



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 02:24 PM JST

PDB ID : 7XXF / pdb_00007xxf
EMDB ID : EMD-33501
Title : Structure of photosynthetic LH1-RC super-complex of Rhodospila globiformis
Authors : Tani, K.; Kanno, R.; Kurosawa, K.; Takaichi, S.; Nagashima, K.V.P.; Hall, M.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2022-05-30
Resolution : 2.24 Å (reported)
Based on initial model : 5Y5S

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 : 1.8.5 (274361), CSD as541be (2020)
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

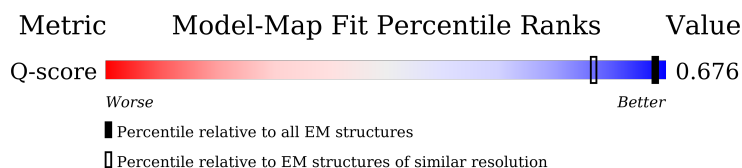
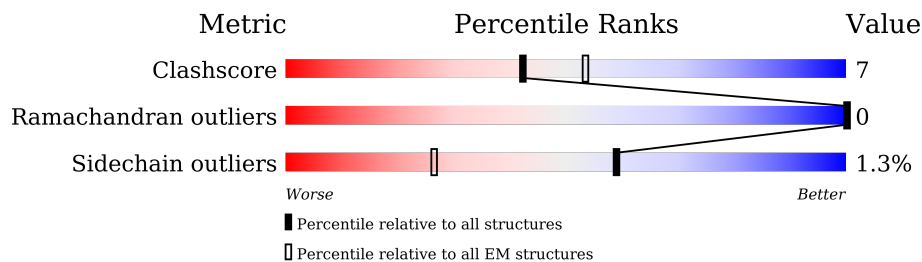
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.24 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	3381 (1.75 - 2.74)

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	C	344	
2	L	275	
3	M	326	
4	H	258	

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Mol	Chain	Length	Quality of chain
5	1	61	
5	3	61	
5	5	61	
5	7	61	
5	9	61	
5	A	61	
5	D	61	
5	F	61	
5	I	61	
5	K	61	
5	O	61	
5	Q	61	
5	S	61	
5	U	61	
5	W	61	
5	Y	61	
6	0	73	
6	2	73	
6	4	73	
6	6	73	
6	8	73	
6	B	73	
6	E	73	
6	G	73	
6	J	73	

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Mol	Chain	Length	Quality of chain
6	N	73	
6	P	73	
6	R	73	
6	T	73	
6	V	73	
6	X	73	
6	Z	73	
7	a	22	
7	b	22	
7	c	22	
7	d	22	
7	e	22	
7	f	22	
7	g	22	
7	h	22	
7	i	22	
7	j	22	
7	k	22	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	HEC	C	401	X	-	-	-
8	HEC	C	402	X	-	-	-
8	HEC	C	403	X	-	-	-
8	HEC	C	404	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 29826 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	343	Total	C	N	O	S	0	0
			2655	1683	471	481	20		

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	274	Total	C	N	O	S	0	0
			2177	1469	353	347	8		

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	320	Total	C	N	O	S	1	0
			2550	1714	421	404	11		

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	258	Total	C	N	O	S	0	0
			2000	1284	332	376	8		

- Molecule 5 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	D	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	F	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	I	46	Total	C	N	O	S	0	0
			394	270	66	56	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	O	45	Total	C	N	O	S	0	0
			389	267	65	55	2		
5	Q	45	Total	C	N	O	S	0	0
			389	267	65	55	2		
5	S	58	Total	C	N	O	S	0	0
			475	321	82	69	3		
5	U	53	Total	C	N	O	S	0	0
			443	299	77	64	3		
5	W	57	Total	C	N	O	S	0	0
			470	318	81	68	3		
5	Y	45	Total	C	N	O	S	0	0
			384	264	63	55	2		
5	1	46	Total	C	N	O	S	0	0
			395	270	67	56	2		
5	3	57	Total	C	N	O	S	0	0
			472	321	79	69	3		
5	5	45	Total	C	N	O	S	0	0
			389	267	65	55	2		
5	7	45	Total	C	N	O	S	0	0
			389	267	65	55	2		
5	9	45	Total	C	N	O	S	1	0
			392	270	64	56	2		

