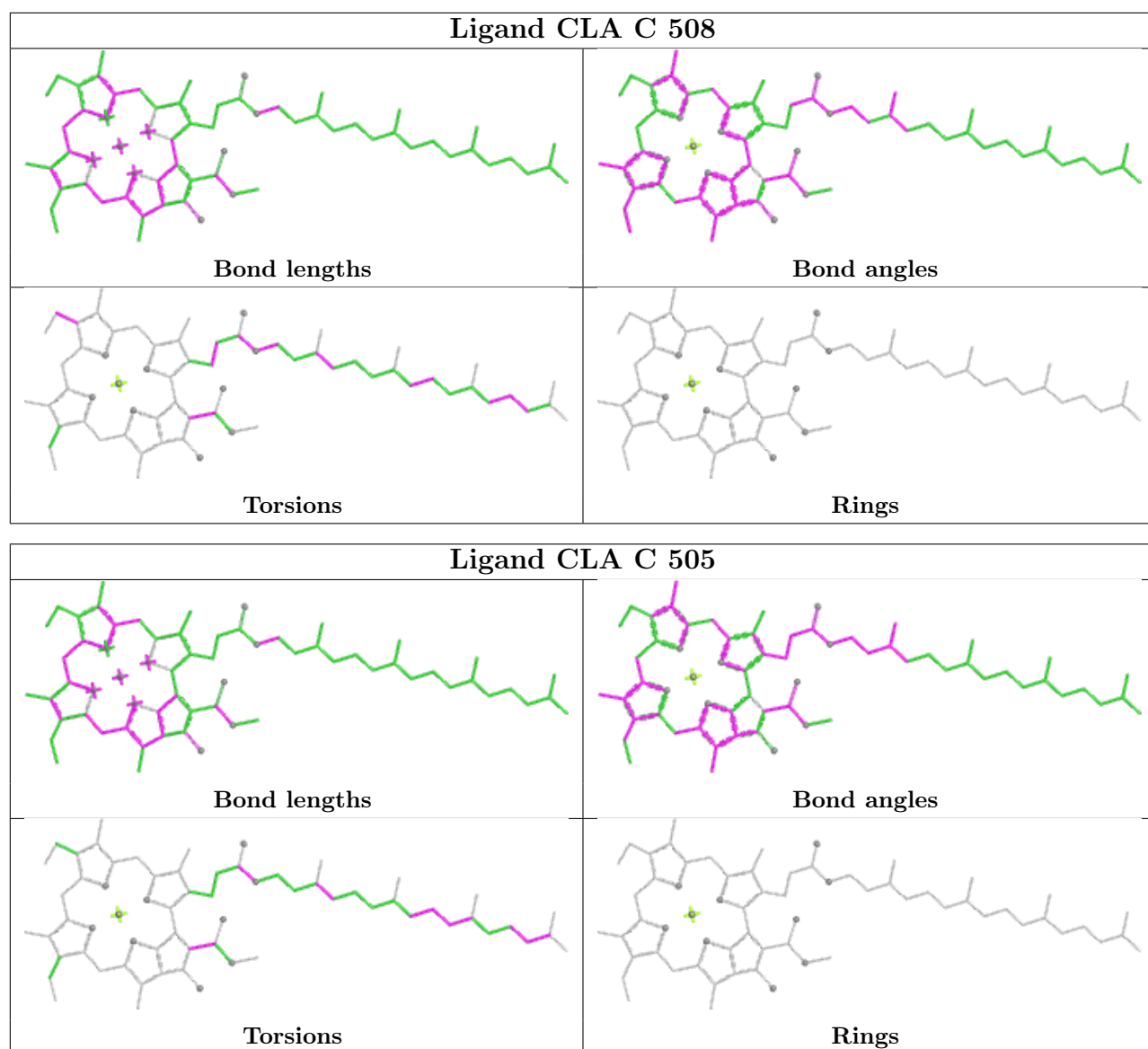
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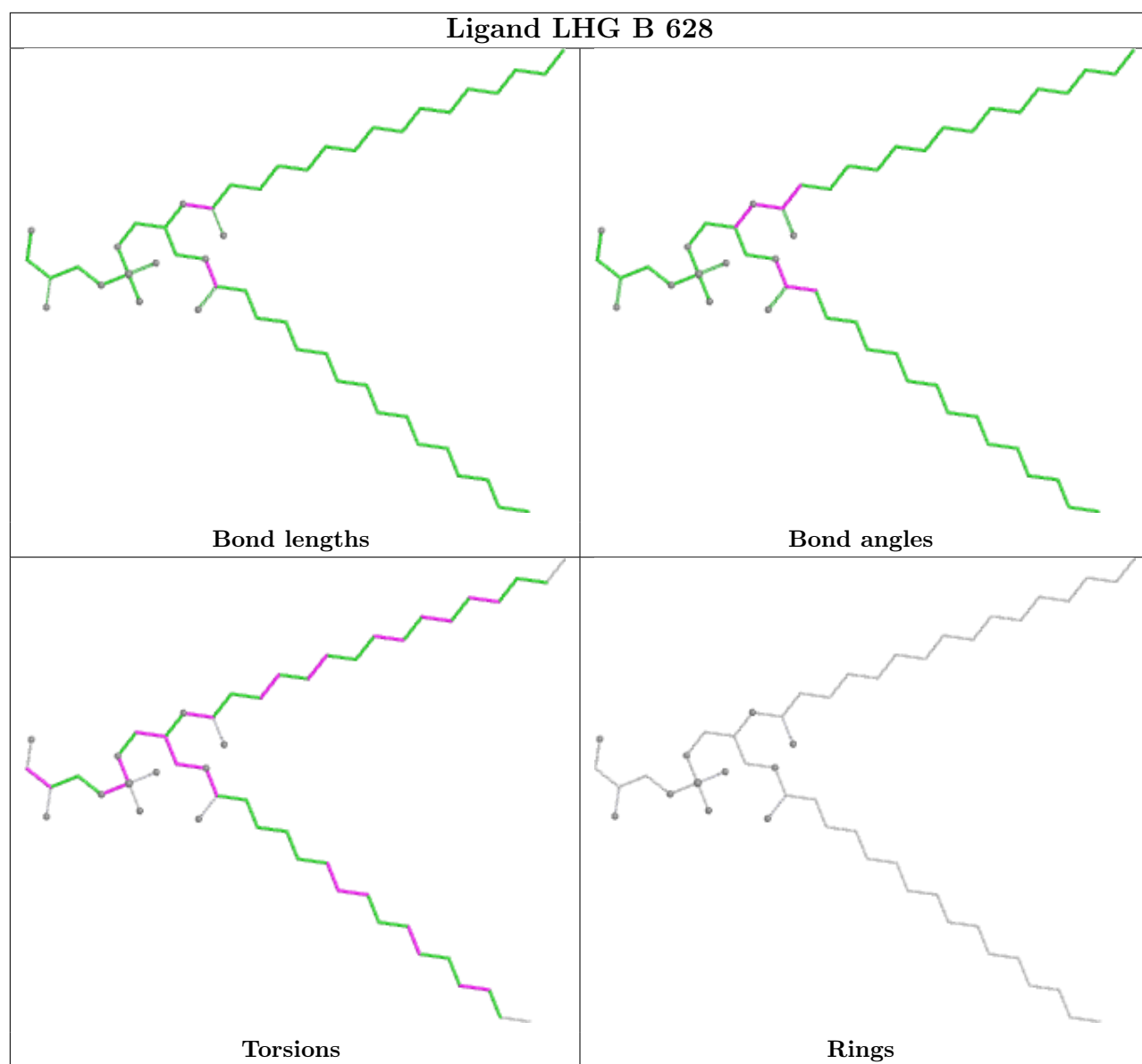


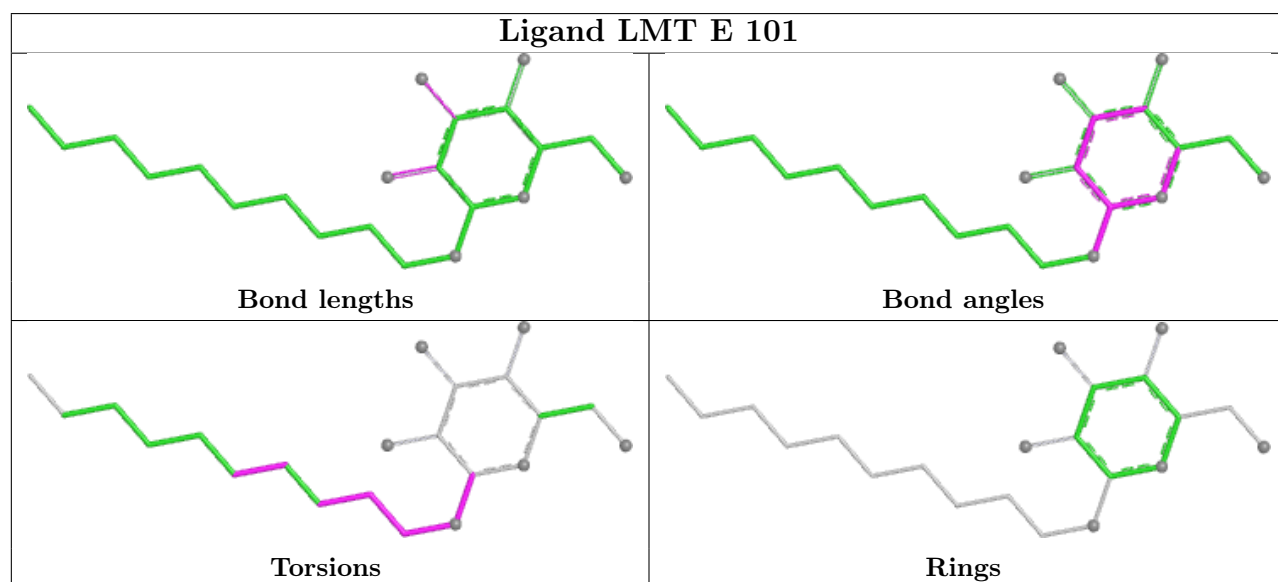
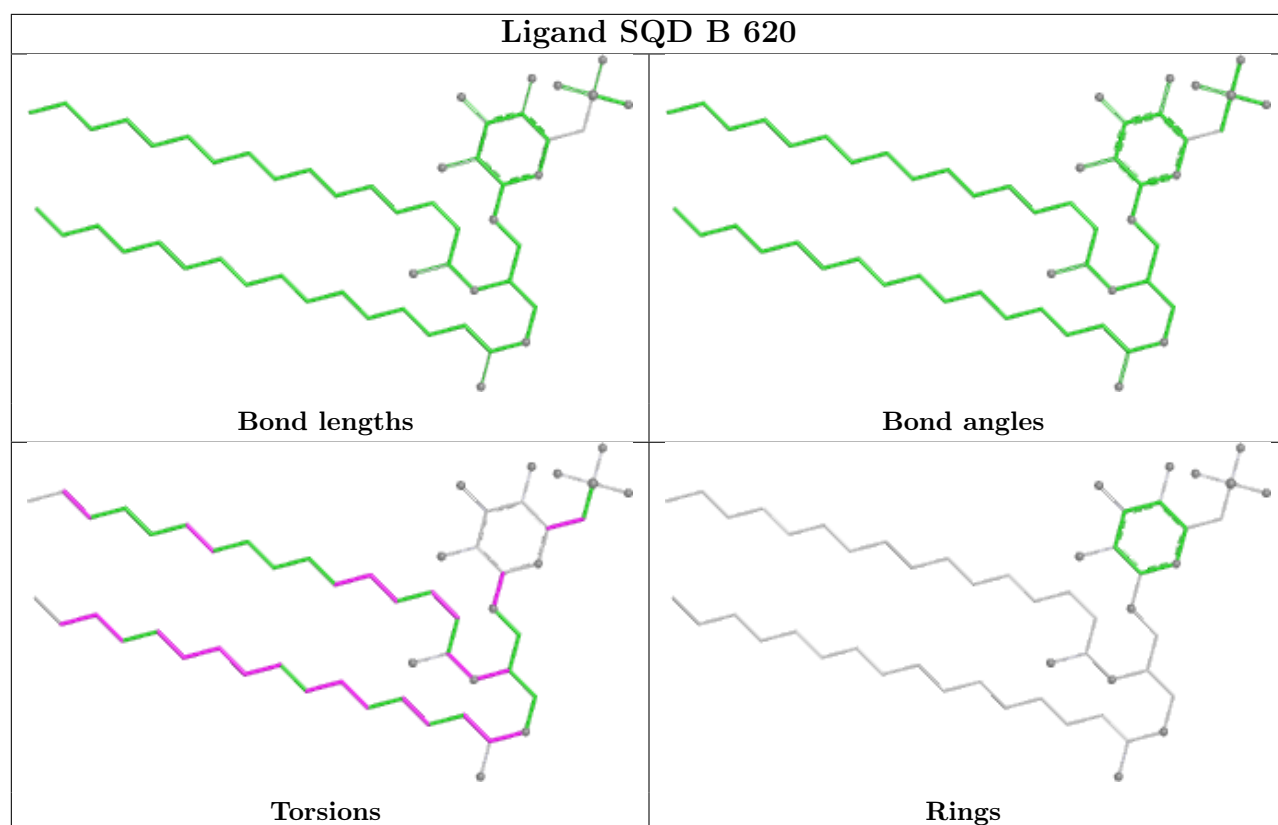
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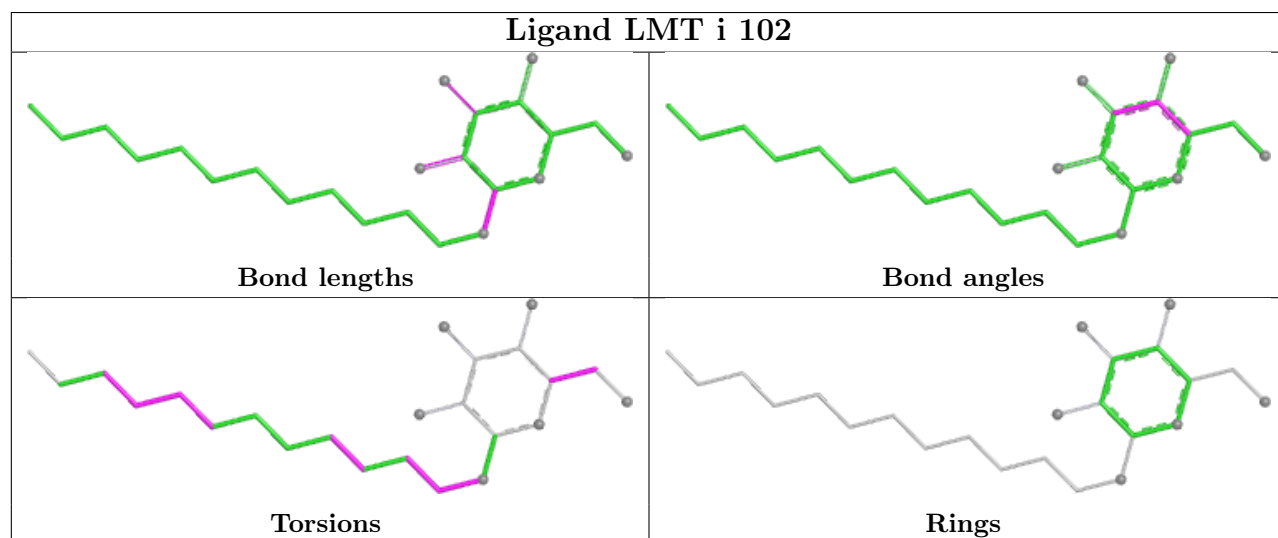
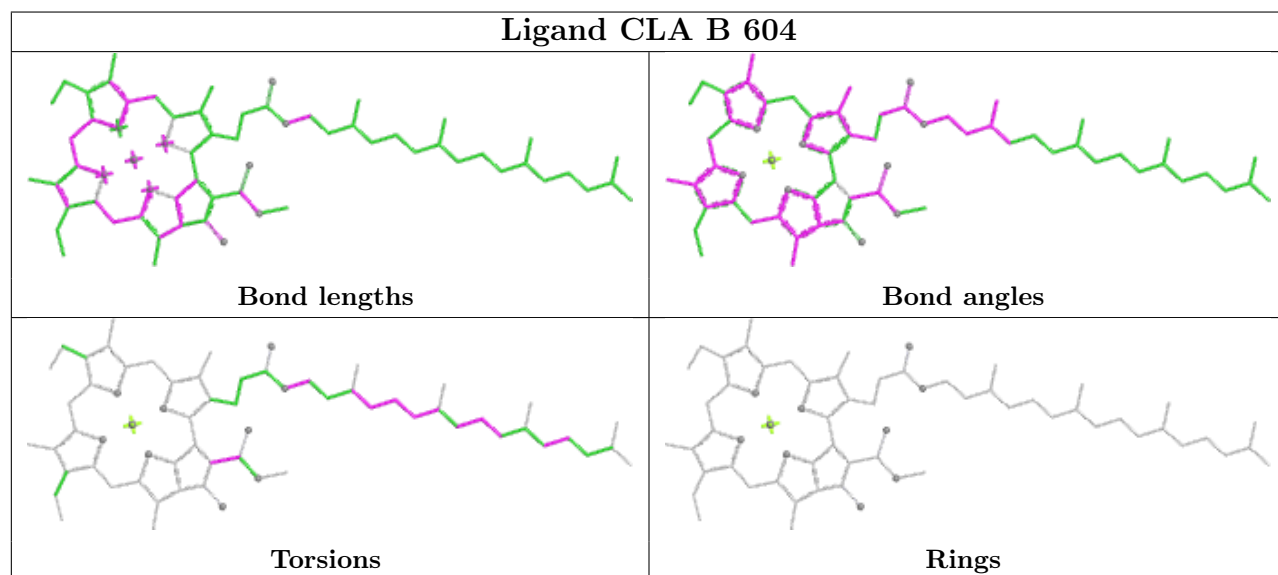
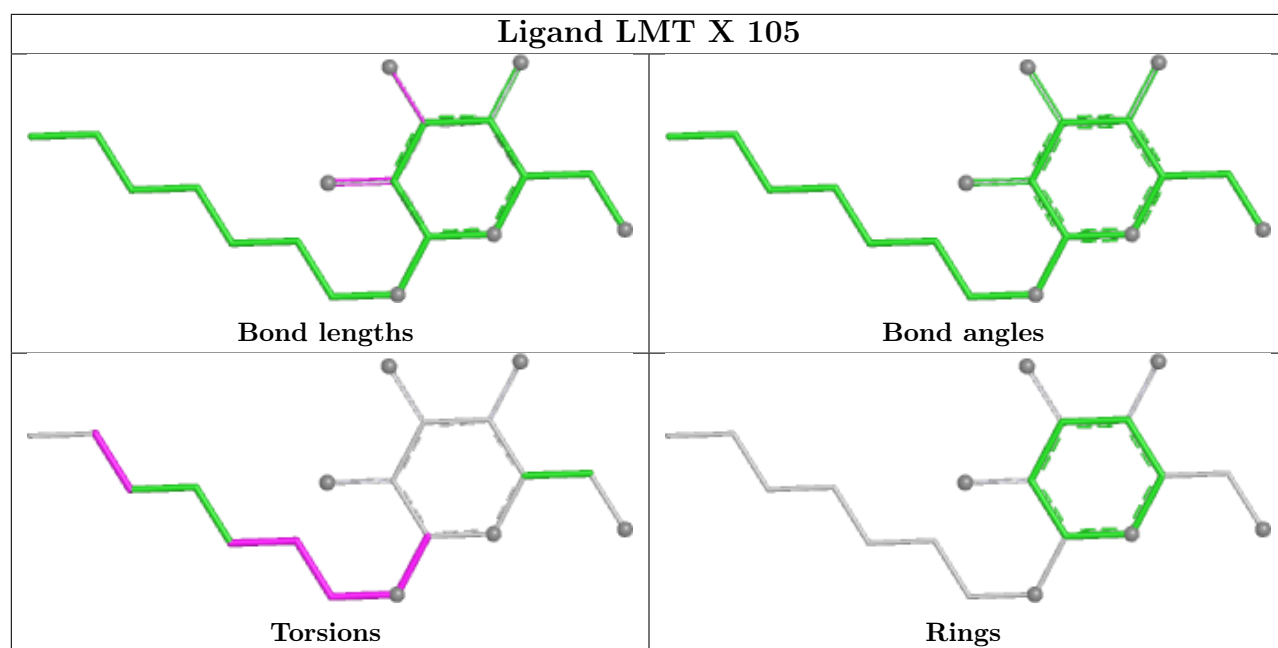


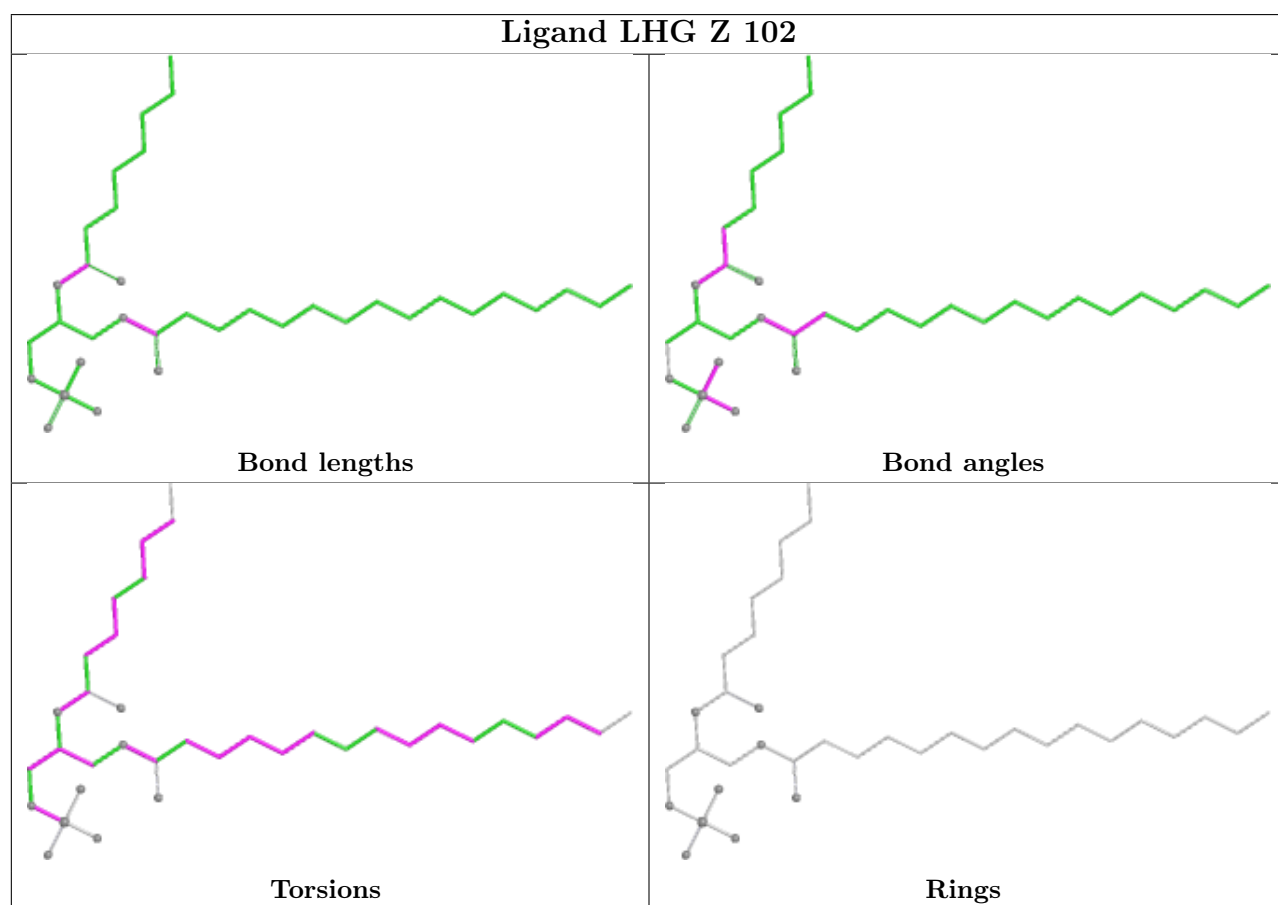
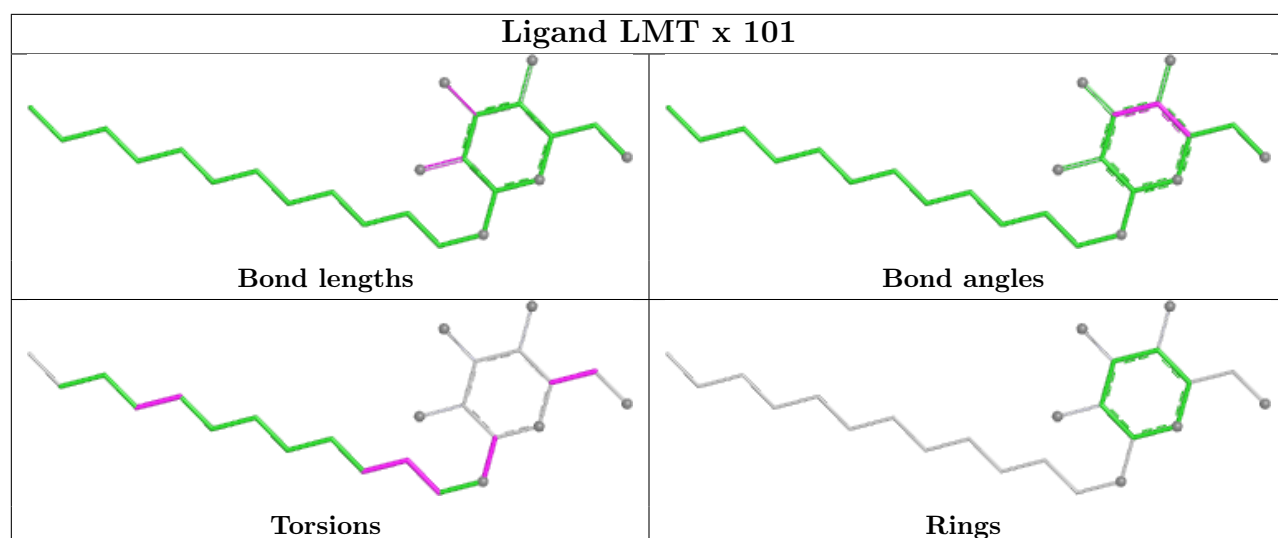


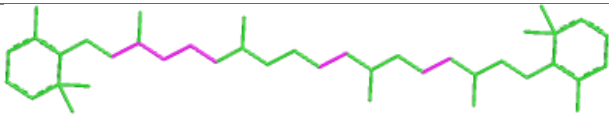
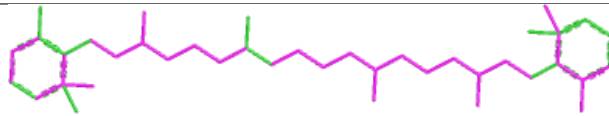
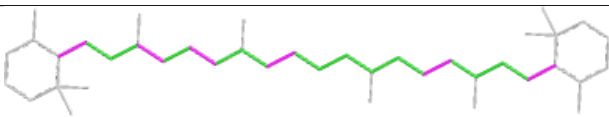
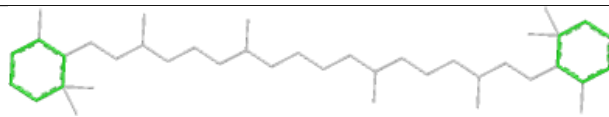


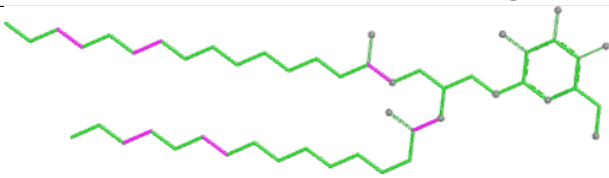
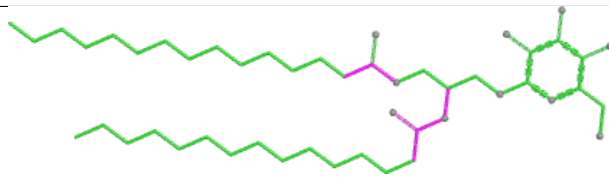
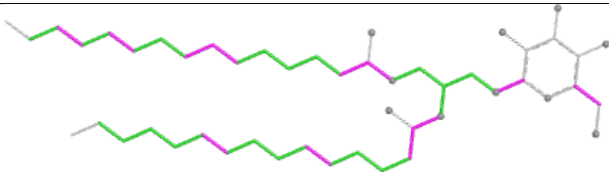
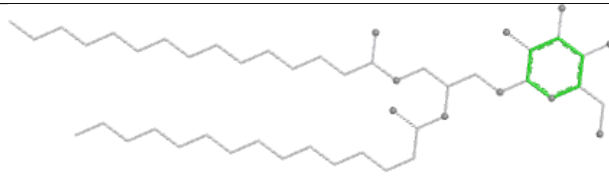


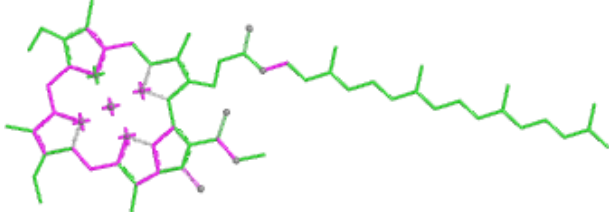
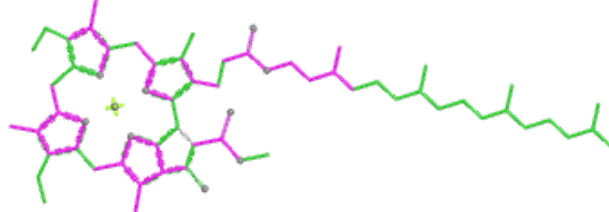
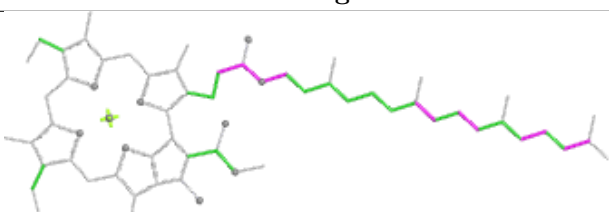
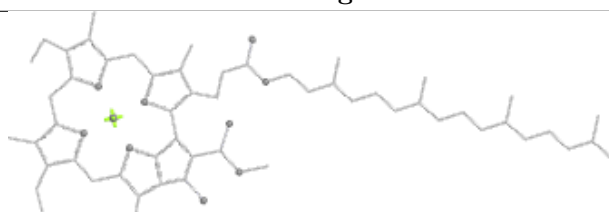


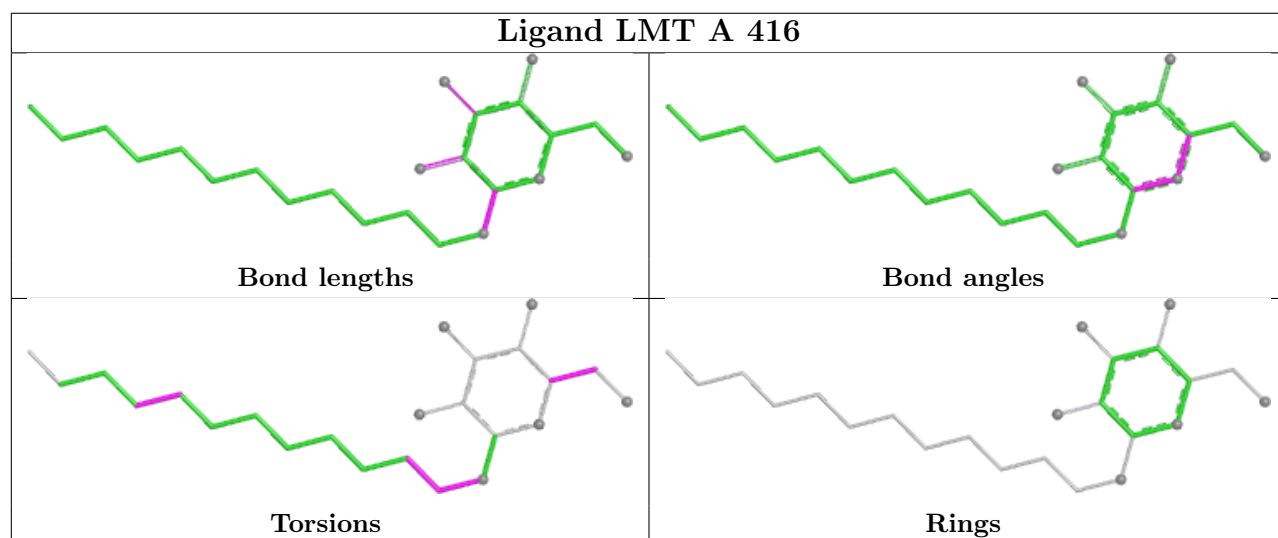
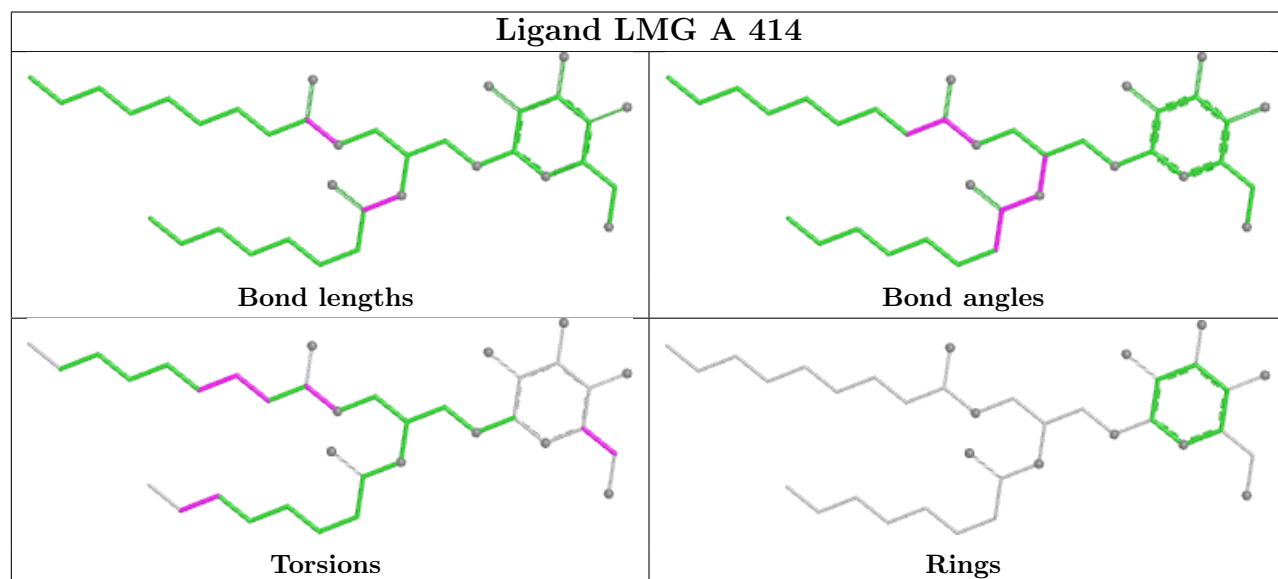
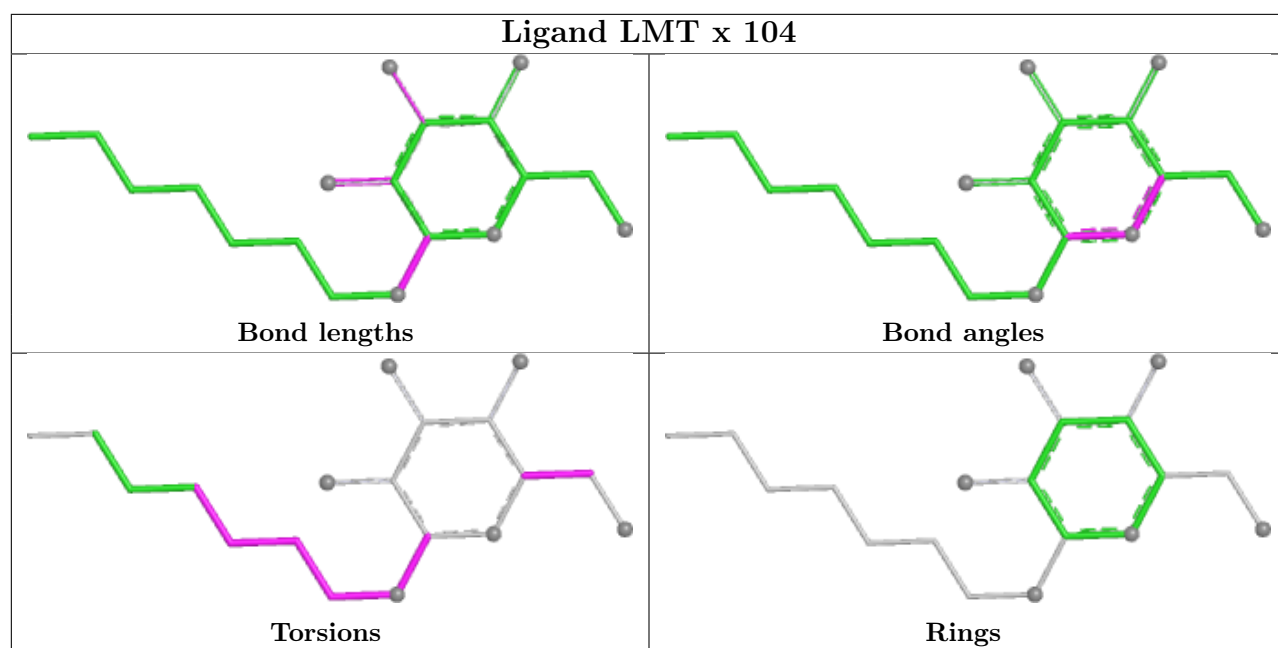


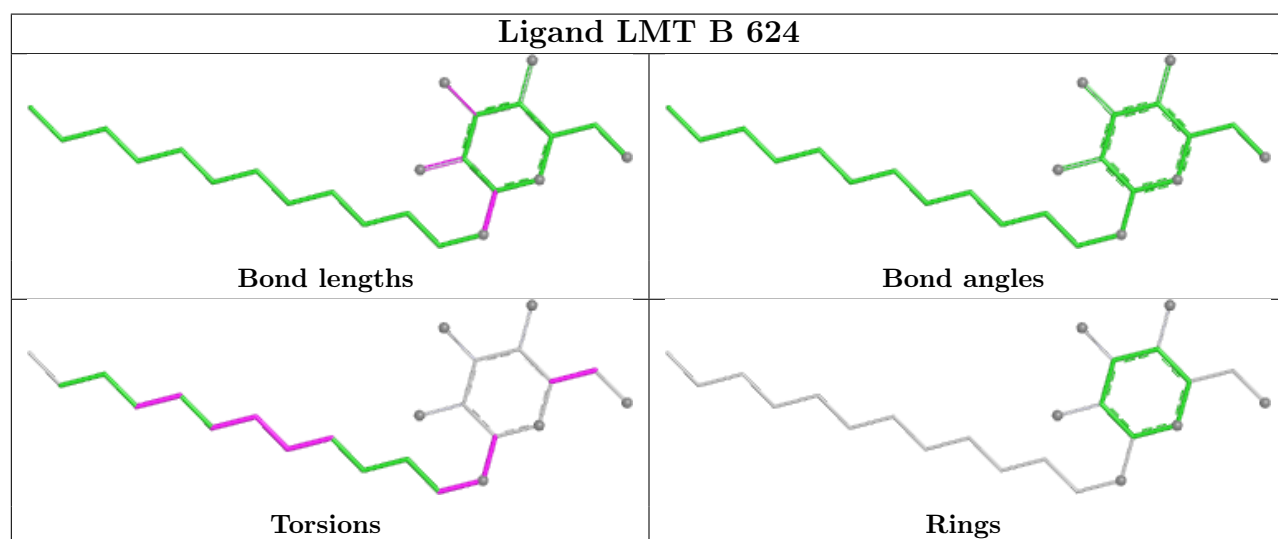
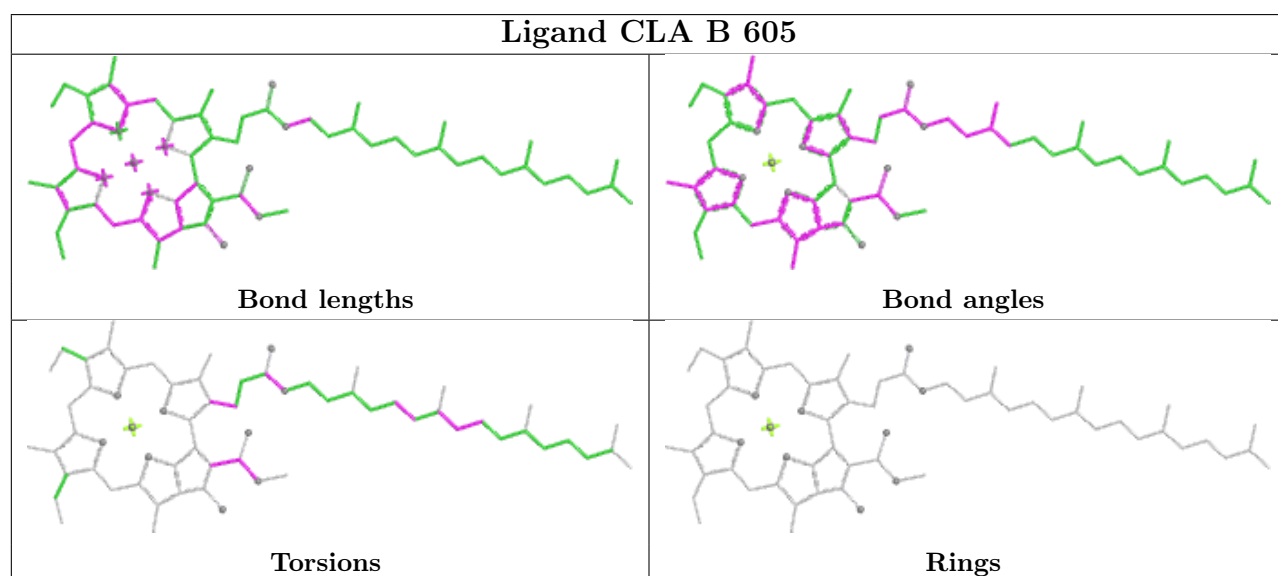
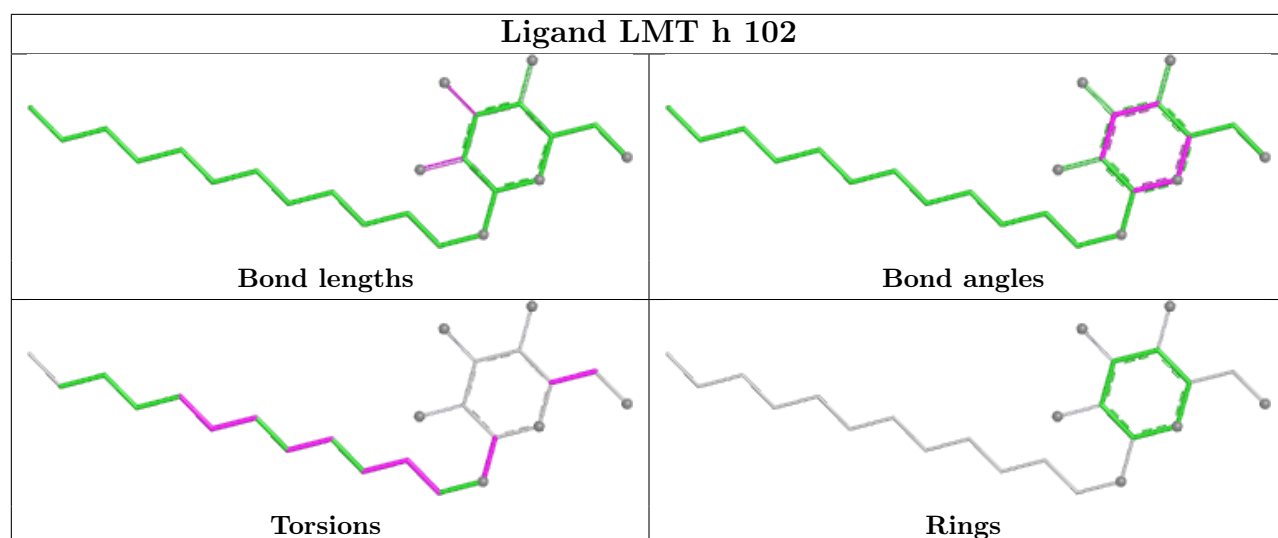


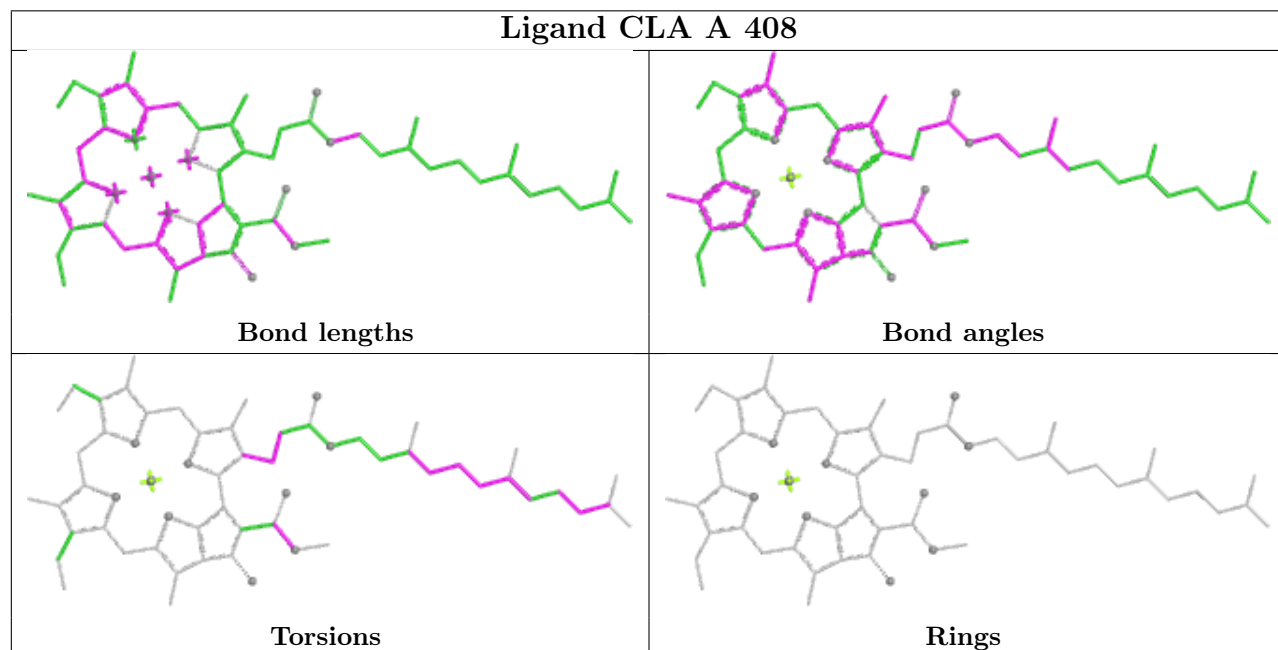
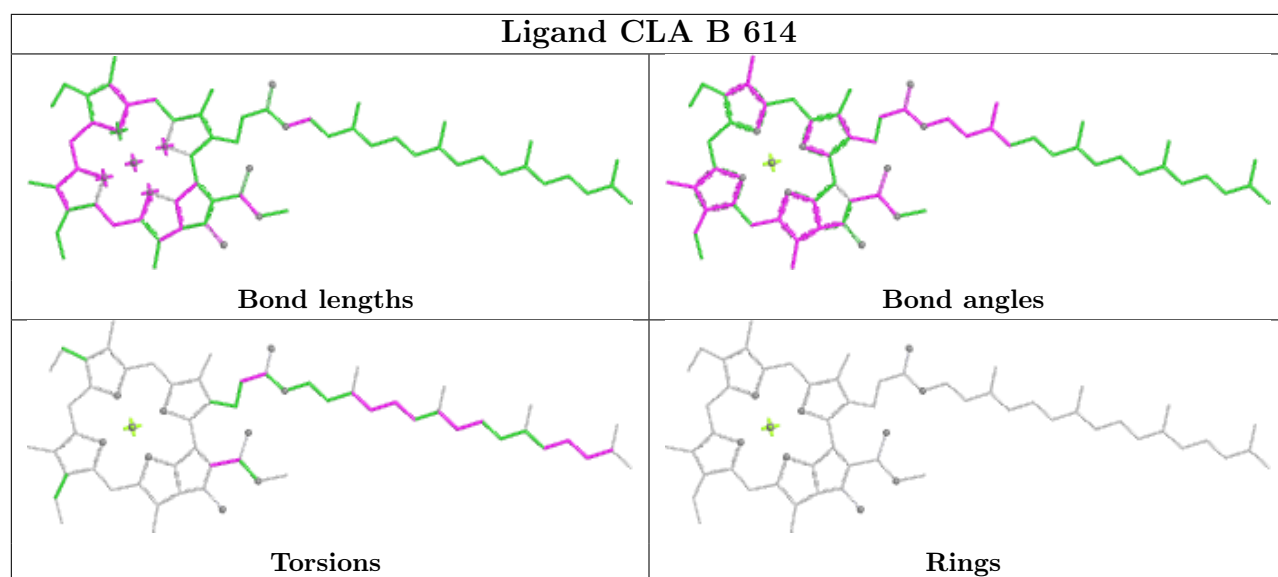
Ligand BCR F 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG C 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

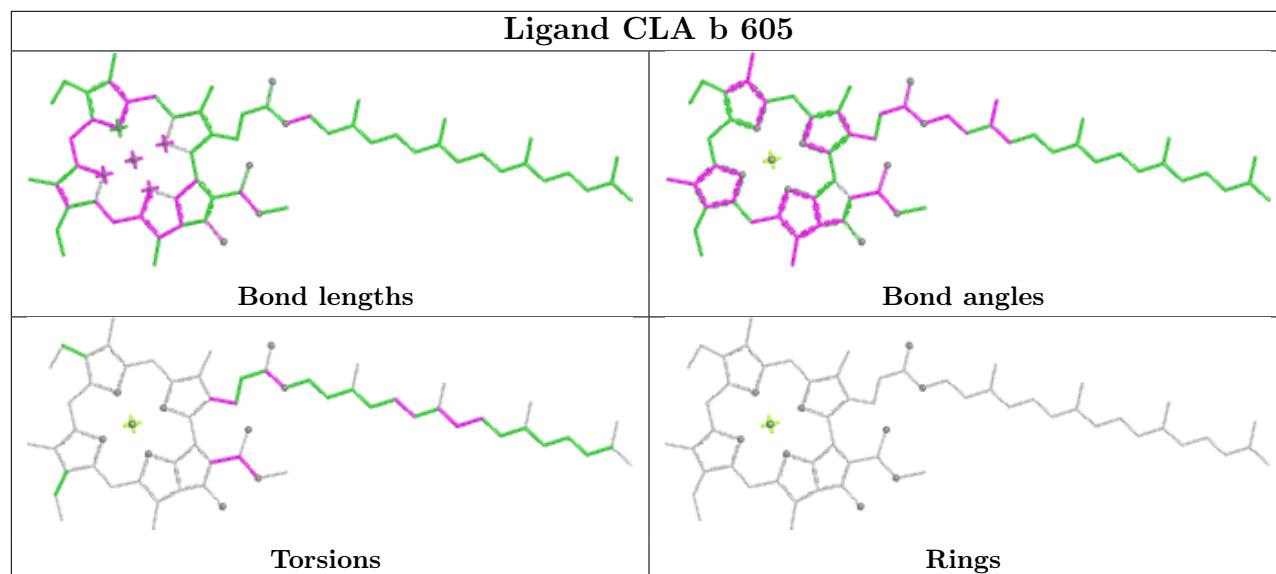
Ligand CLA b 612	
	
Bond lengths	Bond angles
	
Torsions	Rings



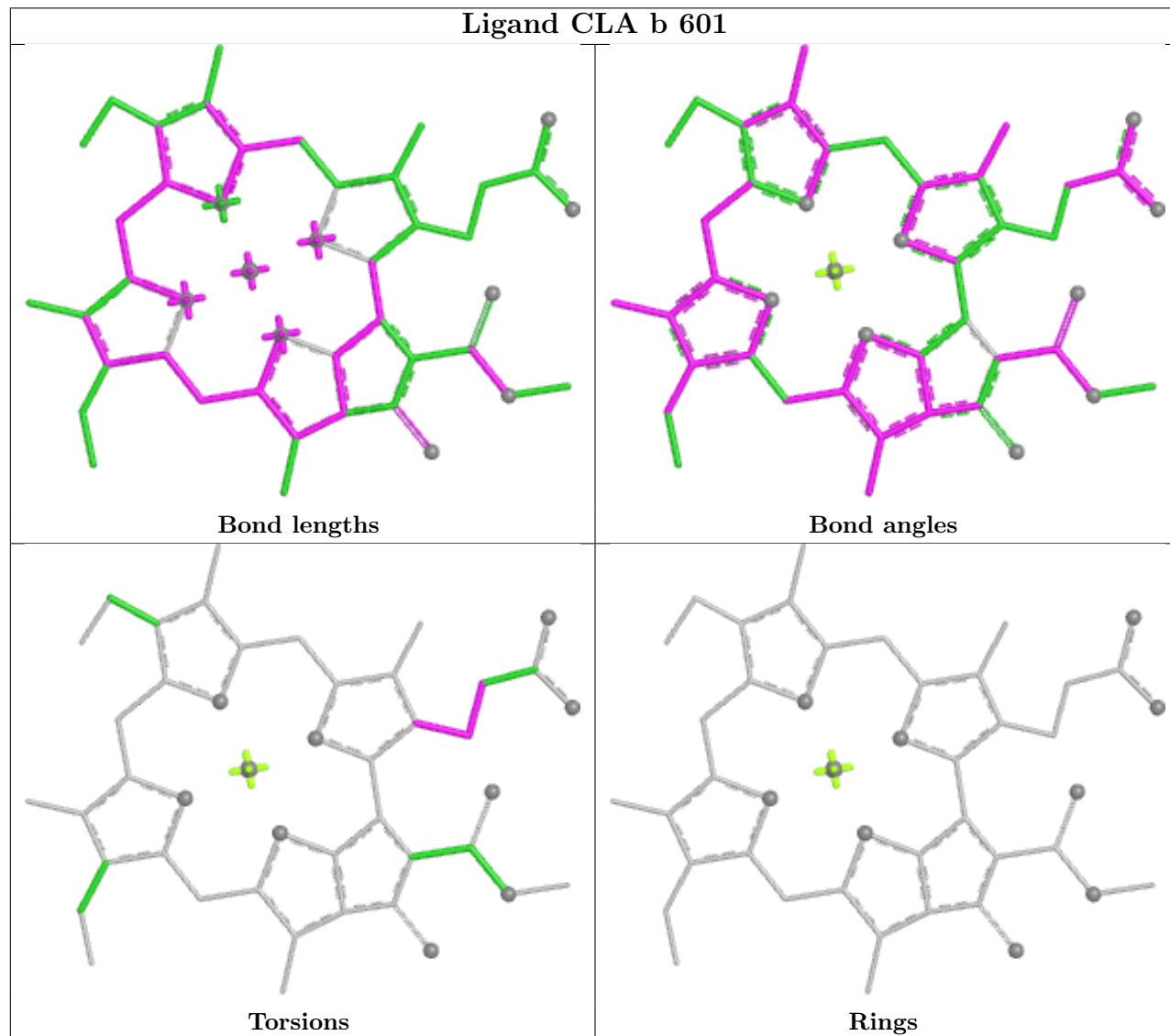


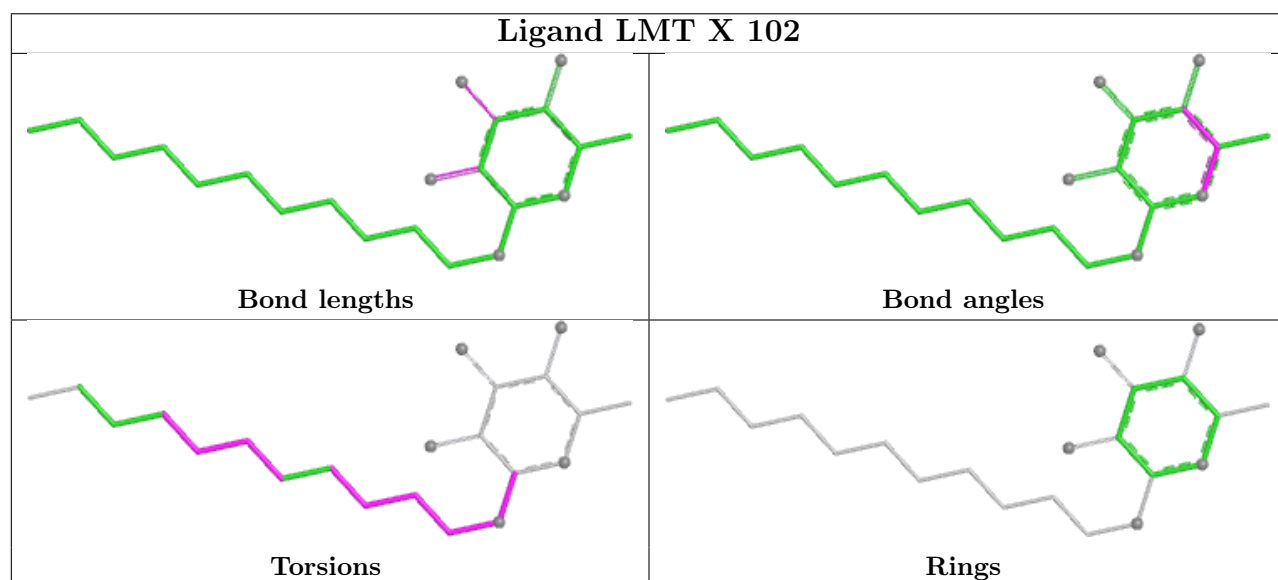
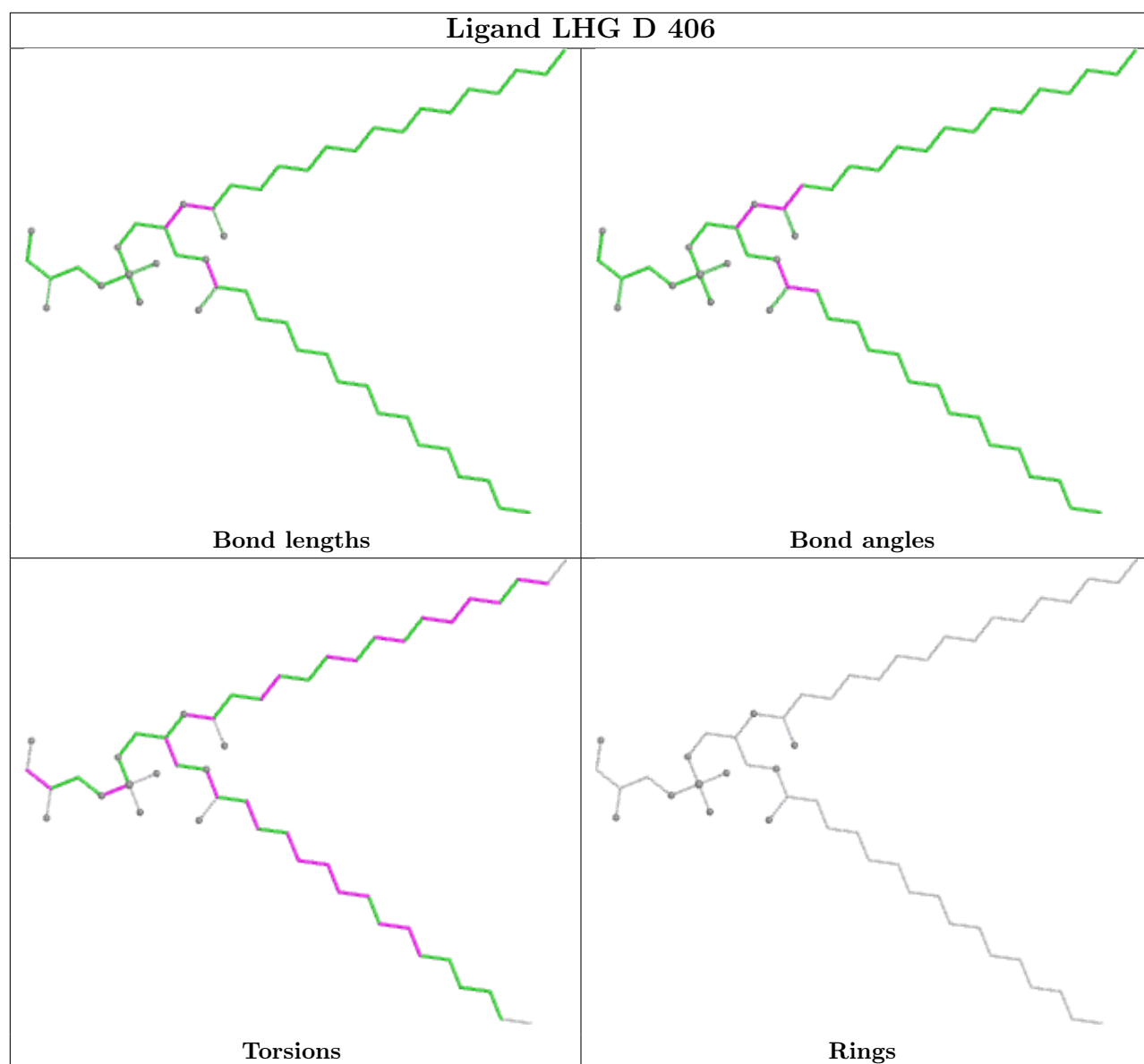


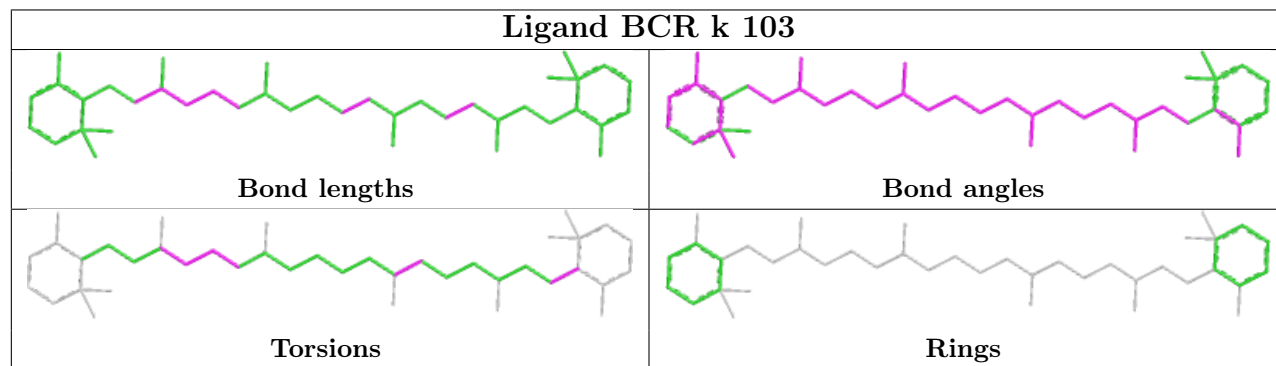
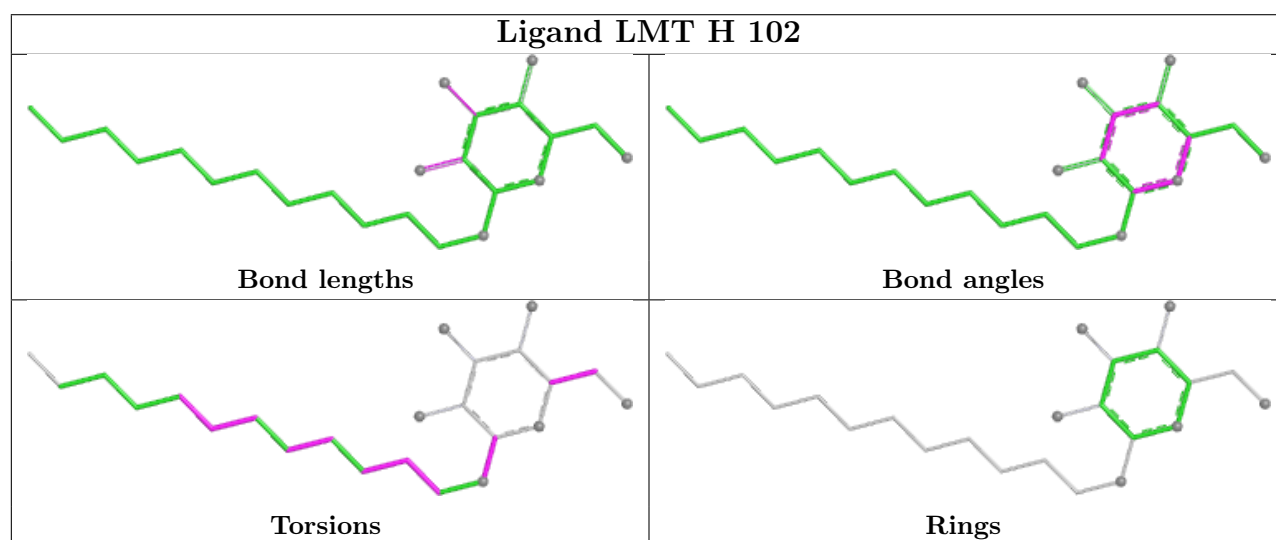
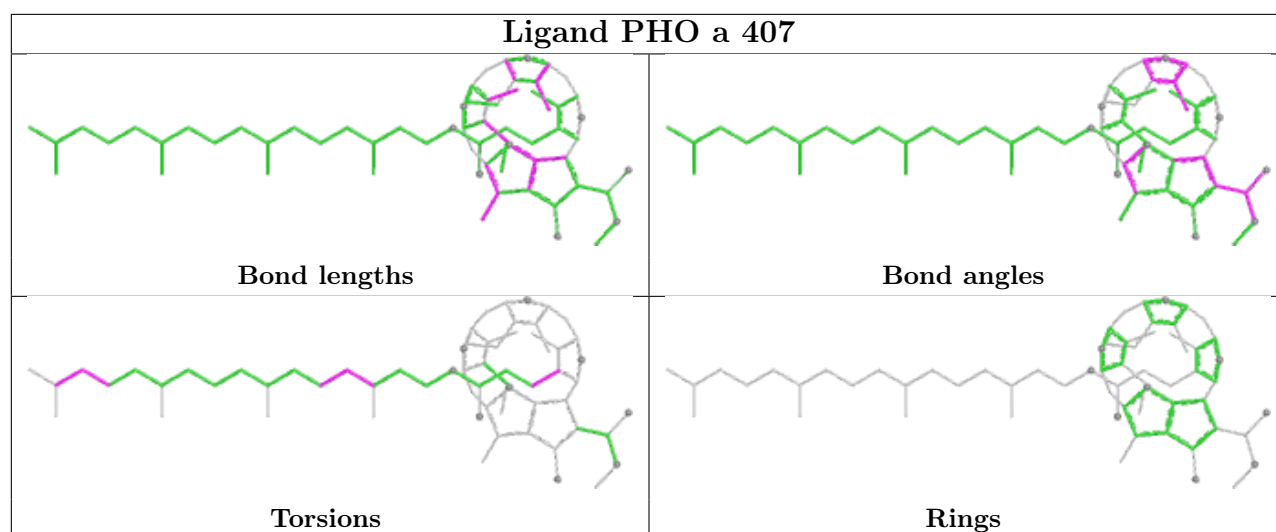
Ligand CLA b 605

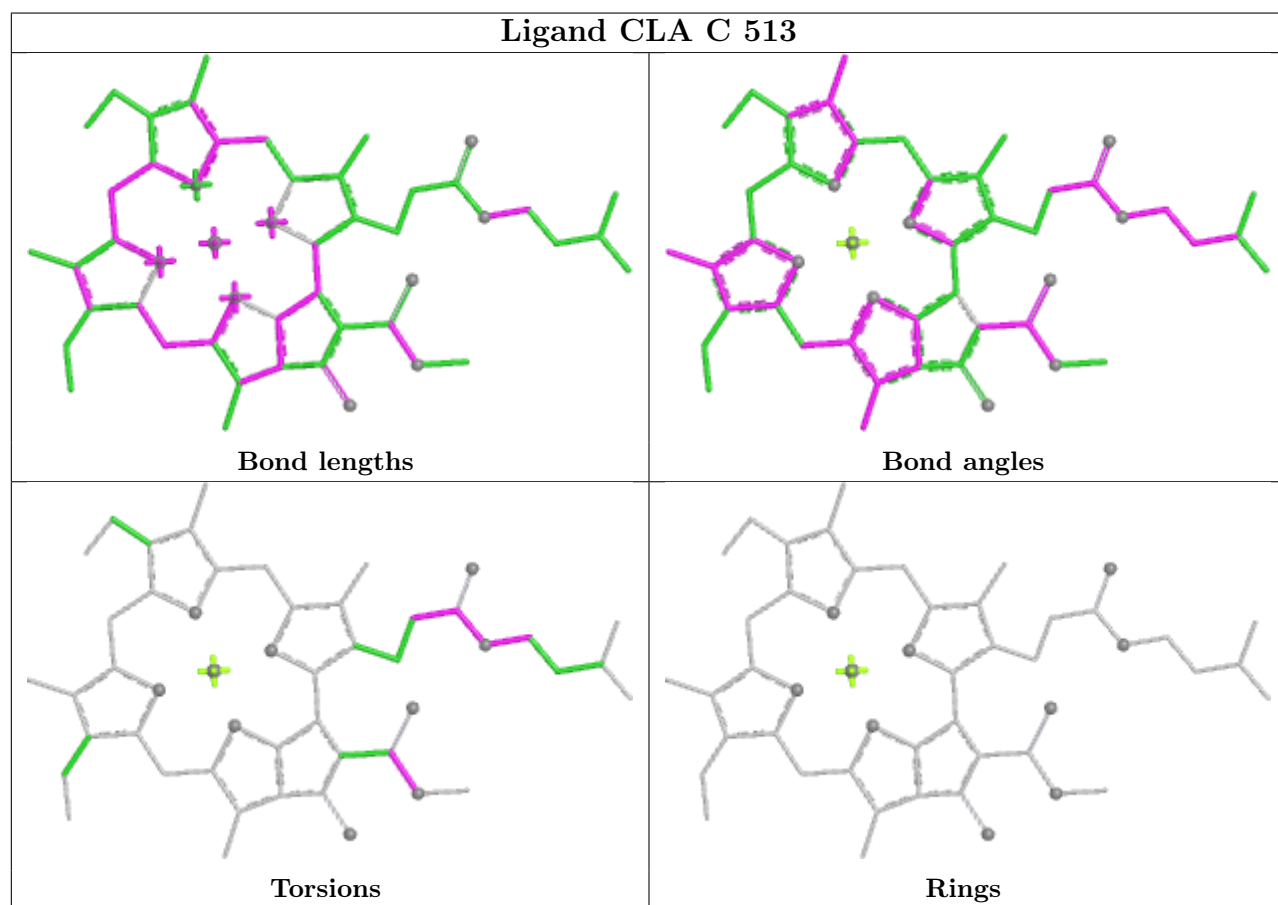
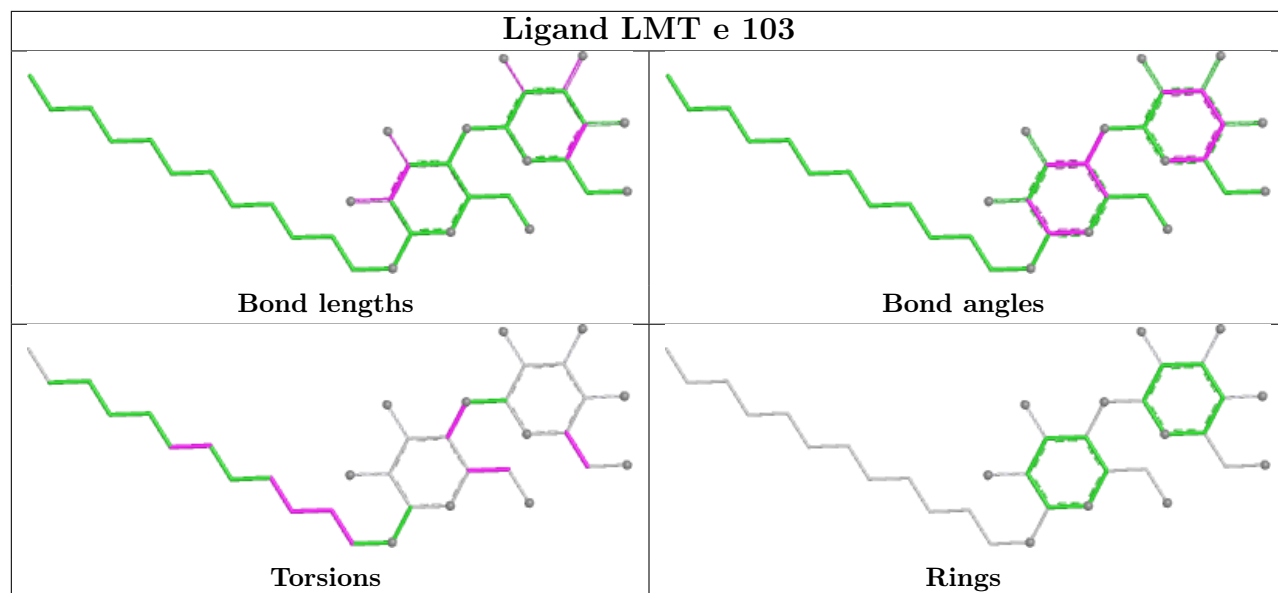


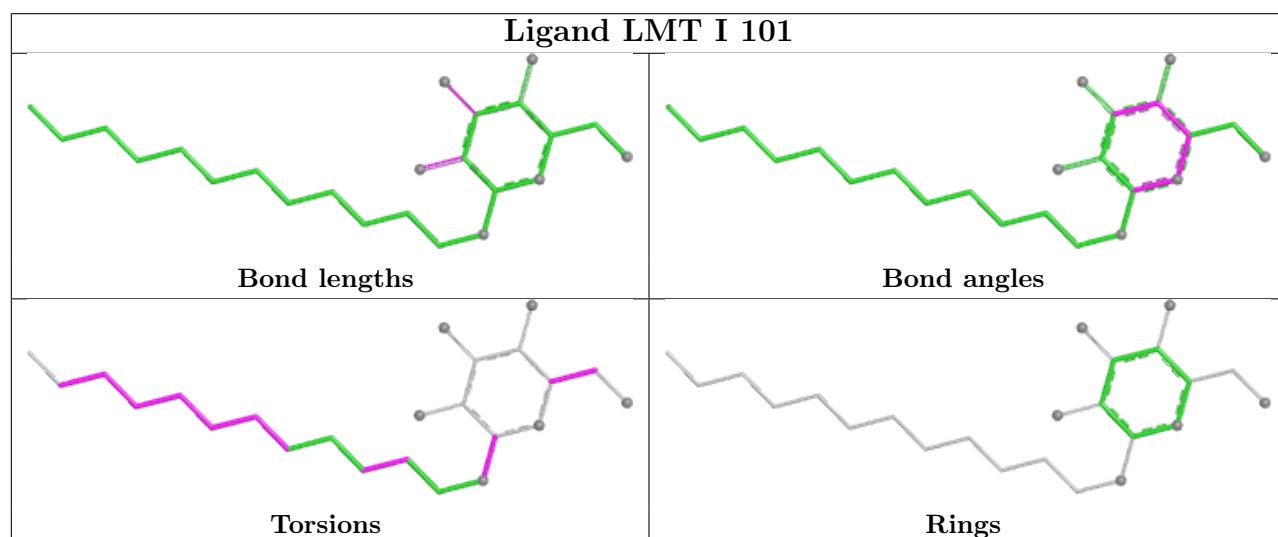
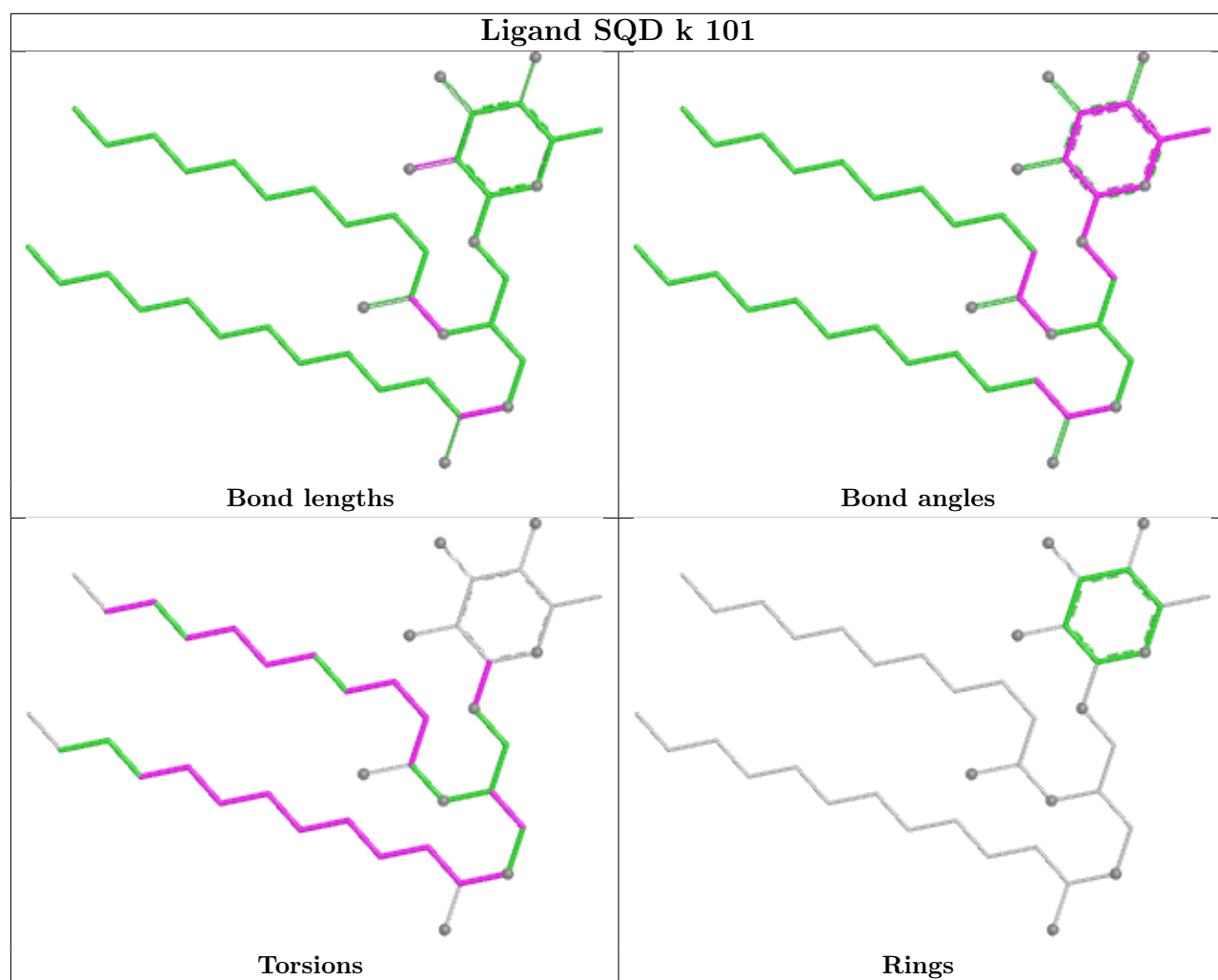
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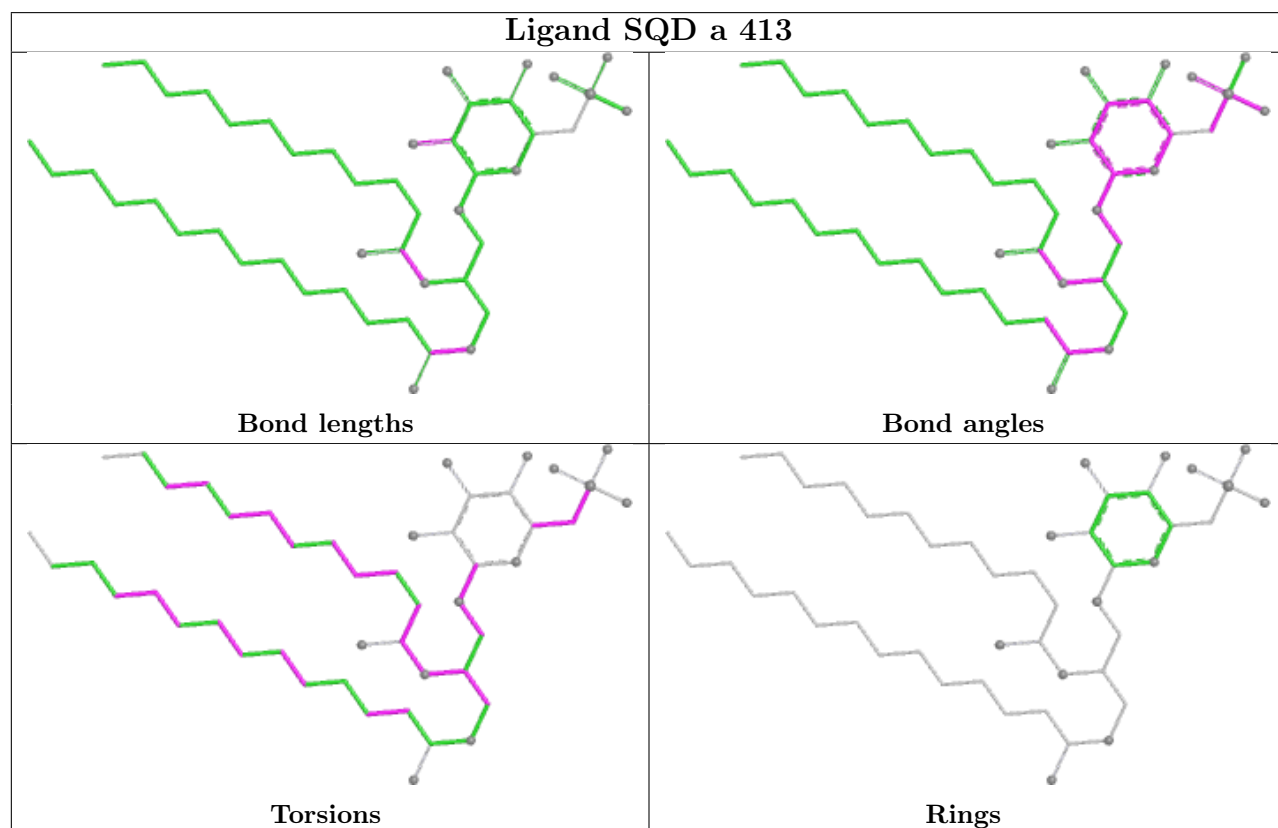
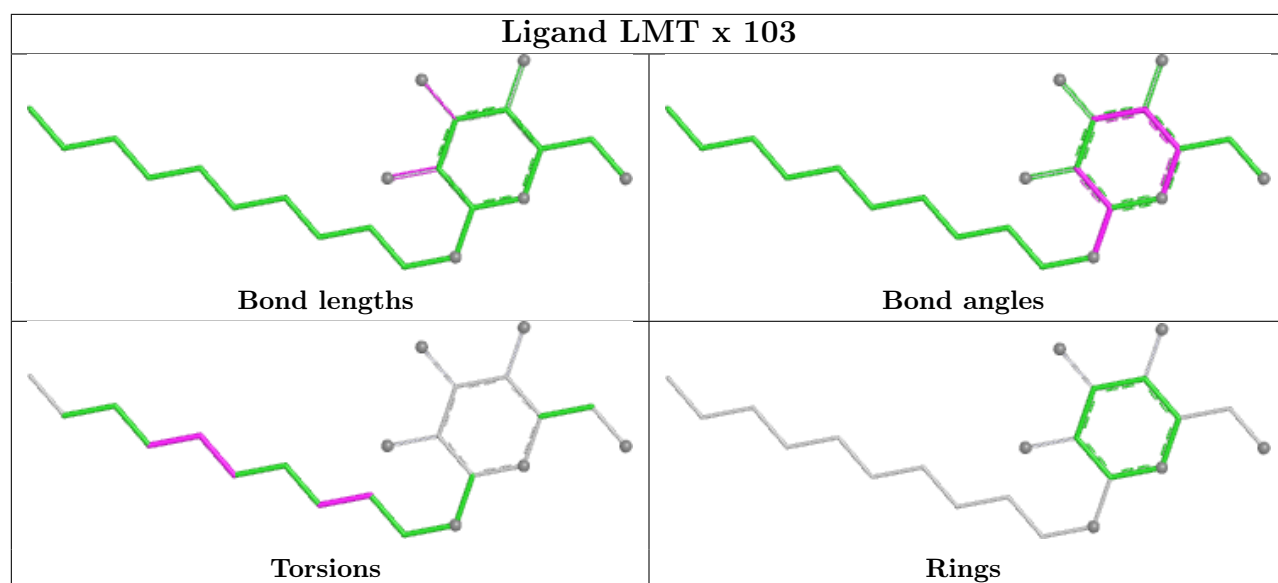


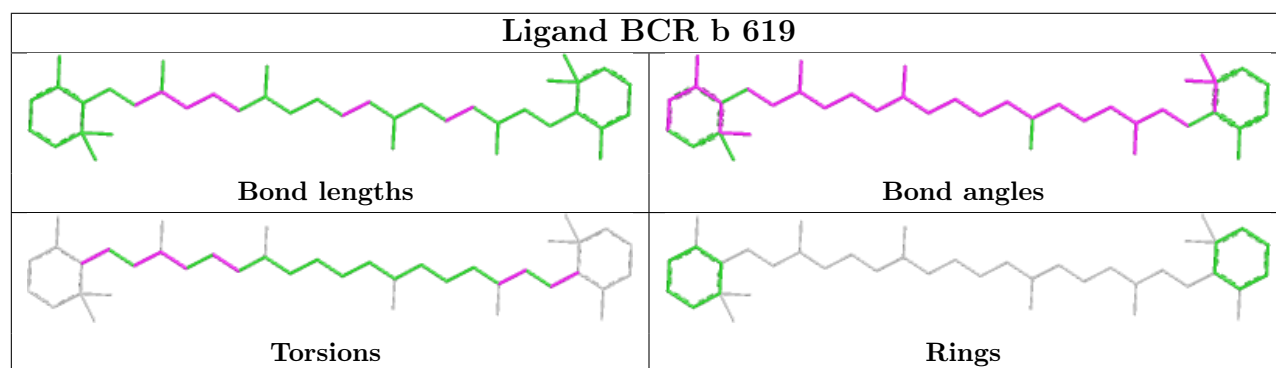
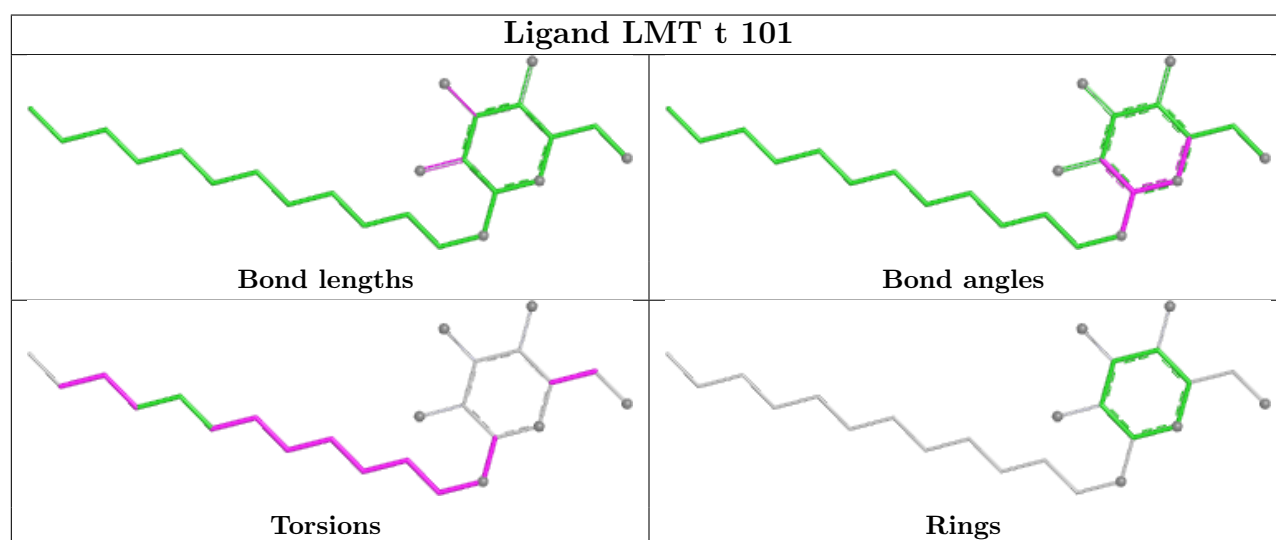
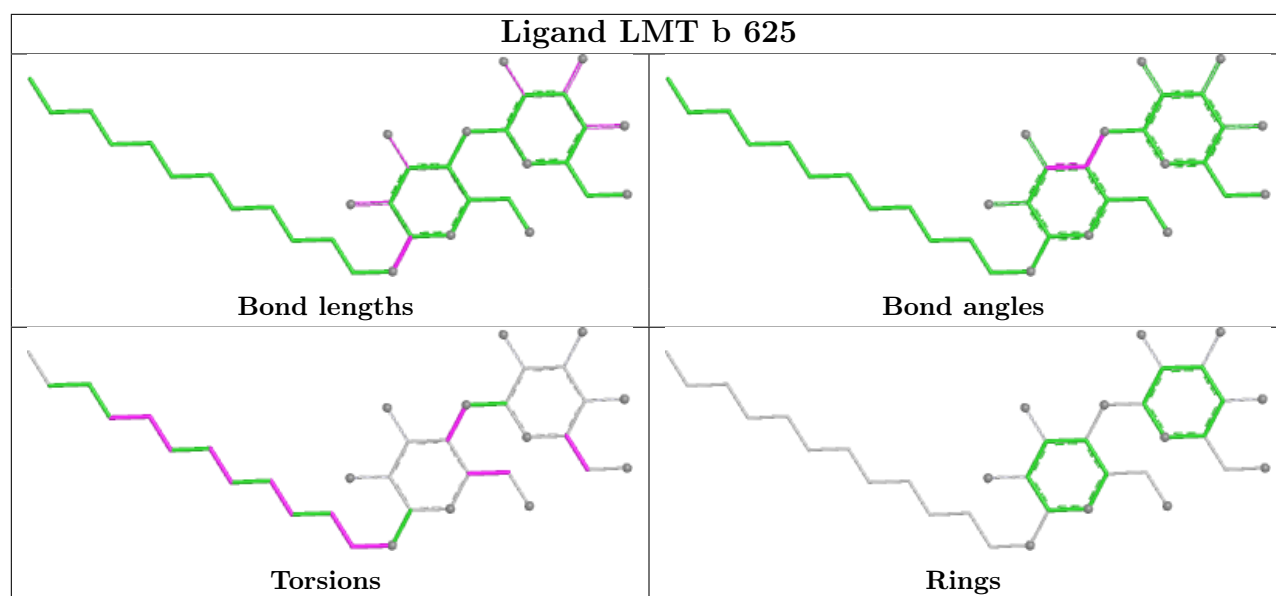


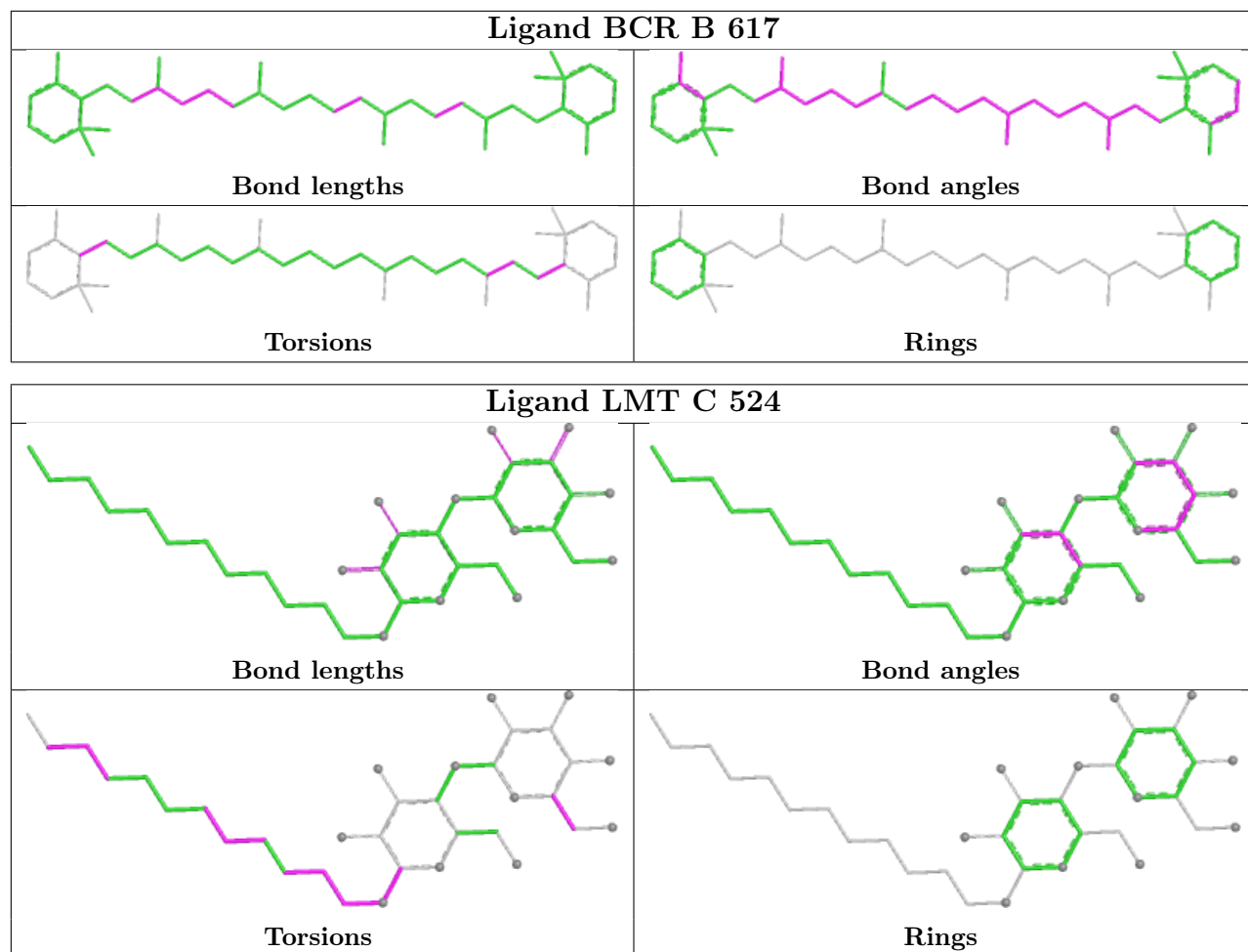


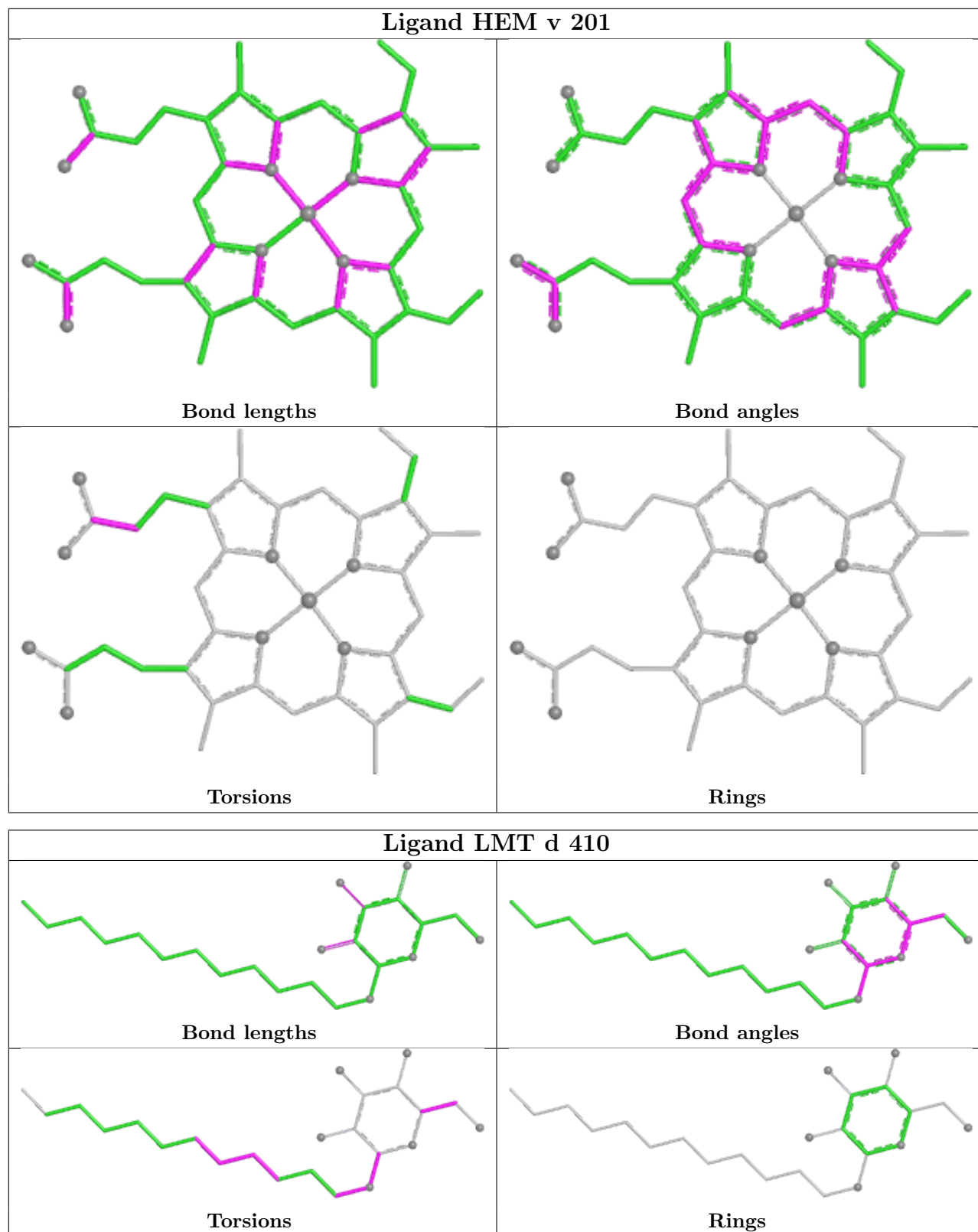


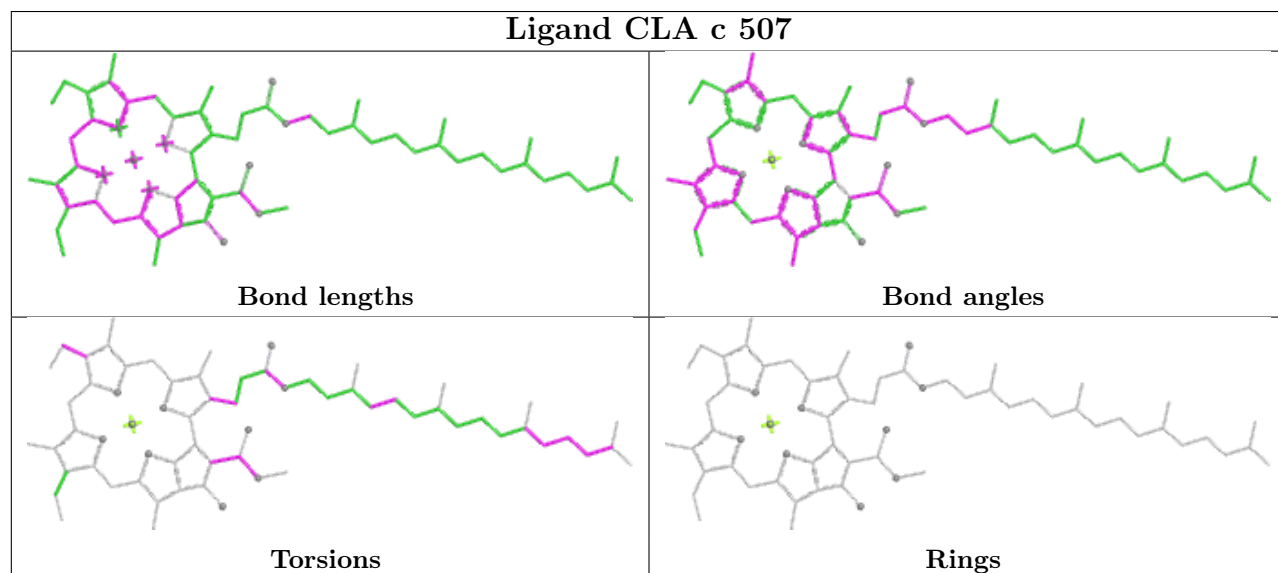
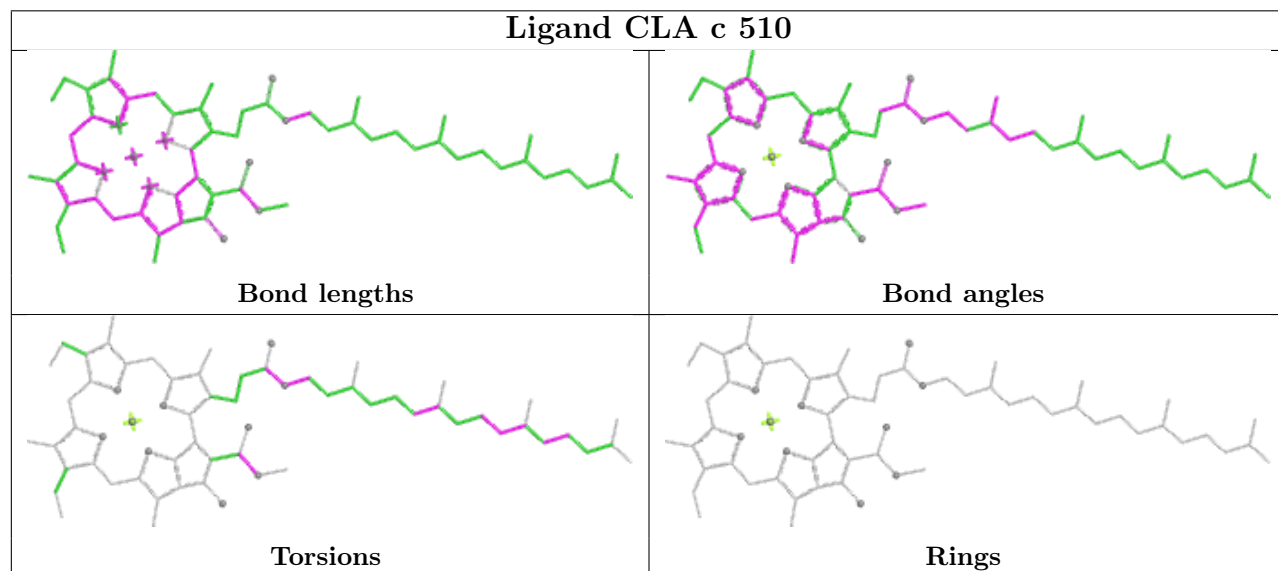
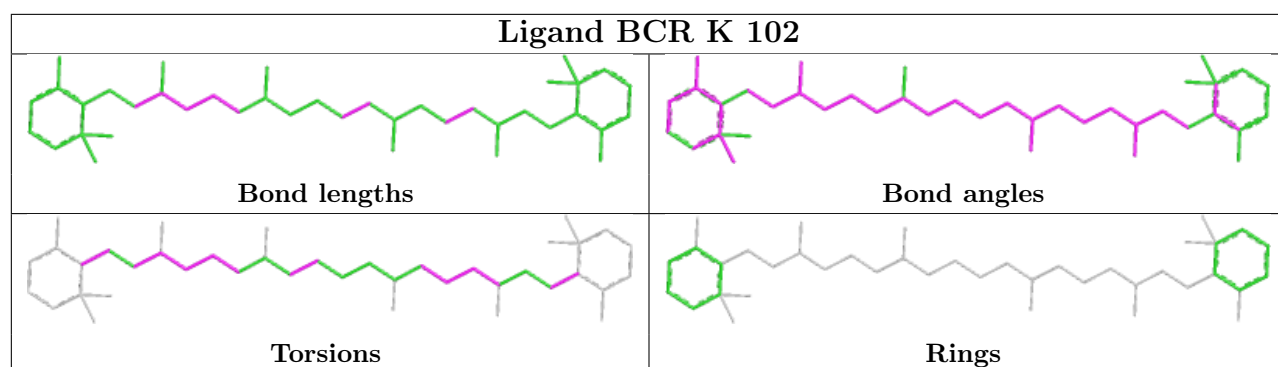


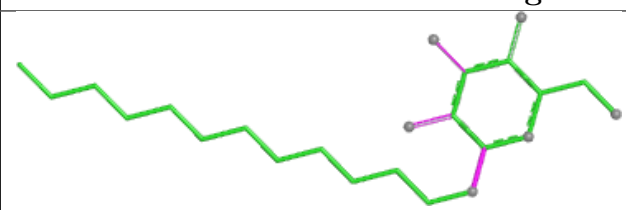
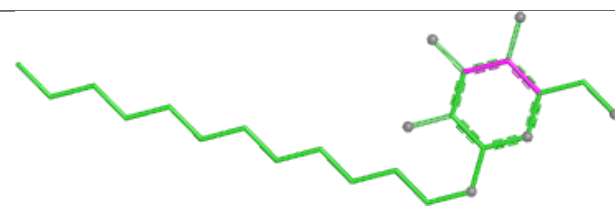
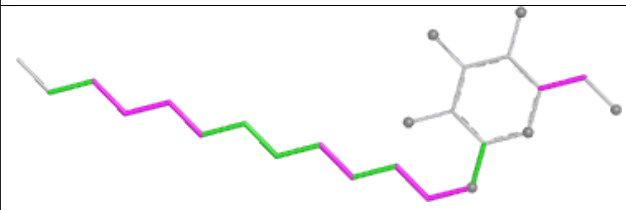
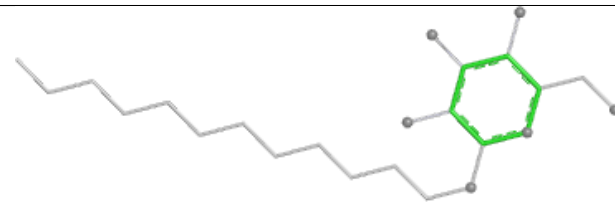


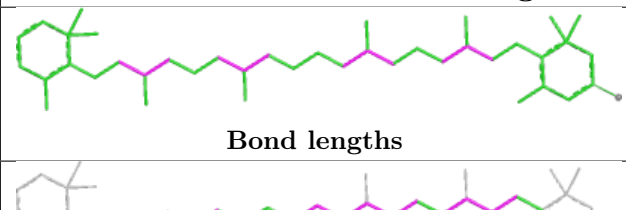
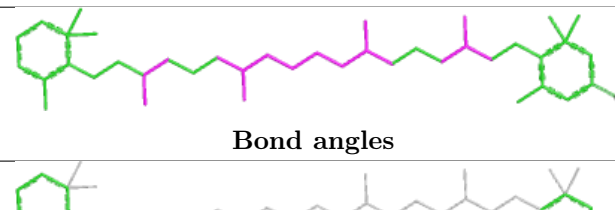
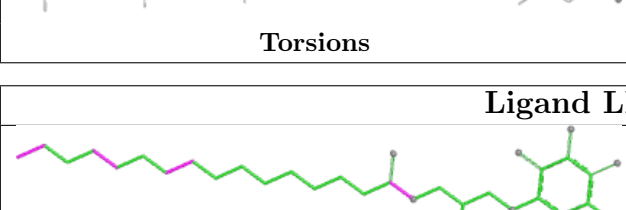
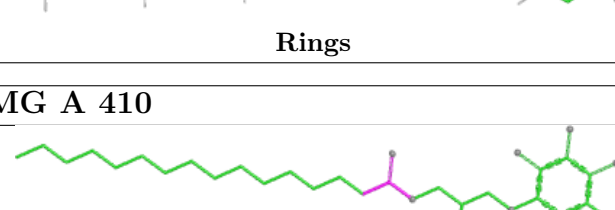


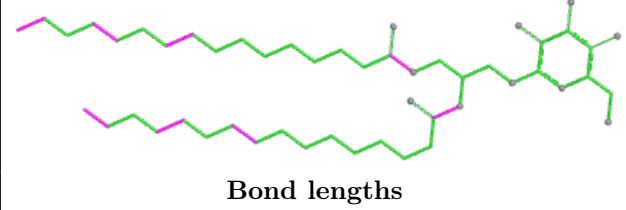
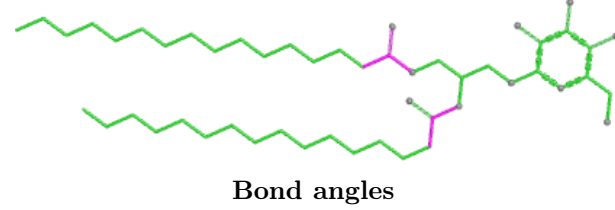


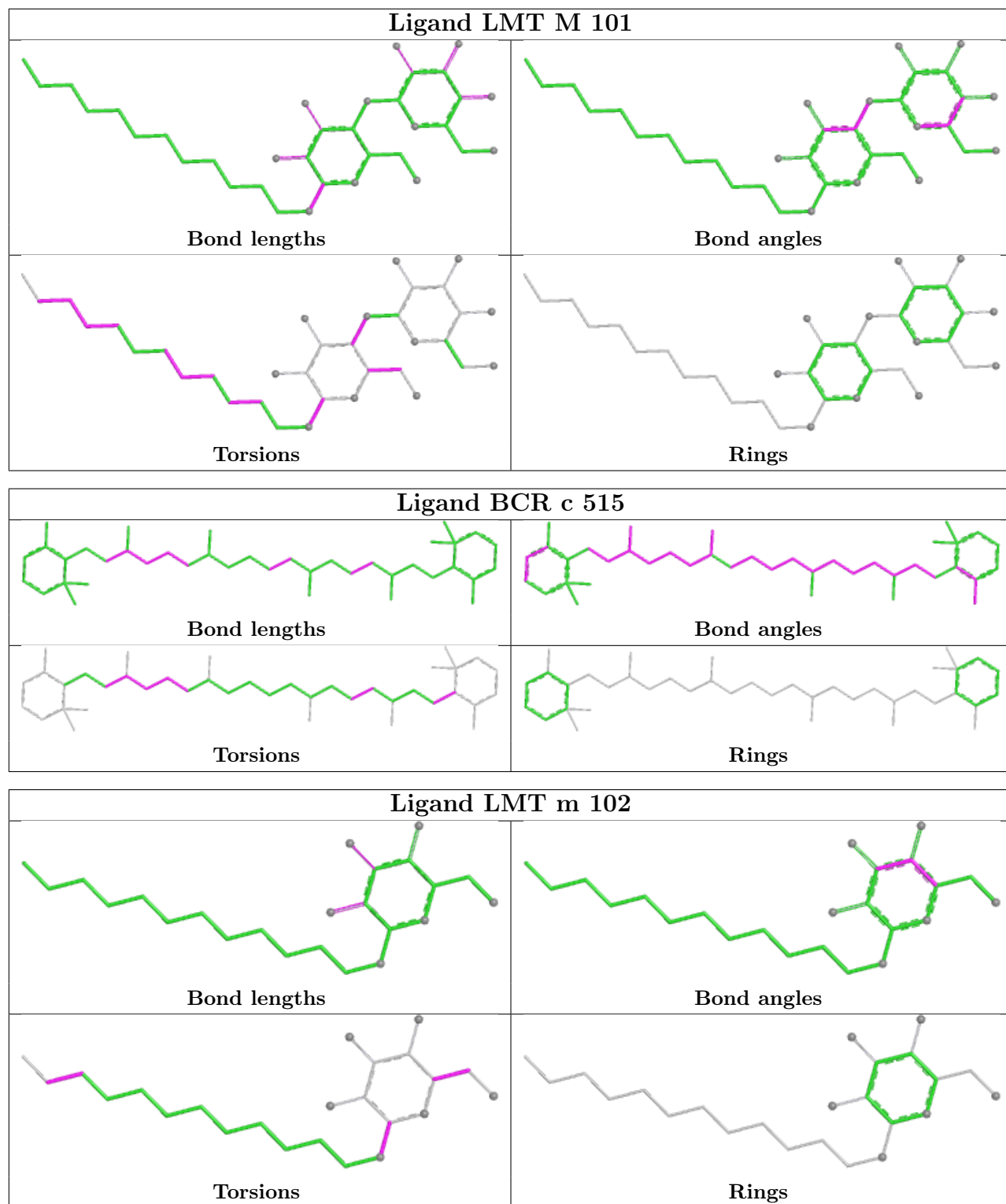




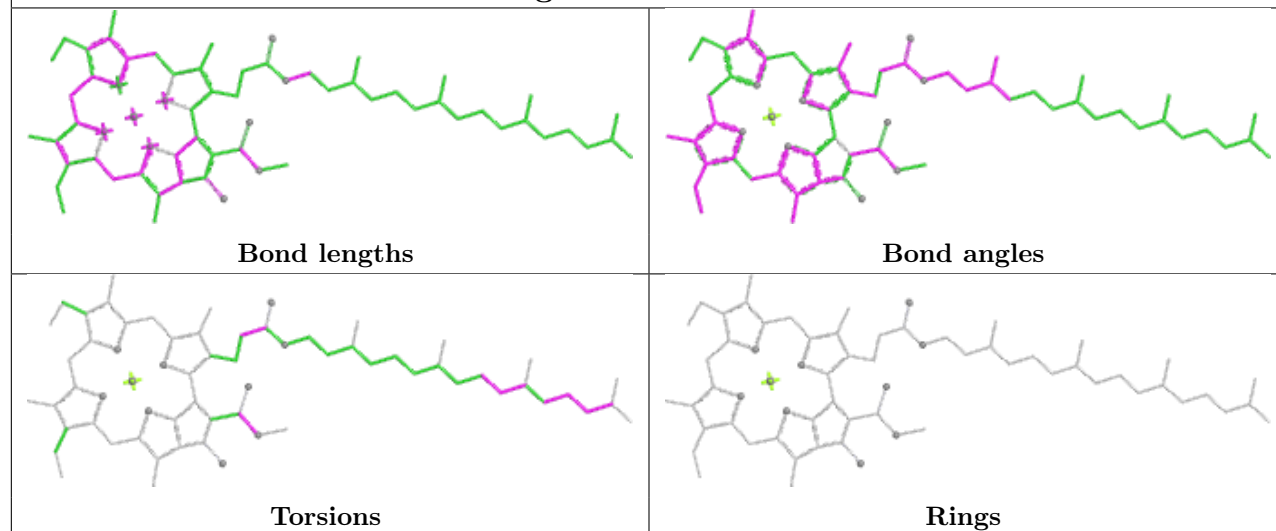
Ligand LMT I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand RRX H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