- Molecule 6 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	B	50	Total	C	N	O	0	0
			396	268	62	66		
6	E	50	Total	C	N	O	0	0
			396	268	62	66		
6	G	50	Total	C	N	O	0	0
			396	268	62	66		
6	J	50	Total	C	N	O	0	0
			396	268	62	66		
6	N	50	Total	C	N	O	0	0
			396	268	62	66		
6	P	50	Total	C	N	O	0	0
			396	268	62	66		
6	R	50	Total	C	N	O	0	0
			396	268	62	66		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	T	50	Total	C	N	O	0	0
			396	268	62	66		
6	V	50	Total	C	N	O	0	0
			396	268	62	66		
6	X	50	Total	C	N	O	0	0
			396	268	62	66		
6	Z	50	Total	C	N	O	0	0
			396	268	62	66		
6	2	50	Total	C	N	O	0	0
			396	268	62	66		
6	4	50	Total	C	N	O	0	0
			396	268	62	66		
6	6	50	Total	C	N	O	0	0
			396	268	62	66		
6	8	50	Total	C	N	O	0	0
			396	268	62	66		
6	0	50	Total	C	N	O	0	0
			396	268	62	66		

- Molecule 7 is a protein called Light-harvesting protein LH1 Gamma-like.

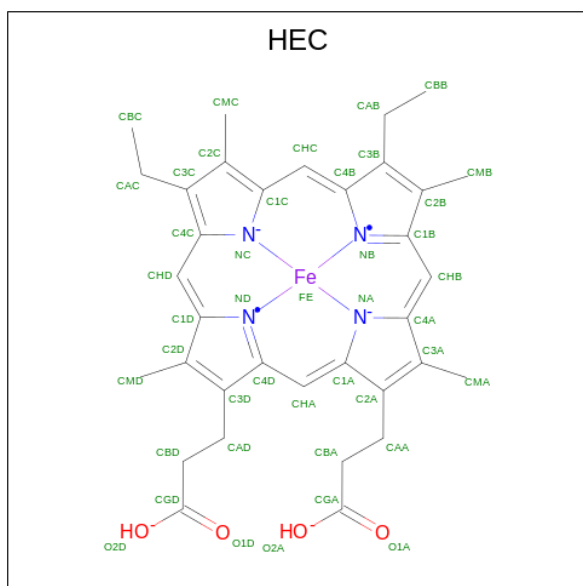
Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	b	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	c	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	d	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	e	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	f	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	g	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	h	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	i	22	Total	C	N	O	S	0	0
			177	120	28	26	3		
7	j	22	Total	C	N	O	S	0	0
			177	120	28	26	3		

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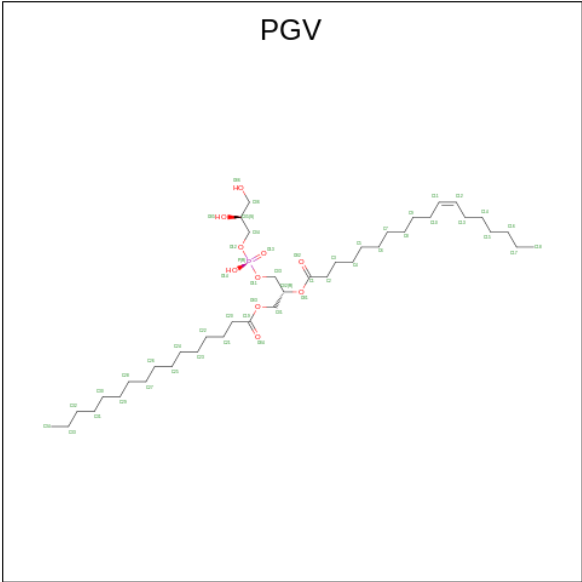
Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	22	Total	C	N	O	S	0	0
			177	120	28	26	3		

- Molecule 8 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 9 is (1R)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