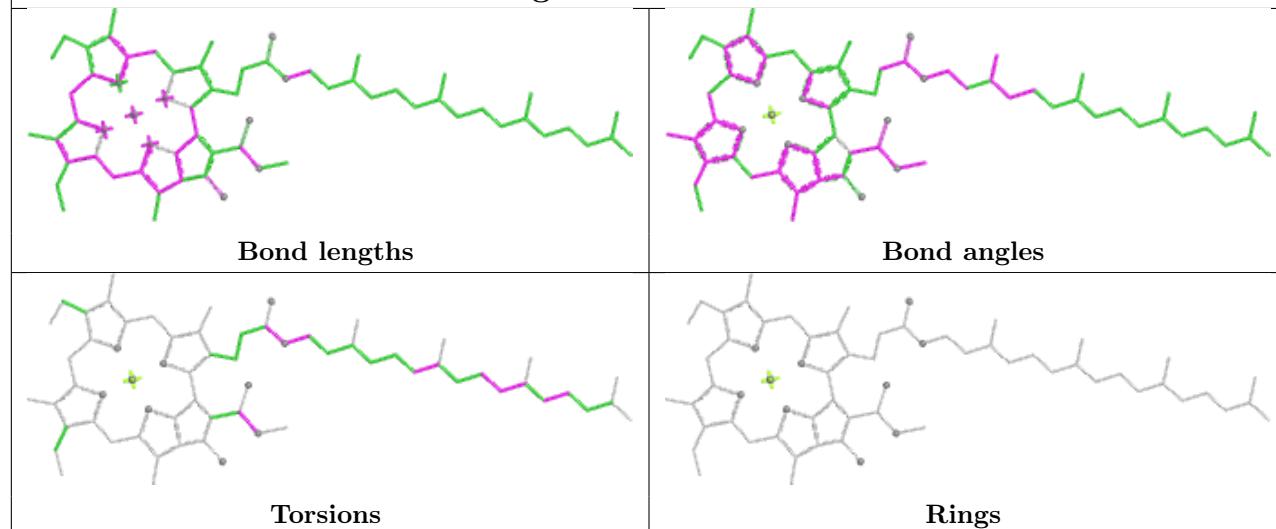
Ligand LMG A 410	
	
Bond lengths	Bond angles
	
Torsions	Rings



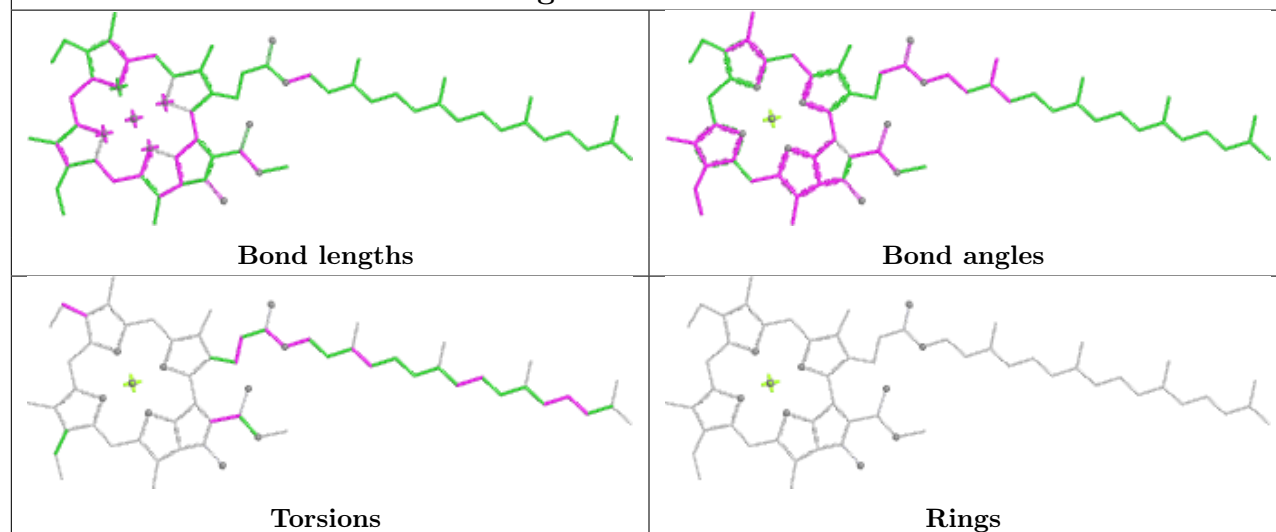
Ligand CLA d 403

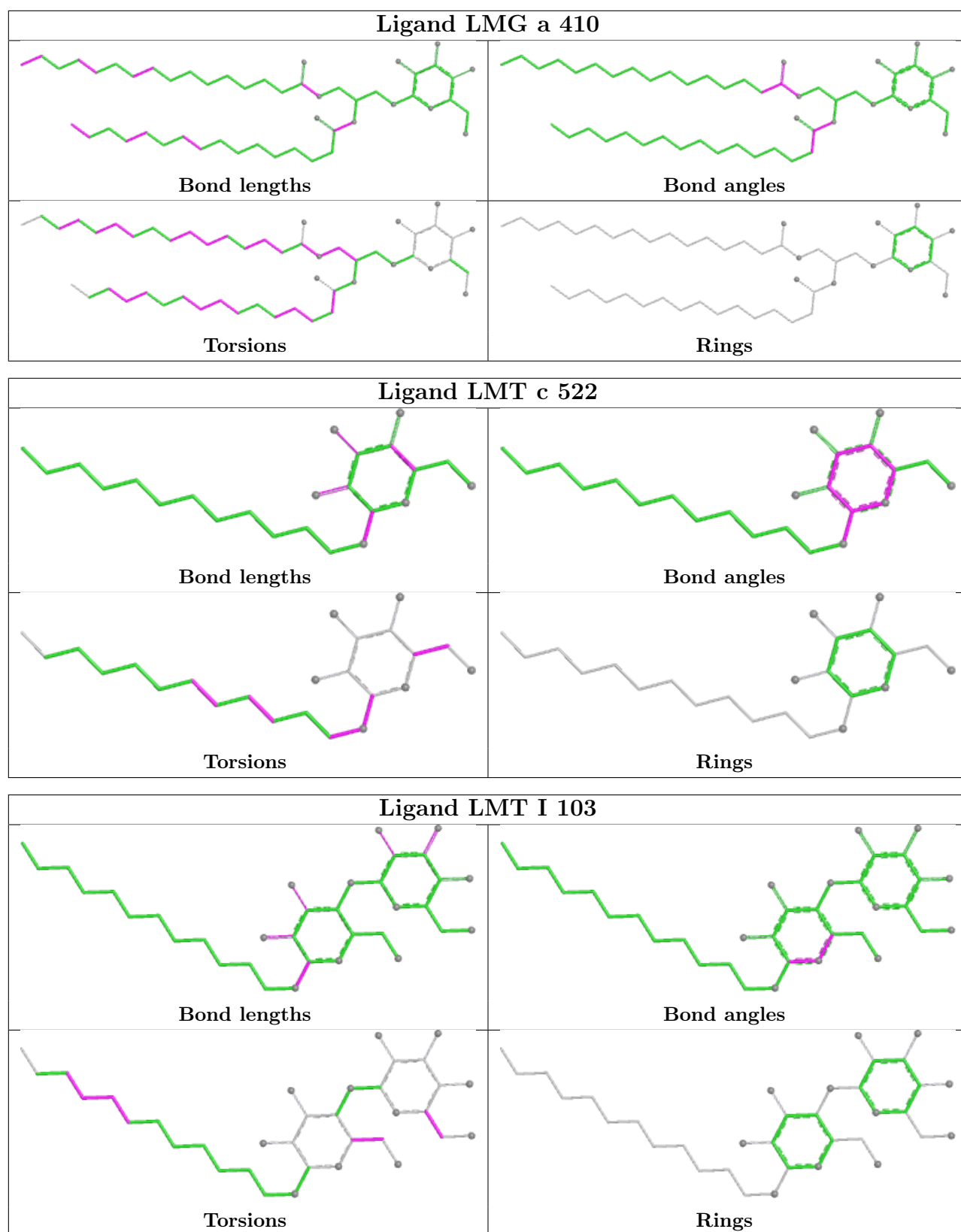


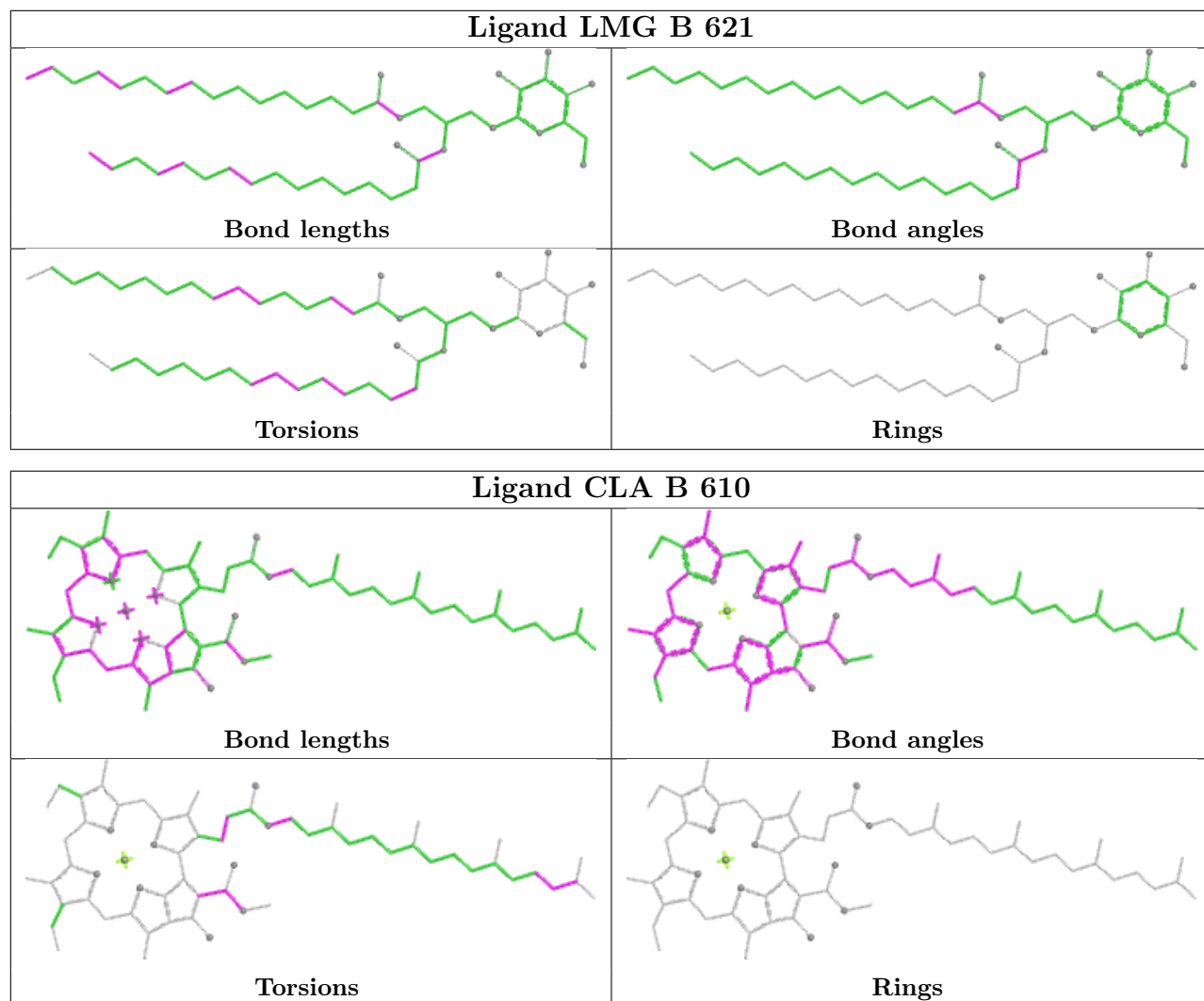
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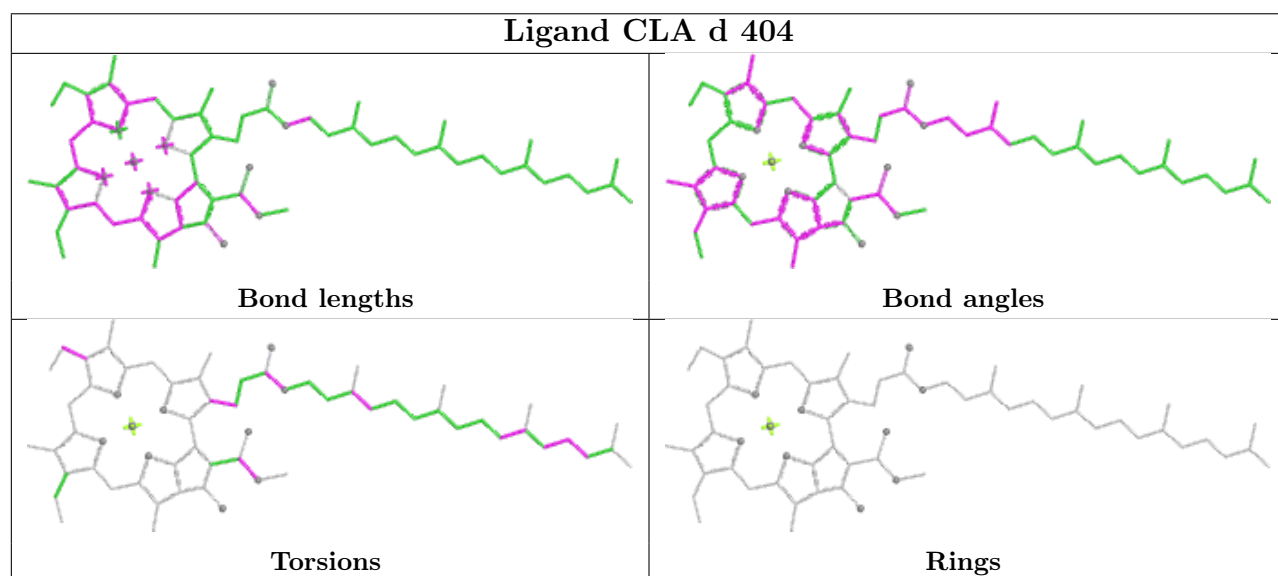
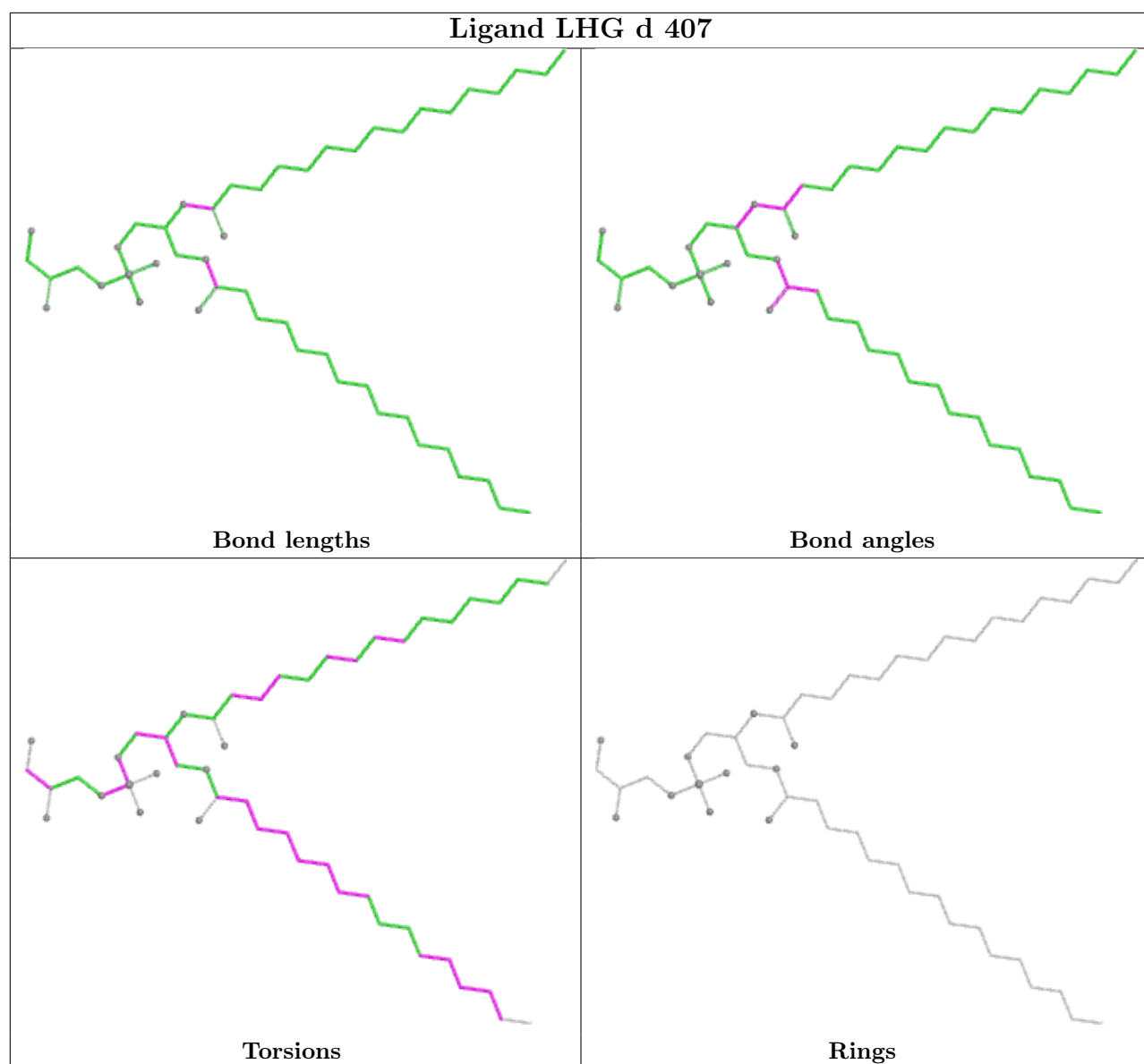


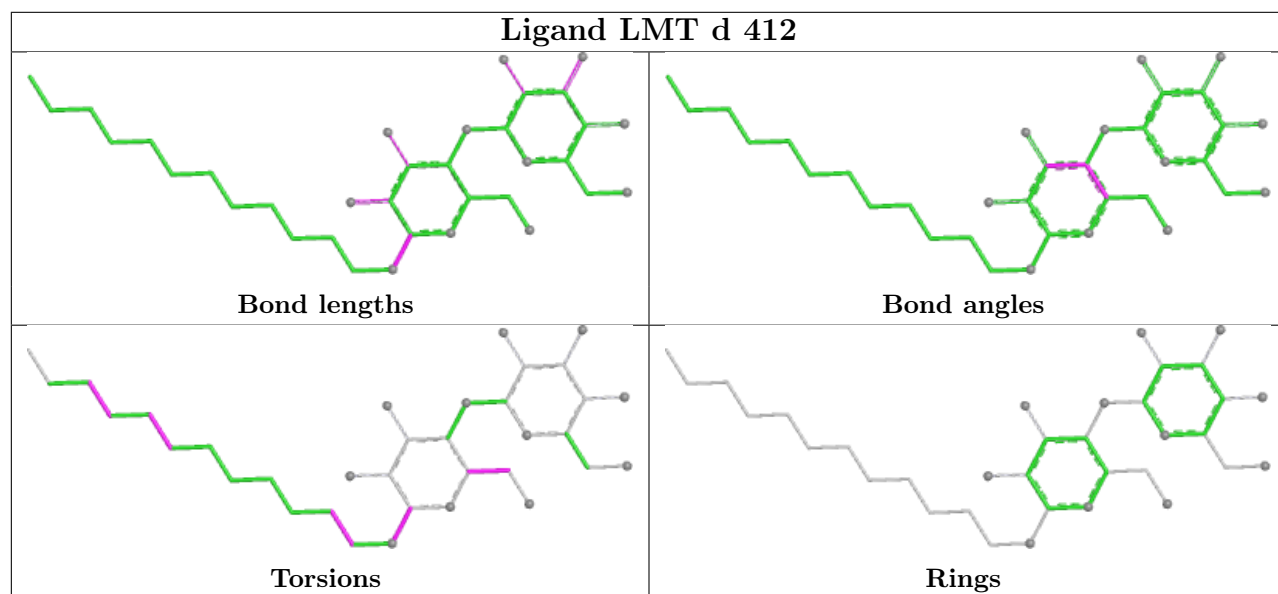
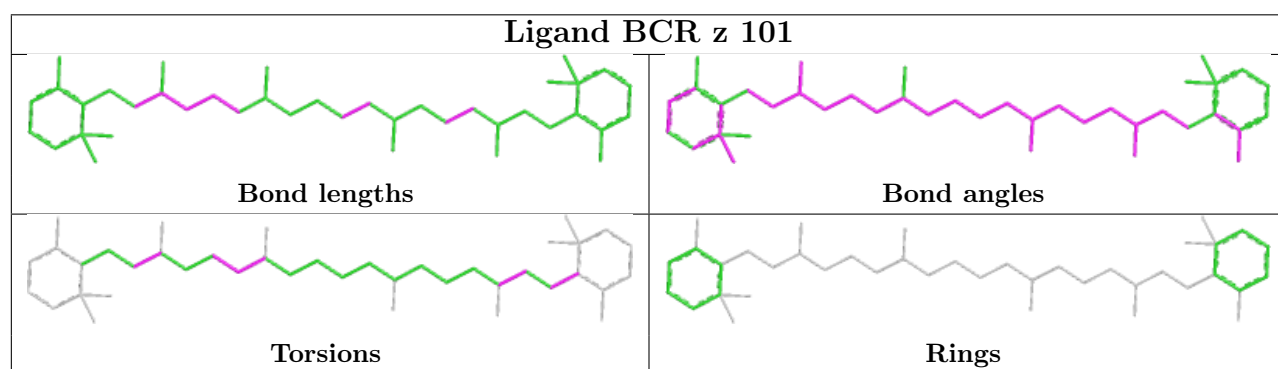
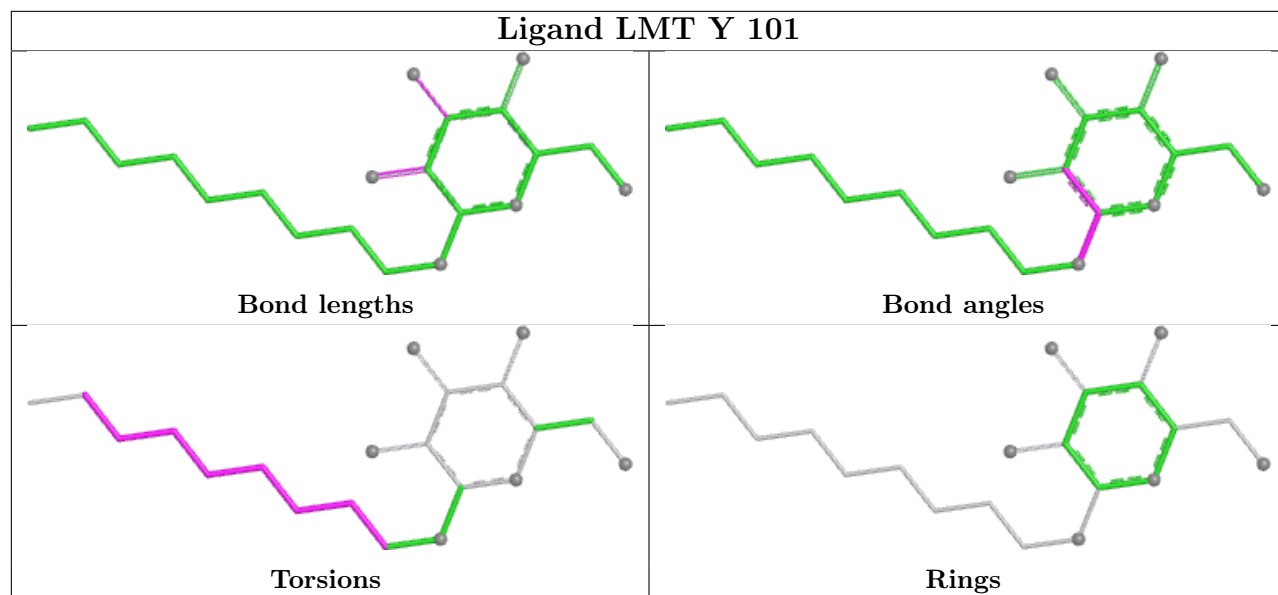
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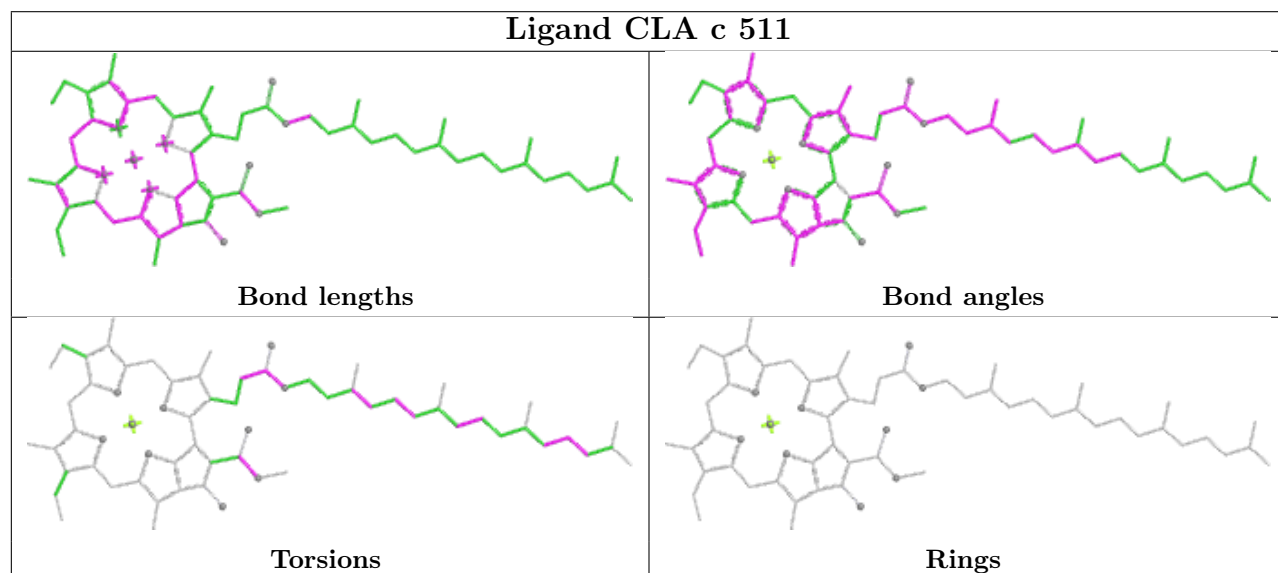
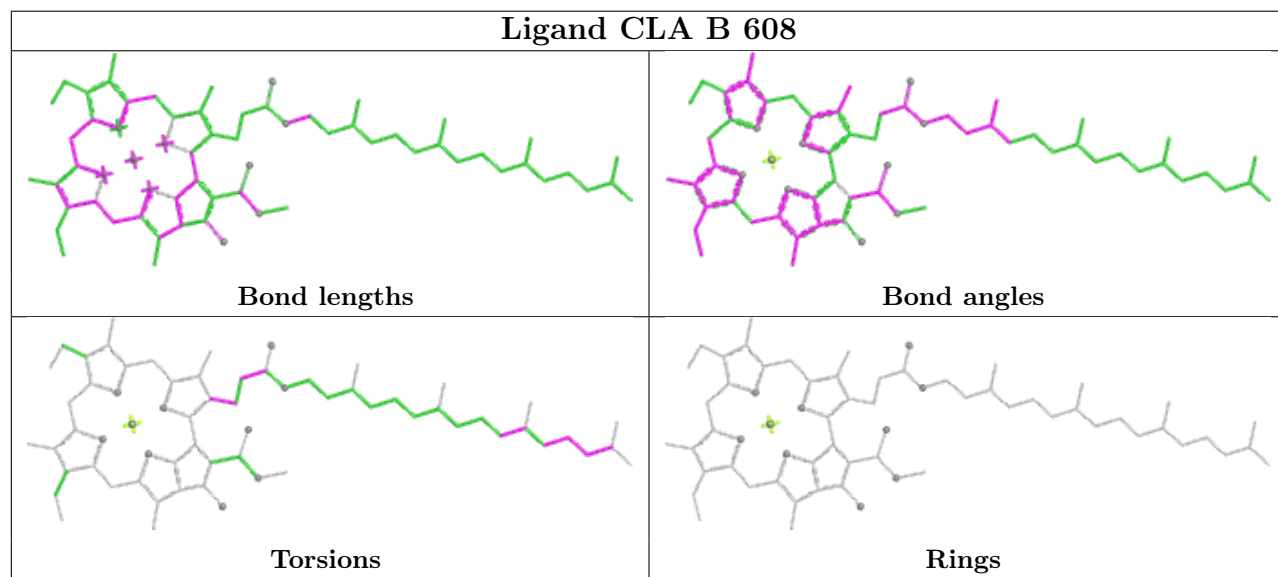
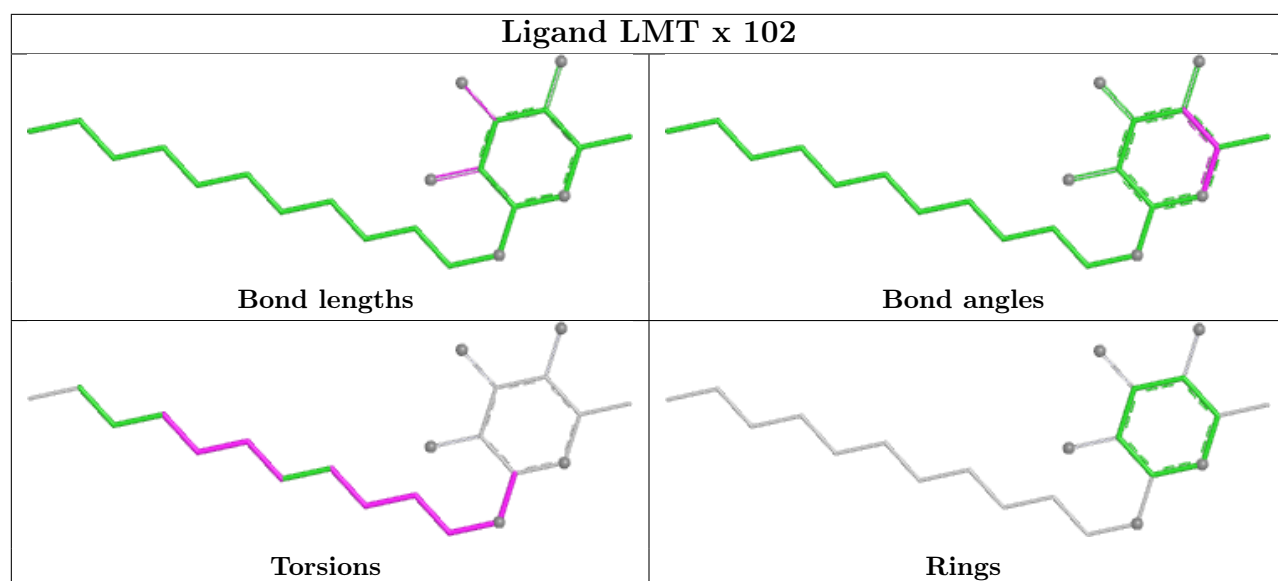


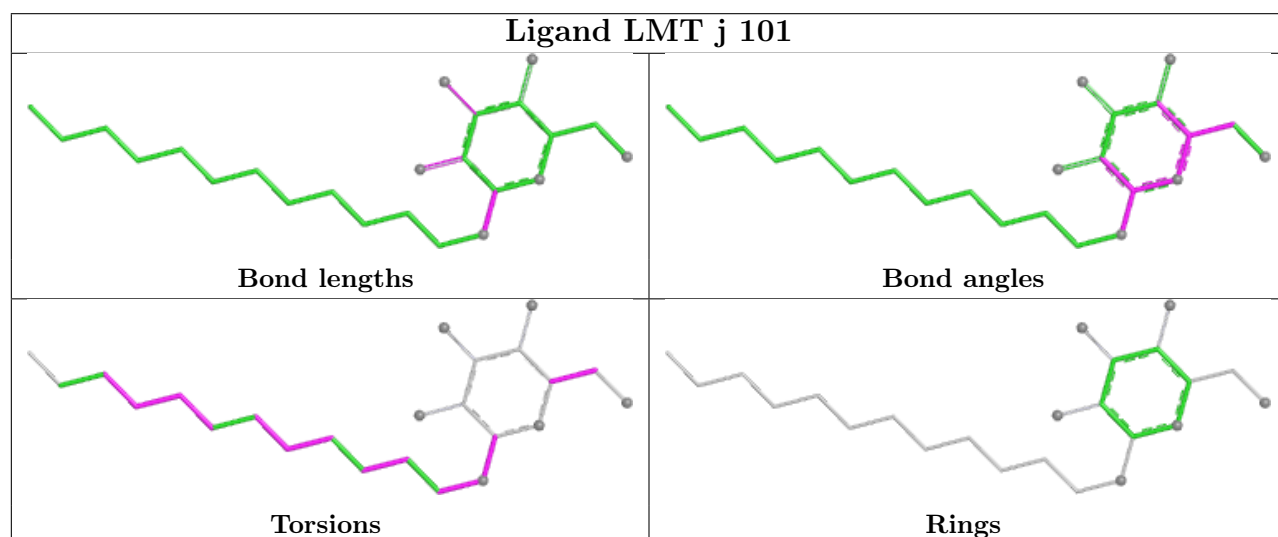
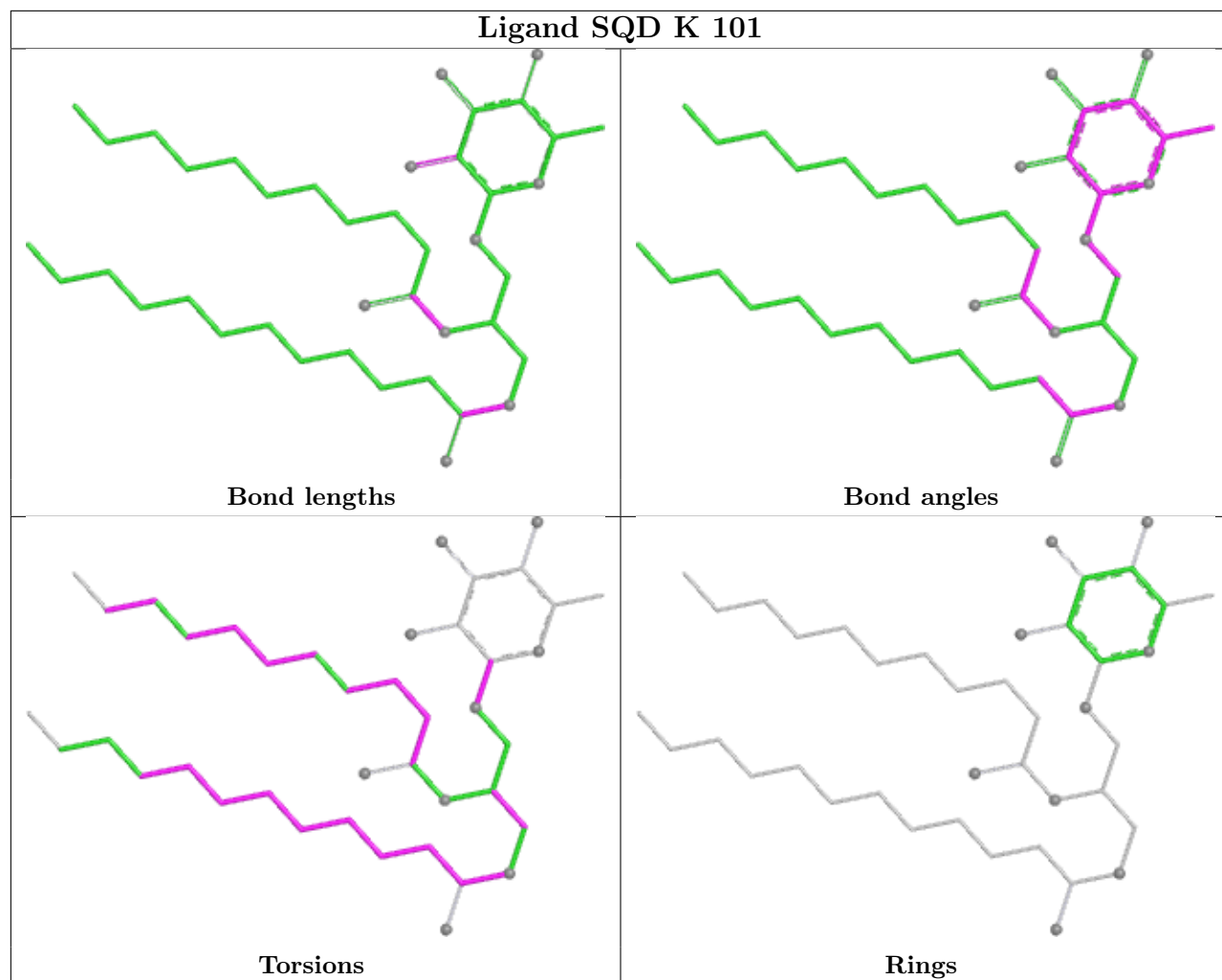


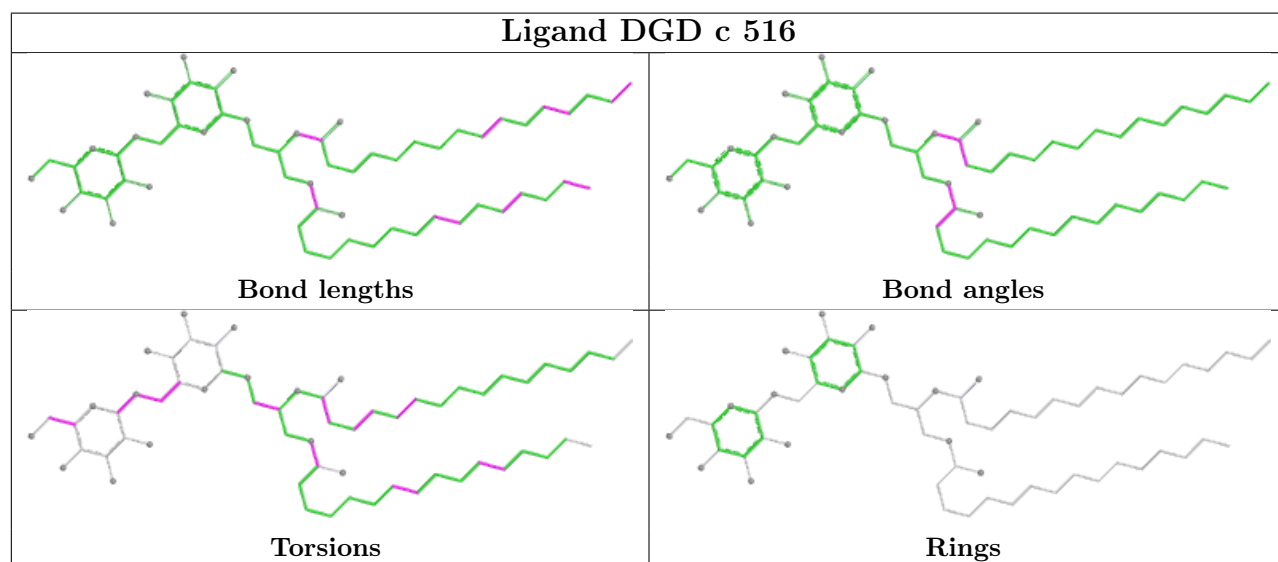
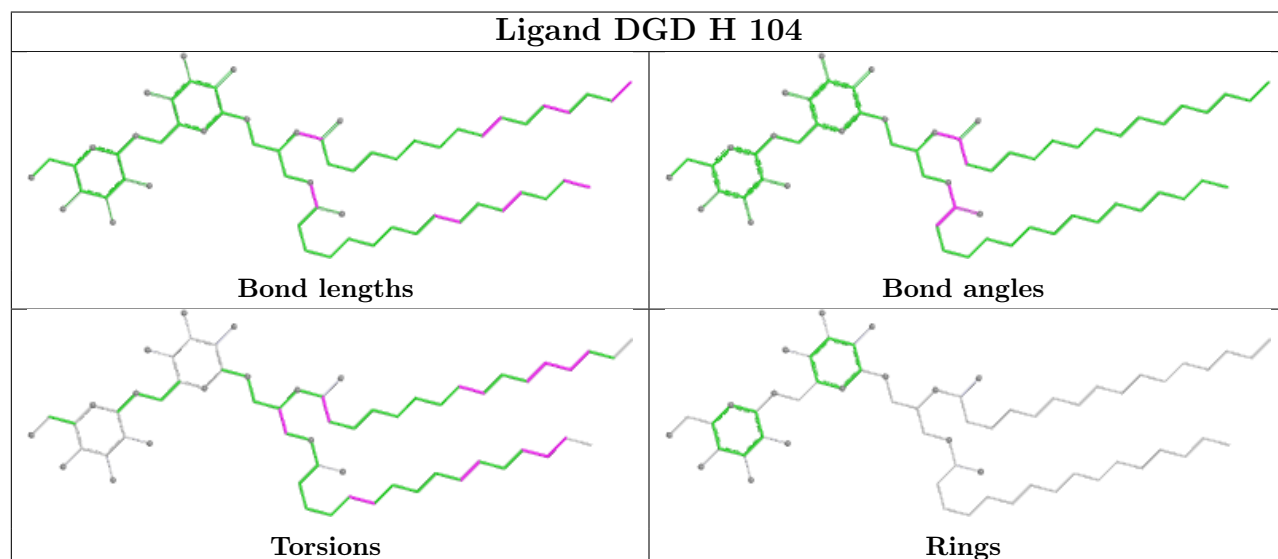
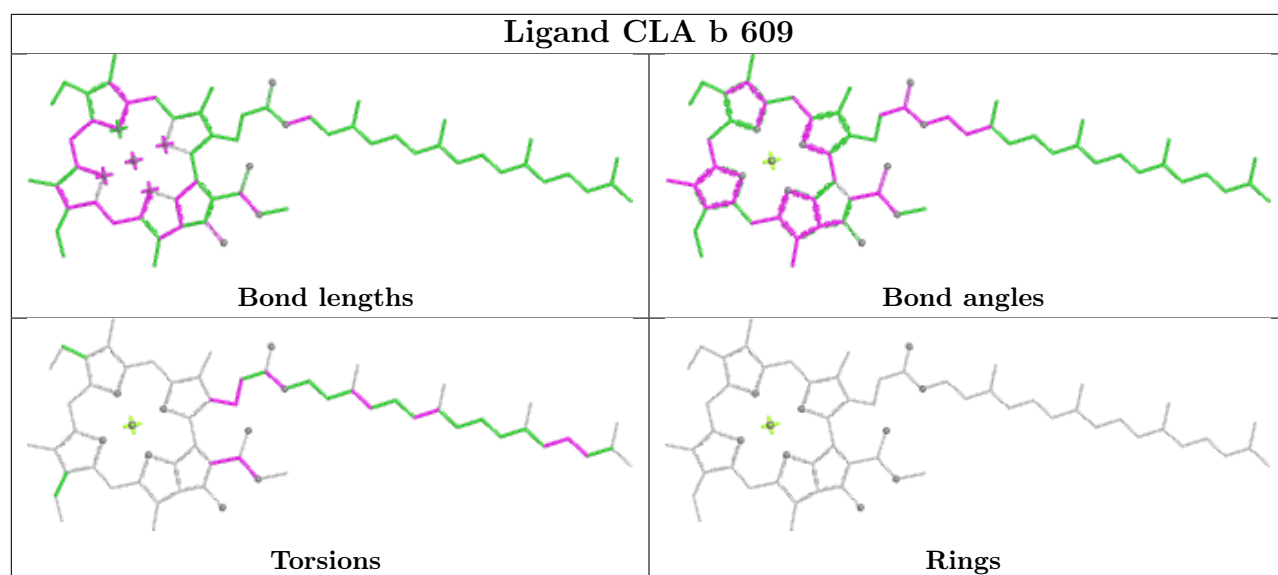


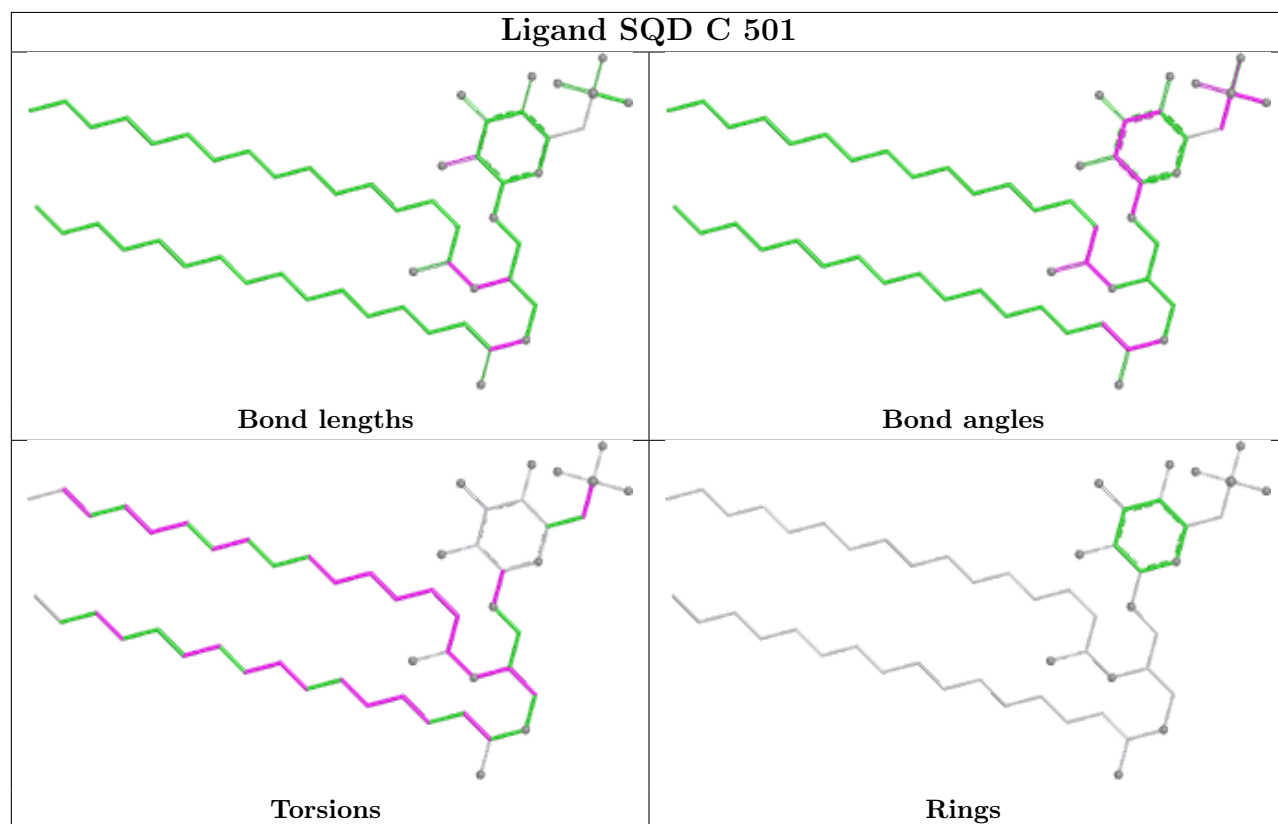
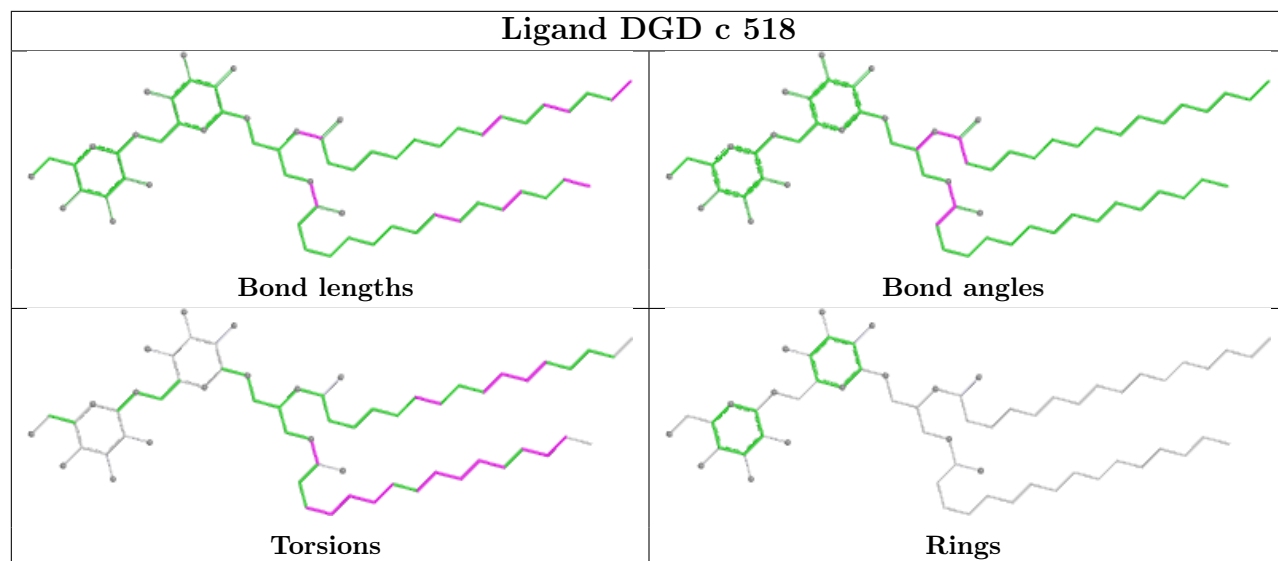


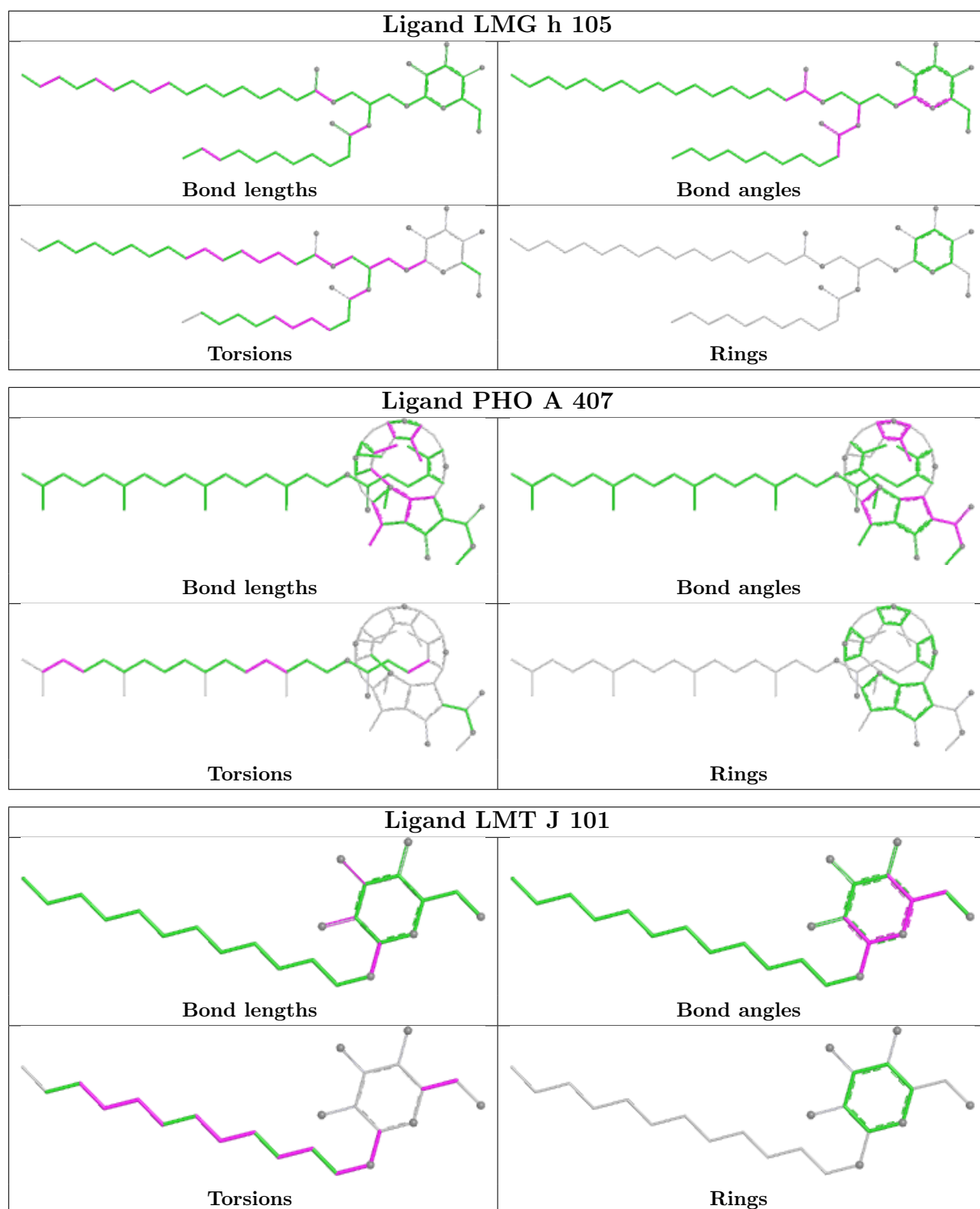


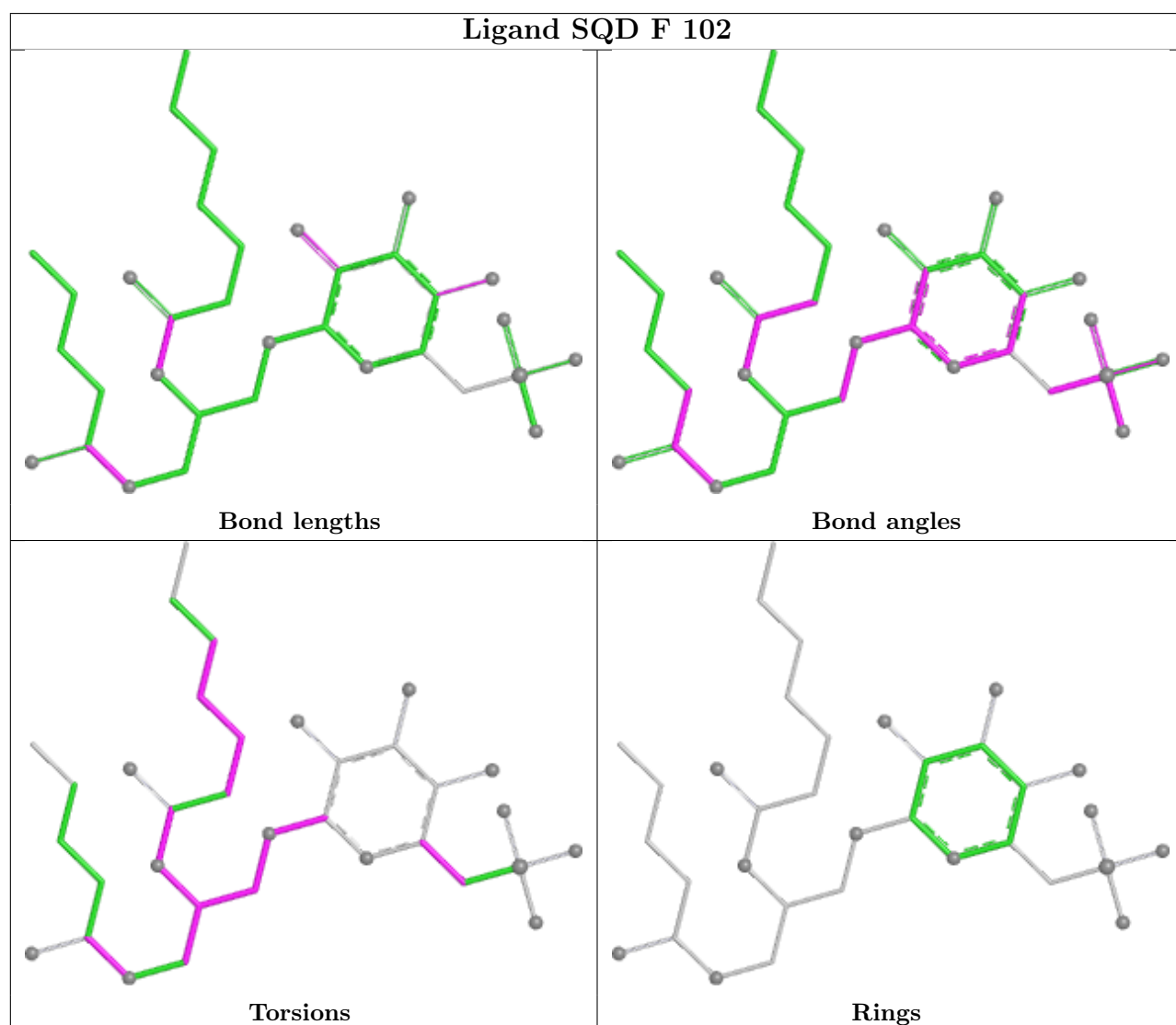
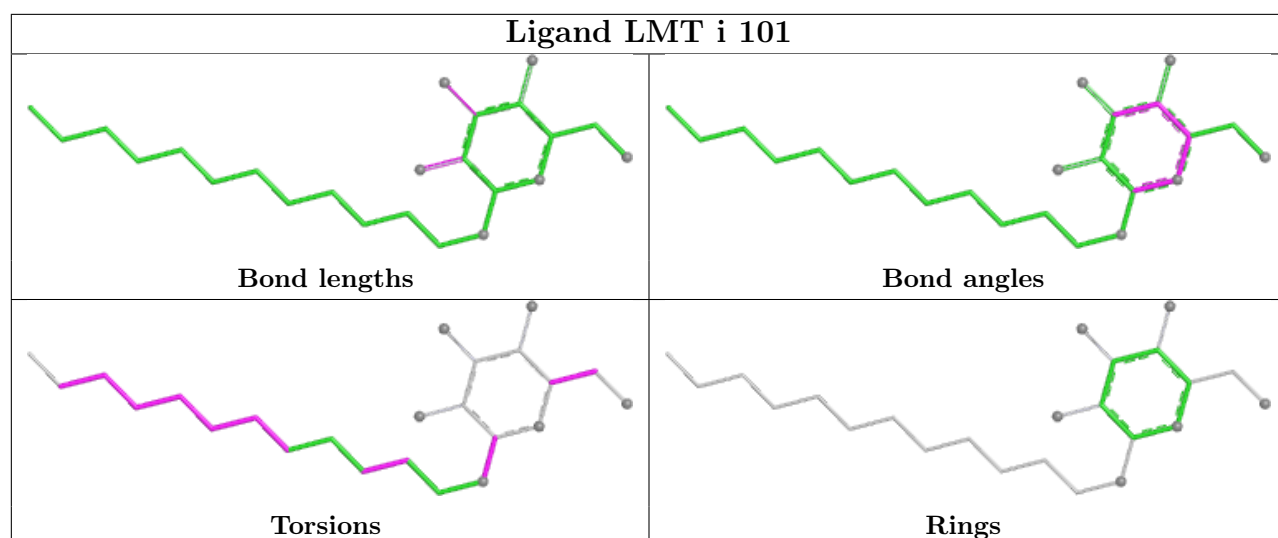




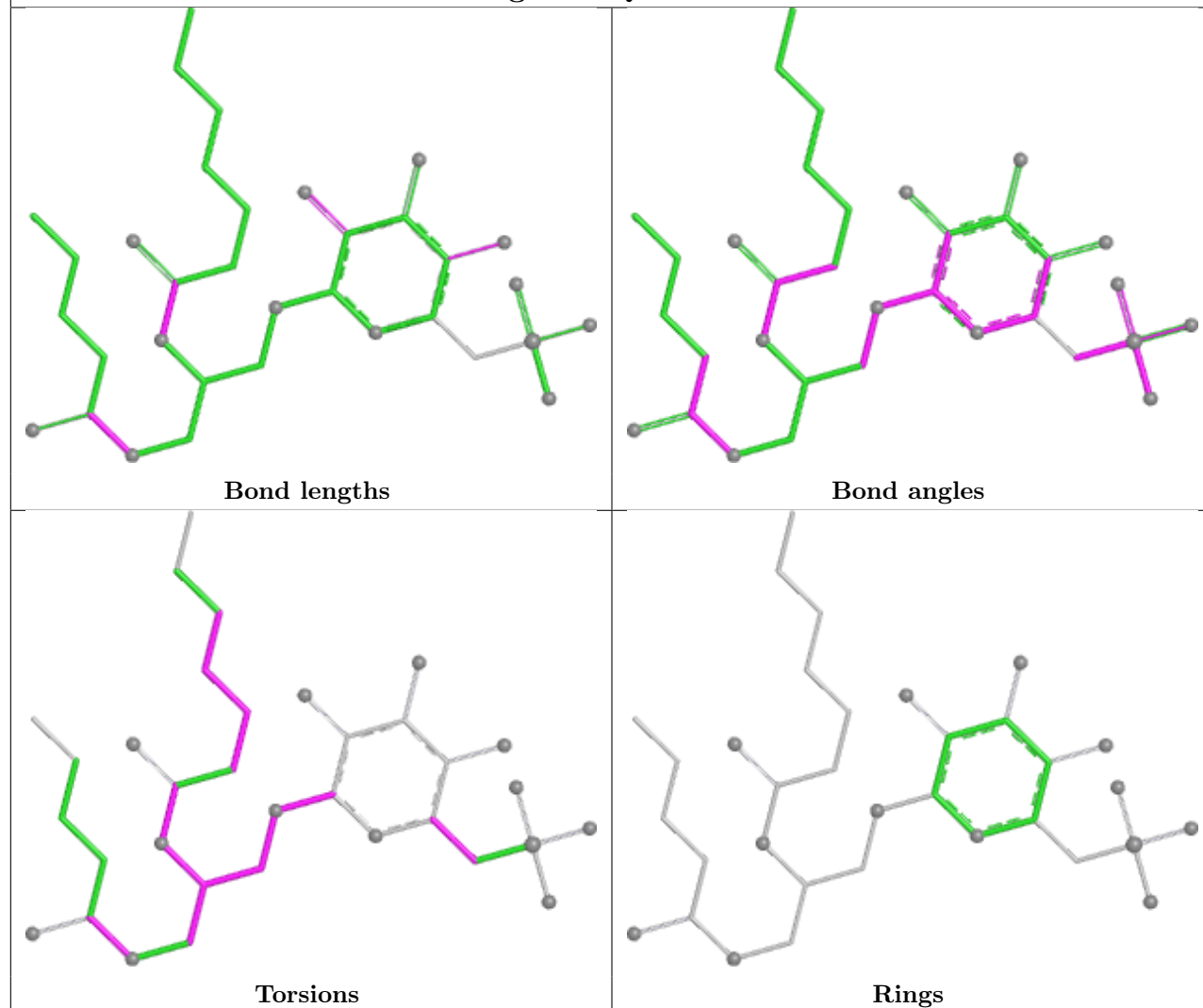




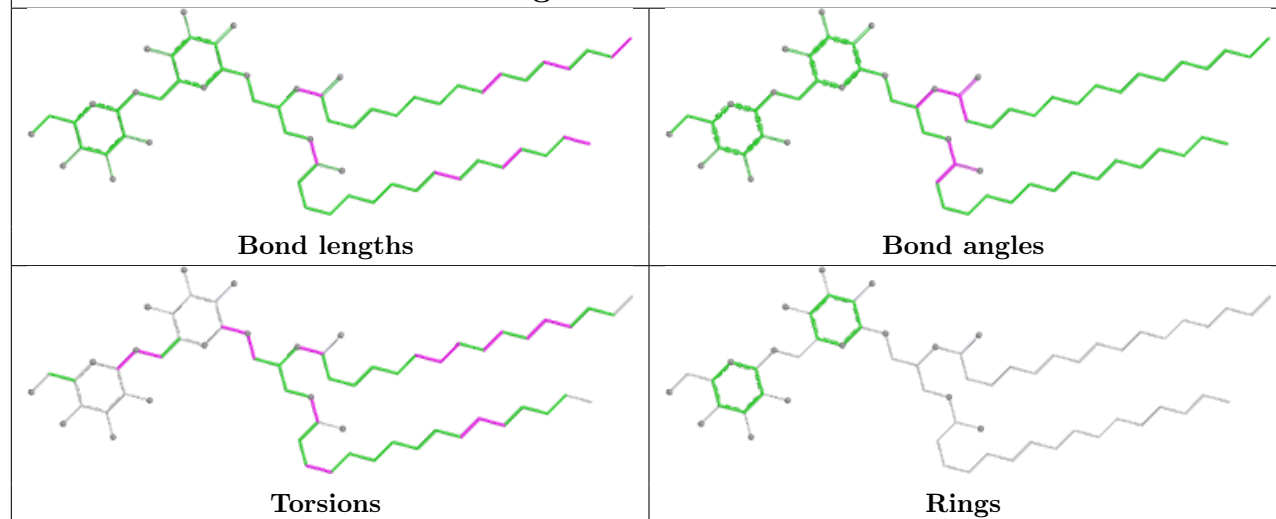


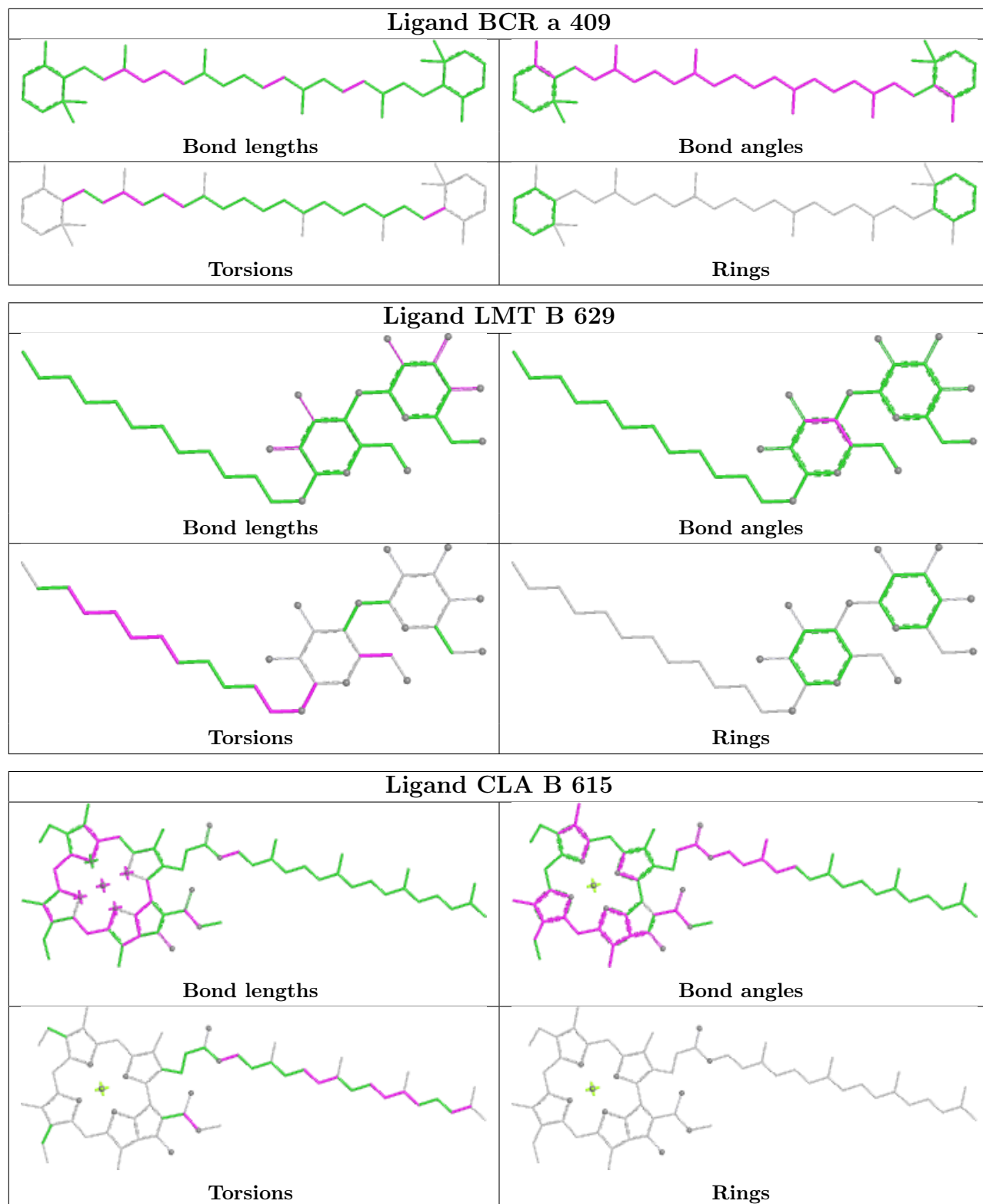


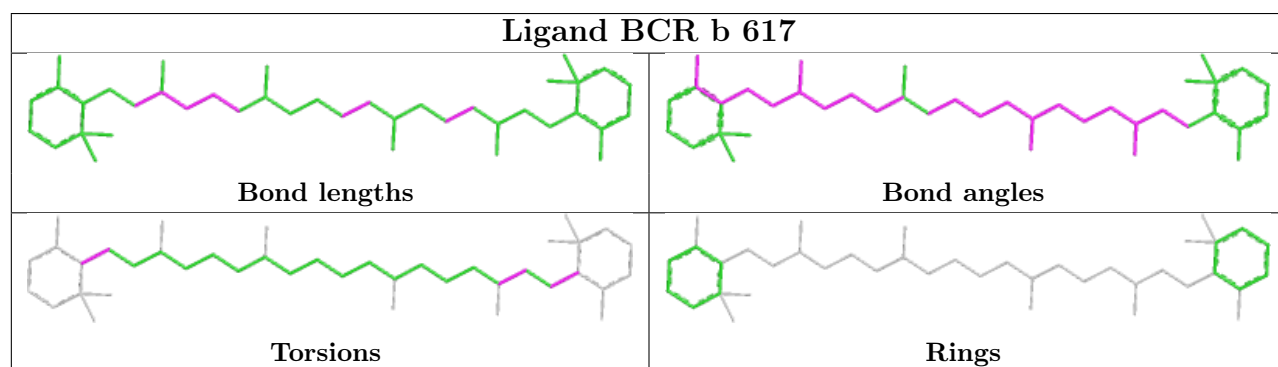
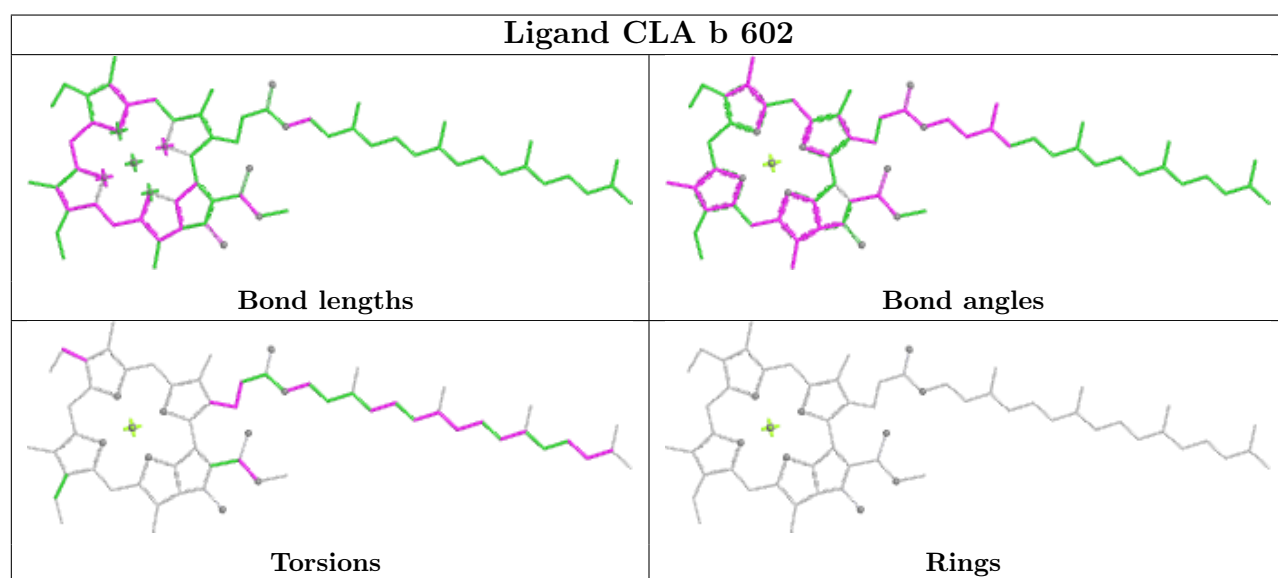
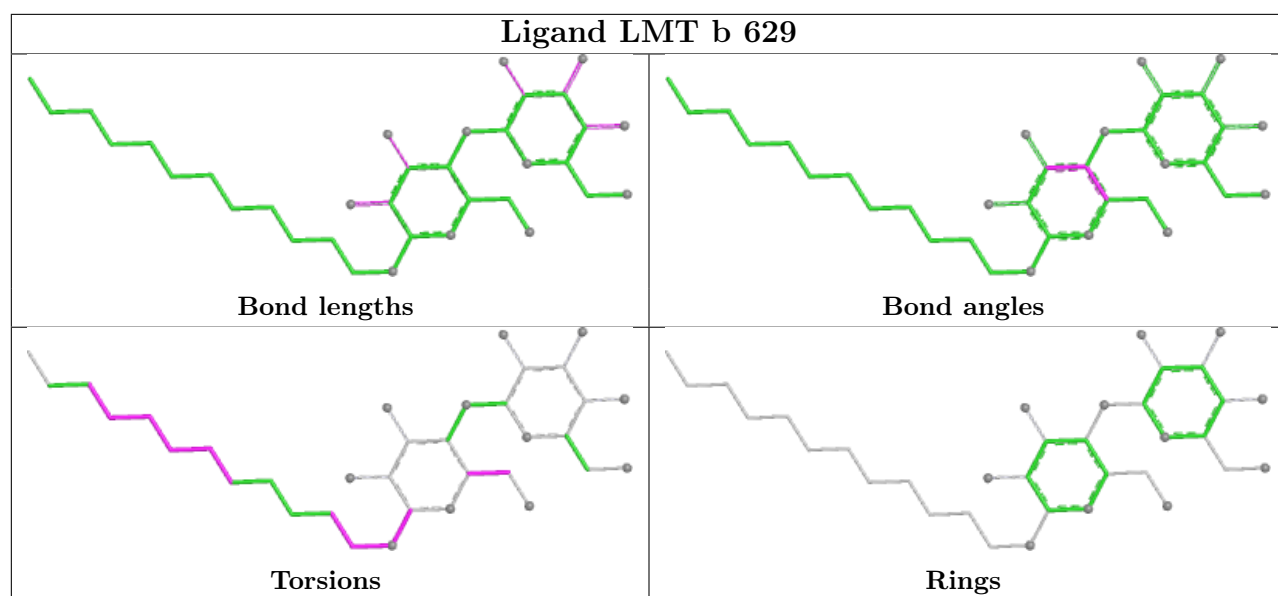
Ligand SQD f 102

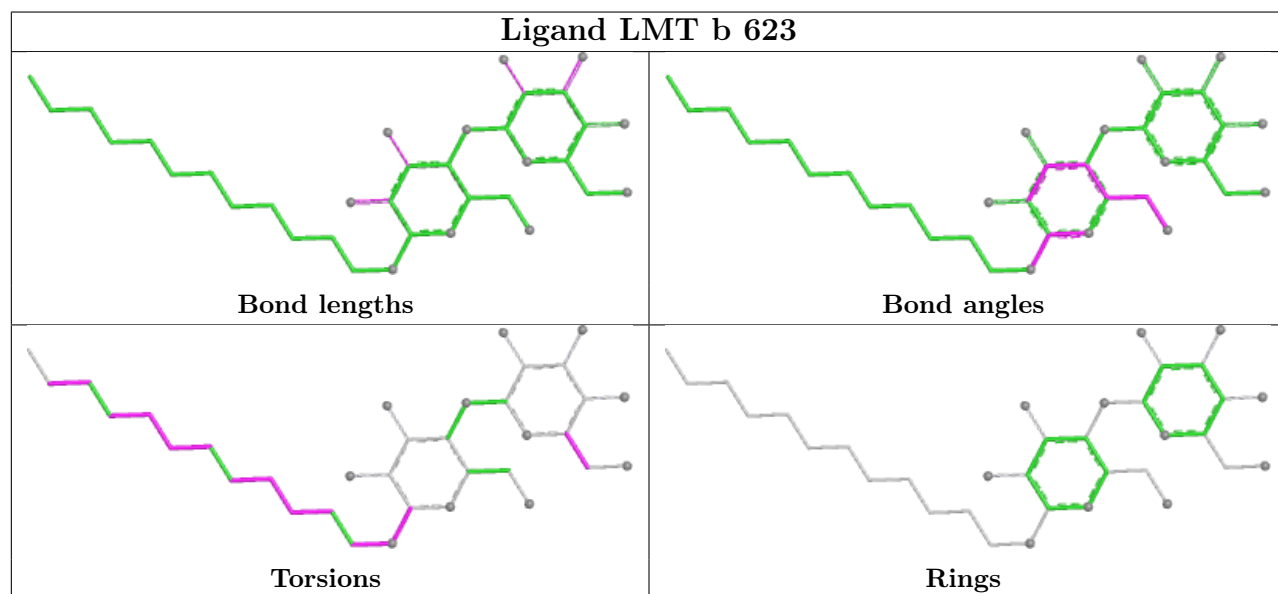
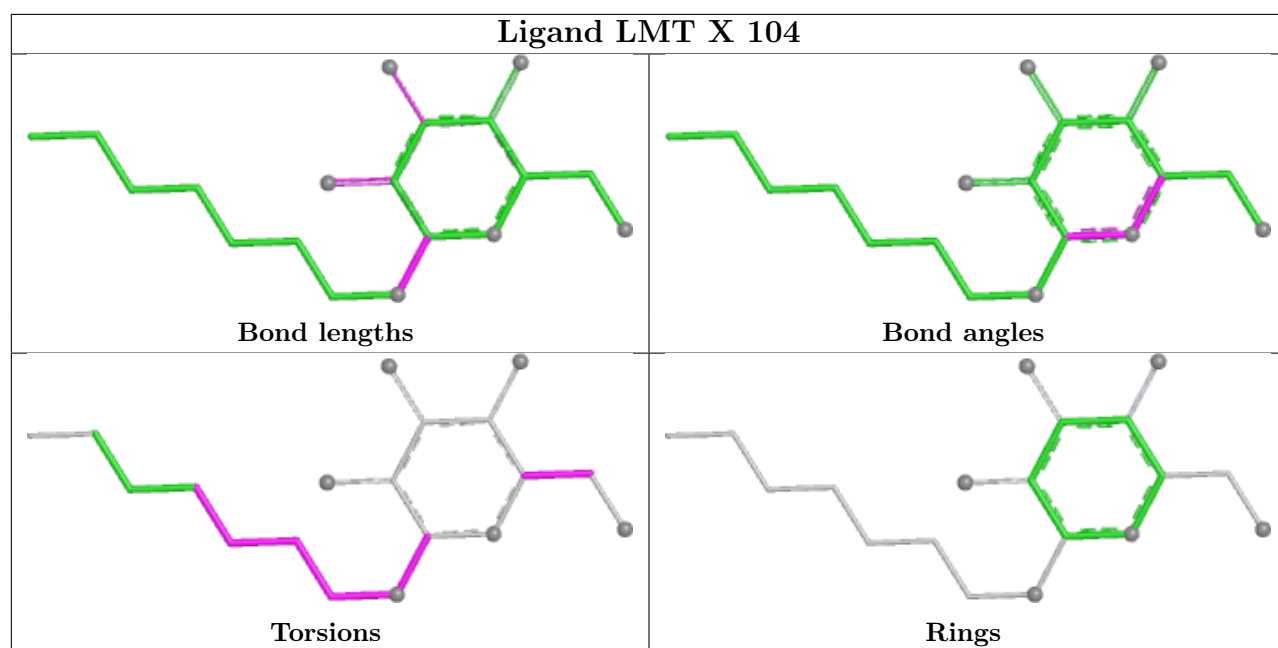


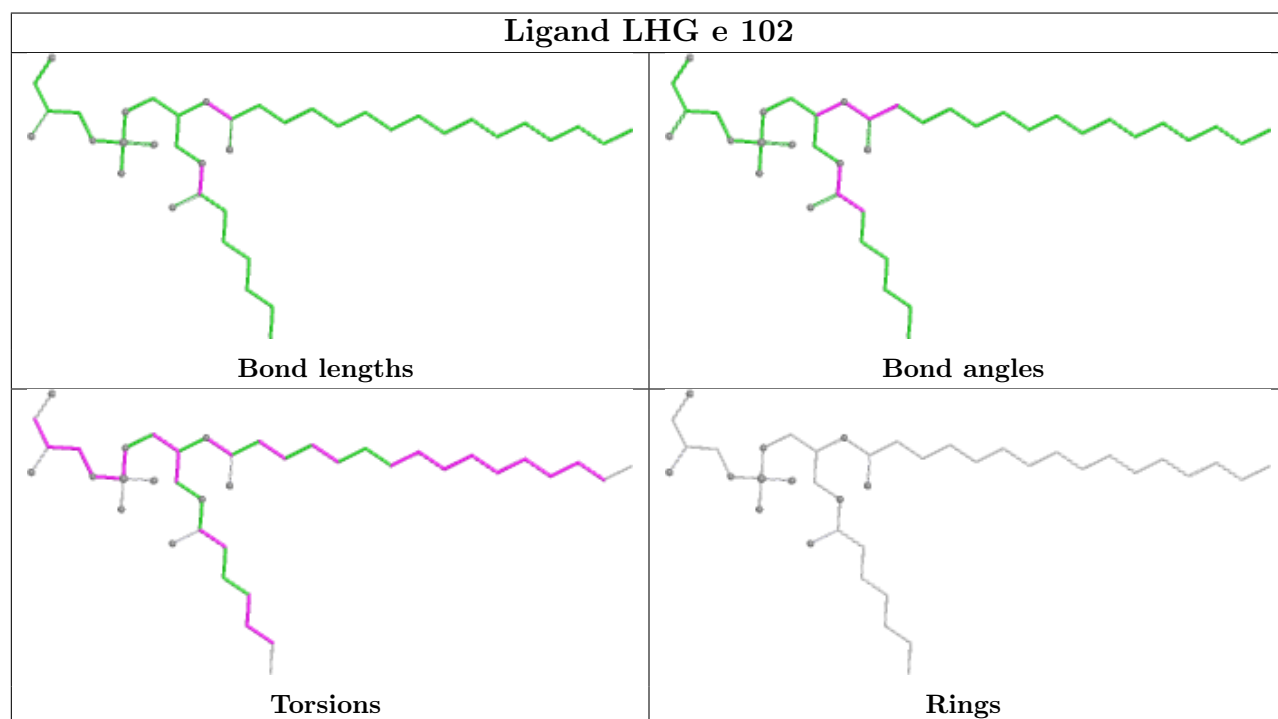
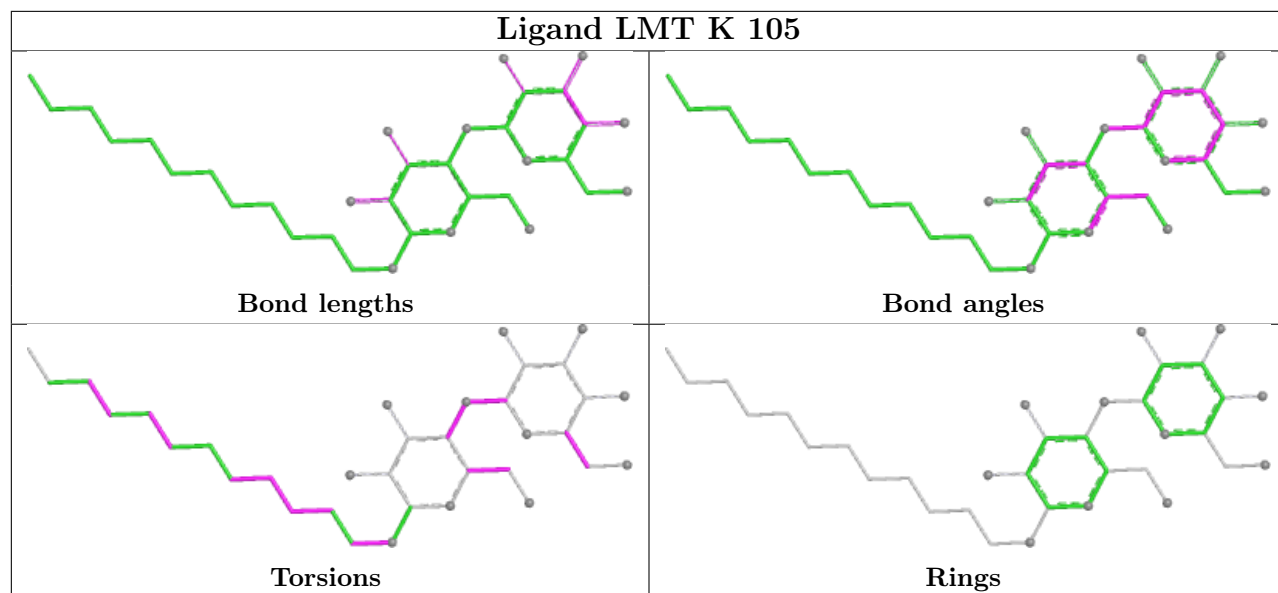
Ligand DGD c 517

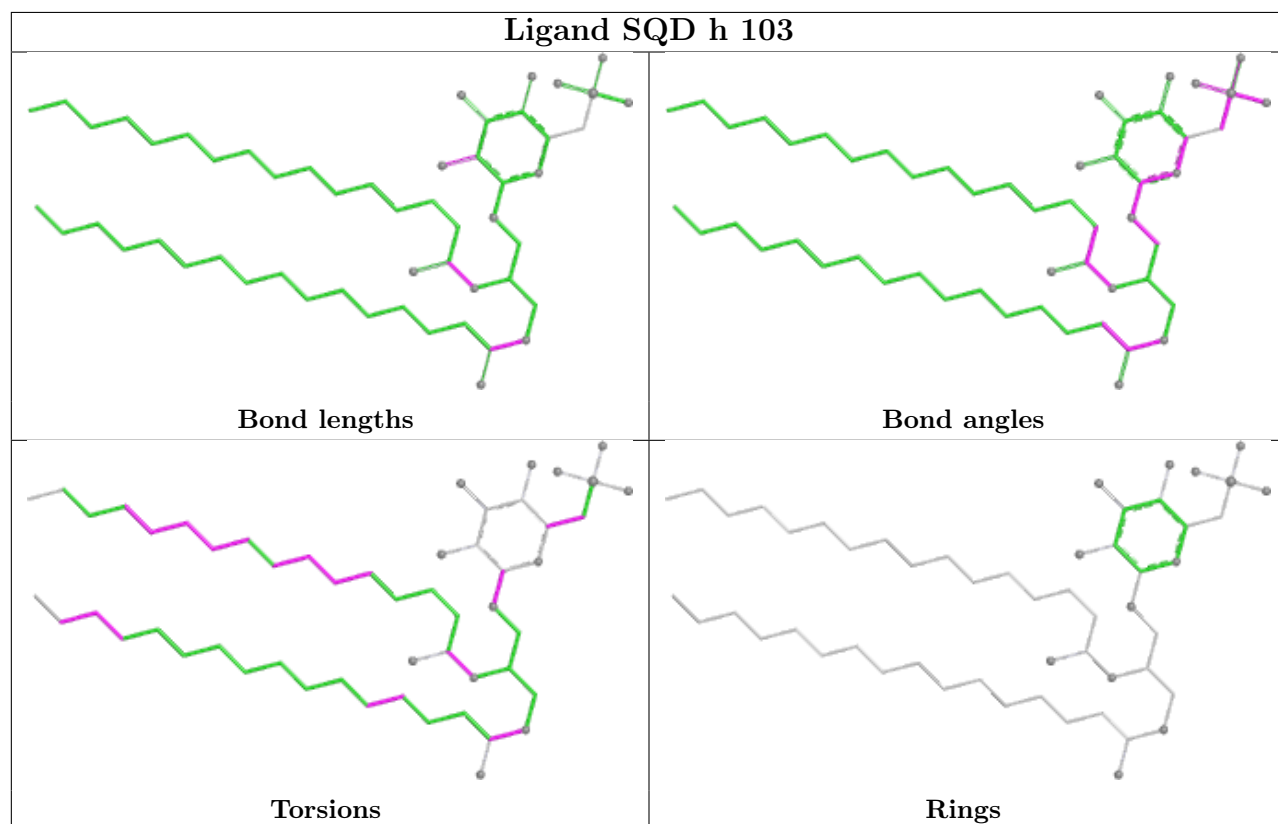
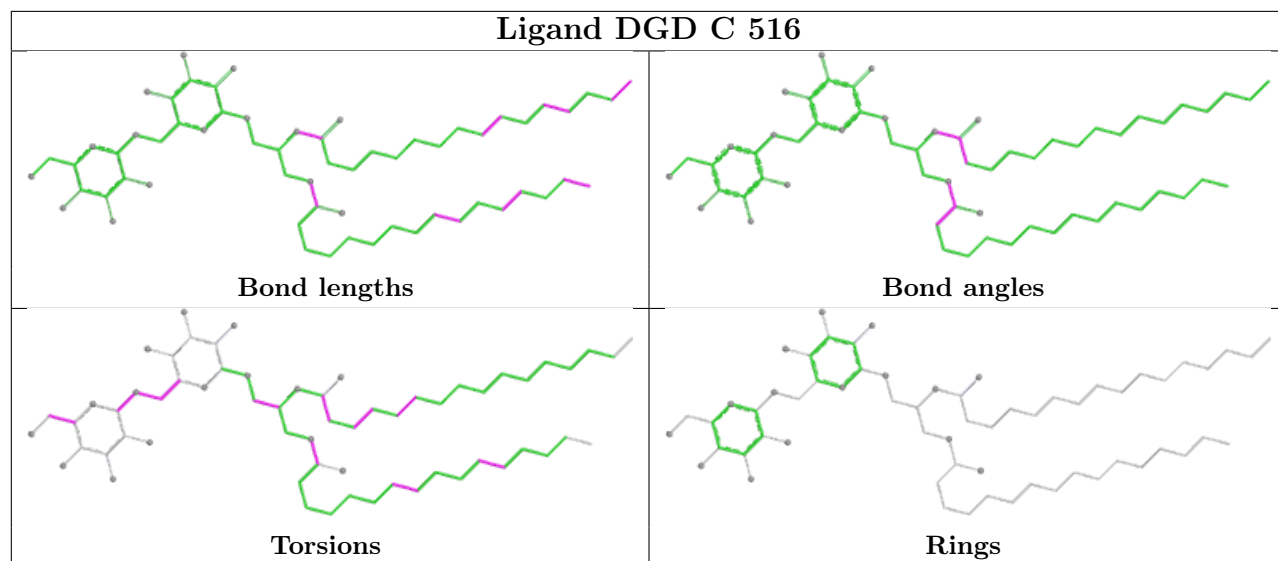




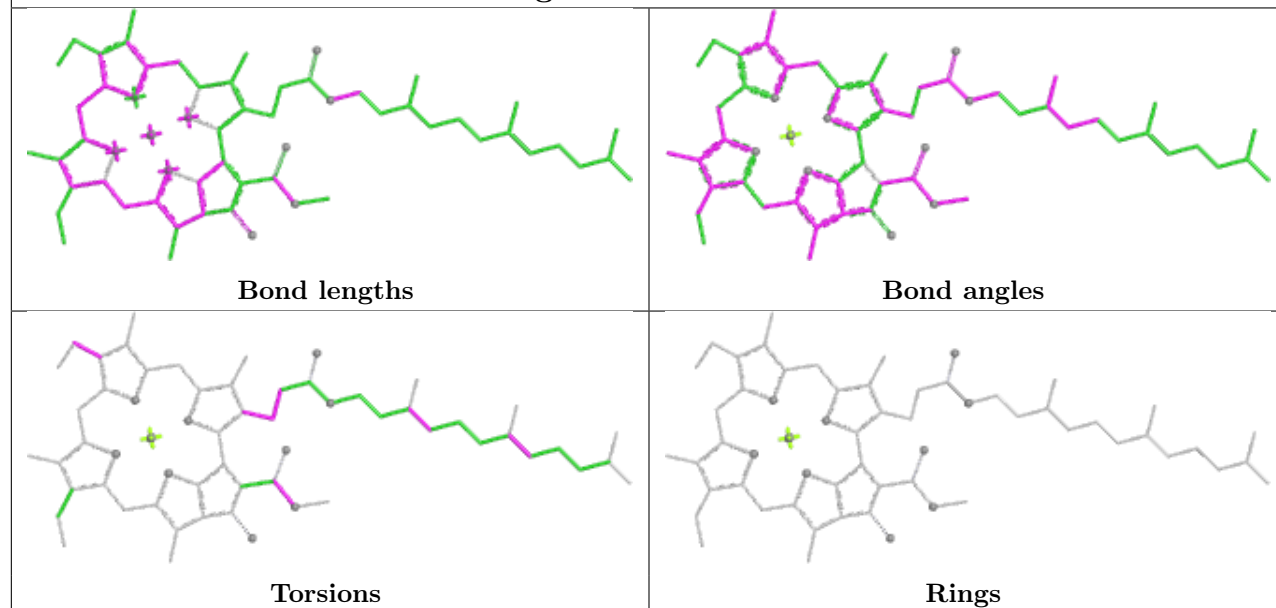




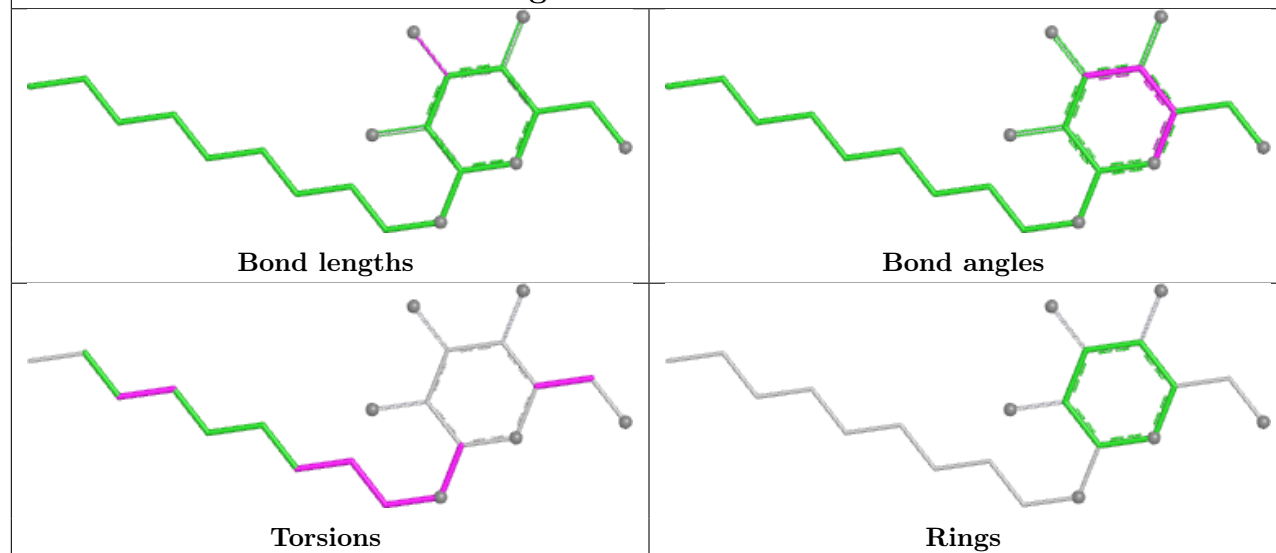


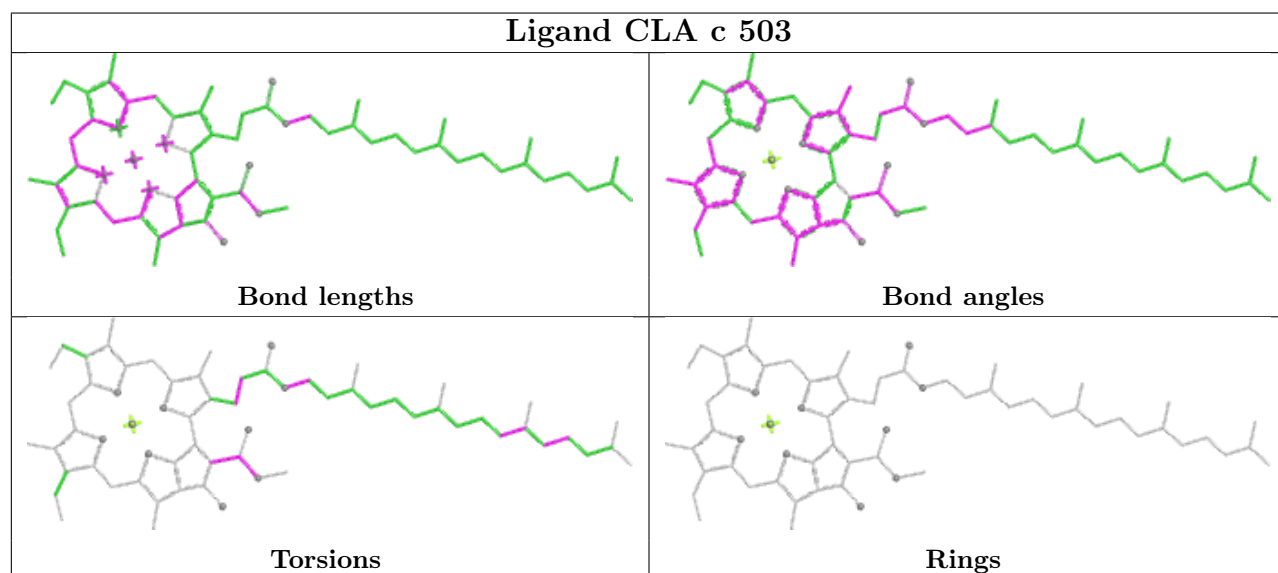
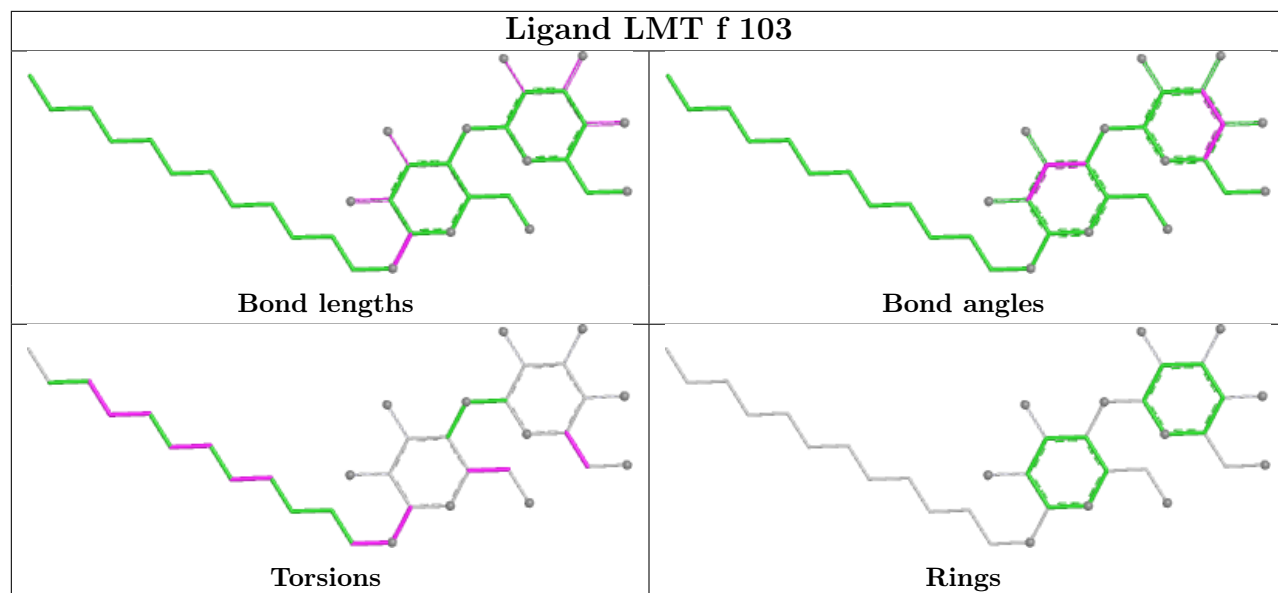


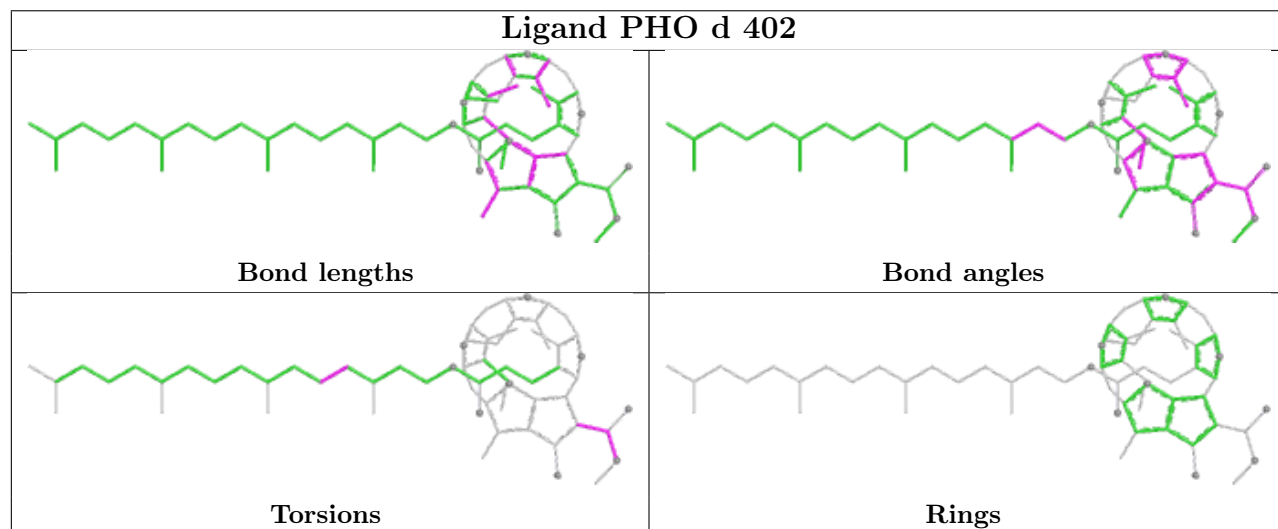
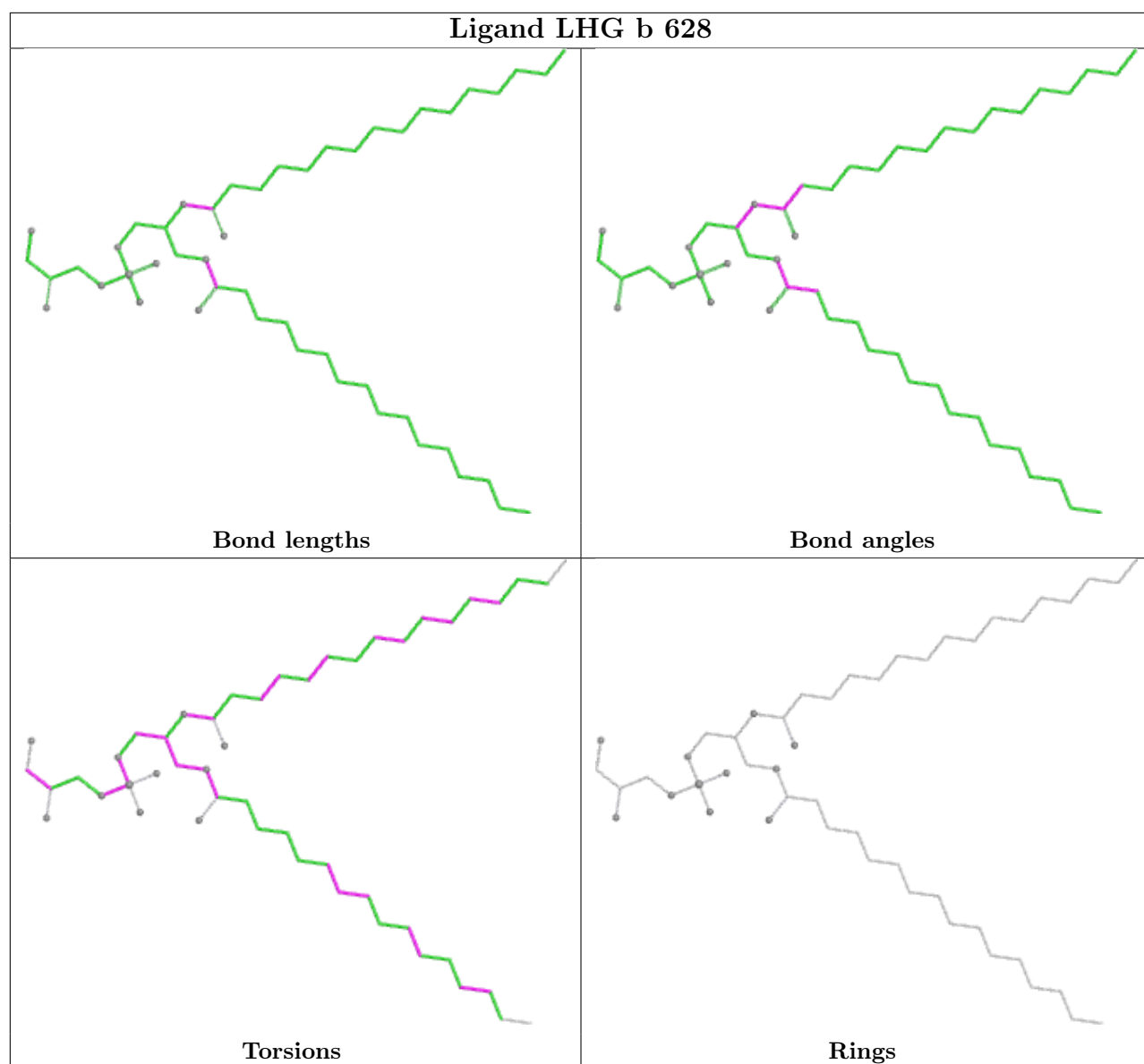
Ligand CLA b 606

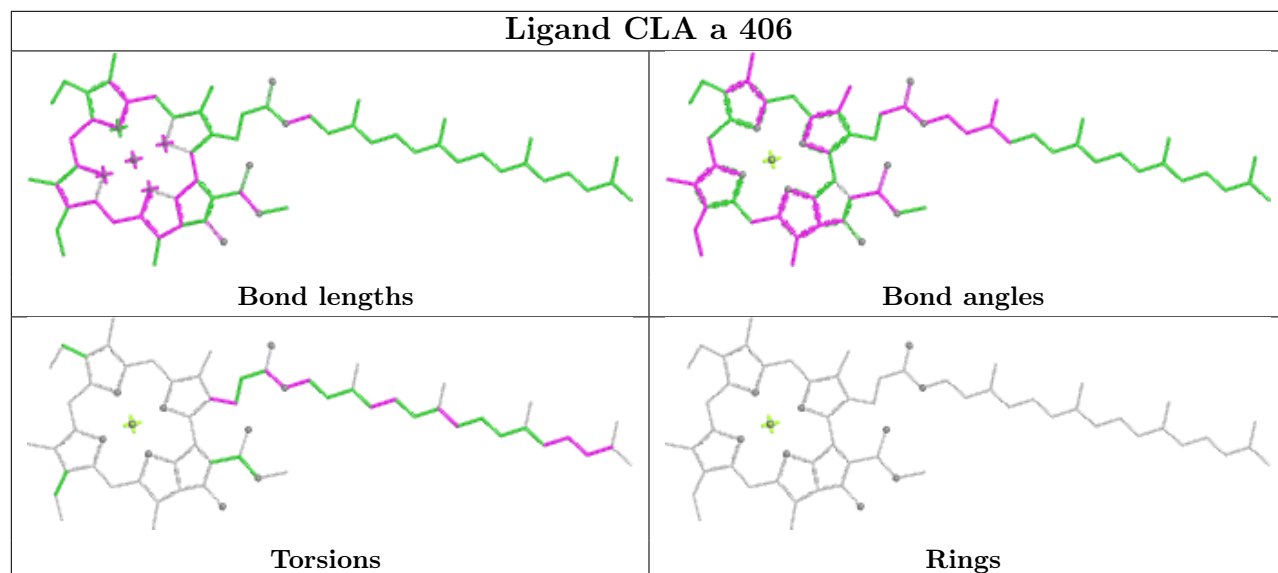
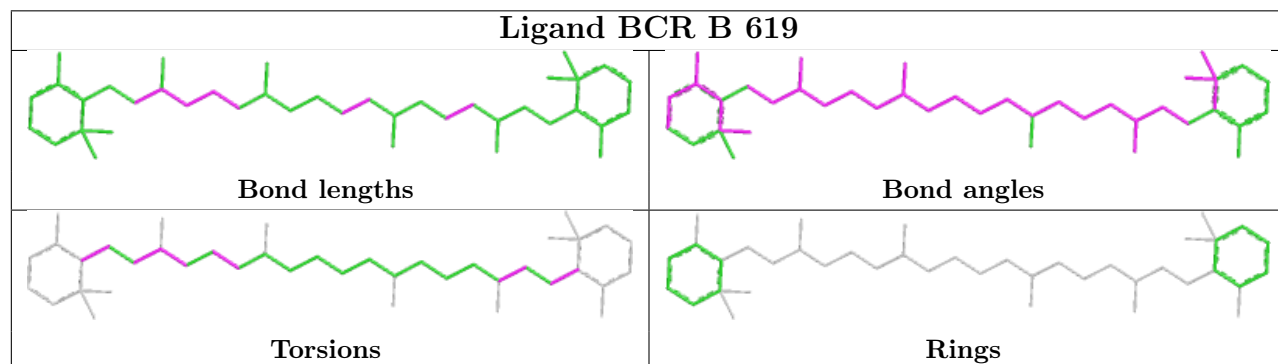
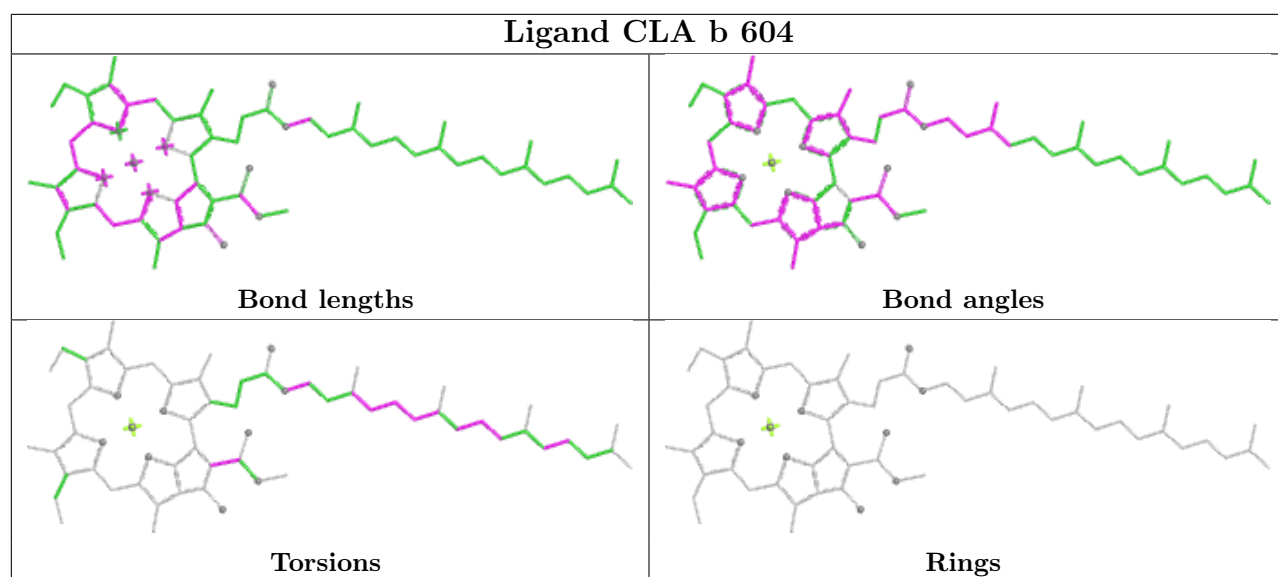