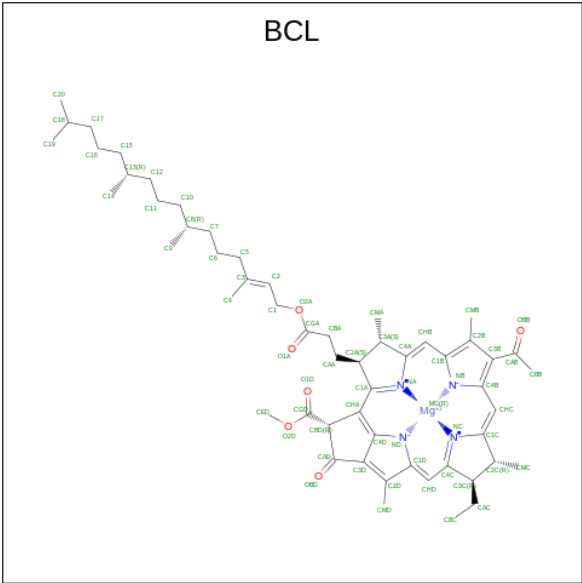
Mol	Chain	Residues	Atoms				AltConf
9	C	1	Total	C	O	P	0
			44	33	10	1	
9	C	1	Total	C	O	P	0
			42	31	10	1	
9	C	1	Total	C	O	P	0
			38	29	8	1	
9	L	1	Total	C	O	P	0
			43	32	10	1	
9	L	1	Total	C	O	P	0
			44	33	10	1	
9	L	1	Total	C	O	P	0
			37	26	10	1	
9	L	1	Total	C	O	P	0
			33	22	10	1	
9	L	1	Total	C	O	P	0
			34	23	10	1	
9	M	1	Total	C	O	P	0
			51	40	10	1	
9	M	1	Total	C	O	P	0
			33	22	10	1	
9	H	1	Total	C	O	P	0
			36	25	10	1	
9	H	1	Total	C	O	P	0
			36	25	10	1	
9	D	1	Total	C	O	P	0
			33	22	10	1	
9	F	1	Total	C	O	P	0
			39	29	9	1	

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Mol	Chain	Residues	Atoms				AltConf
9	K	1	Total	C	O	P	0
			39	28	10	1	
9	5	1	Total	C	O	P	0
			37	28	8	1	
9	5	1	Total	C	O	P	0
			37	28	8	1	
9	5	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 10 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	D	1	Total 66	C 55	Mg 1	N 4	O 6	0

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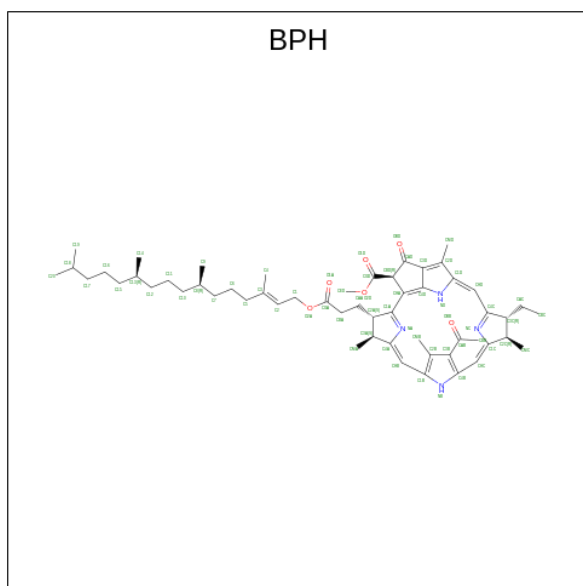
Mol	Chain	Residues	Atoms					AltConf
10	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
10	2	1	Total 66	C 55	Mg 1	N 4	O 6	0