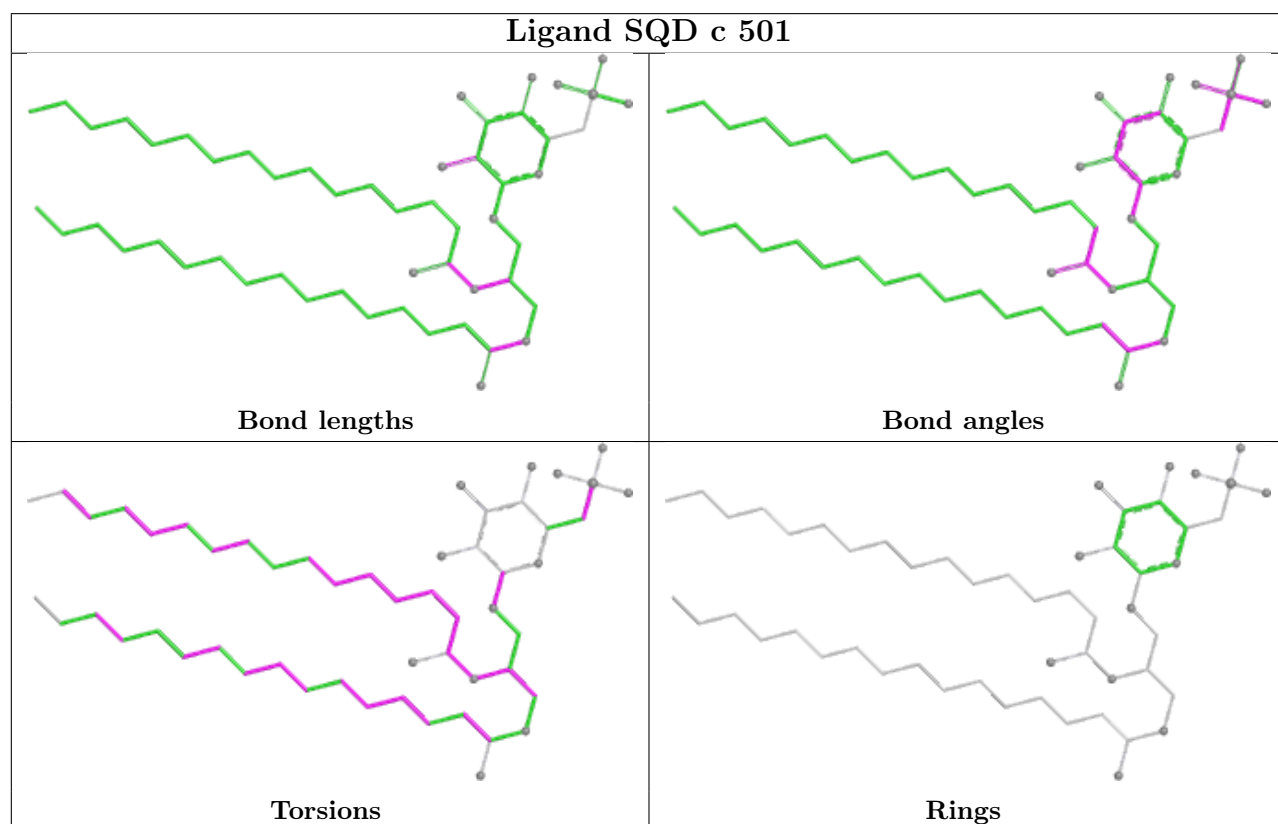
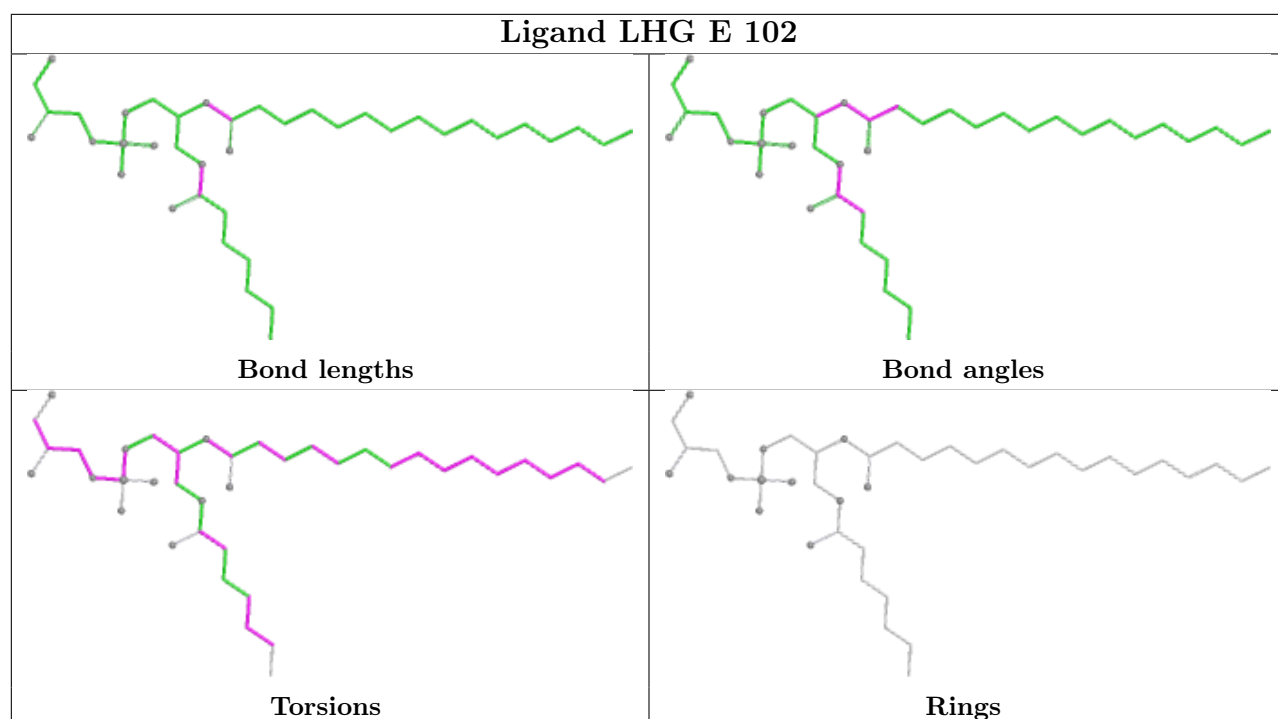
Ligand LMT C 525

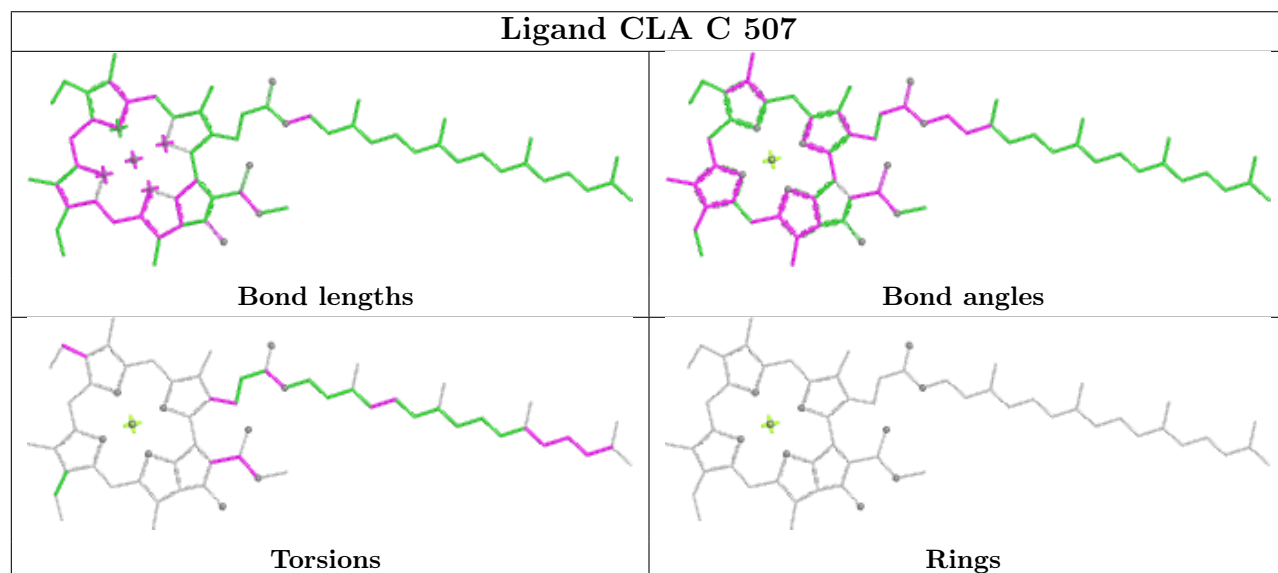
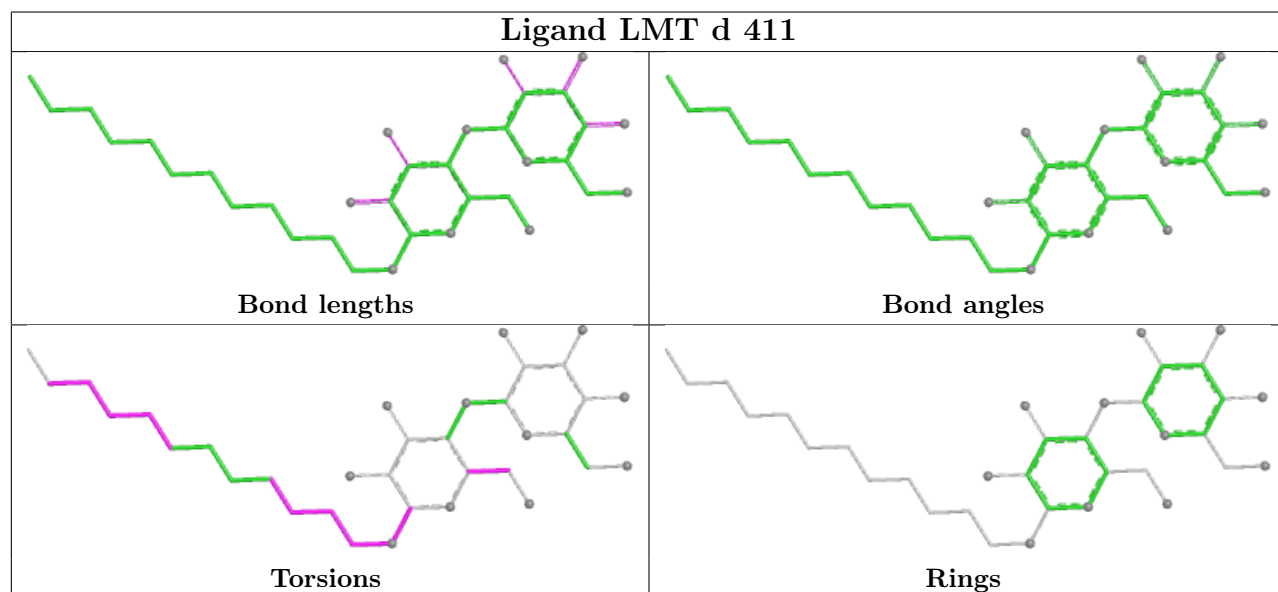
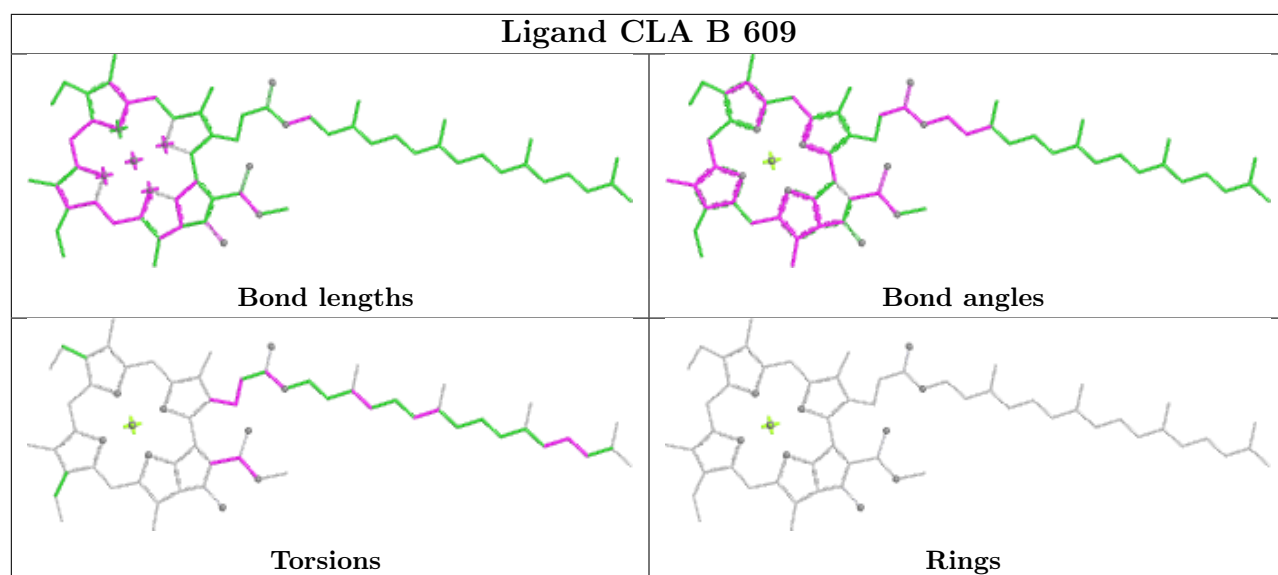


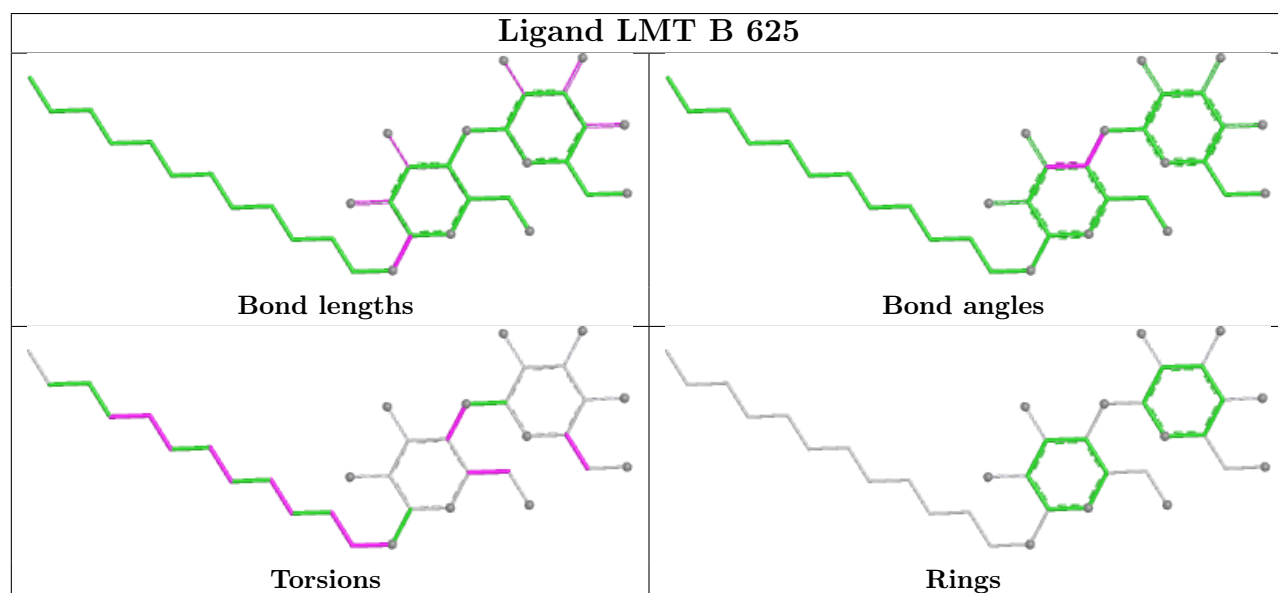
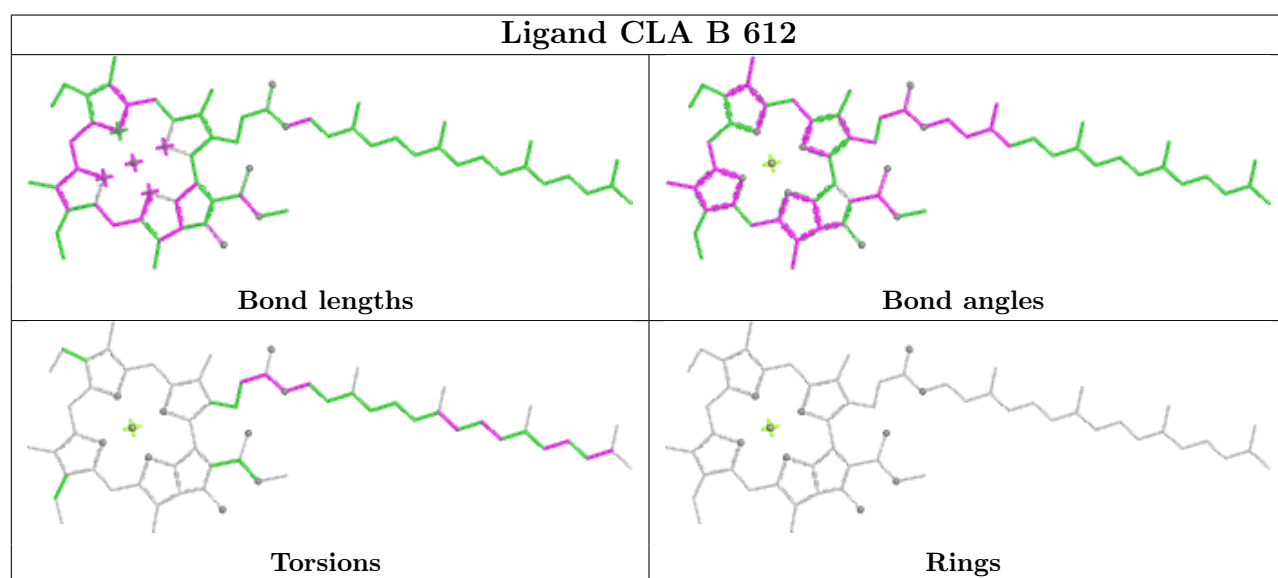
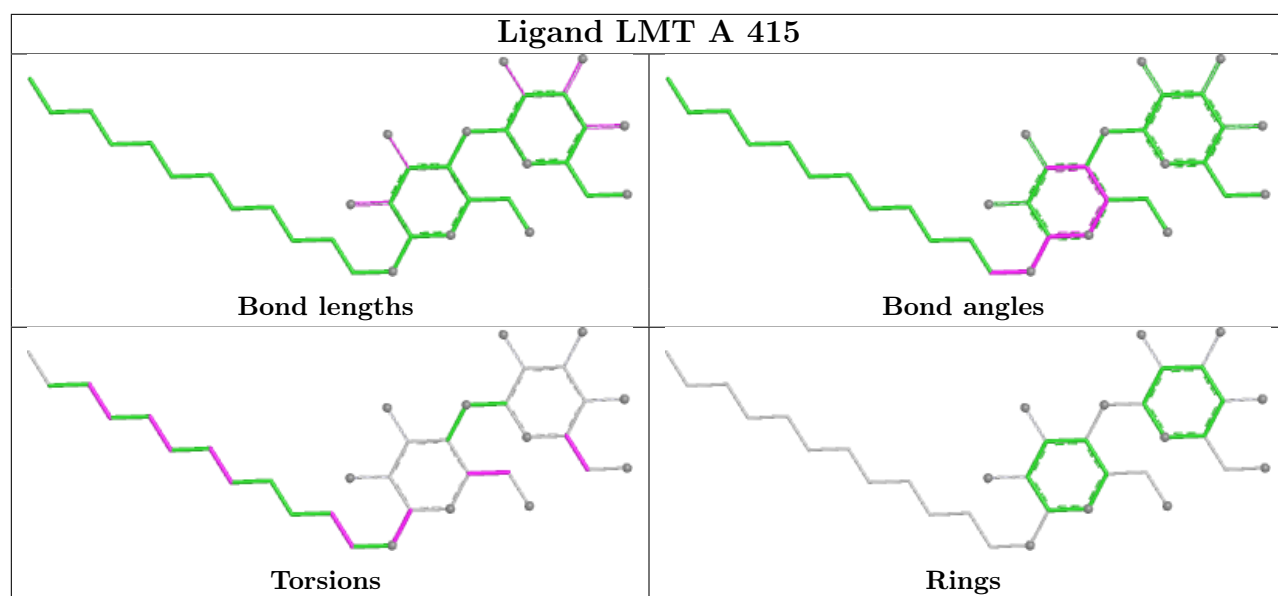


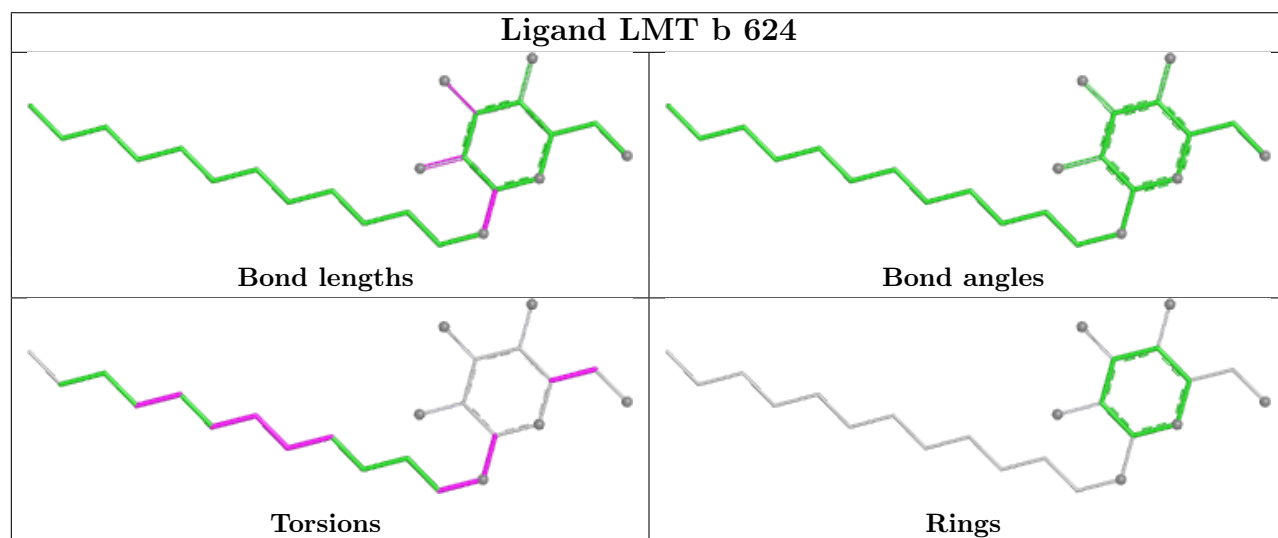
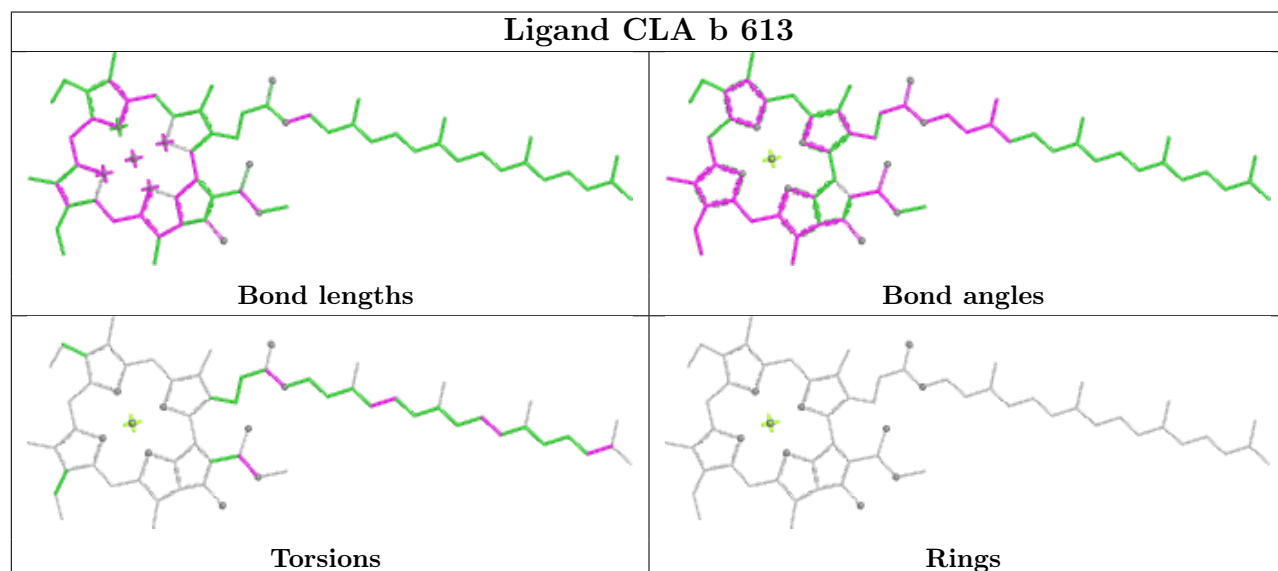
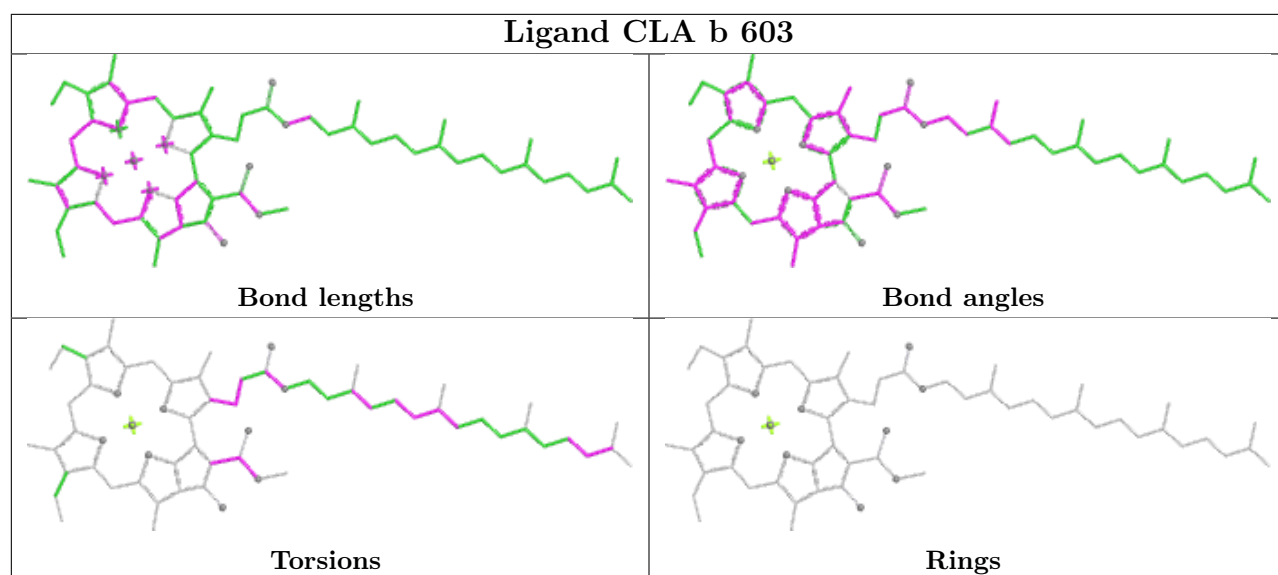


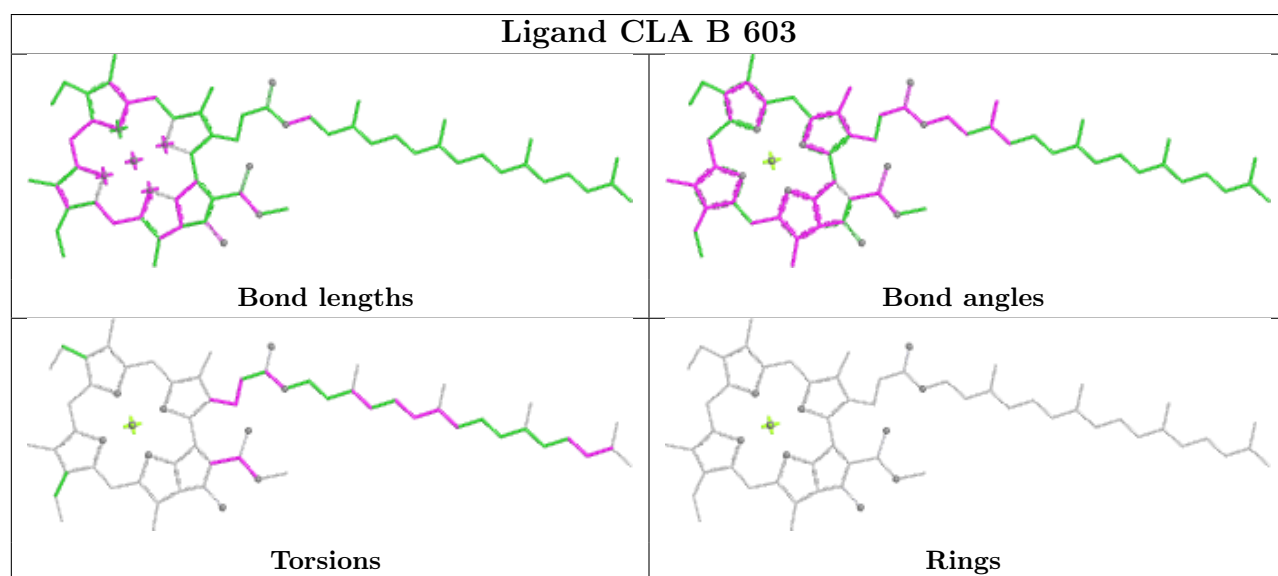
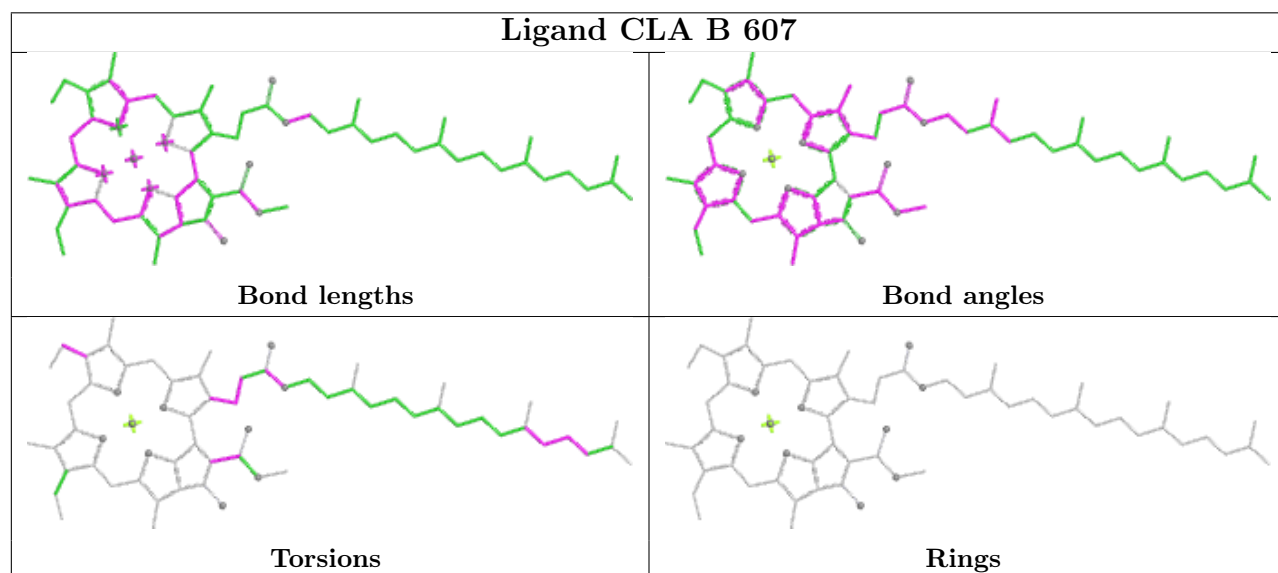
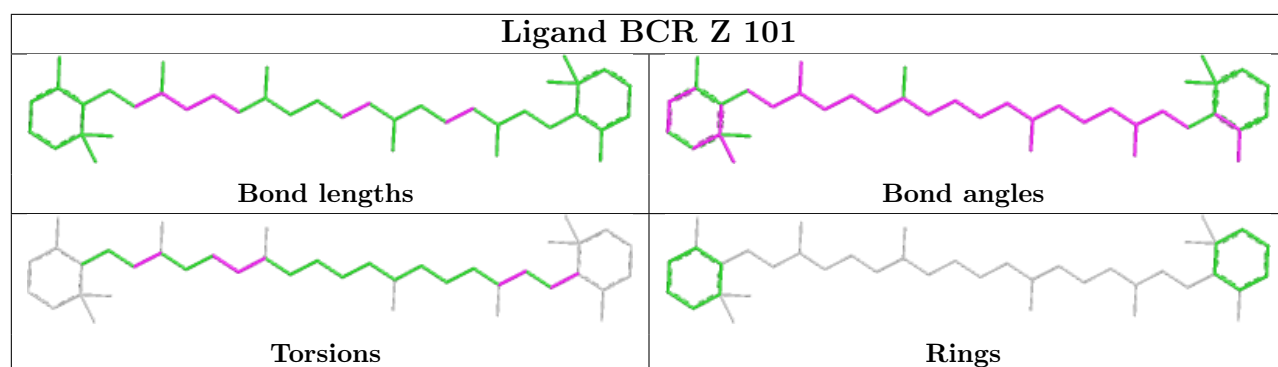


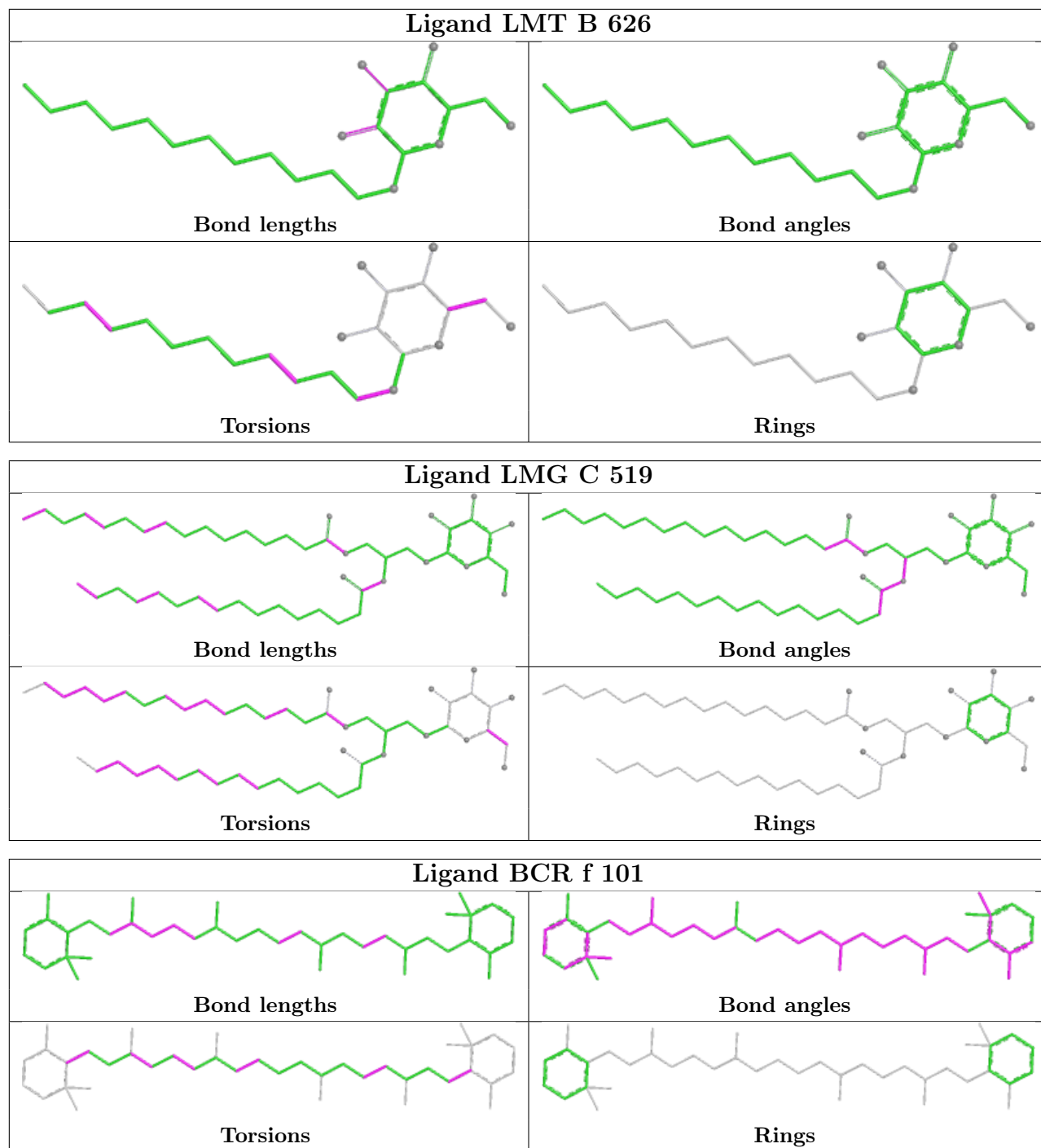


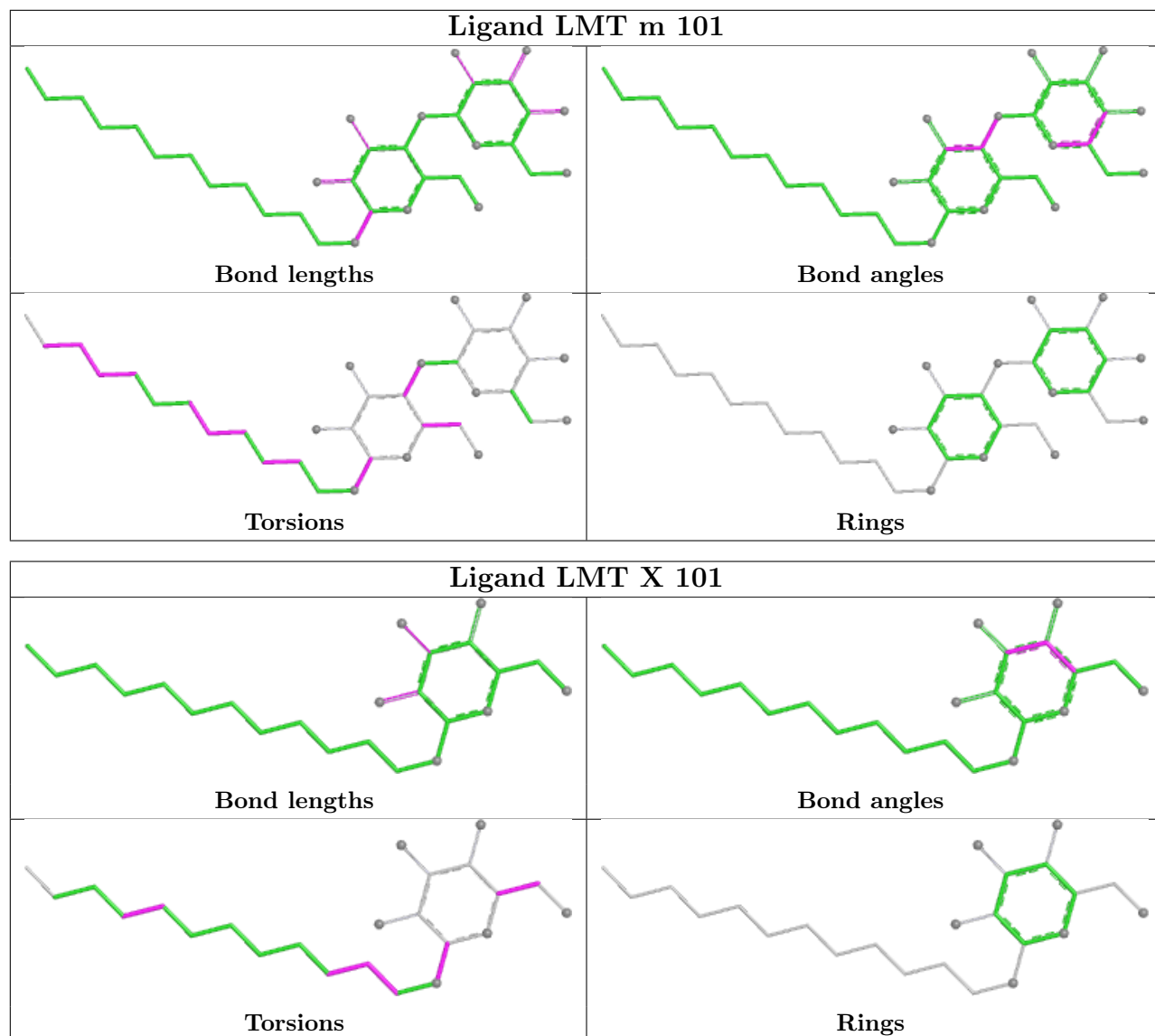


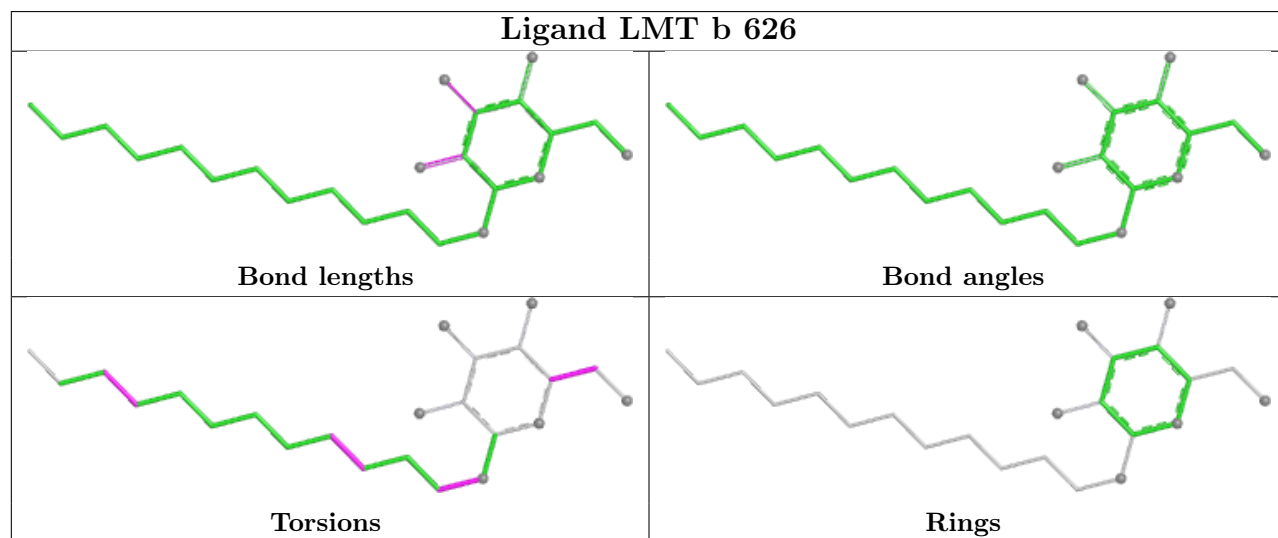
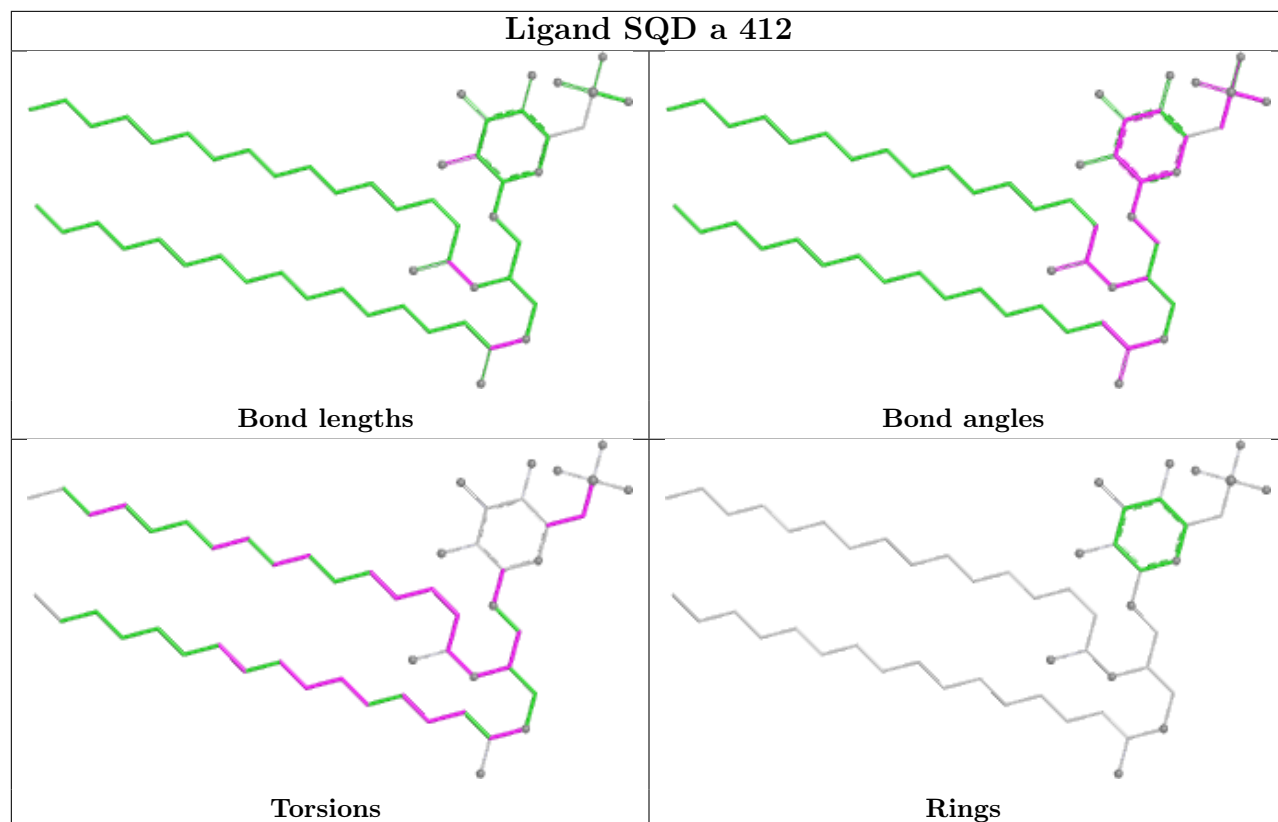


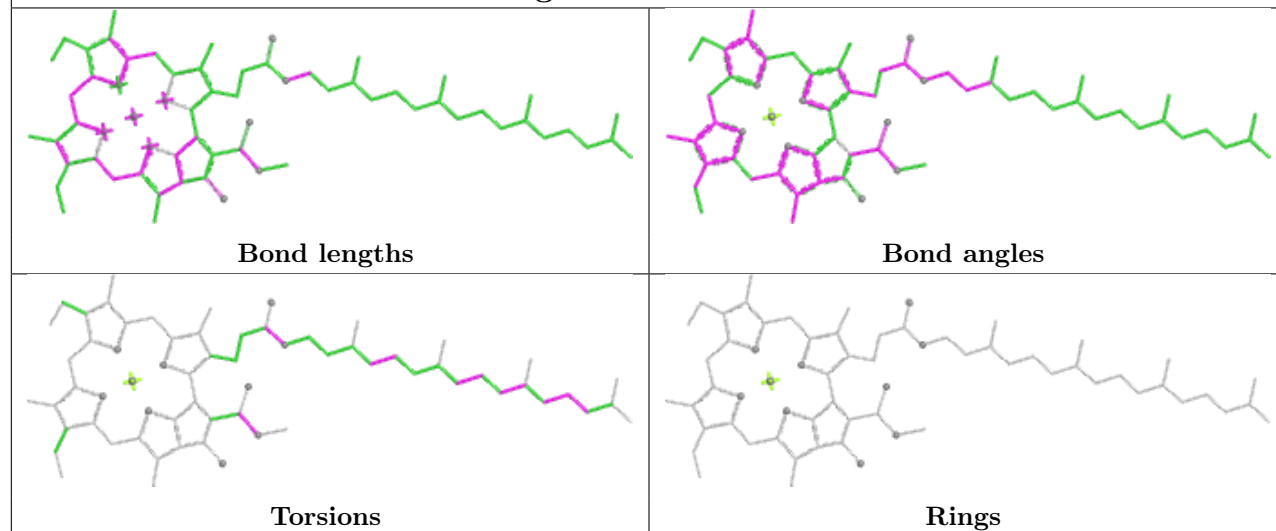
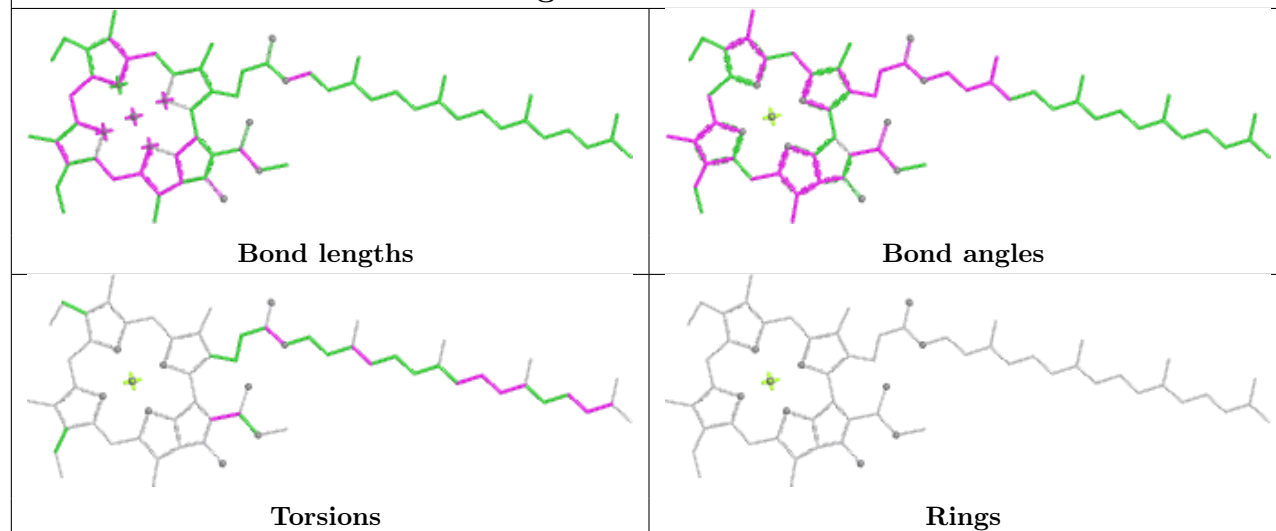




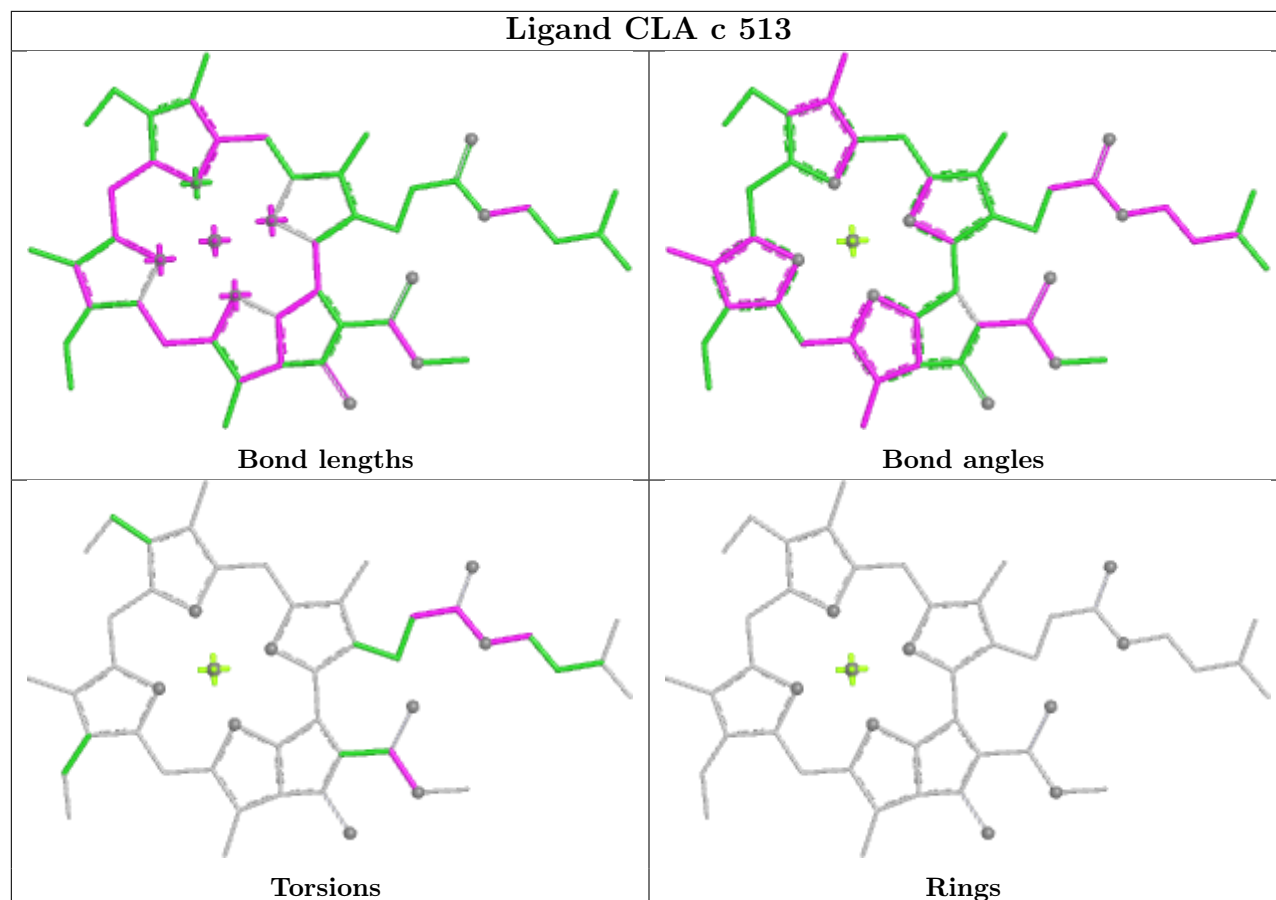




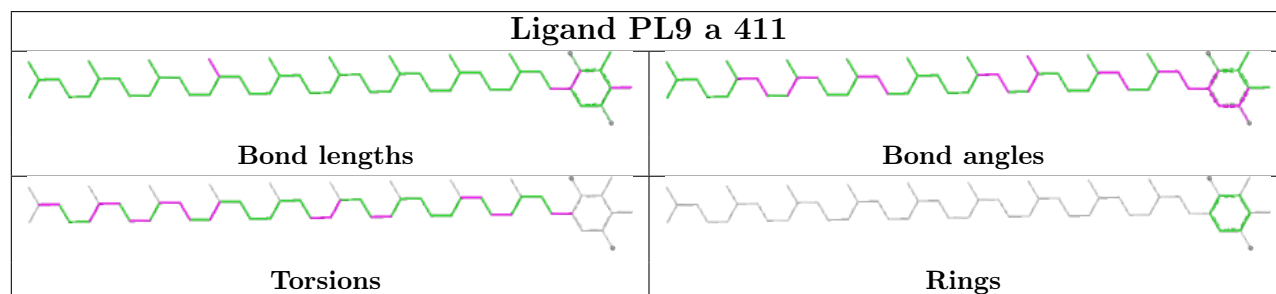


Ligand CLA b 611**Ligand CLA c 505**

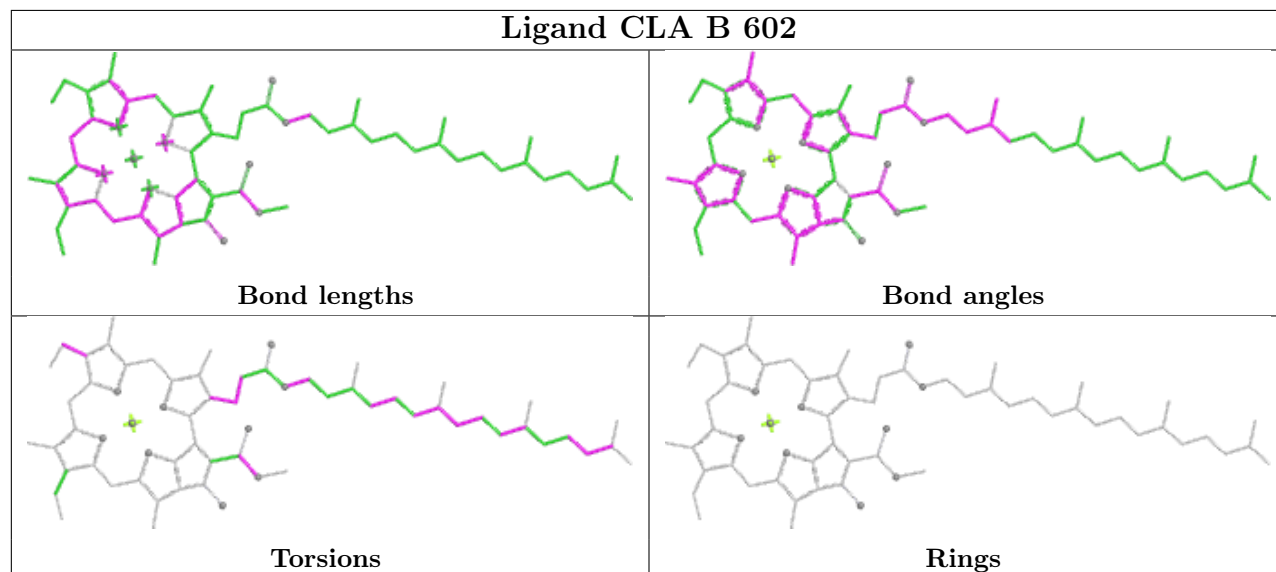
Ligand CLA c 513

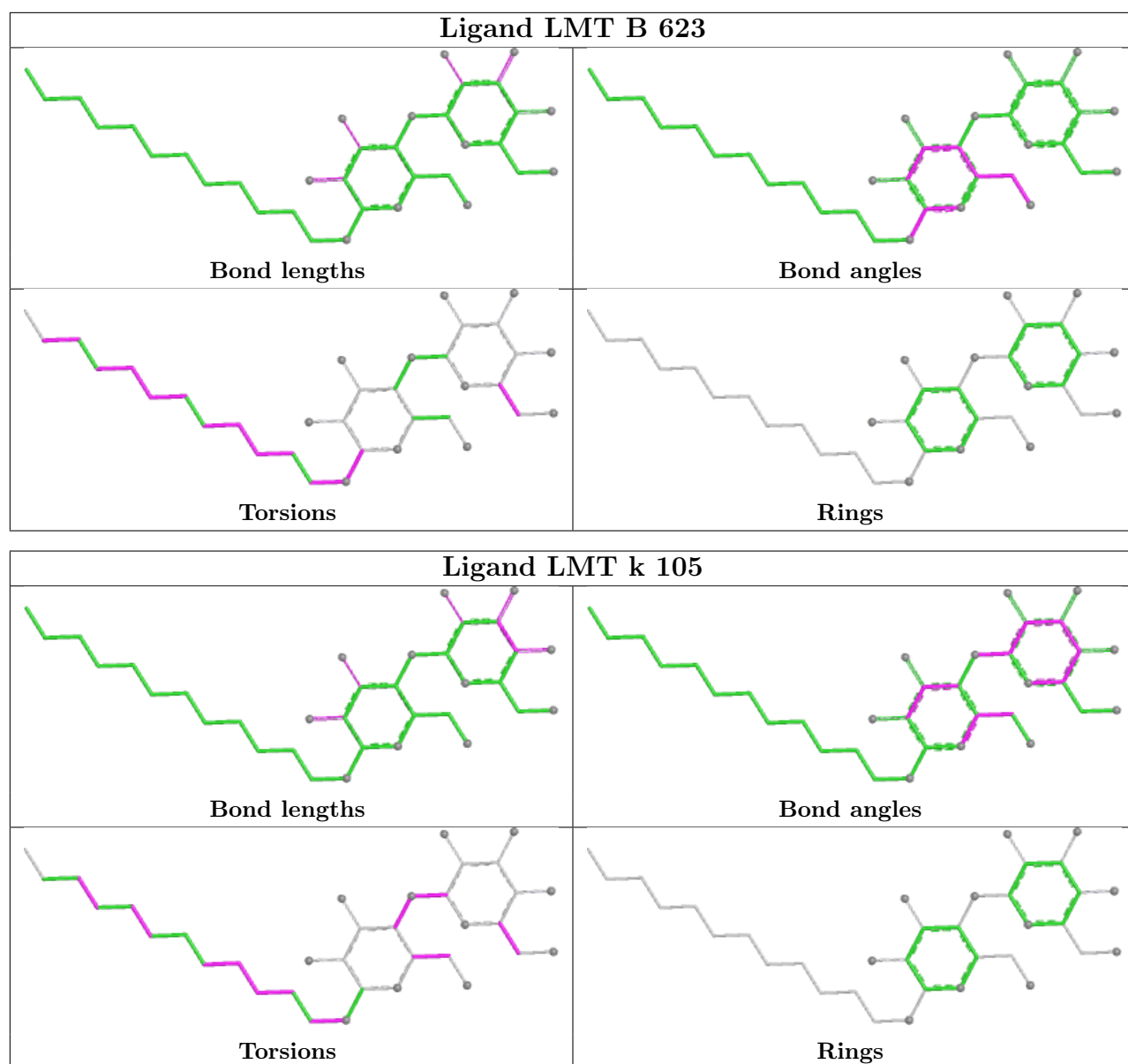


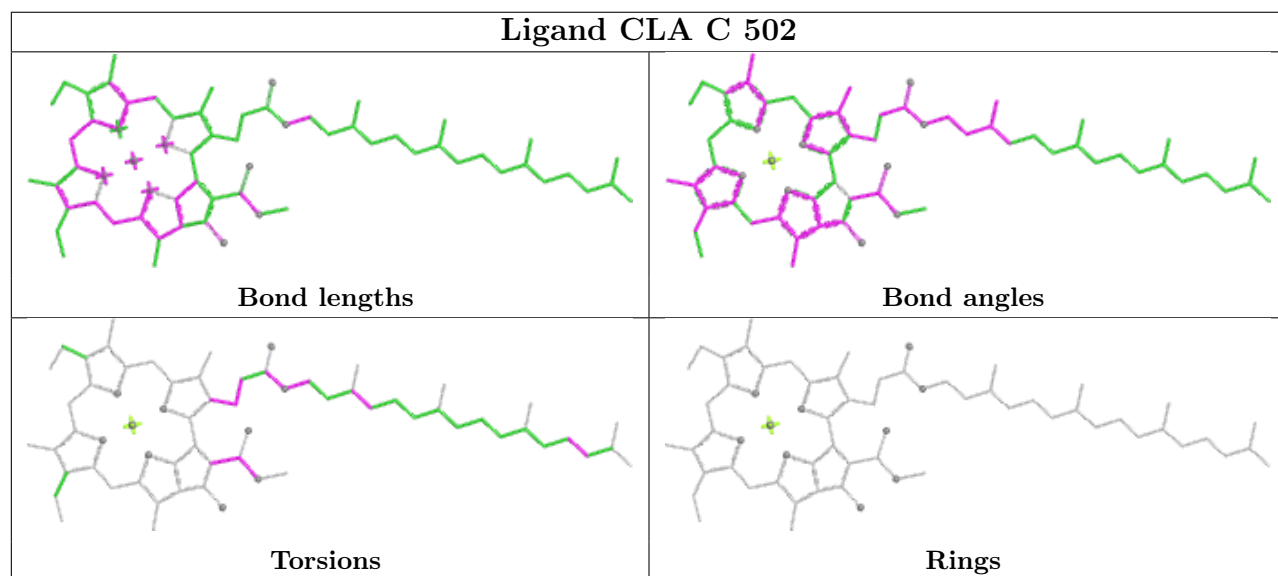
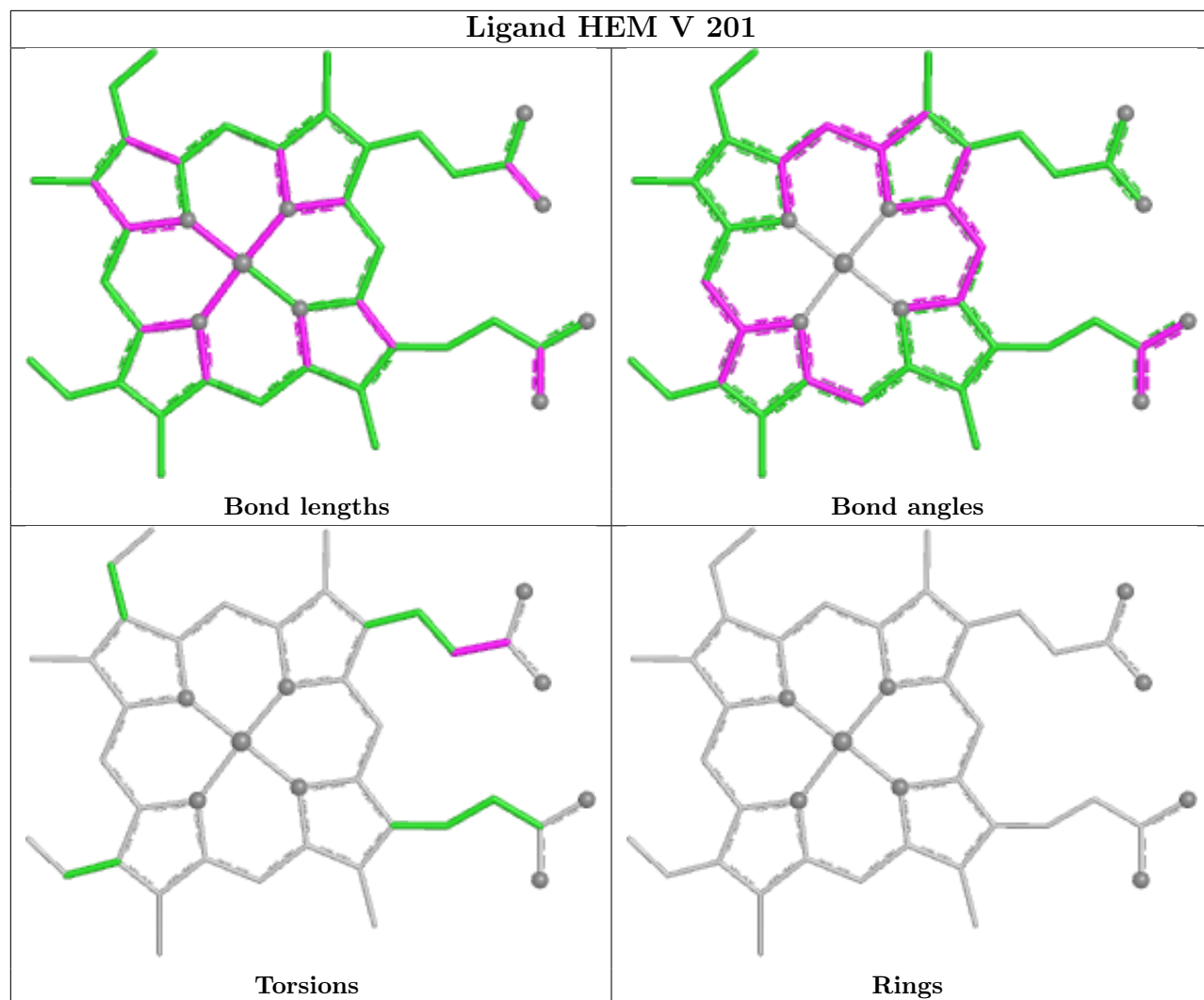
Ligand PL9 a 411

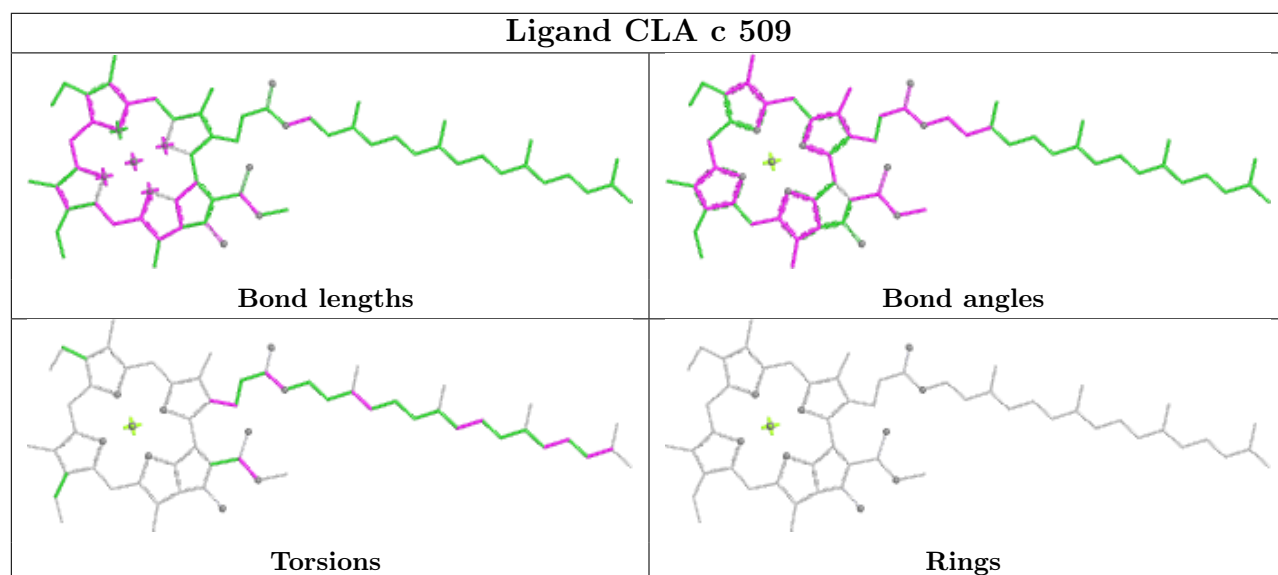
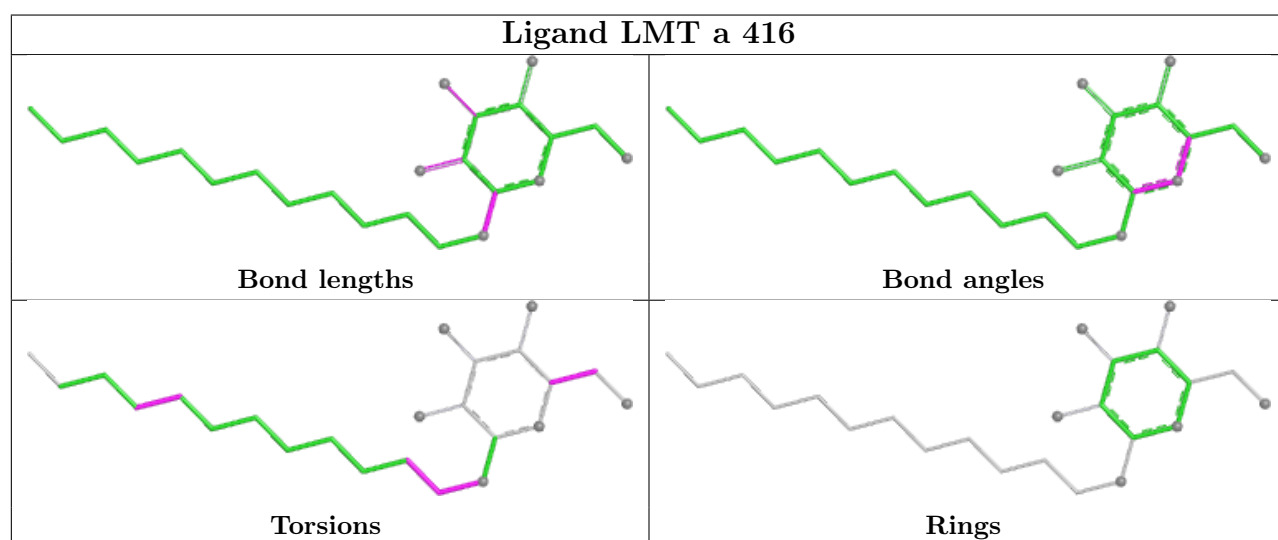
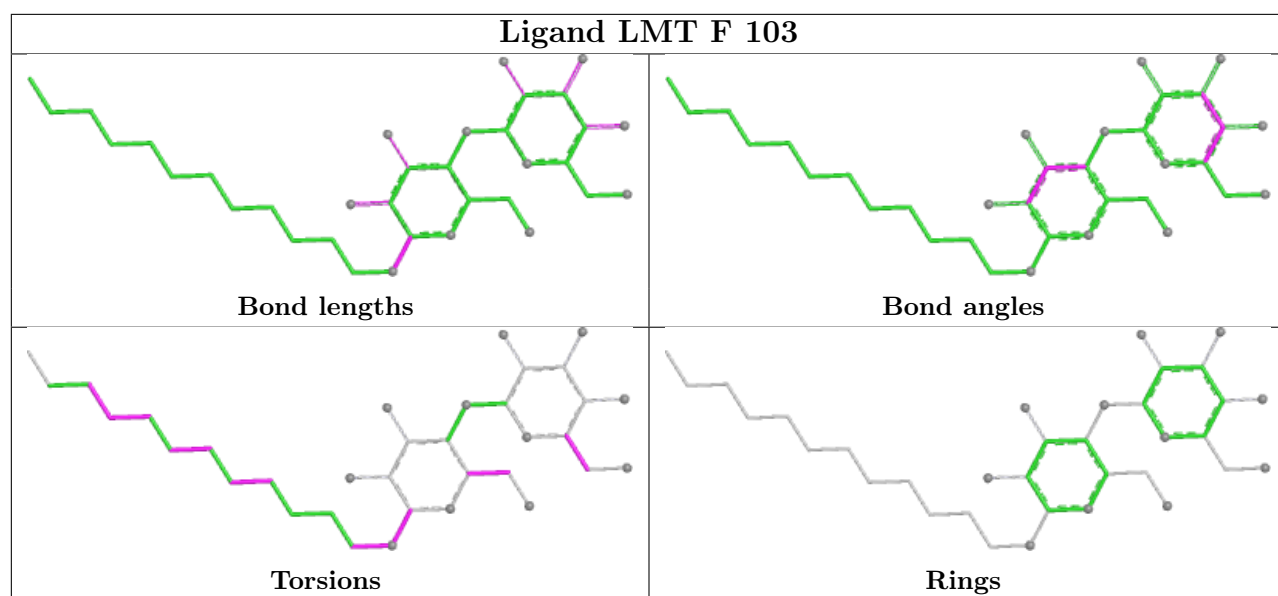


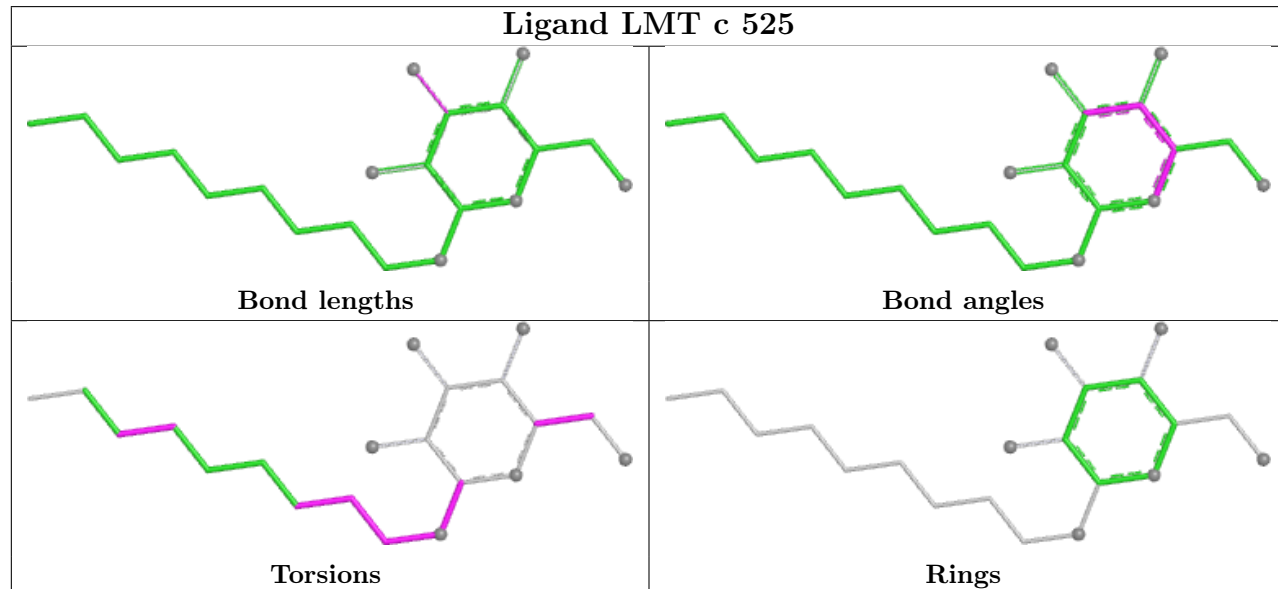
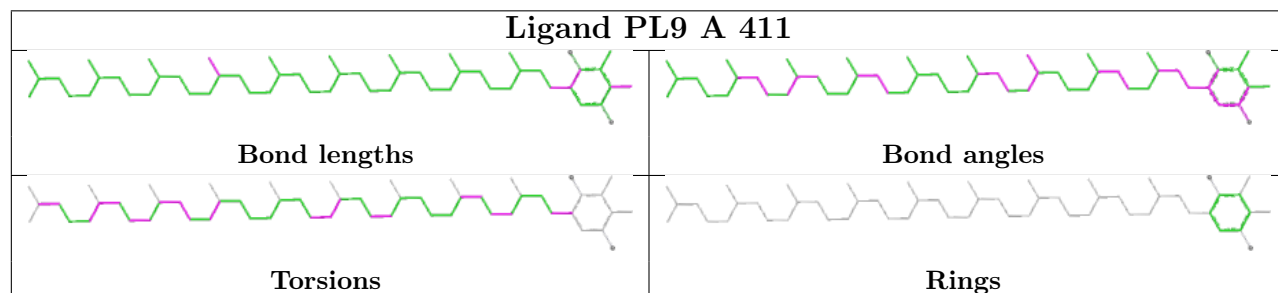
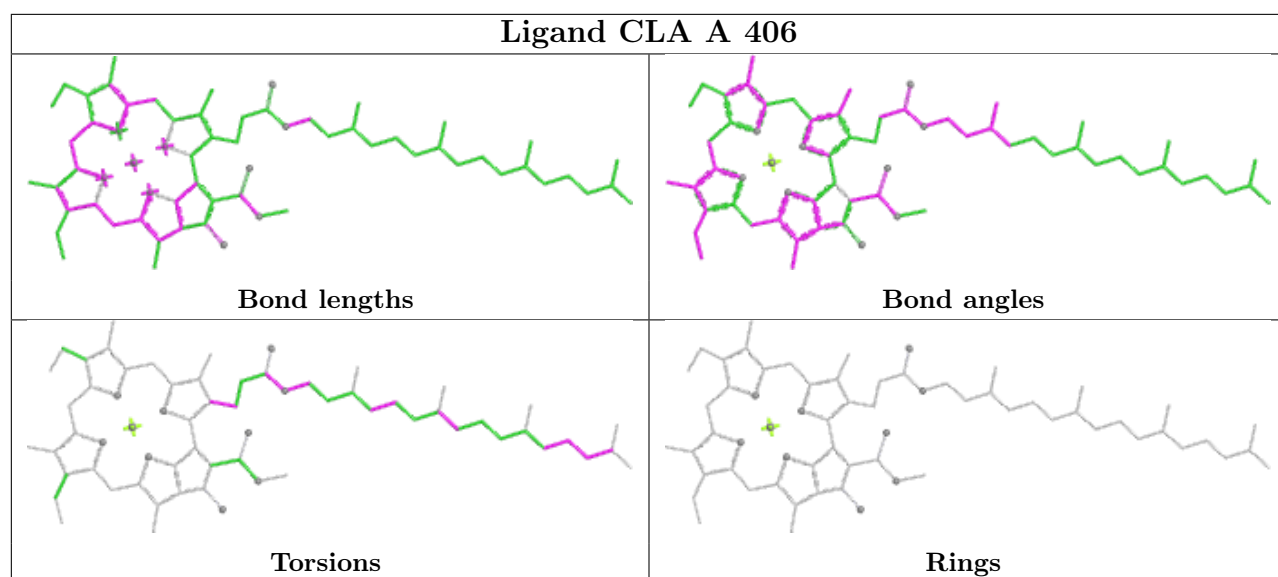
Ligand CLA B 602

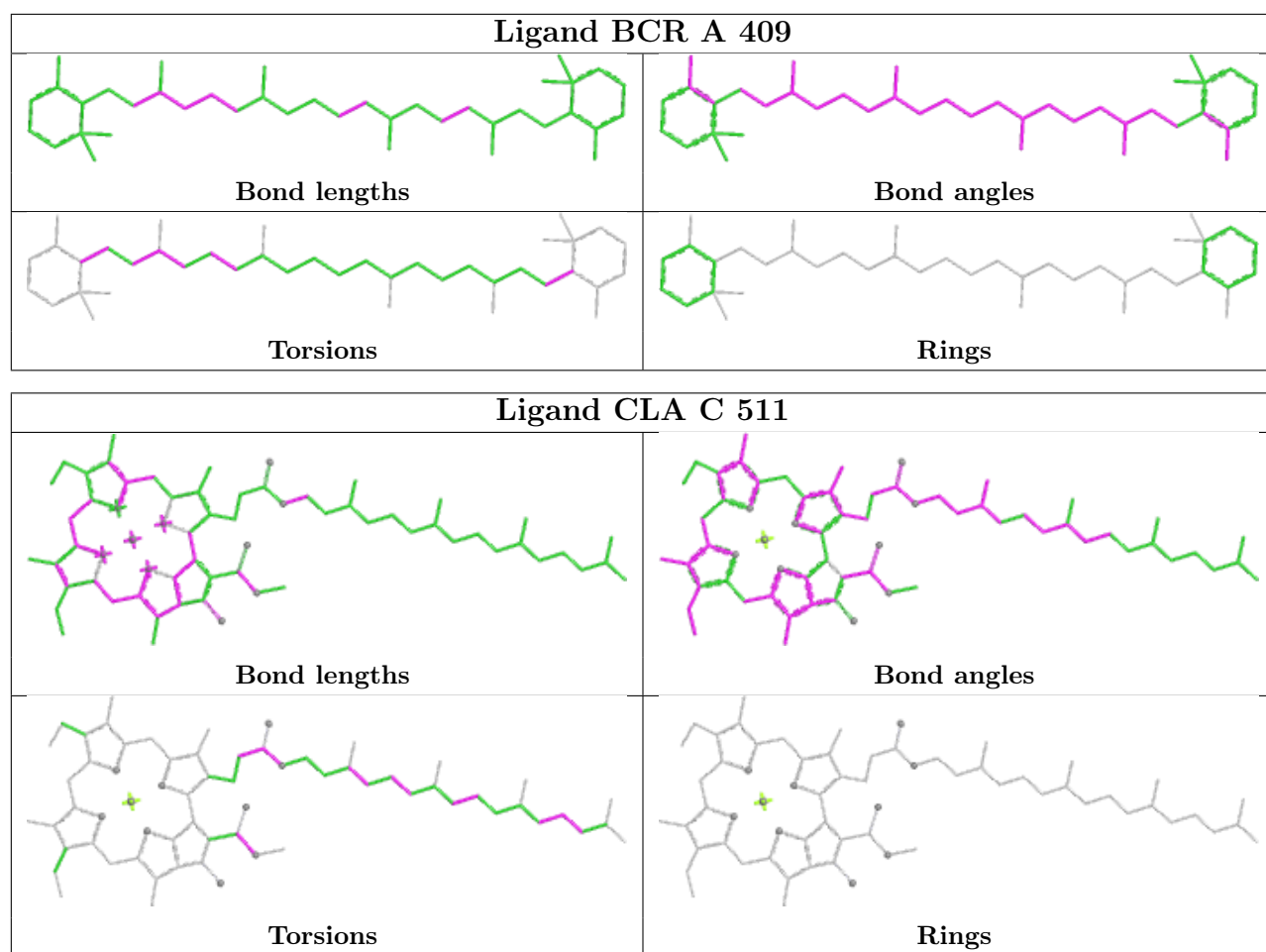


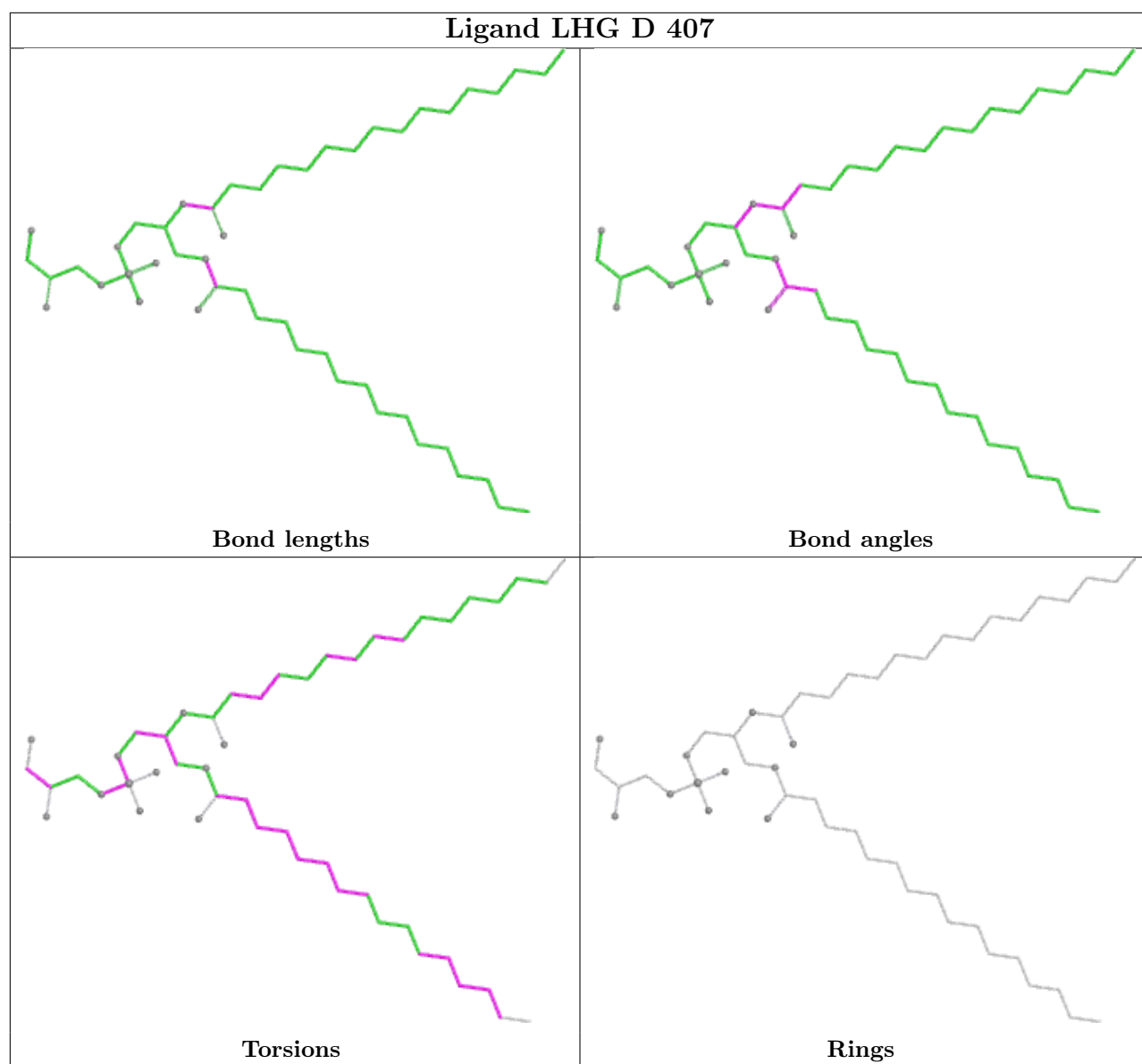


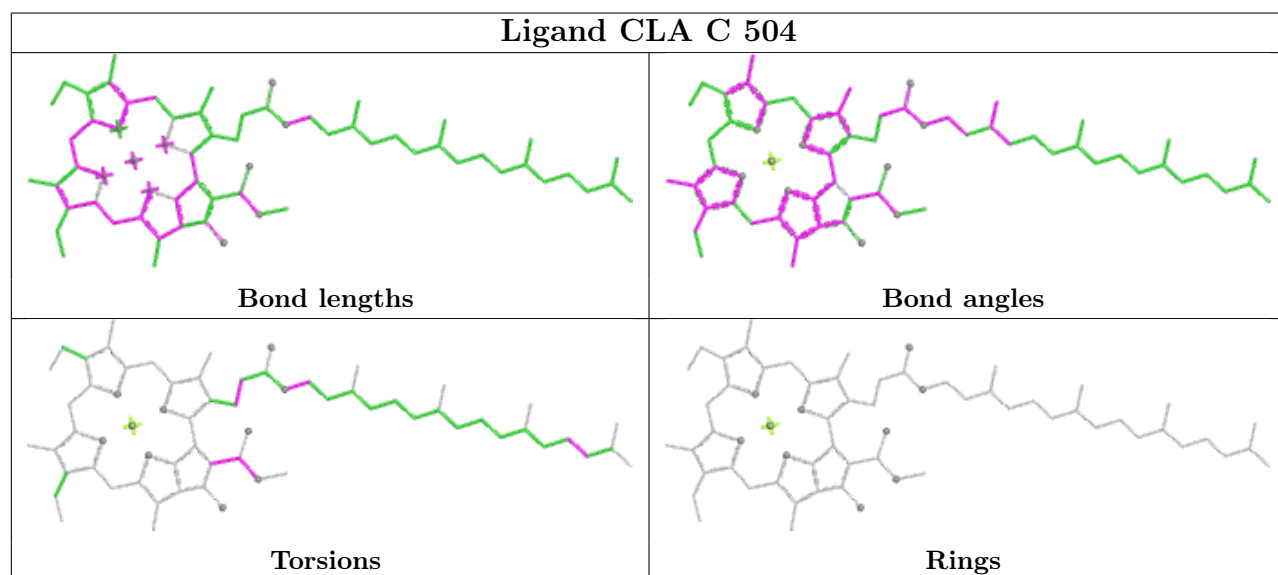
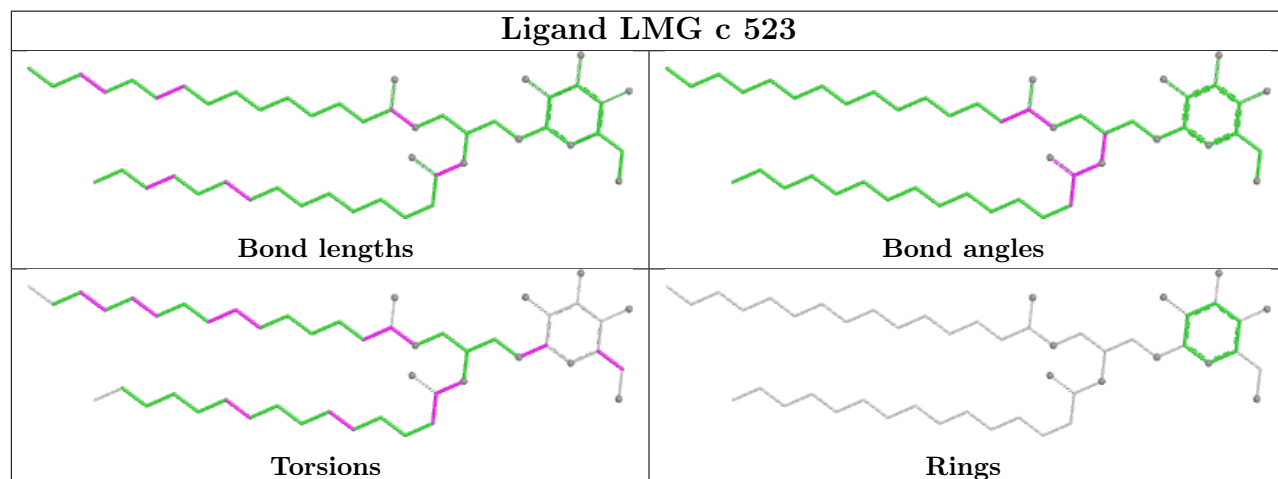
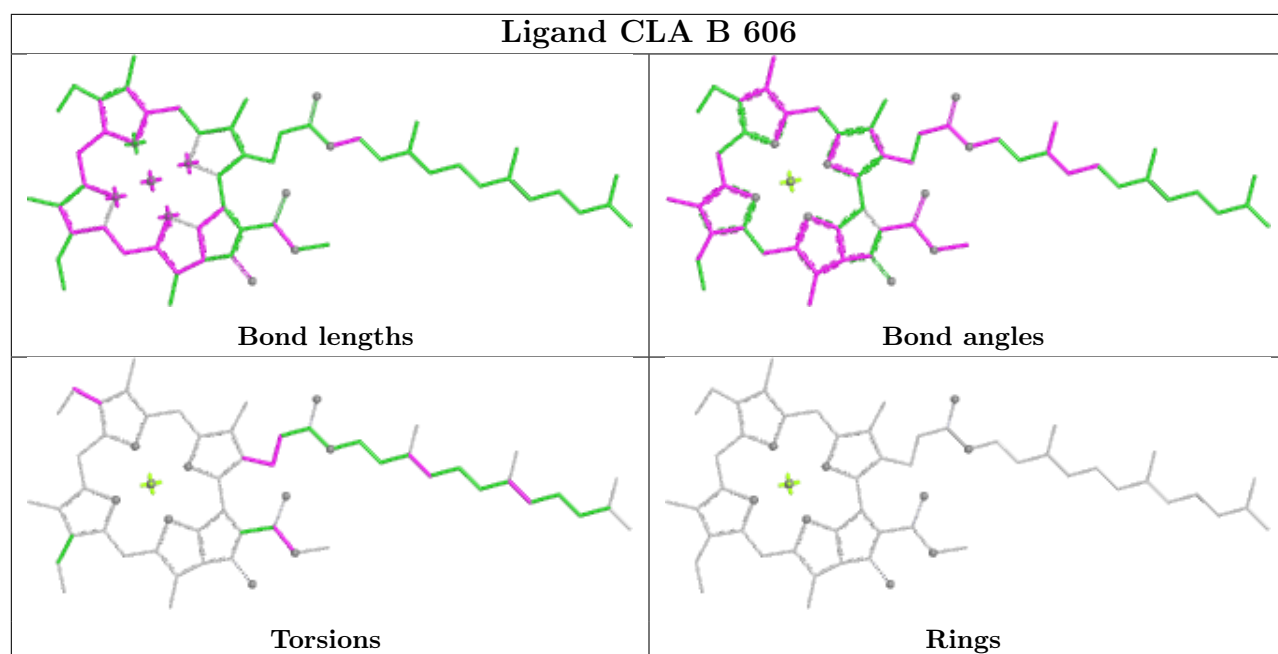


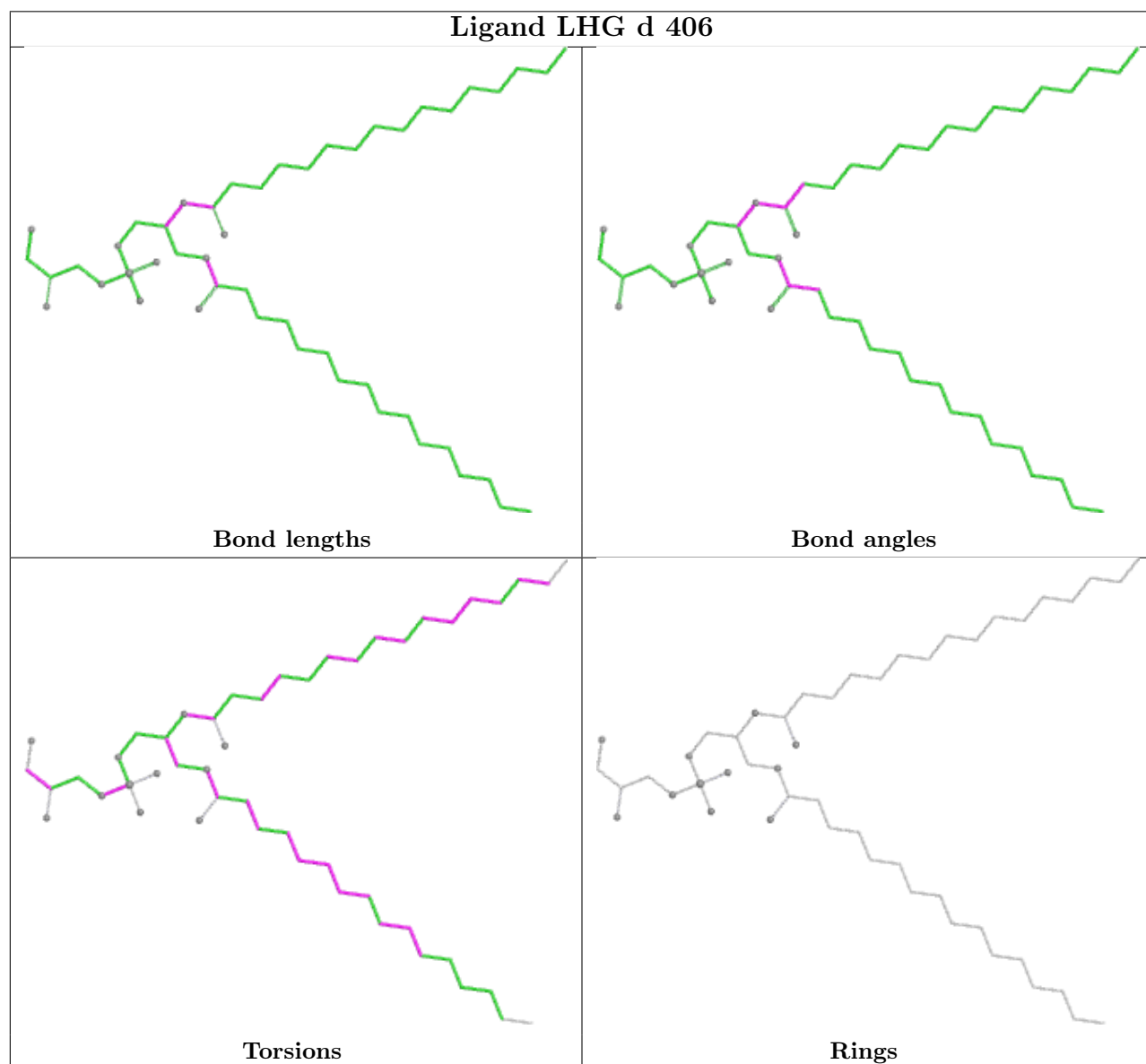
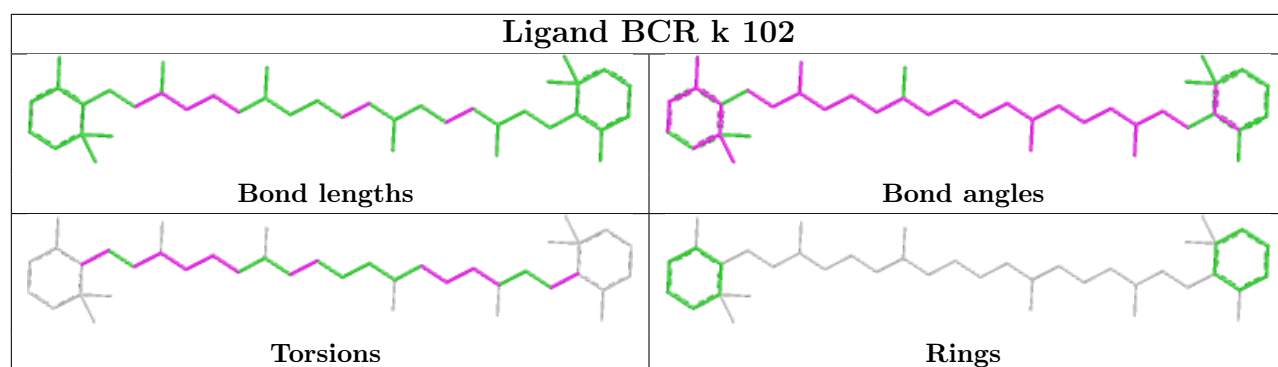


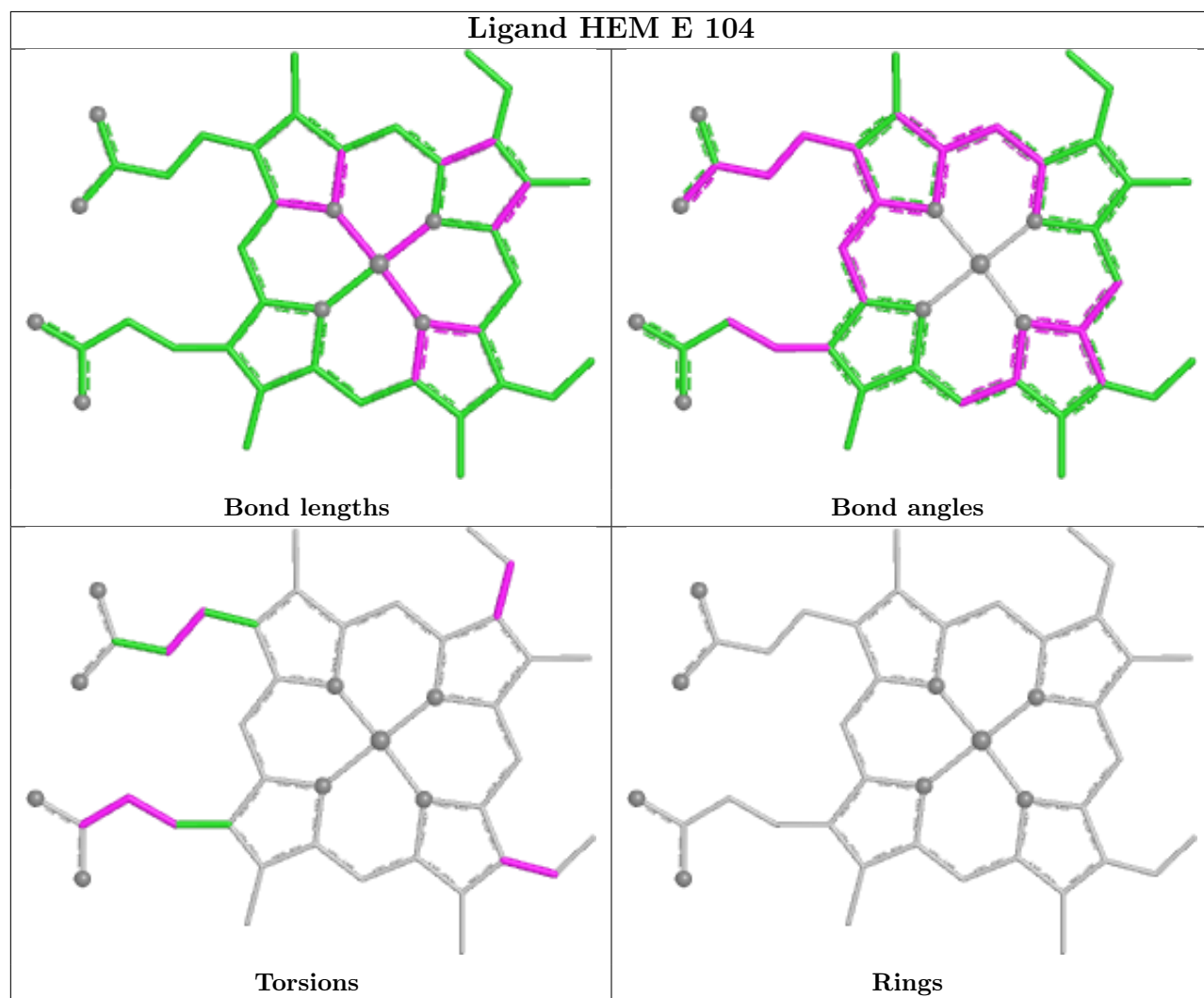
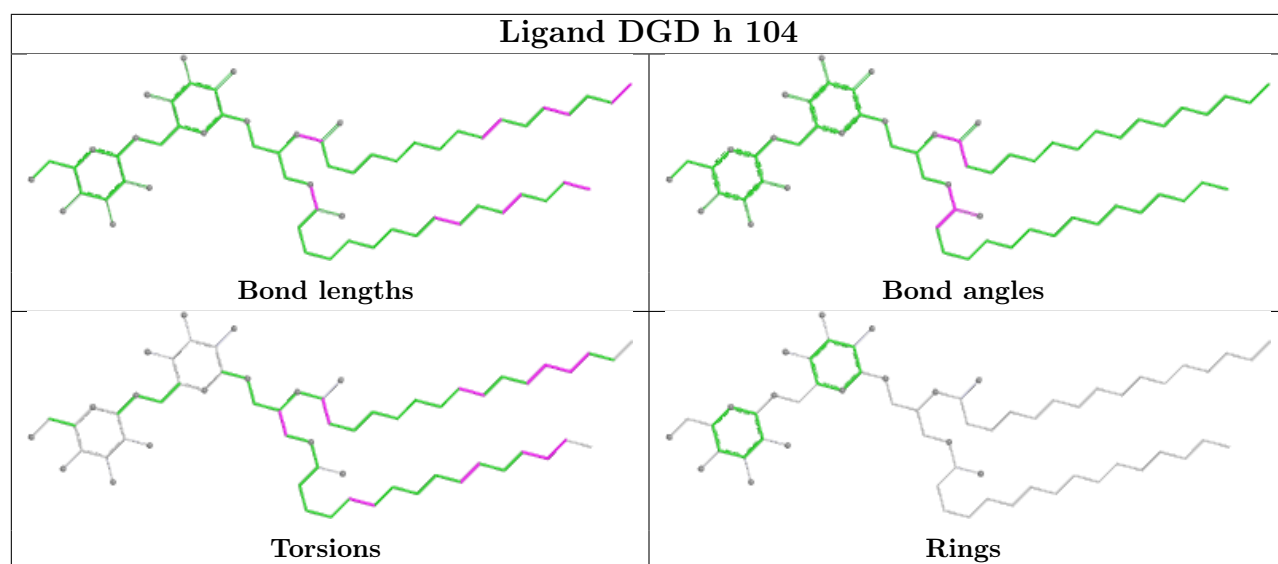


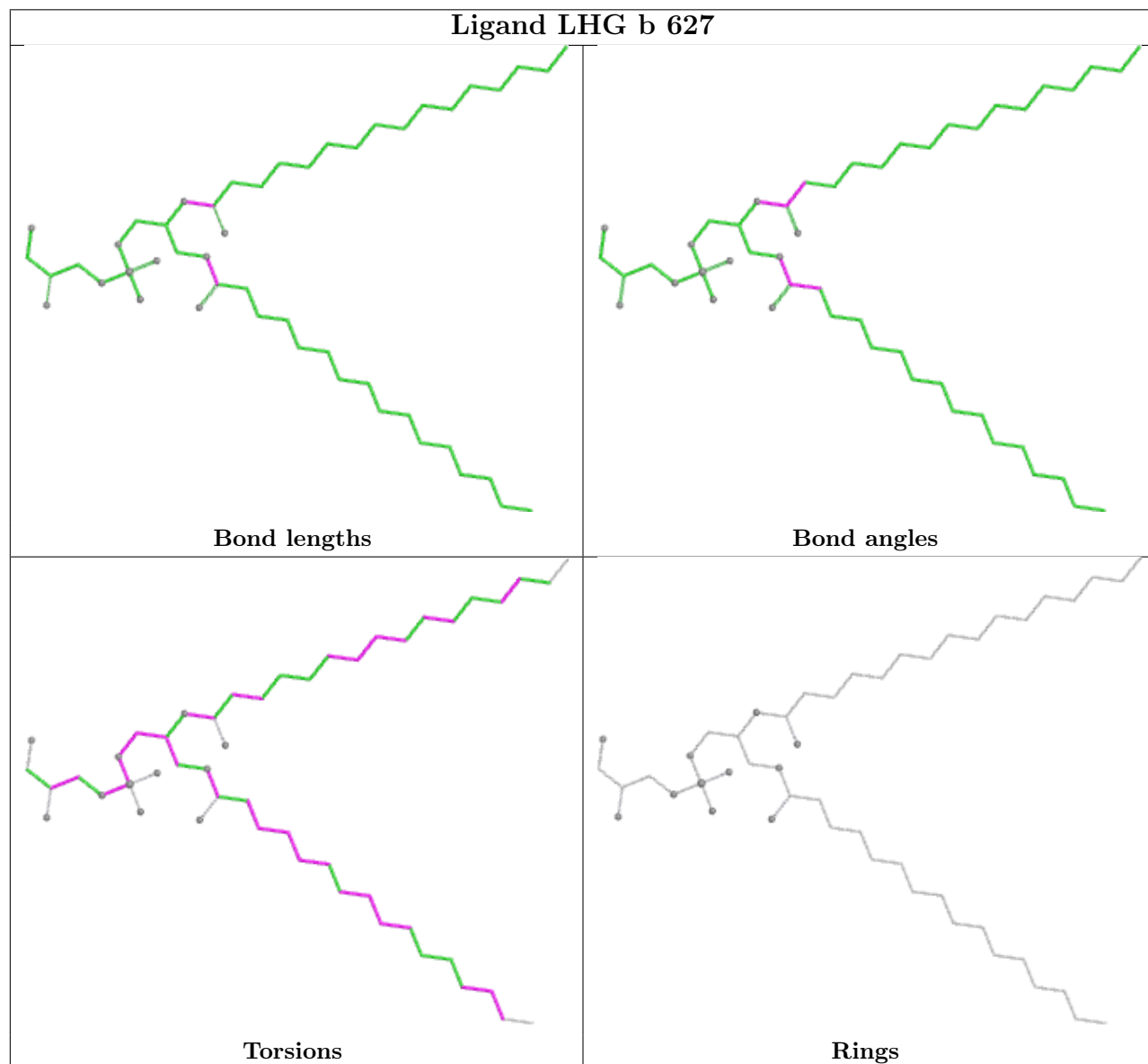
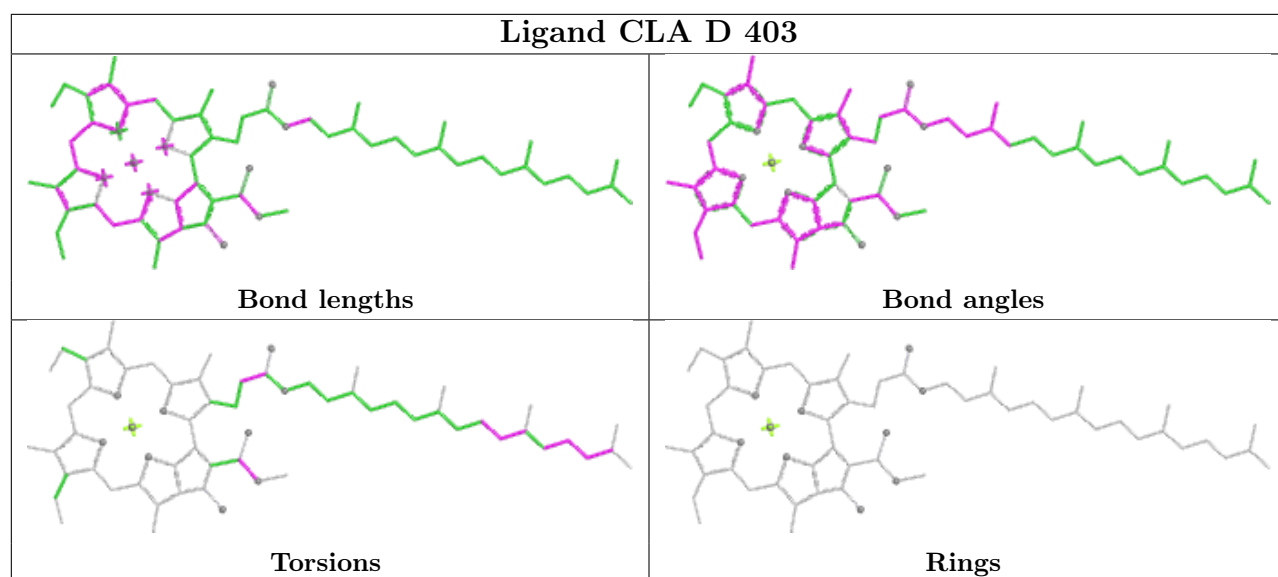


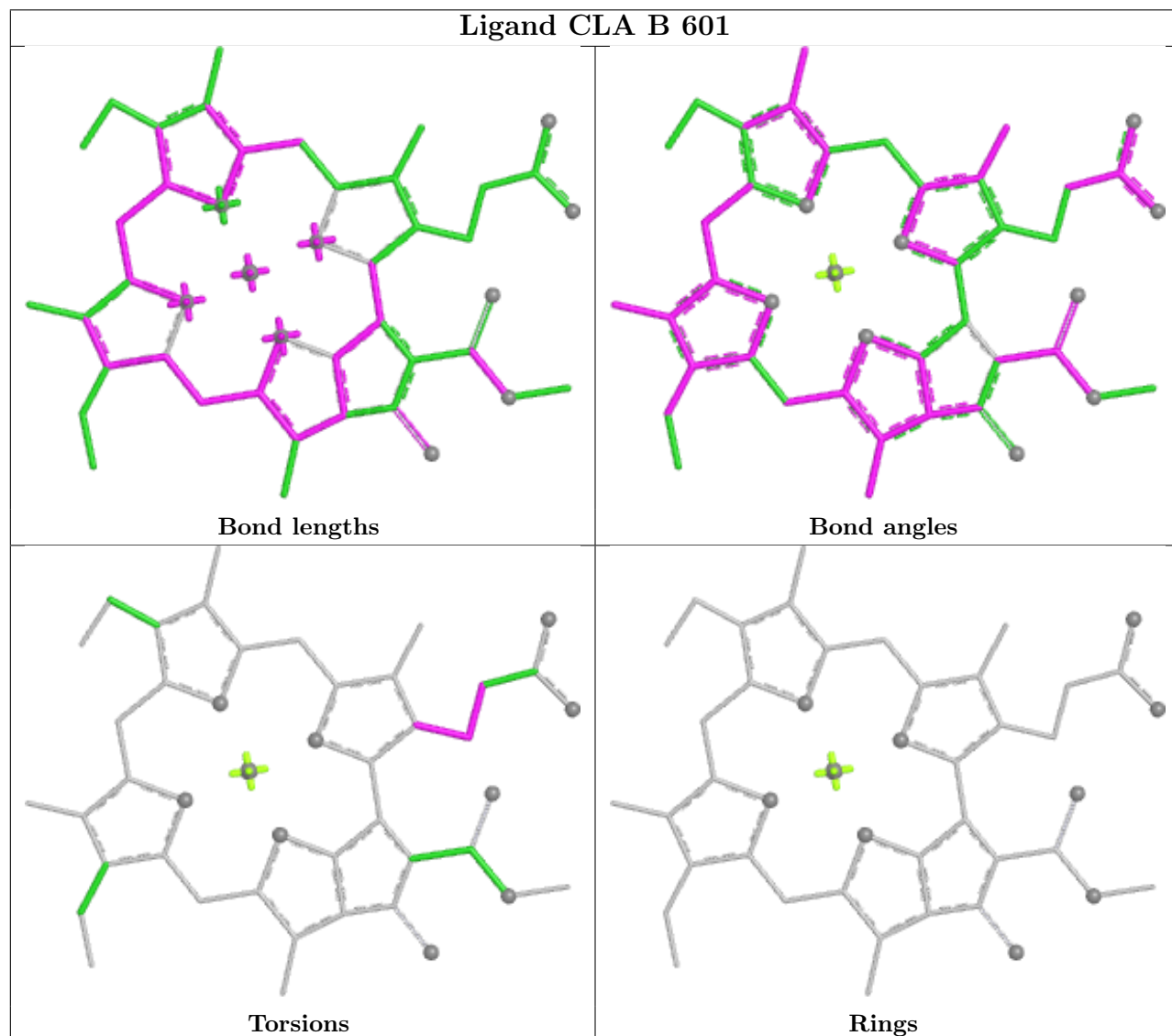
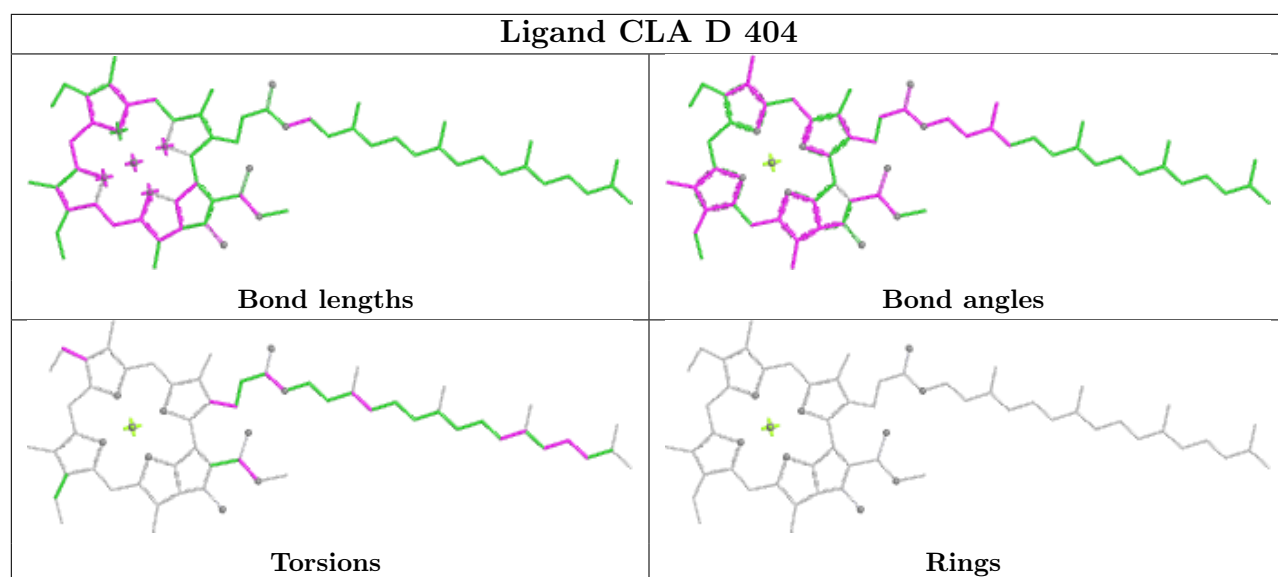