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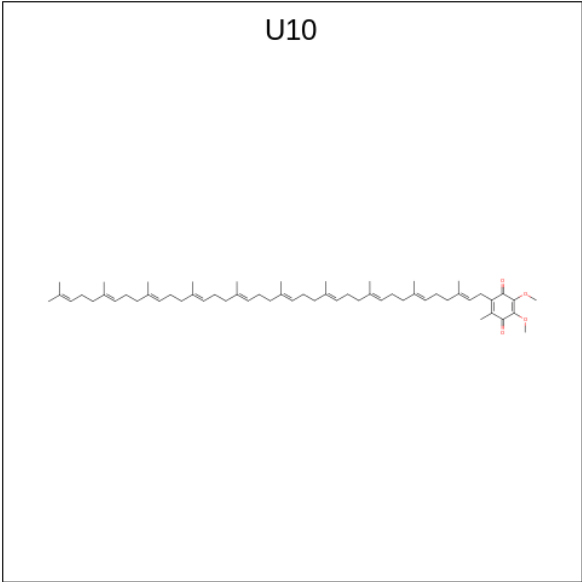
Mol	Chain	Residues	Atoms					AltConf
10	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
10	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 11 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



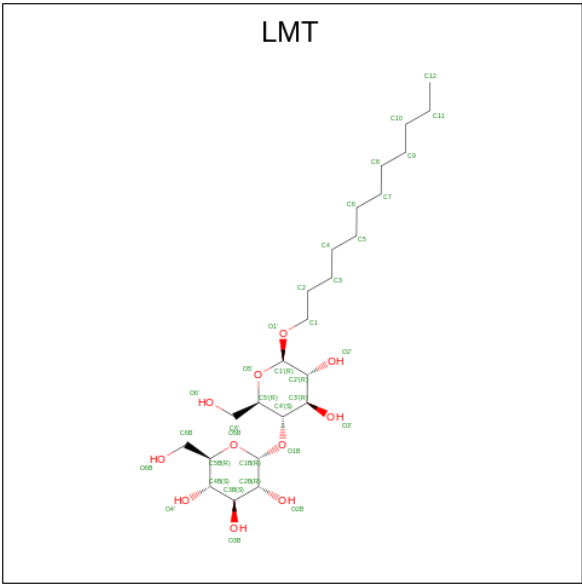
Mol	Chain	Residues	Atoms				AltConf
11	L	1	Total	C	N	O	0
			65	55	4	6	
11	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			36	32	4	
12	L	1	Total	C	O	0
			15	11	4	
12	L	1	Total	C	O	0
			35	31	4	
12	7	1	Total	C	O	0
			63	59	4	

- Molecule 13 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

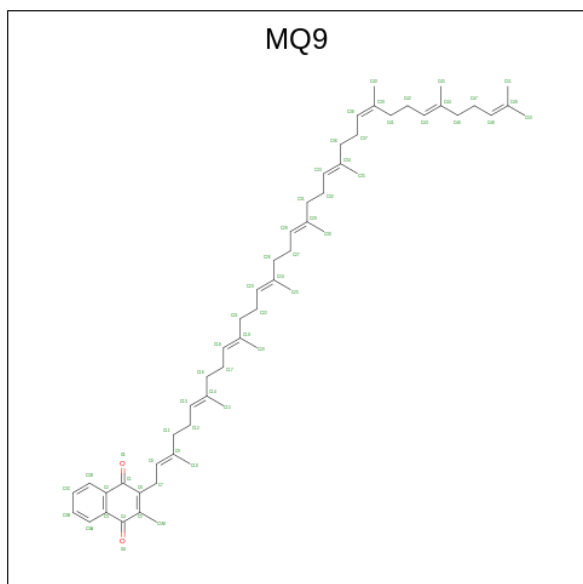


Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			30	19	11	
13	L	1	Total	C	O	0
			35	24	11	
13	I	1	Total	C	O	0
			33	22	11	
13	1	1	Total	C	O	0
			35	24	11	
13	3	1	Total	C	O	0
			31	20	11	

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe).

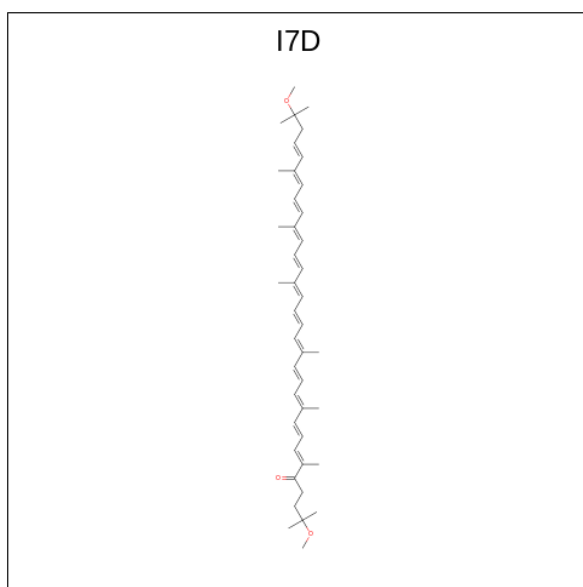
Mol	Chain	Residues	Atoms		AltConf
14	M	1	Total	Fe	0
			1	1	

- Molecule 15 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).



Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			39	37	2	

- Molecule 16 is (6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E},26 {E},28 {E})-2,31-dimethoxy-2,6,10,14,19,23,27,31-octamethyl-dotriaconta-6,8,10,12,14,16,18,20,22,24,26,28-dodecaen-5-one (CCD ID: I7D) (formula: C₄₂H₆₀O₃) (labeled as "Ligand of Interest" by depositor).



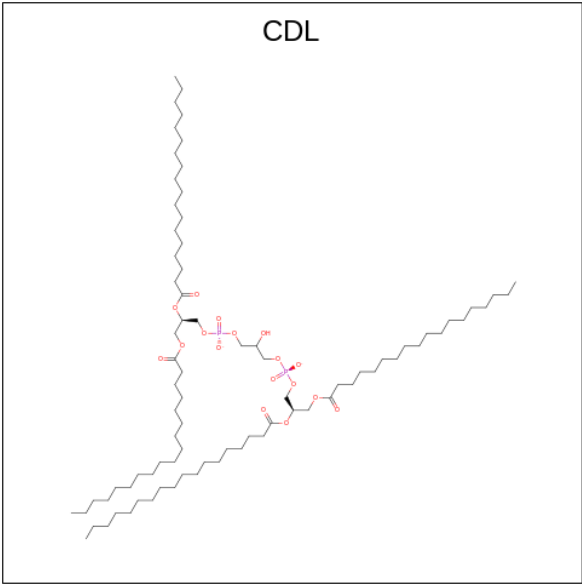
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			45	42	3	
16	A	1	Total	C	O	0
			45	42	3	
16	D	1	Total	C	O	0
			45	42	3	
16	E	1	Total	C	O	0
			45	42	3	
16	I	1	Total	C	O	0
			45	42	3	
16	K	1	Total	C	O	0
			45	42	3	
16	N	1	Total	C	O	0
			45	42	3	
16	Q	1	Total	C	O	0
			45	42	3	
16	R	1	Total	C	O	0
			45	42	3	
16	T	1	Total	C	O	0
			45	42	3	
16	V	1	Total	C	O	0
			45	42	3	
16	X	1	Total	C	O	0
			45	42	3	
16	1	1	Total	C	O	0
			45	42	3	
16	3	1	Total	C	O	0
			45	42	3	

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Mol	Chain	Residues	Atoms			AltConf
16	4	1	Total	C	O	0
			45	42	3	
16	6	1	Total	C	O	0
			45	42	3	
16	8	1	Total	C	O	0
			45	42	3	

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



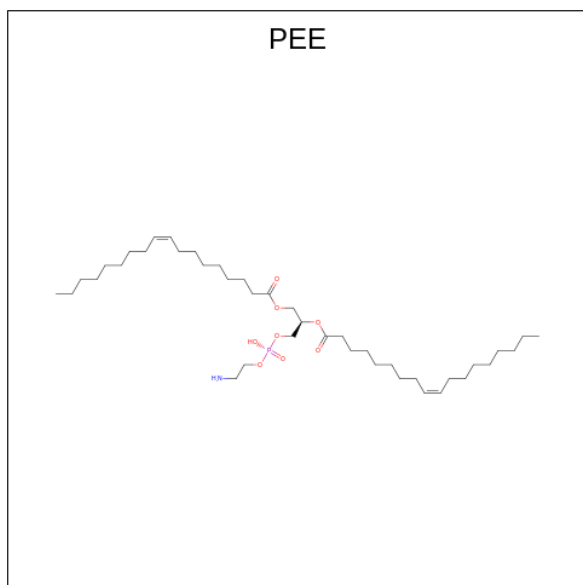
Mol	Chain	Residues	Atoms				AltConf
17	M	1	Total	C	O	P	0
			35	17	16	2	
17	M	1	Total	C	O	P	0
			69	50	17	2	
17	H	1	Total	C	O	P	0
			72	53	17	2	
17	A	1	Total	C	O	P	0
			58	39	17	2	
17	T	1	Total	C	O	P	0
			72	53	17	2	
17	2	1	Total	C	O	P	0
			72	53	17	2	
17	6	1	Total	C	O	P	0
			69	50	17	2	
17	6	1	Total	C	O	P	0
			63	44	17	2	