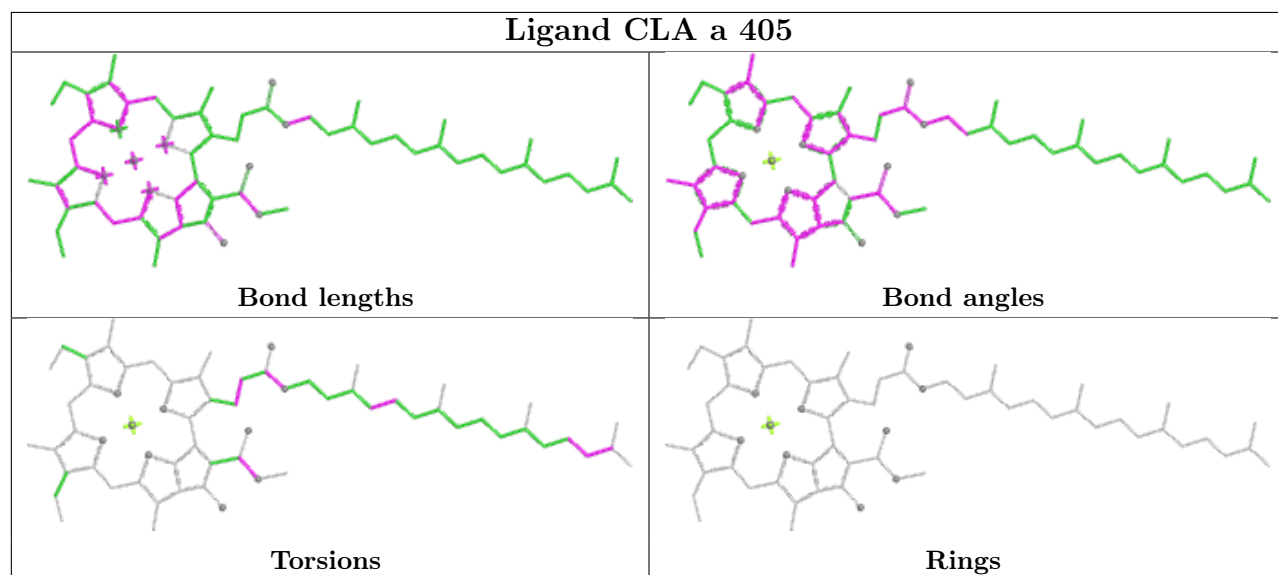
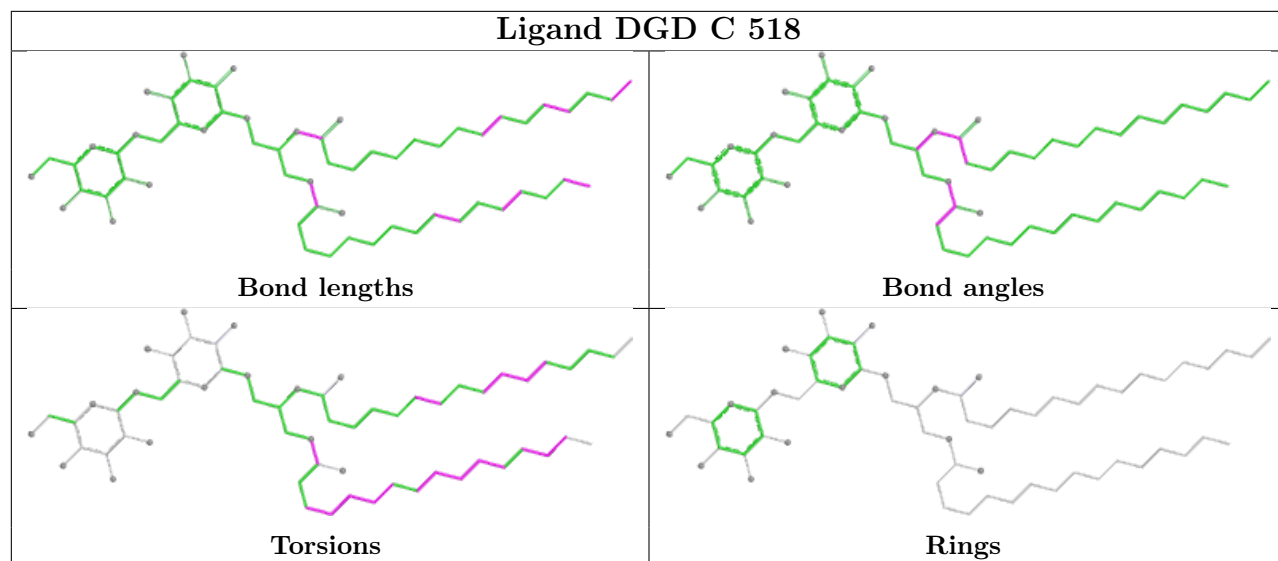


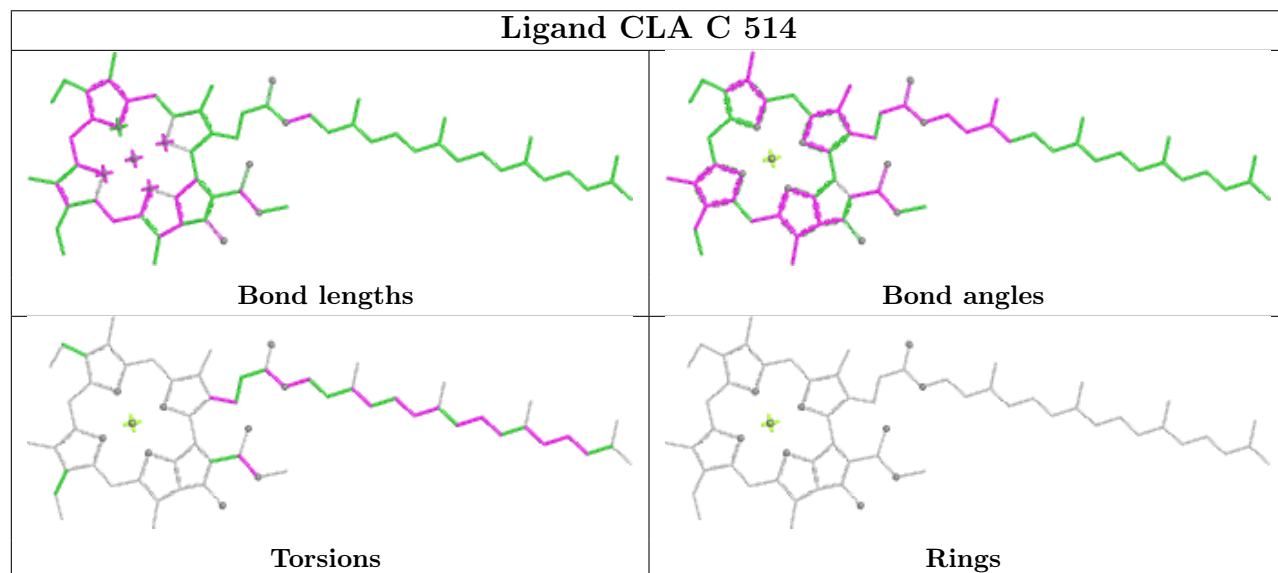
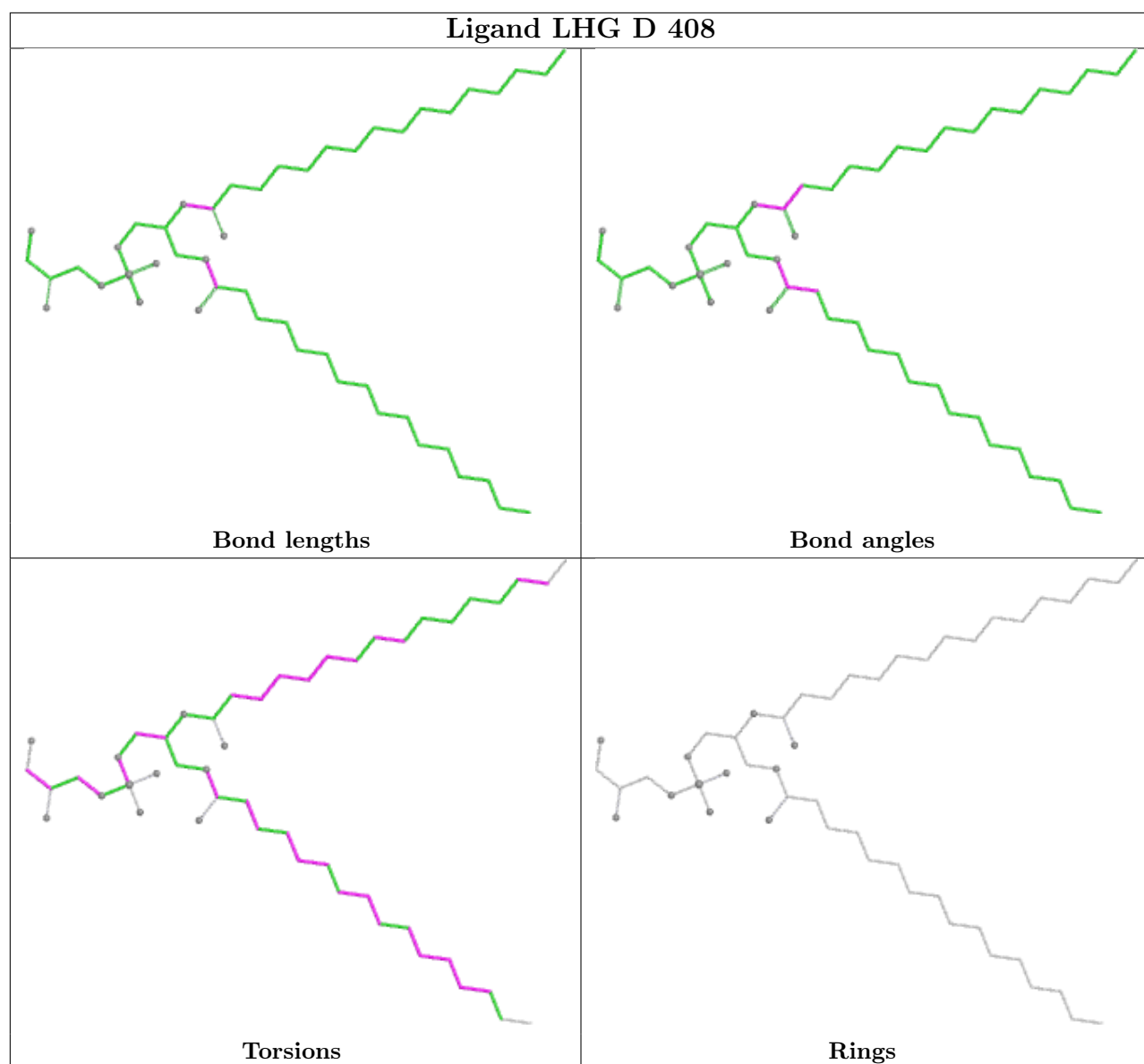


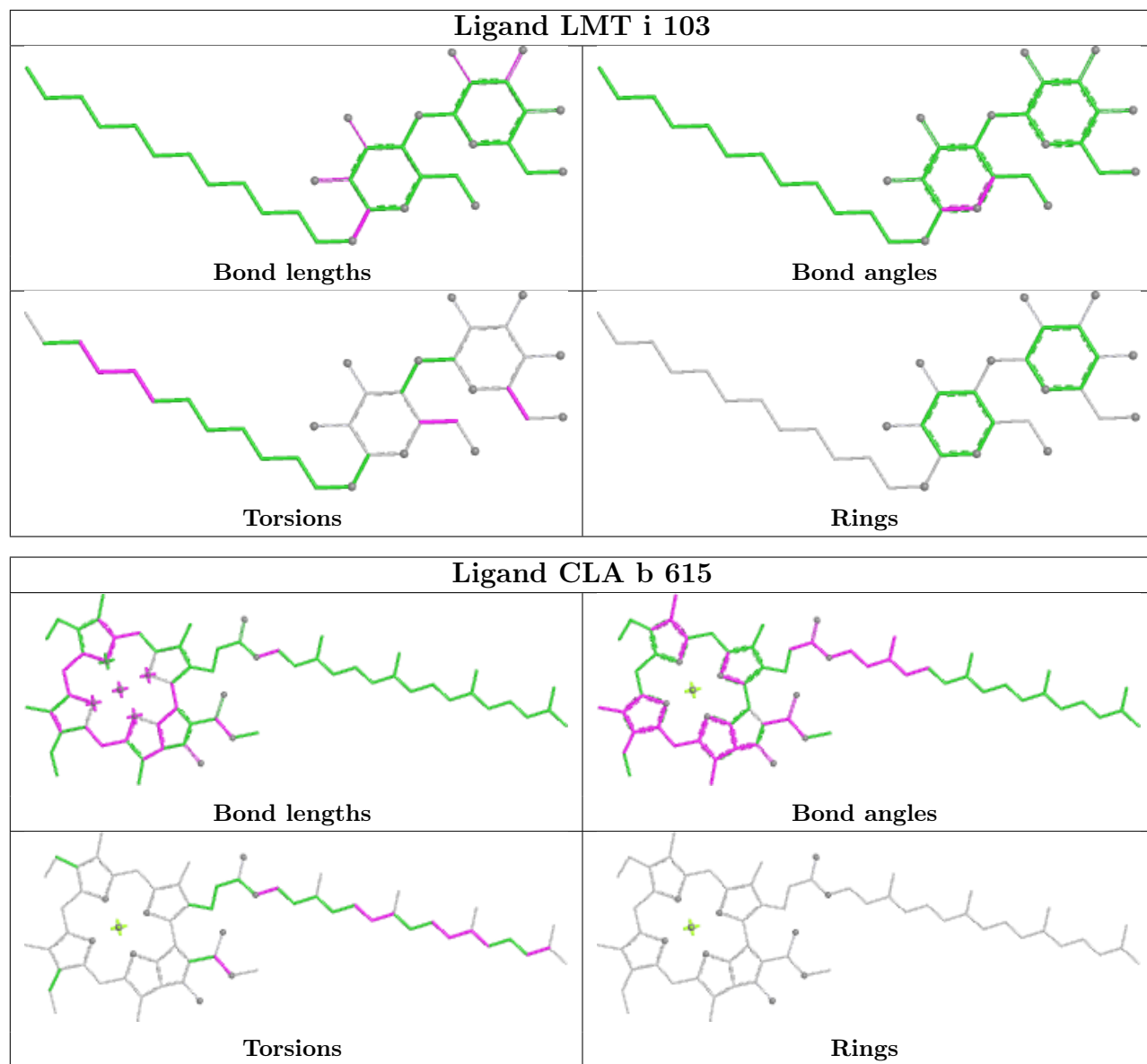




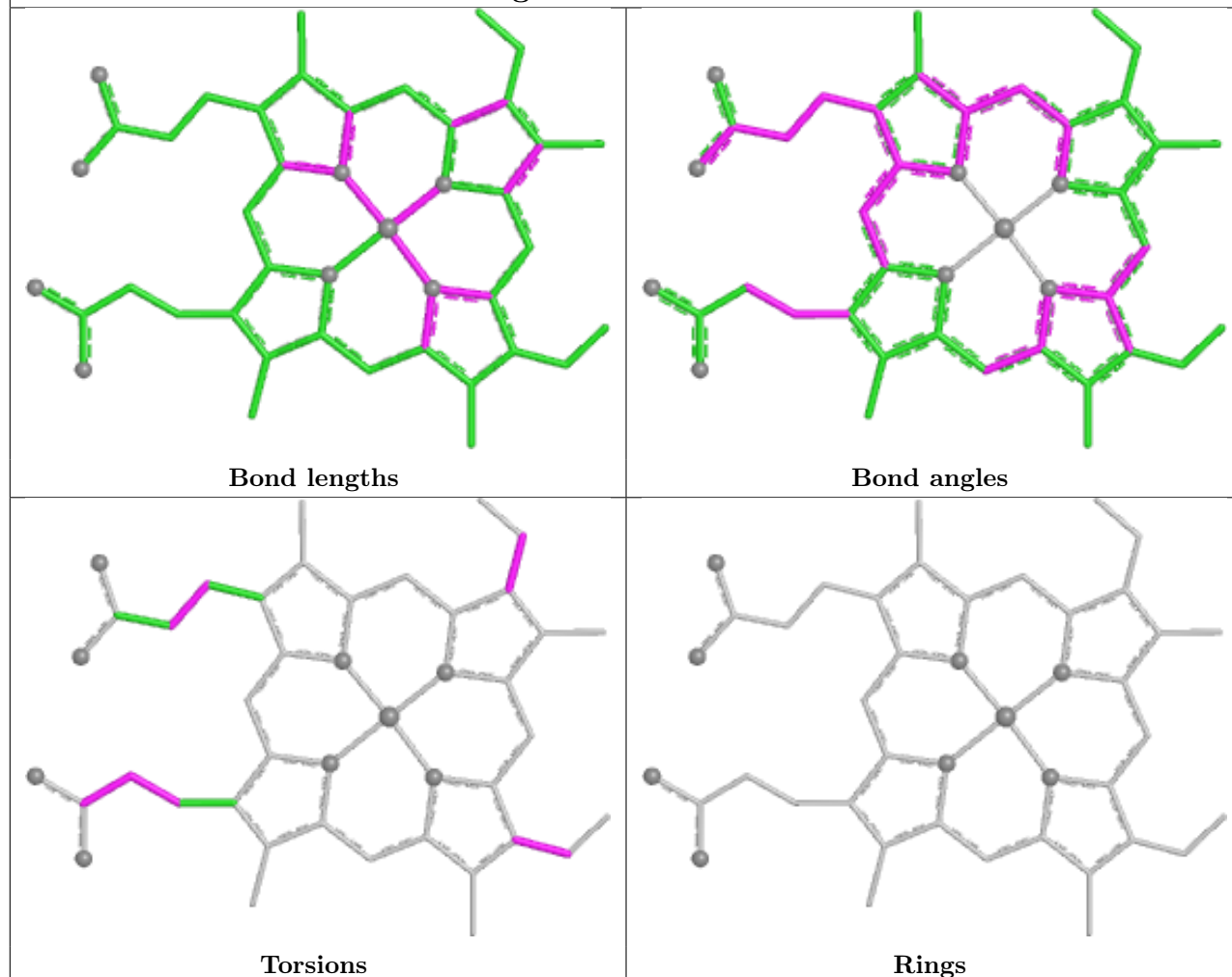




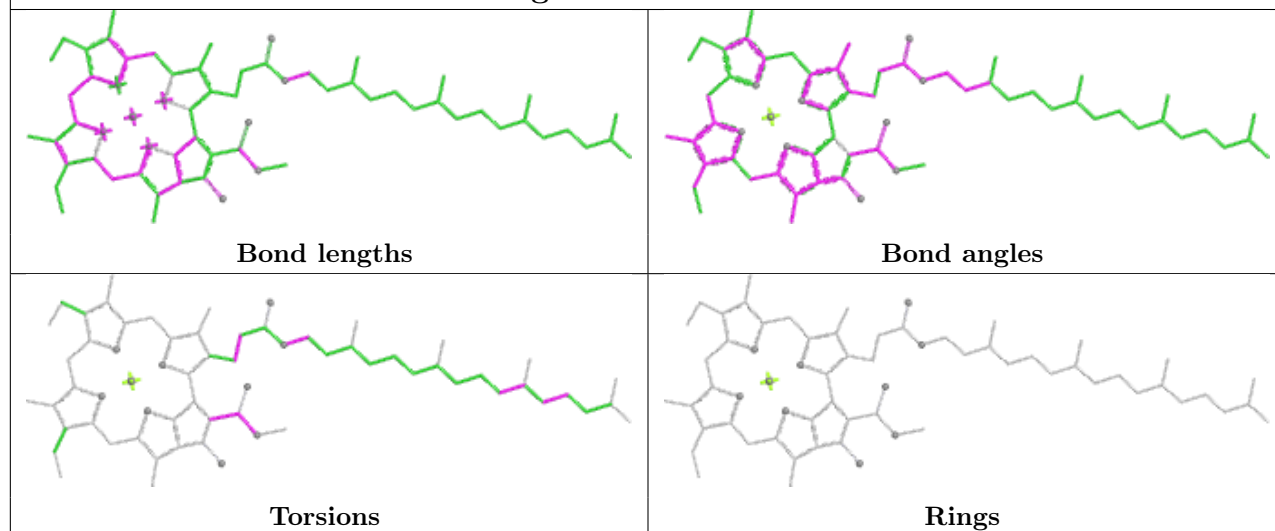


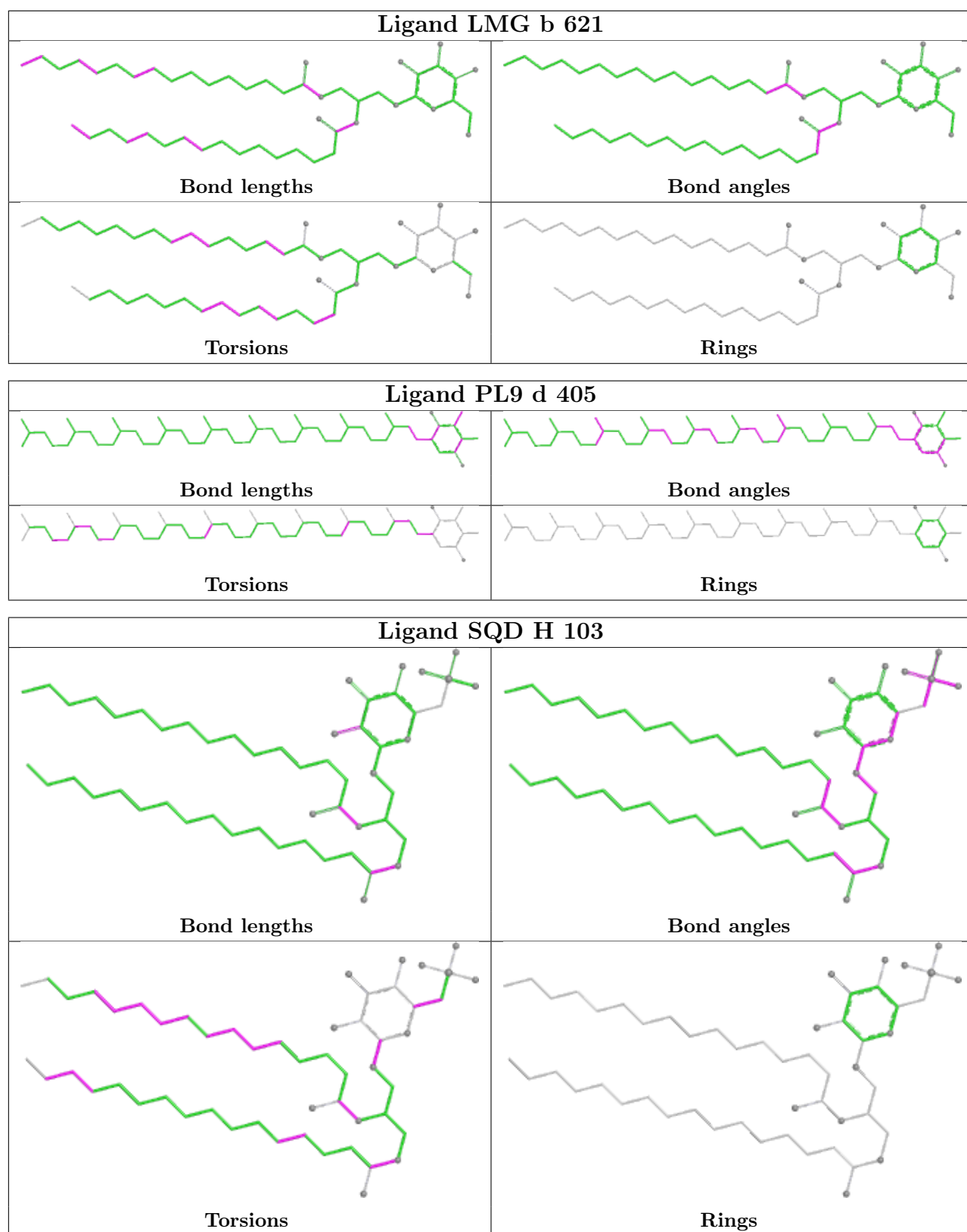


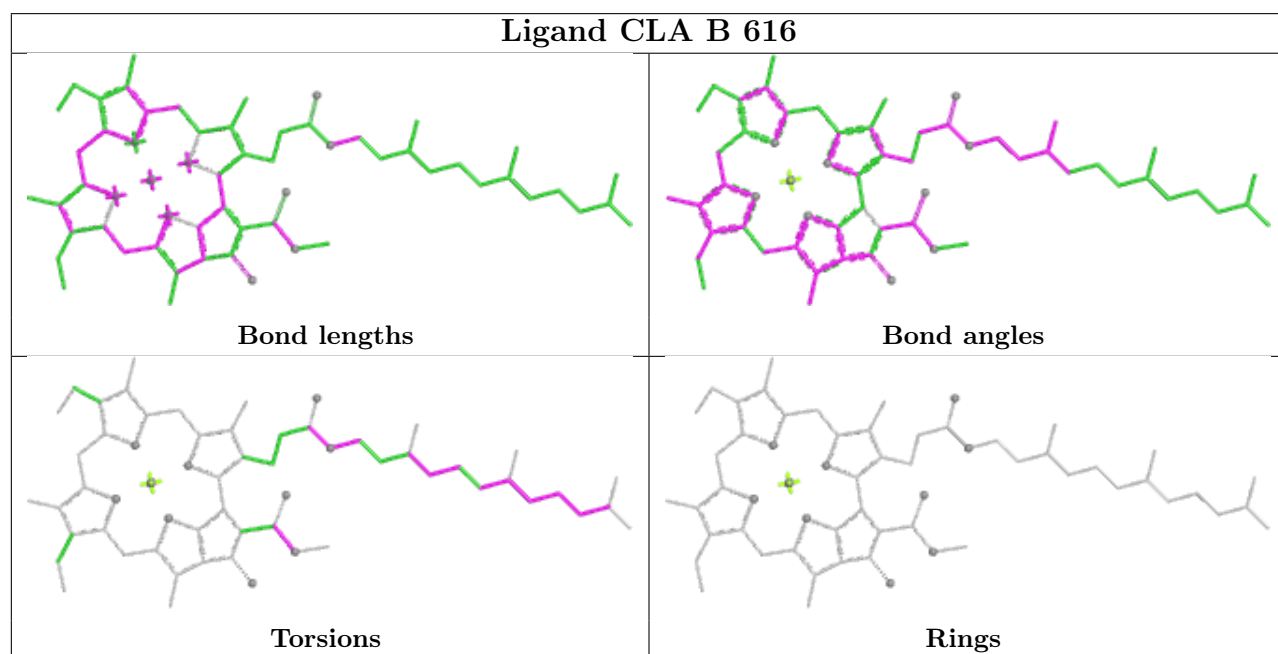
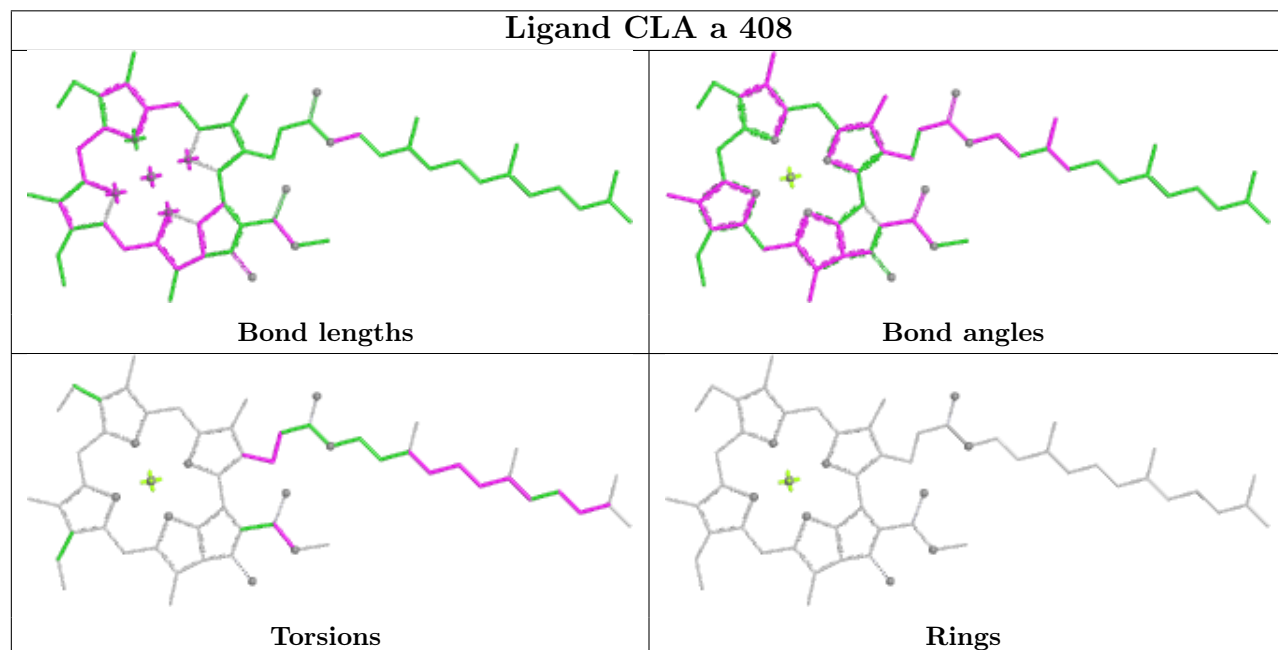
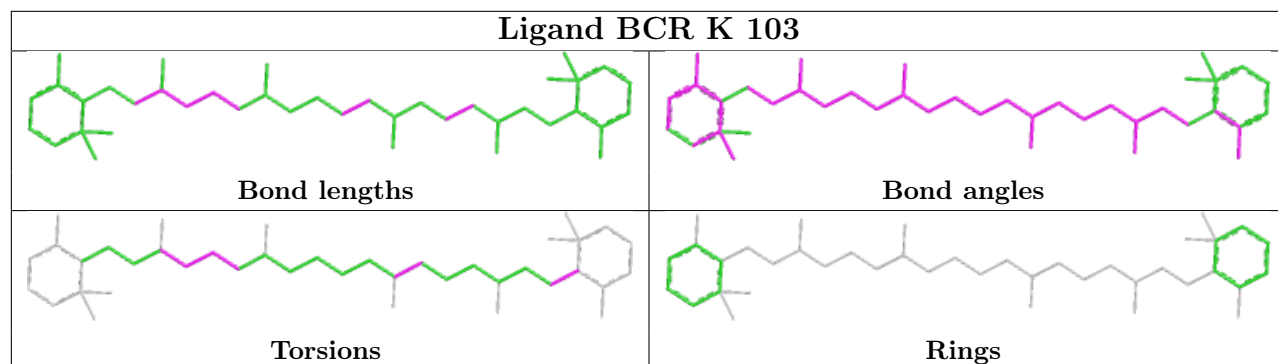
Ligand HEM e 104

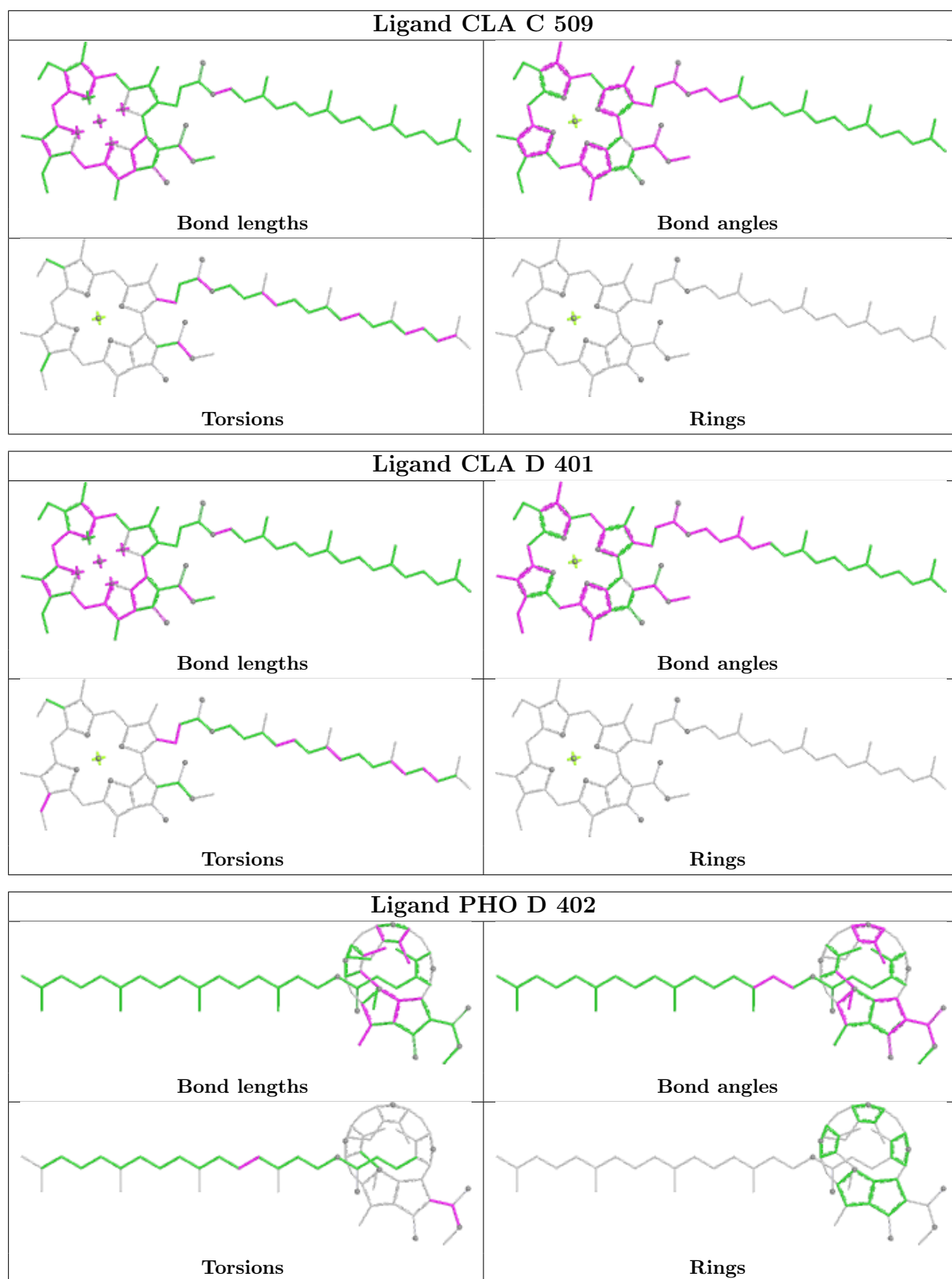


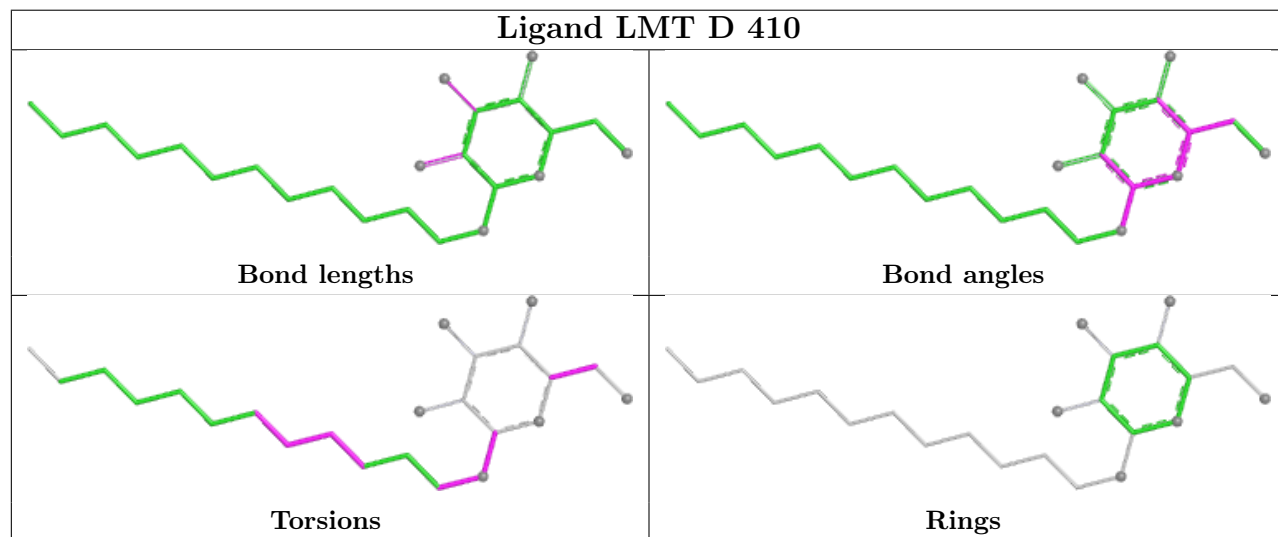
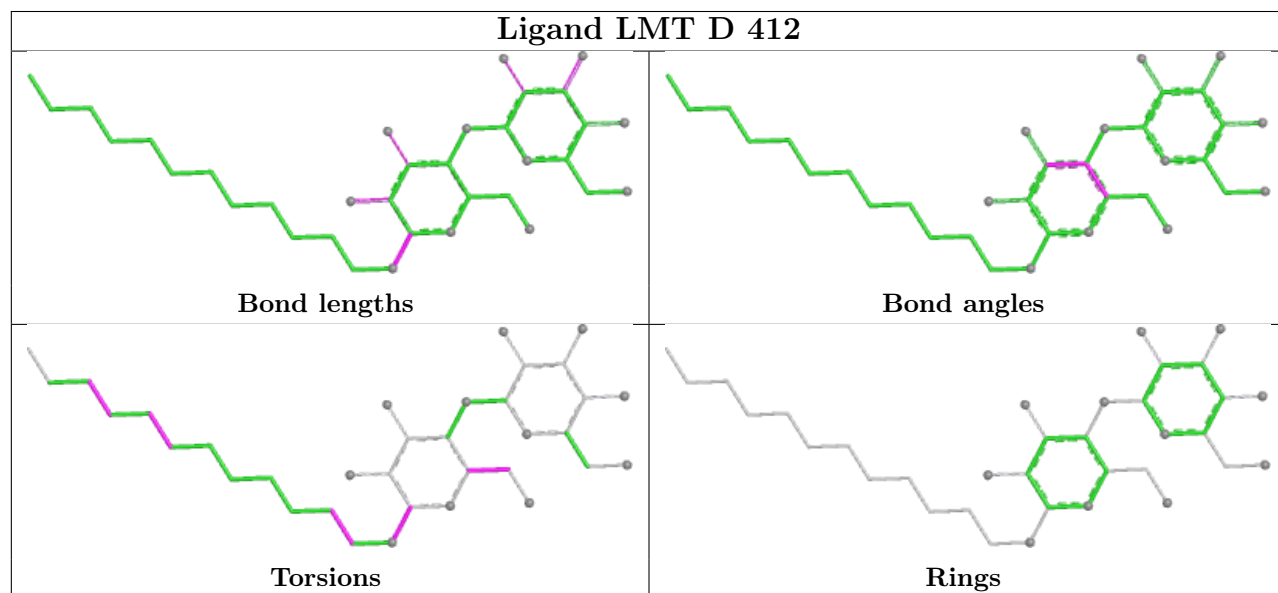
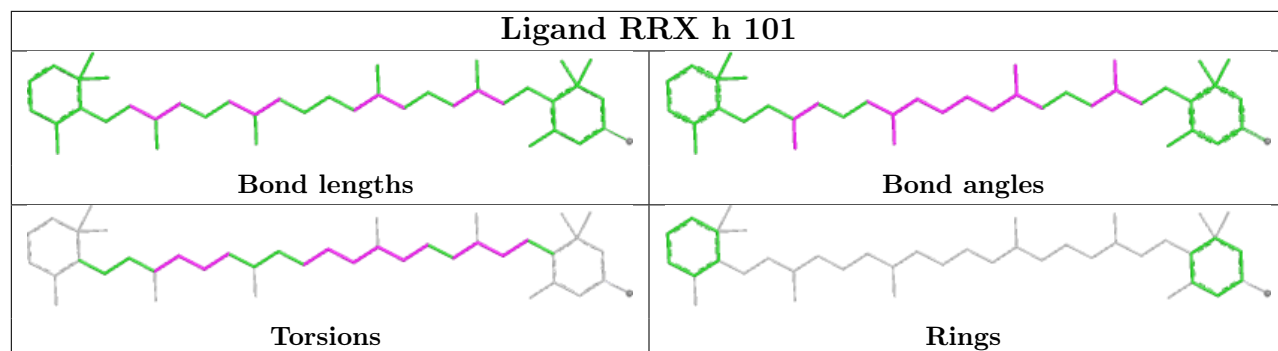
Ligand CLA C 503

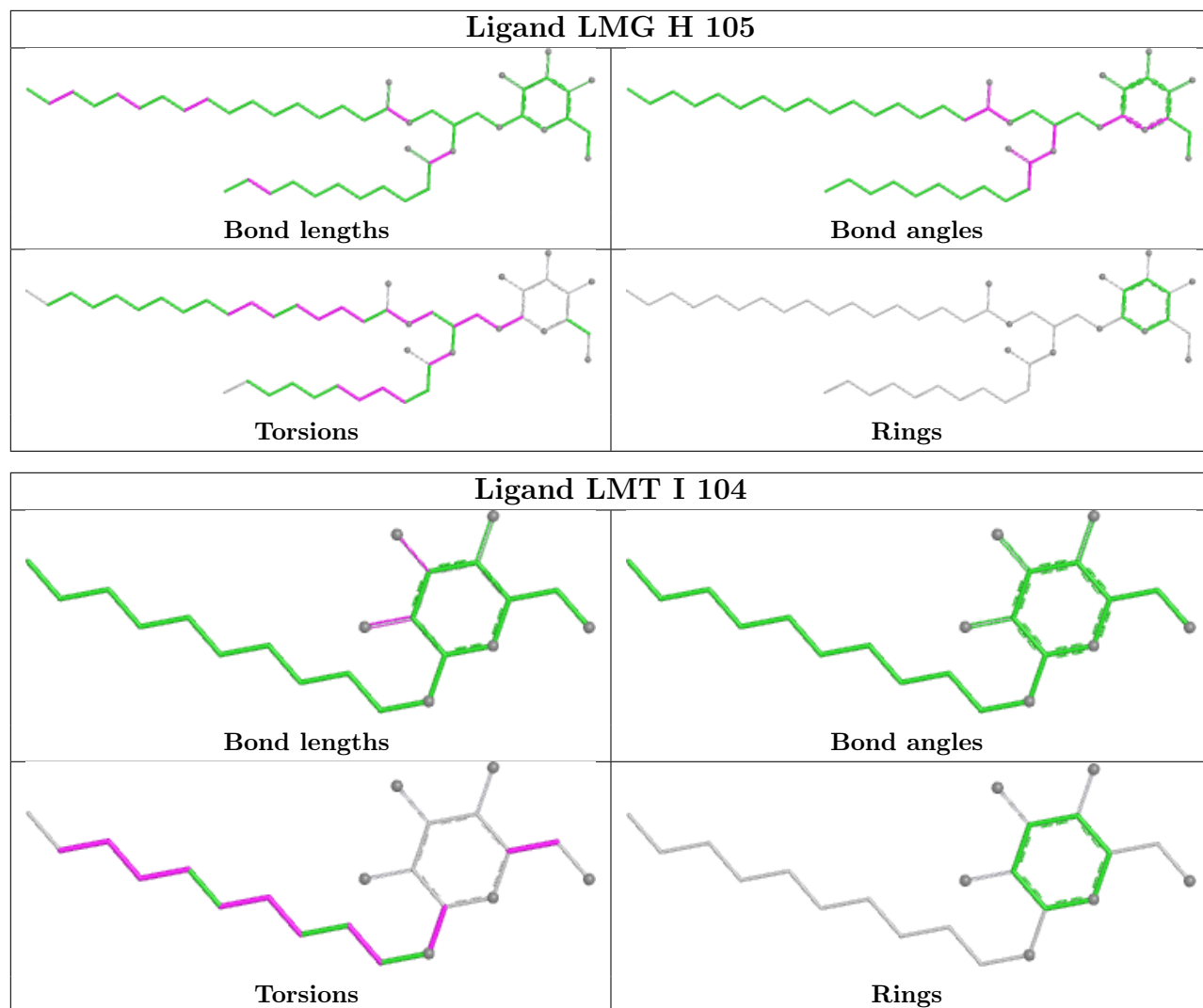


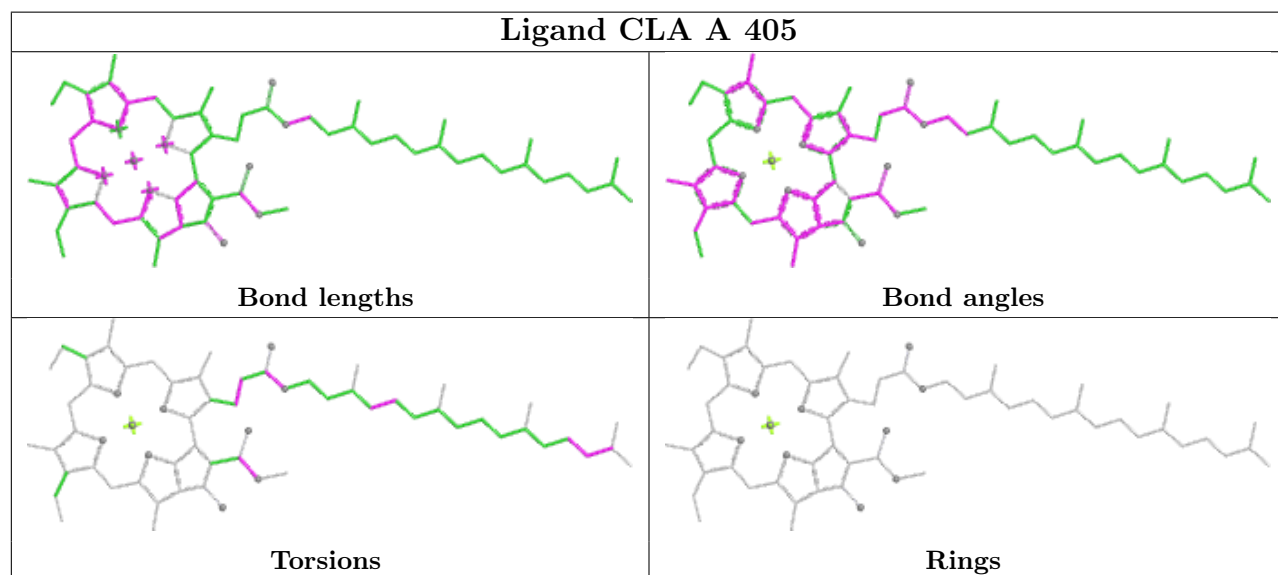
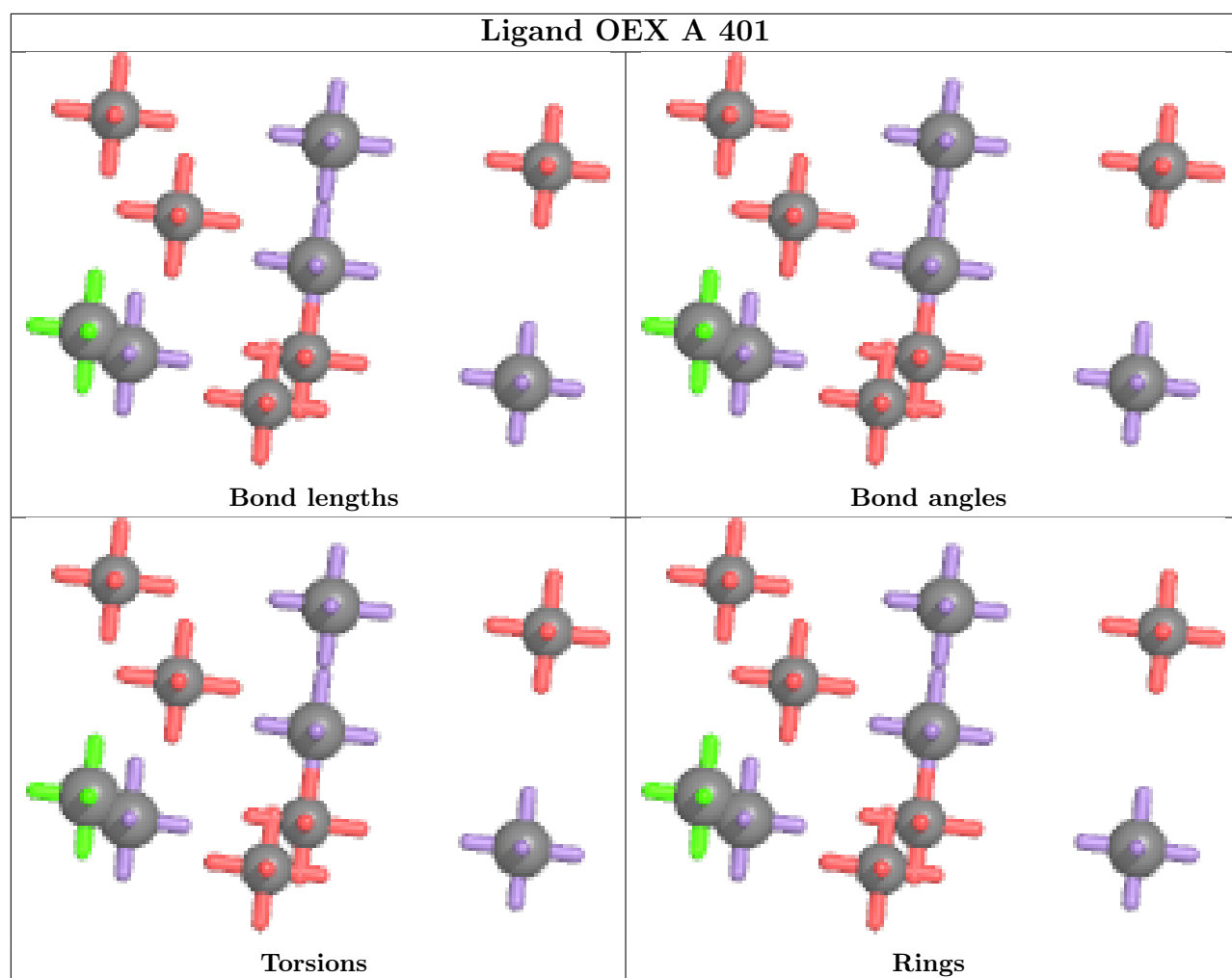


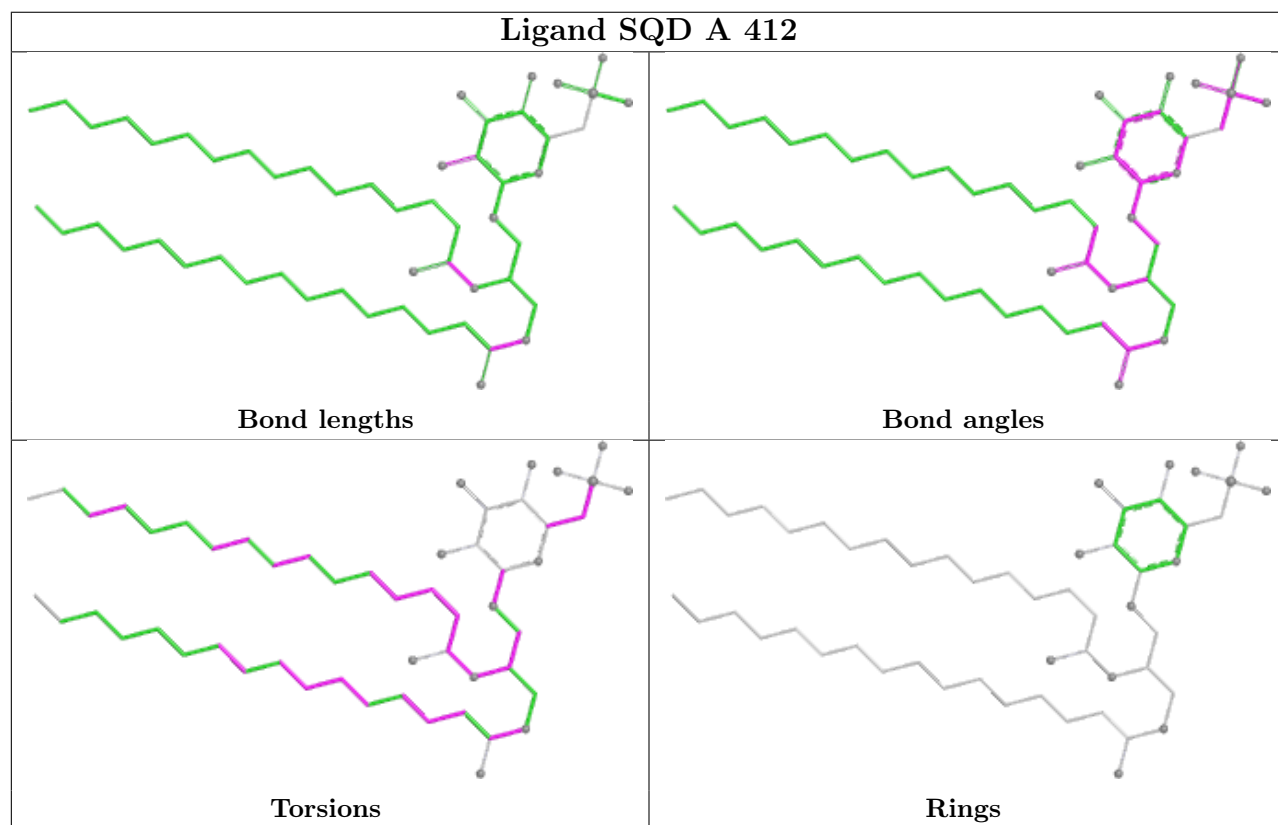
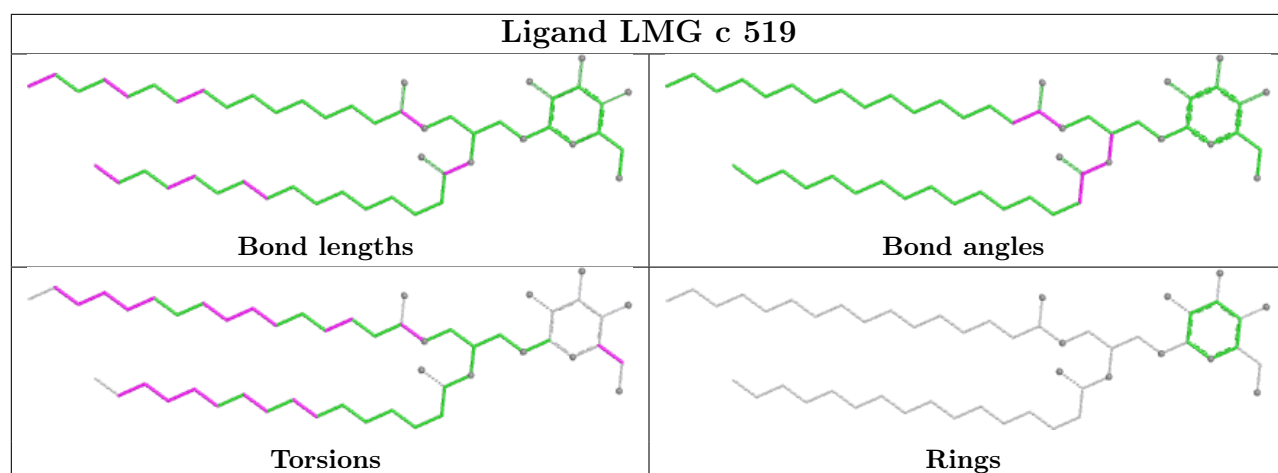


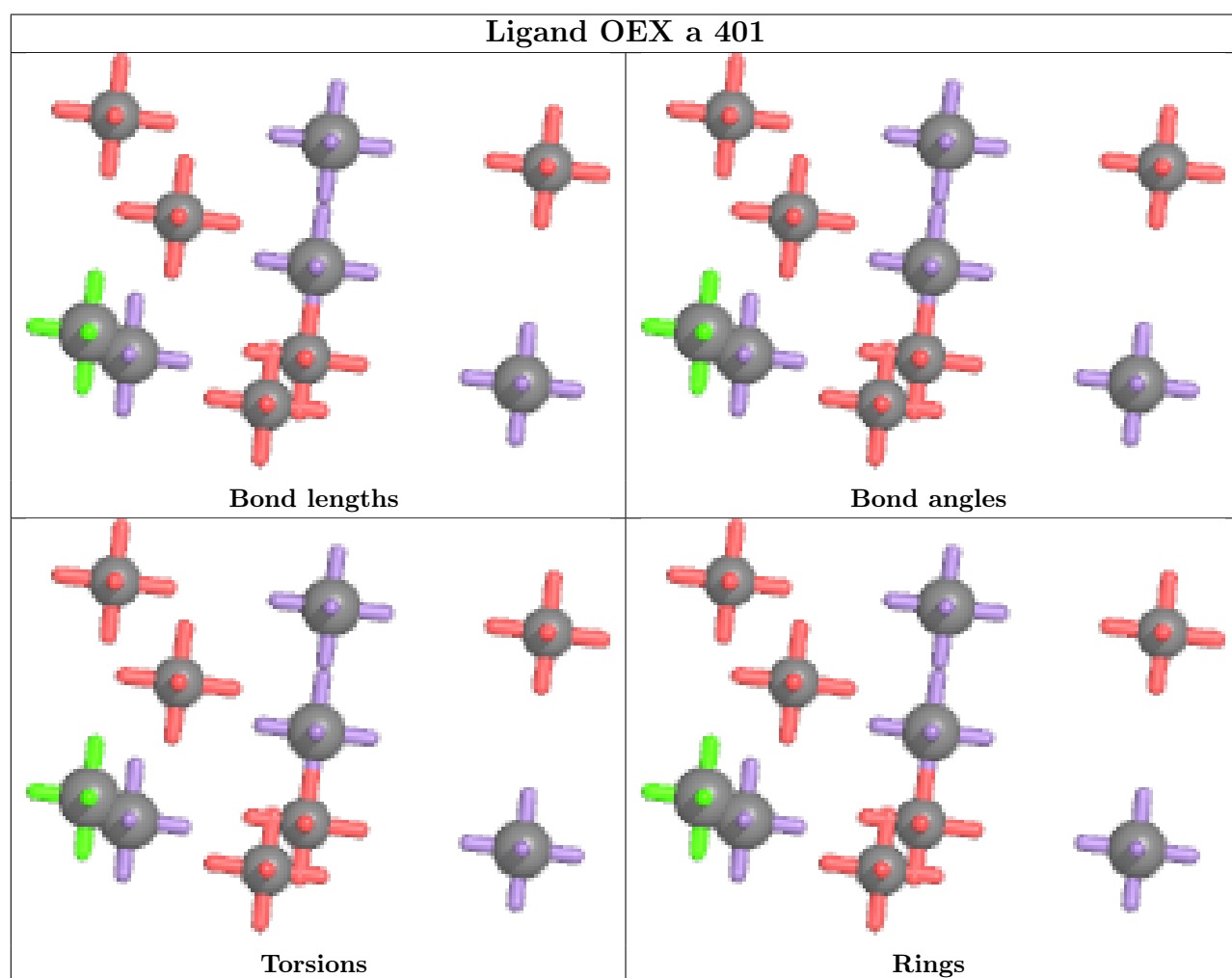
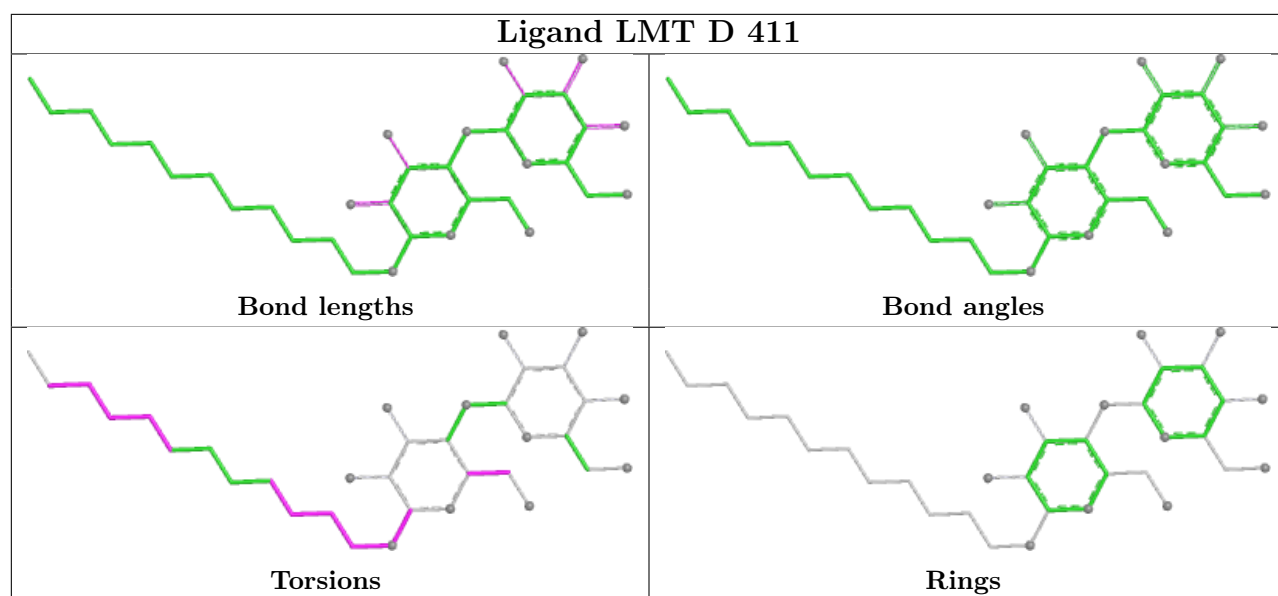


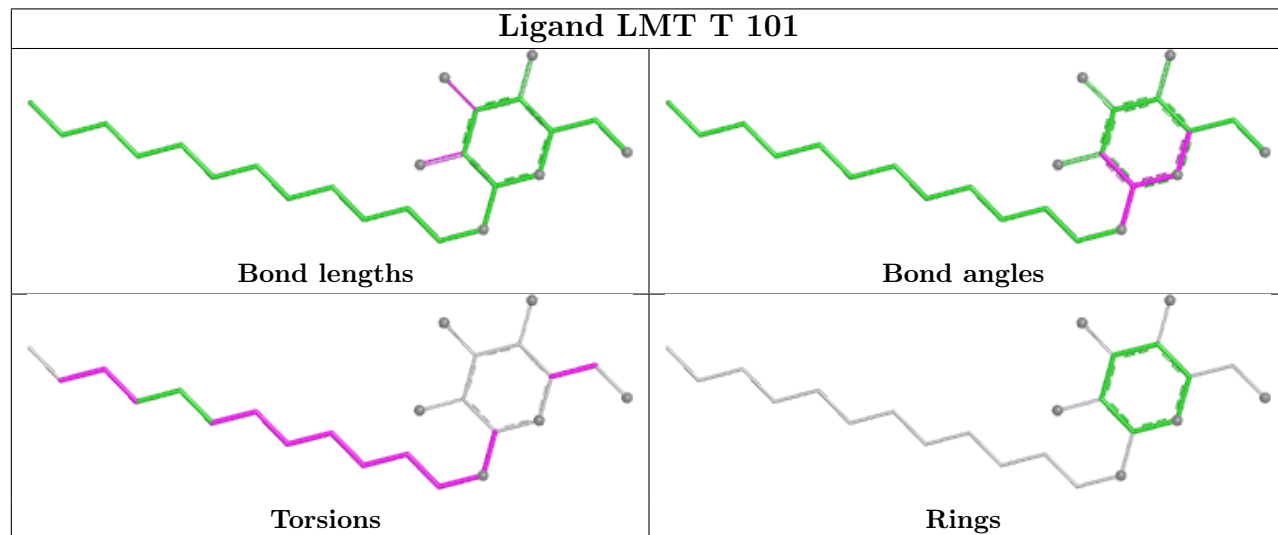
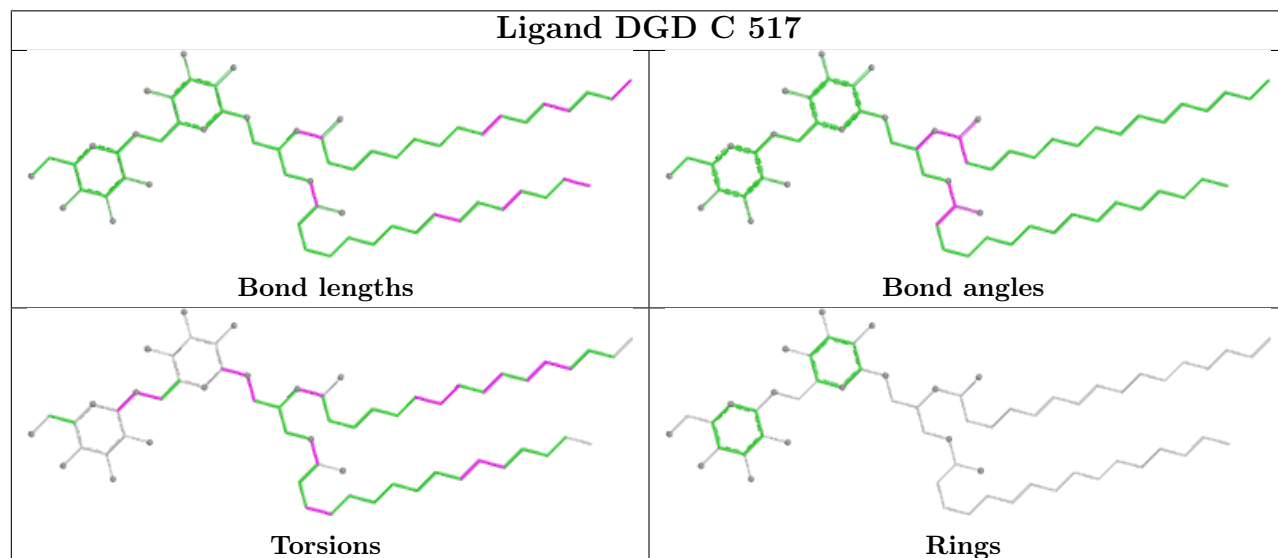
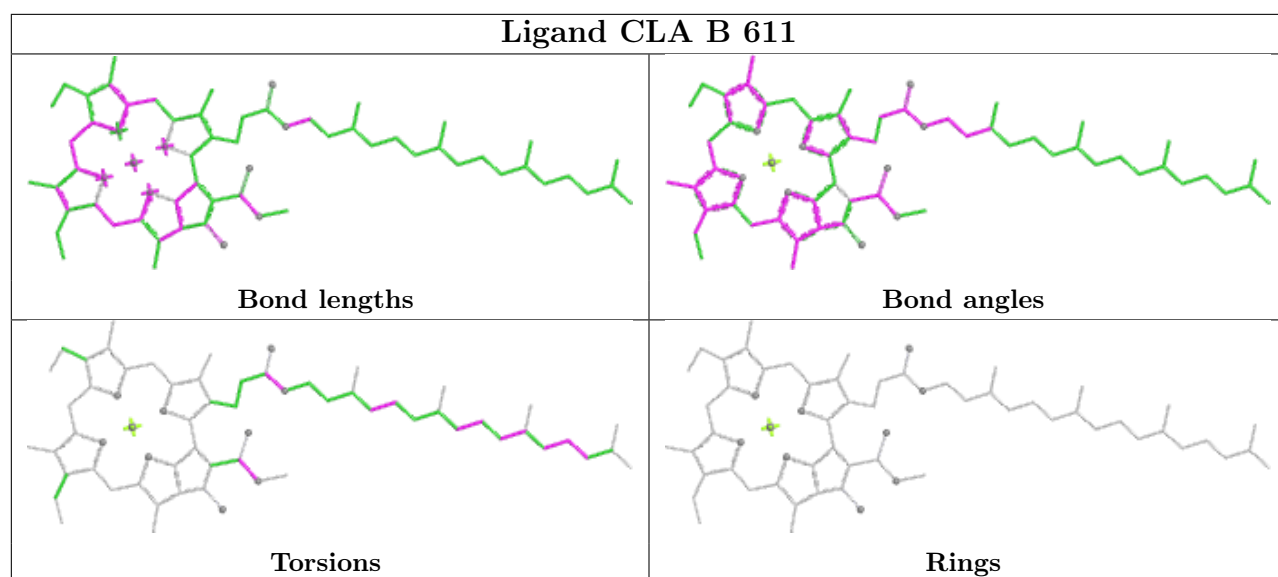


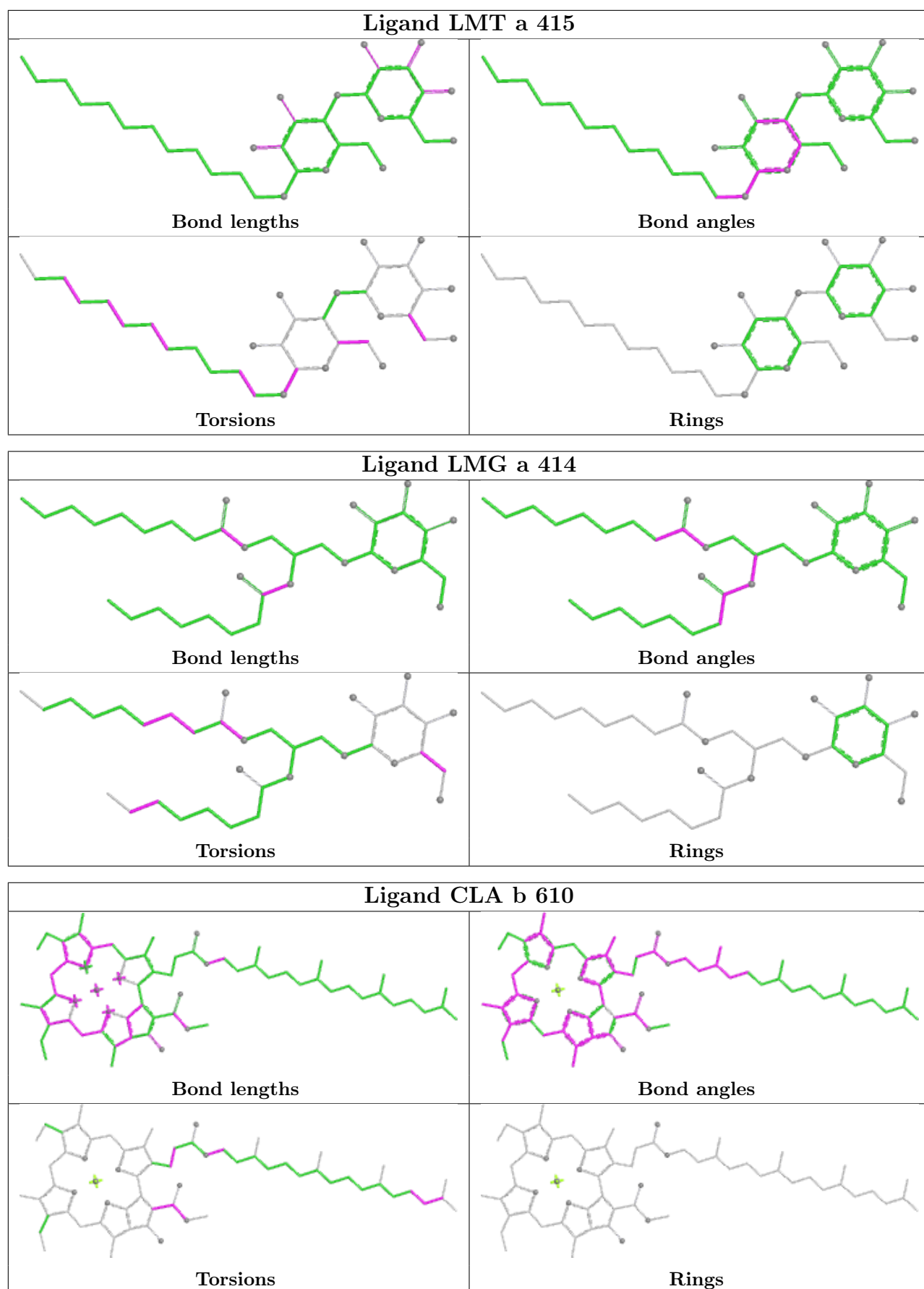












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

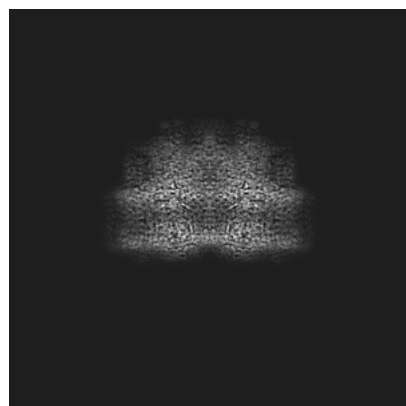
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41460. These allow visual inspection of the internal detail of the map and identification of artifacts.

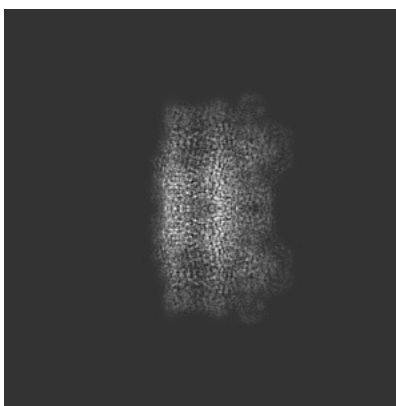
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

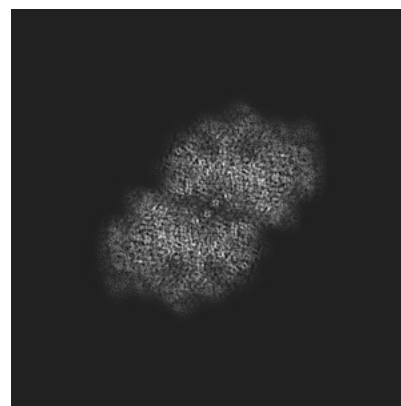
6.1.1 Primary map



X

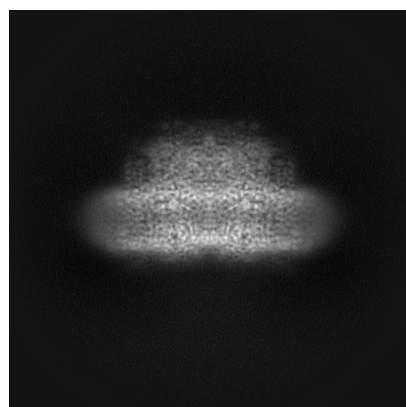


Y

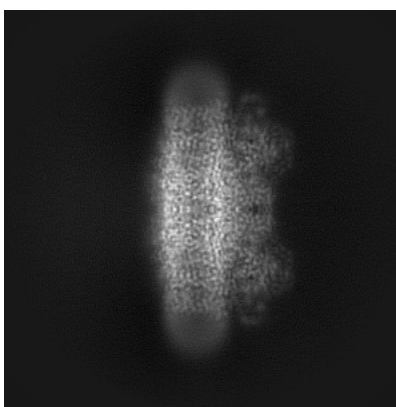


Z

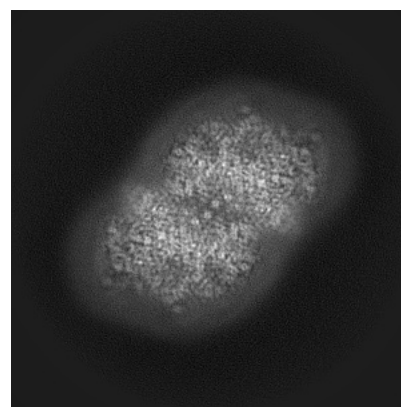
6.1.2 Raw map



X



Y



Z

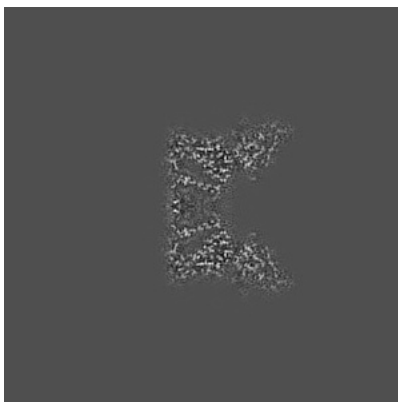
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

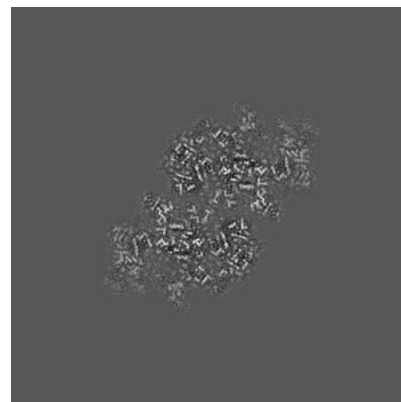
6.2.1 Primary map



X Index: 180

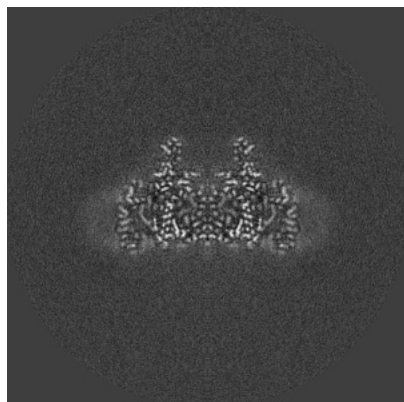


Y Index: 180

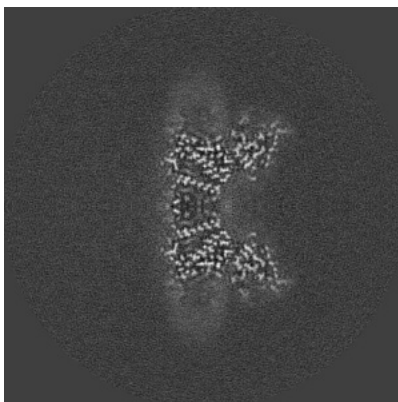


Z Index: 180

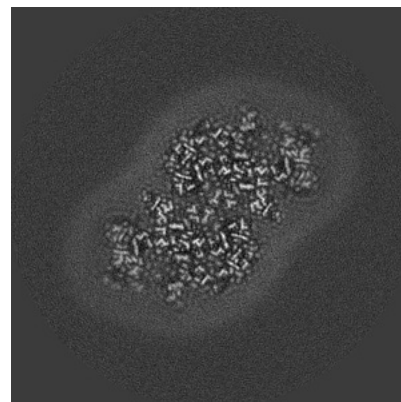
6.2.2 Raw map



X Index: 180



Y Index: 180

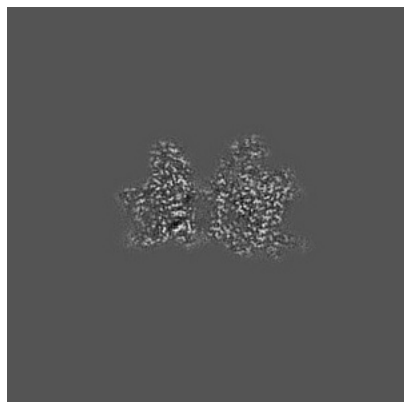


Z Index: 180

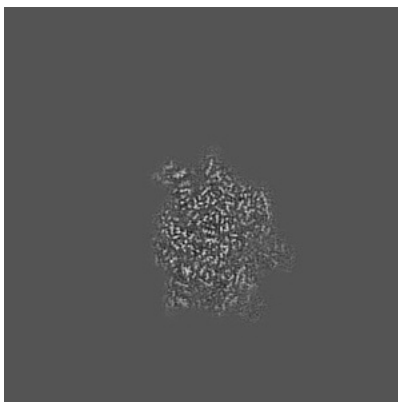
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

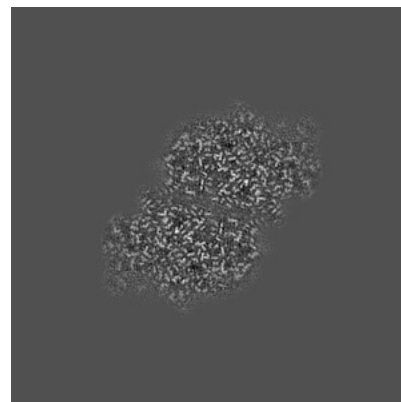
6.3.1 Primary map



X Index: 192

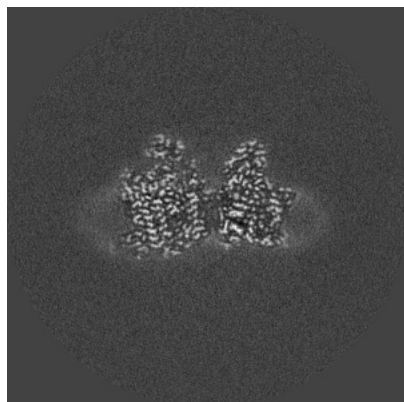


Y Index: 146

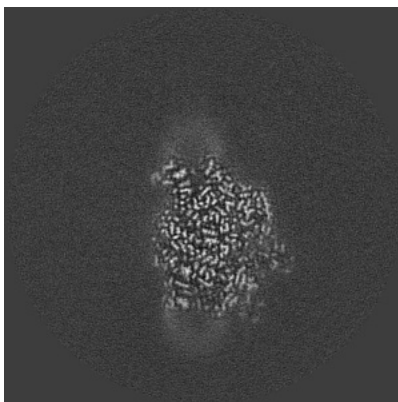


Z Index: 191

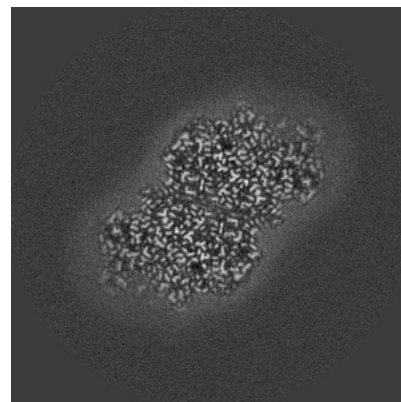
6.3.2 Raw map



X Index: 168



Y Index: 146

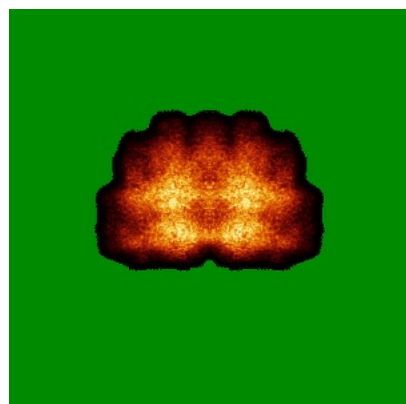


Z Index: 191

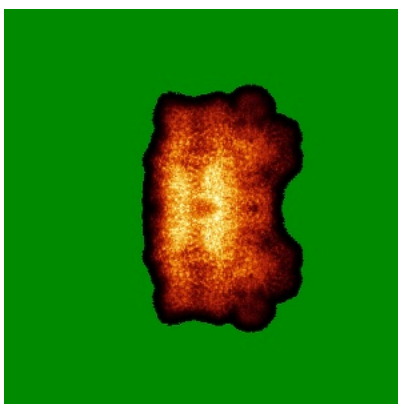
The images above show the largest variance slices of the map in three orthogonal directions.

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

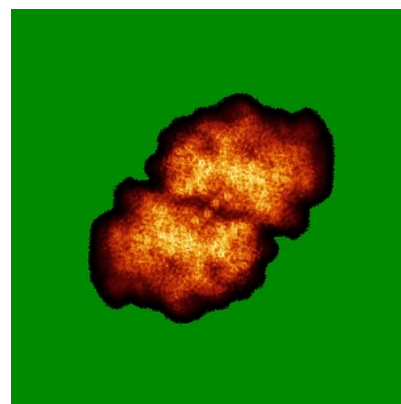
6.4.1 Primary map



X

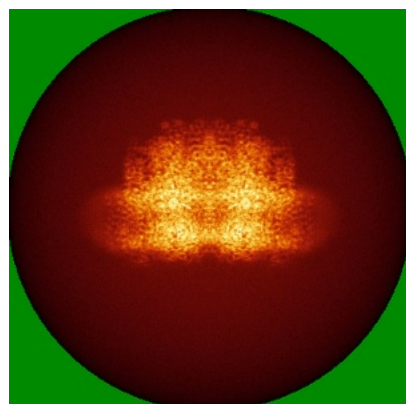


Y

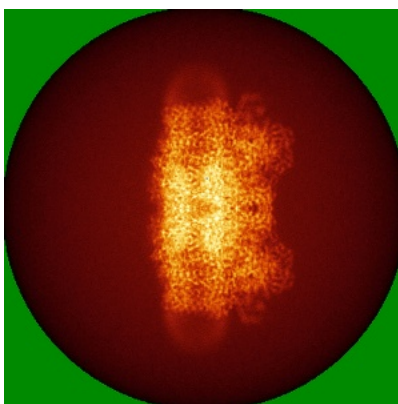


Z

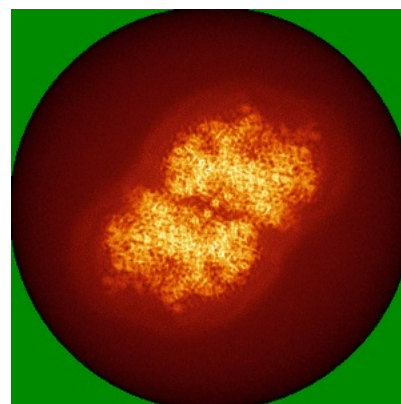
6.4.2 Raw map



X



Y

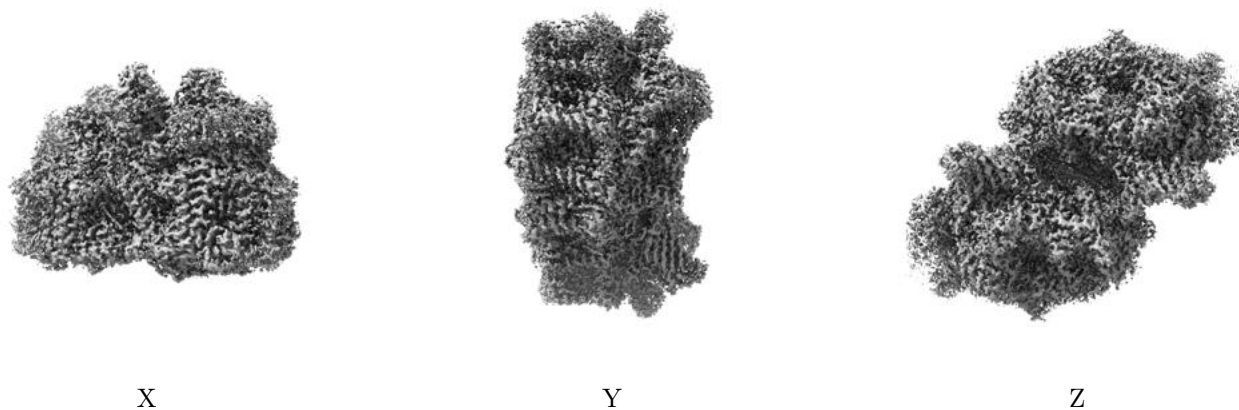


Z

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

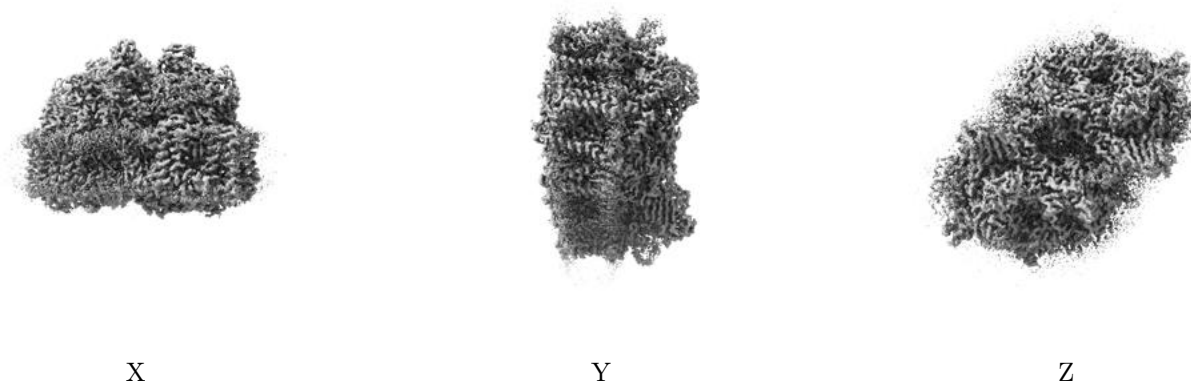
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00432. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

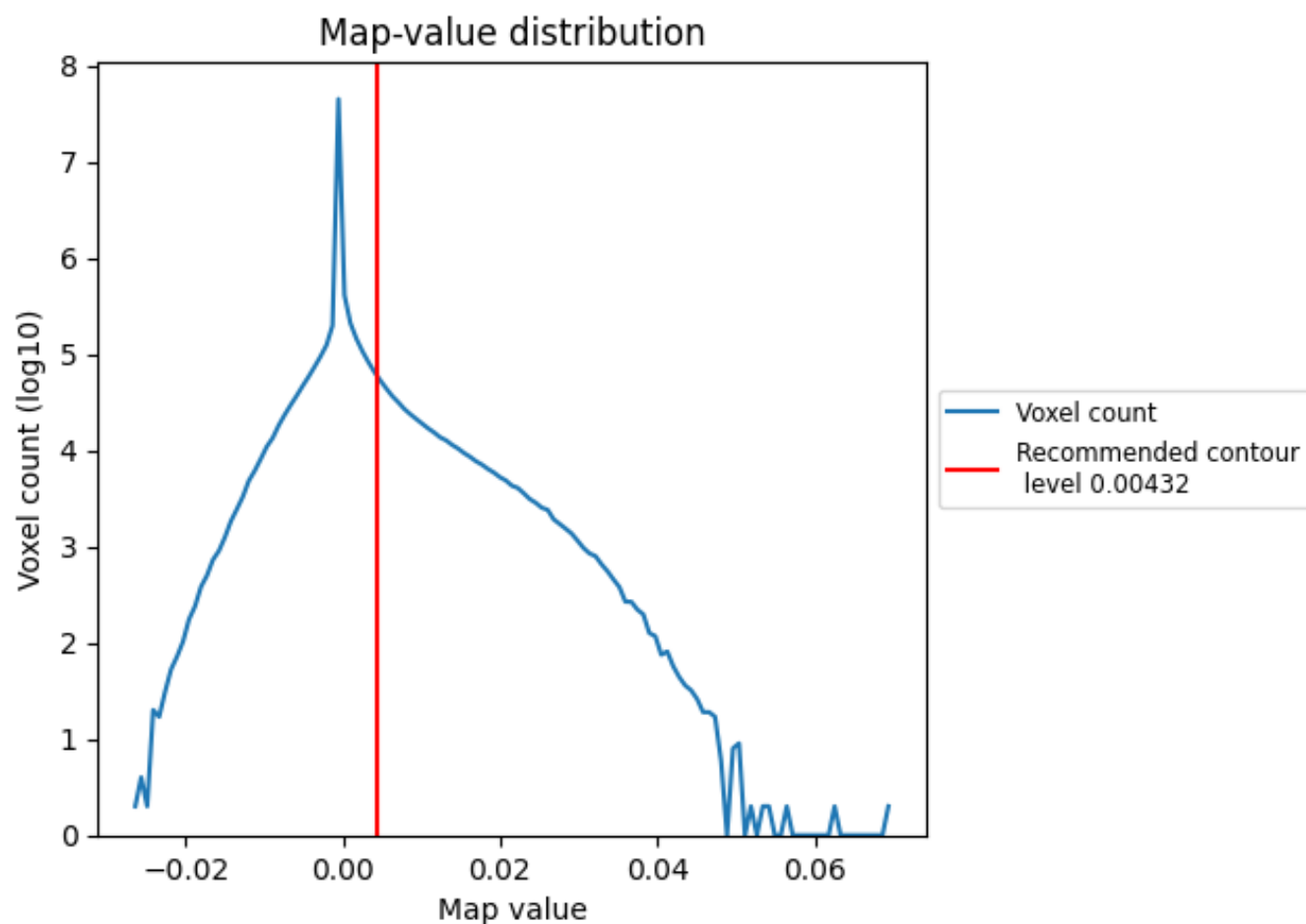
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

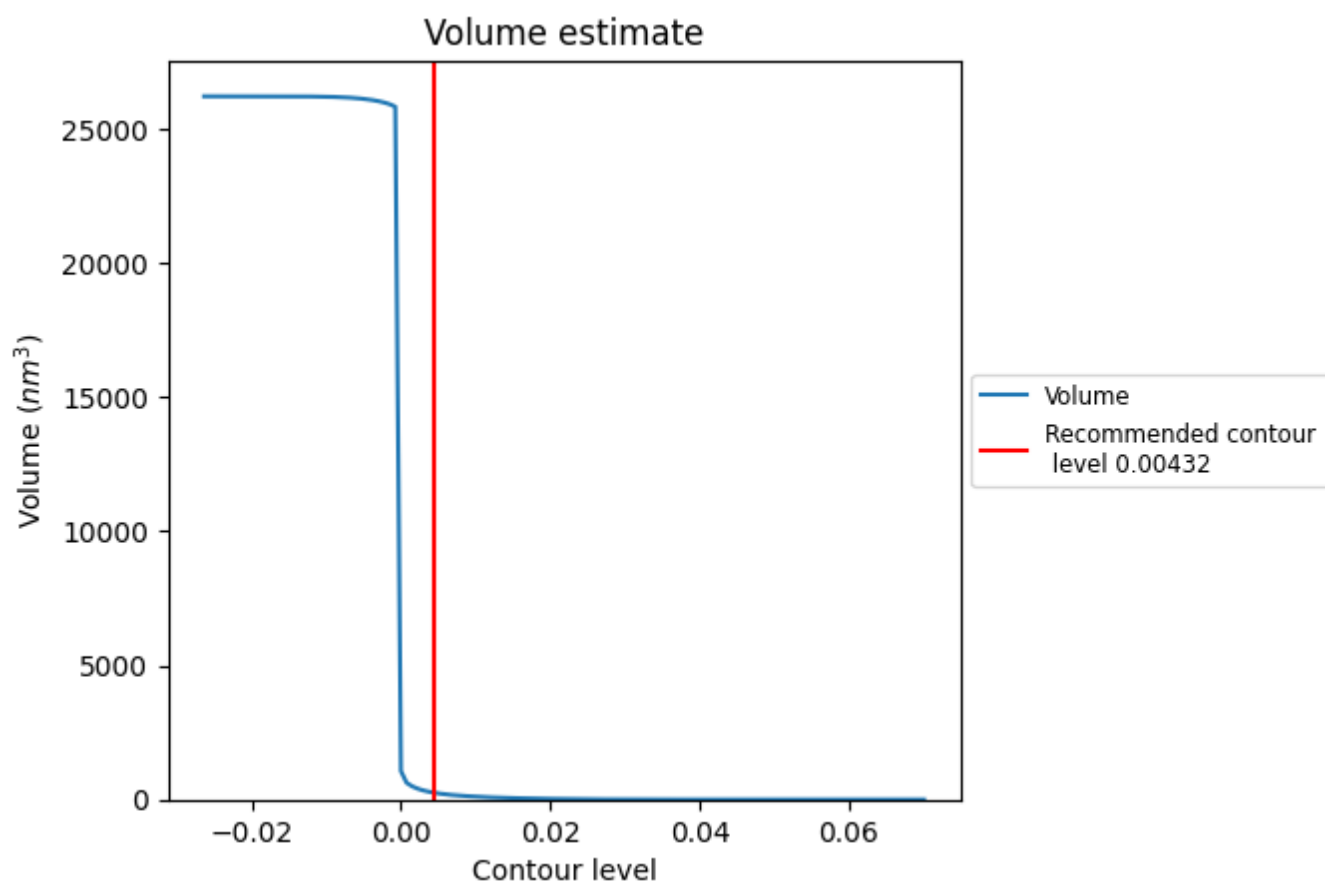
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

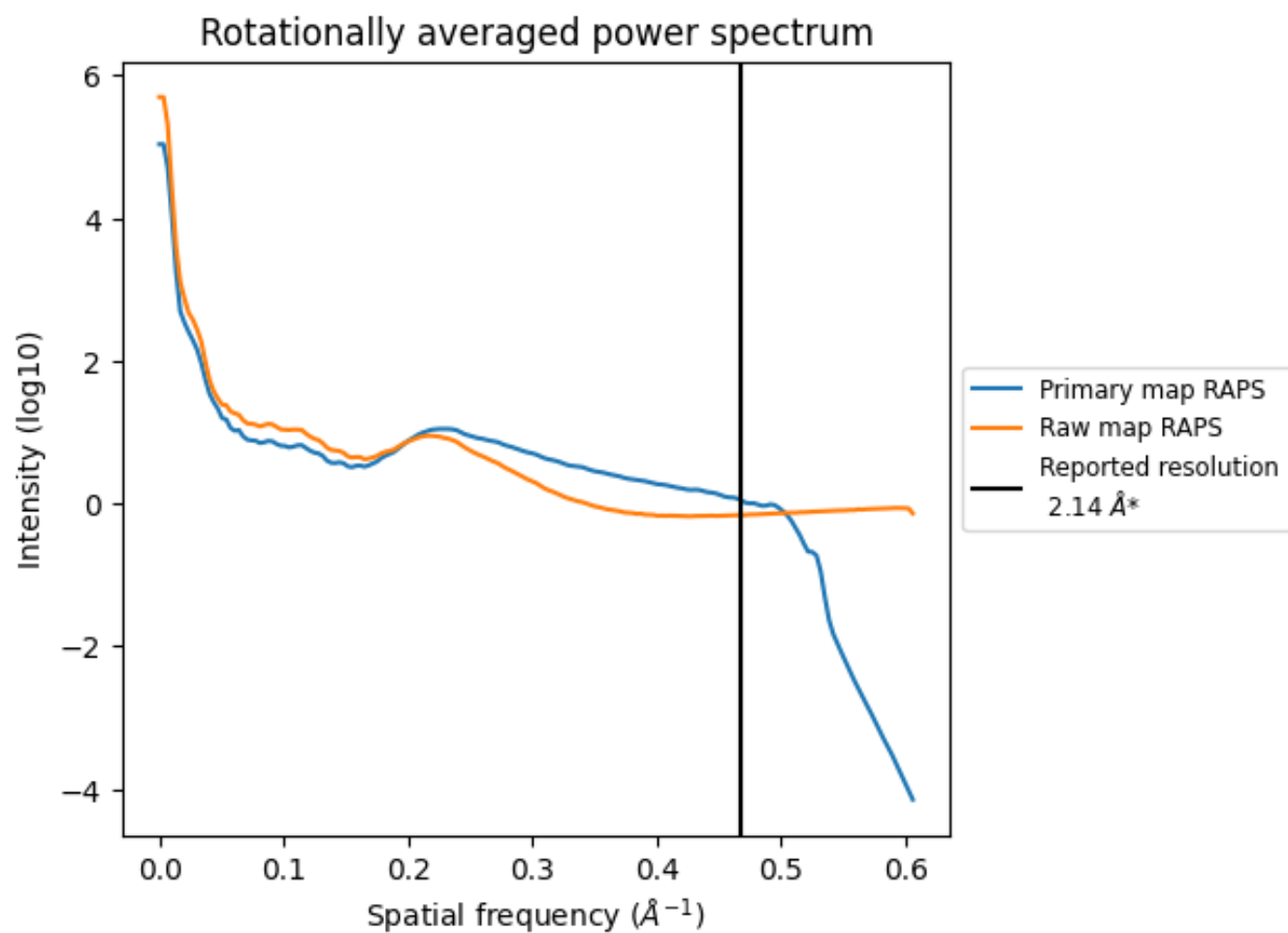
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm^3 ; this corresponds to an approximate mass of 237 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

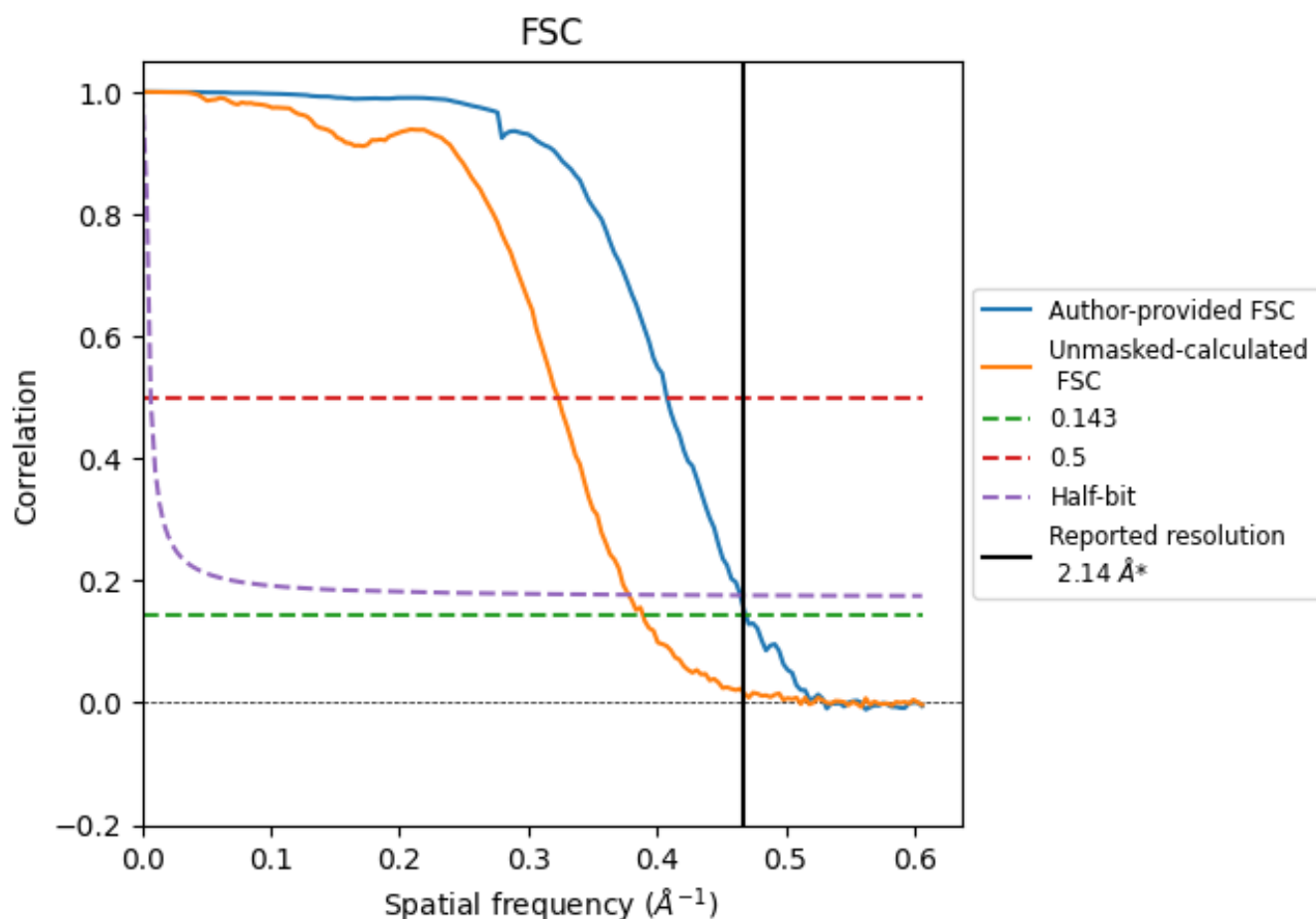


*Reported resolution corresponds to spatial frequency of 0.467 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.467 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

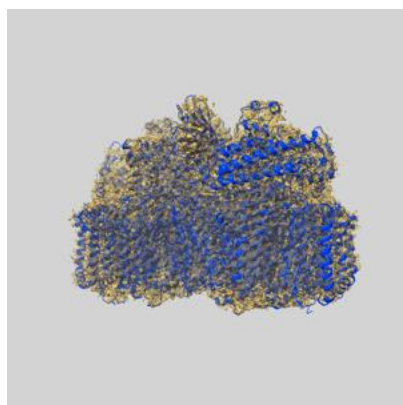
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.13	2.45	2.15
Unmasked-calculated*	2.57	3.09	2.65

*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 2.57 differs from the reported value 2.14 by more than 10 %

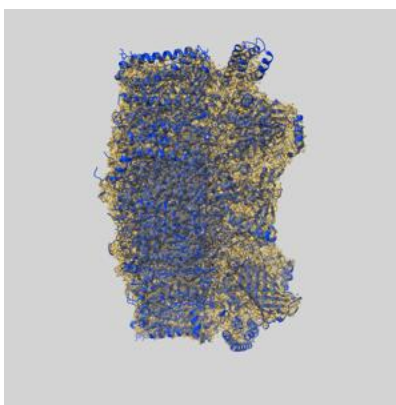
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41460 and PDB model 8TOW. Per-residue inclusion information can be found in section [3](#) on page [30](#).

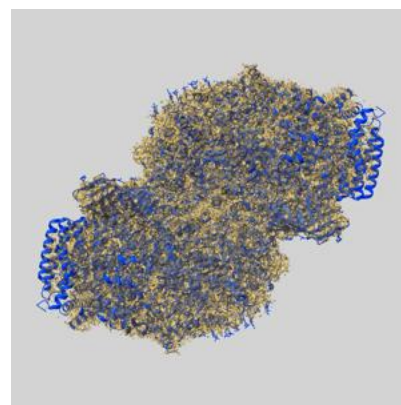
9.1 Map-model overlay [i](#)



X



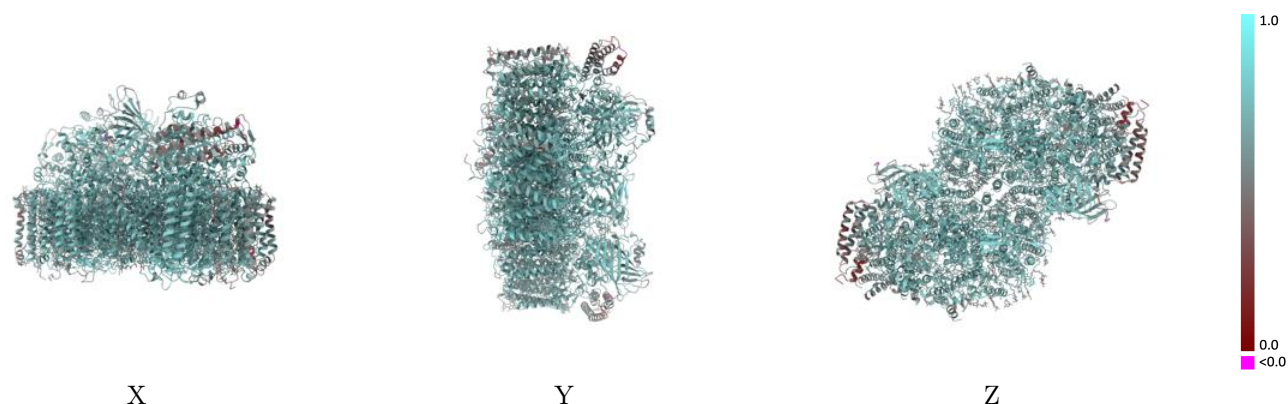
Y



Z

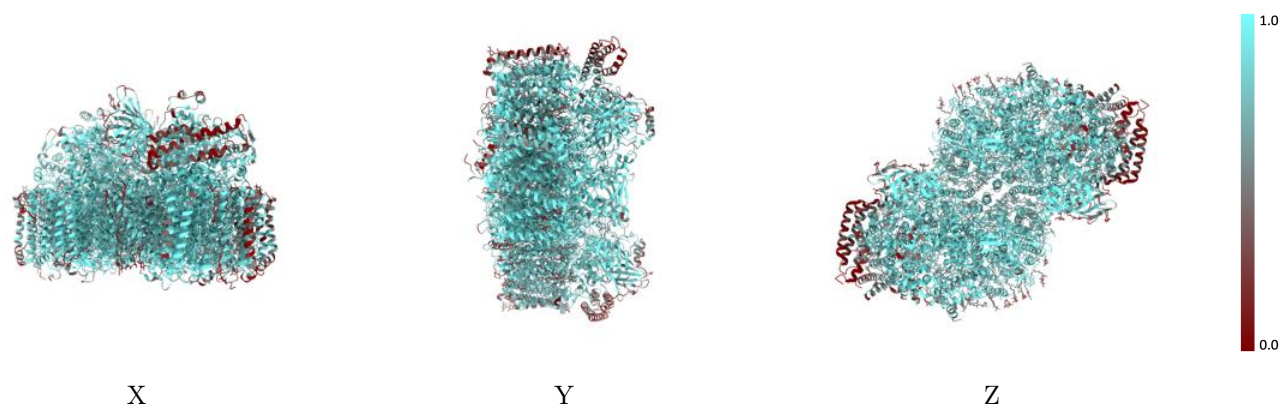
The images above show the 3D surface view of the map at the recommended contour level 0.00432 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



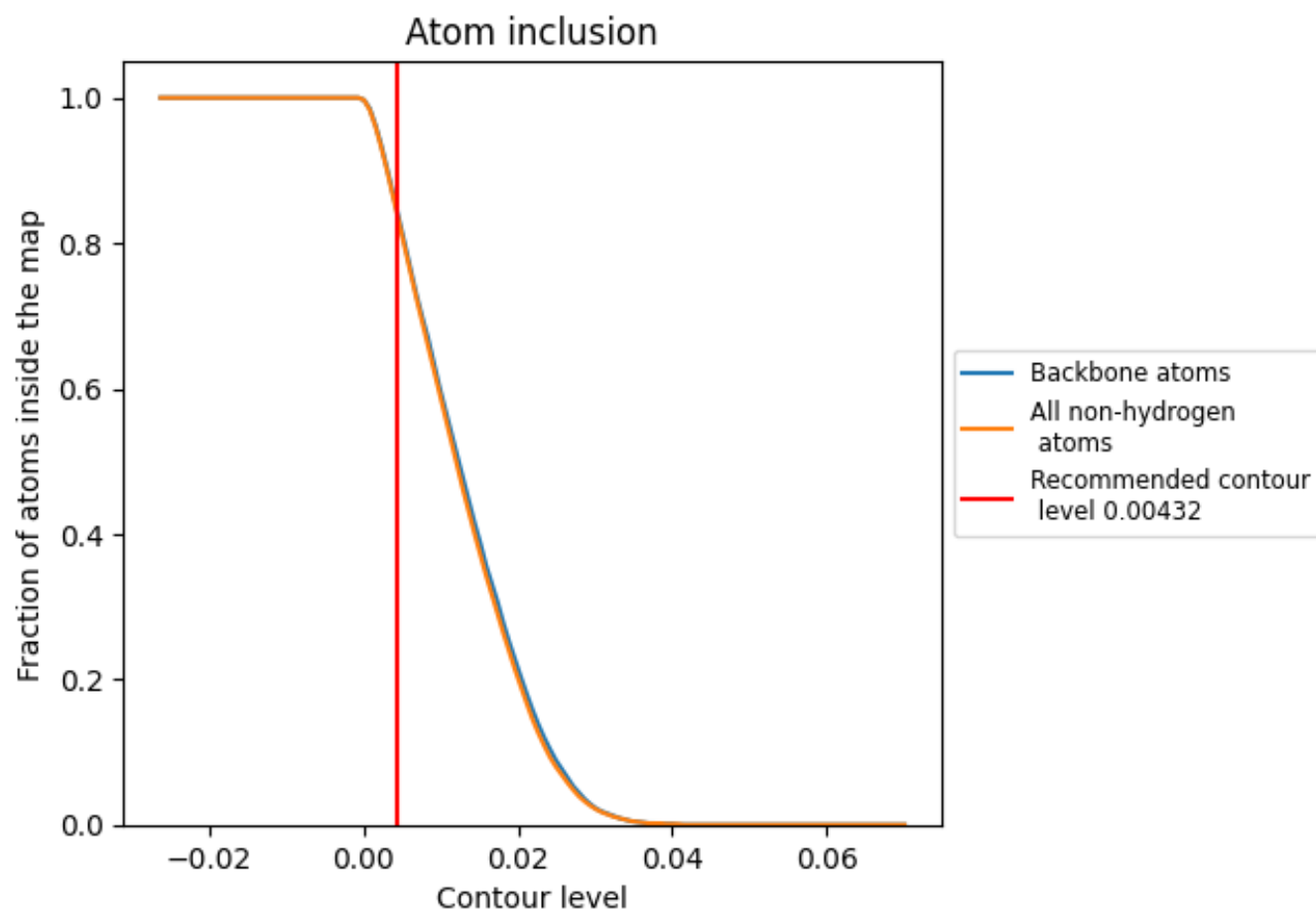
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00432).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00432) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.6860
A	 0.9280	 0.7330
B	 0.9220	 0.7210
C	 0.8760	 0.6950
D	 0.9540	 0.7430
E	 0.8100	 0.6680
F	 0.7770	 0.6340
H	 0.8390	 0.6850
I	 0.6350	 0.6560
J	 0.7250	 0.6350
K	 0.7770	 0.6040
L	 0.9680	 0.7420
M	 0.8880	 0.6880
O	 0.7630	 0.6520
Q	 0.3080	 0.4660
R	 0.5280	 0.5230
T	 0.9040	 0.7030
U	 0.7290	 0.6390
V	 0.8060	 0.6640
X	 0.6730	 0.6300
Y	 0.6020	 0.5660
Z	 0.4320	 0.5510
a	 0.9270	 0.7340
b	 0.9220	 0.7210
c	 0.8770	 0.6960
d	 0.9540	 0.7430
e	 0.8090	 0.6670
f	 0.7800	 0.6360
h	 0.8360	 0.6850
i	 0.6370	 0.6550
j	 0.7280	 0.6340
k	 0.7800	 0.6020
l	 0.9640	 0.7440
m	 0.8850	 0.6900
o	 0.7610	 0.6540



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Chain	Atom inclusion	Q-score
q	 0.3070	 0.4660
r	 0.5280	 0.5180
t	 0.9040	 0.7080
u	 0.7290	 0.6370
v	 0.8080	 0.6650
x	 0.6780	 0.6360
y	 0.5900	 0.5640
z	 0.4320	 0.5470