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Mol	Chain	Residues	Atoms				AltConf
17	0	1	Total	C	O	P	0
			63	44	17	2	

- Molecule 18 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
18	M	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	C	136	Total	O	0
			136	136	
19	L	65	Total	O	0
			65	65	
19	M	81	Total	O	0
			81	81	
19	H	81	Total	O	0
			81	81	
19	A	4	Total	O	0
			4	4	
19	B	7	Total	O	0
			7	7	
19	D	3	Total	O	0
			3	3	

Continued on next page...

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Mol	Chain	Residues	Atoms		AltConf
19	E	3	Total 3	O 3	0
19	F	4	Total 4	O 4	0
19	G	2	Total 2	O 2	0
19	I	6	Total 6	O 6	0
19	J	3	Total 3	O 3	0
19	K	3	Total 3	O 3	0
19	N	4	Total 4	O 4	0
19	O	7	Total 7	O 7	0
19	P	5	Total 5	O 5	0
19	Q	9	Total 9	O 9	0
19	R	12	Total 12	O 12	0
19	S	16	Total 16	O 16	0
19	T	6	Total 6	O 6	0
19	U	8	Total 8	O 8	0
19	V	5	Total 5	O 5	0
19	W	11	Total 11	O 11	0
19	X	3	Total 3	O 3	0
19	Y	6	Total 6	O 6	0
19	Z	3	Total 3	O 3	0
19	1	2	Total 2	O 2	0
19	2	4	Total 4	O 4	0

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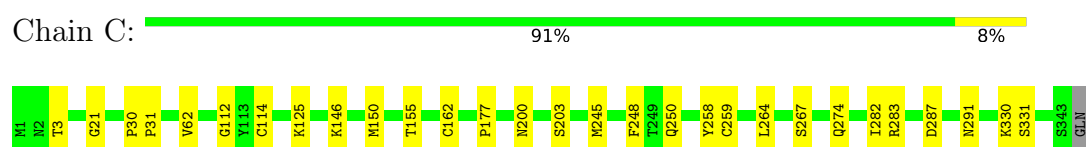
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
19	3	7	Total 7	O 7	0
19	4	7	Total 7	O 7	0
19	5	3	Total 3	O 3	0
19	6	4	Total 4	O 4	0
19	7	7	Total 7	O 7	0
19	8	2	Total 2	O 2	0
19	9	7	Total 7	O 7	0
19	0	1	Total 1	O 1	0
19	b	1	Total 1	O 1	0

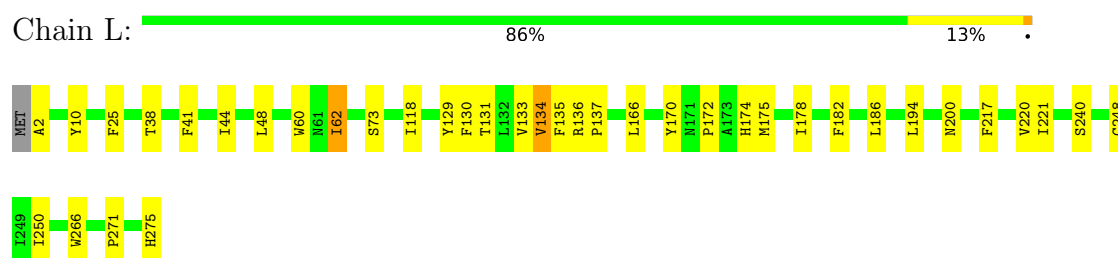
3 Residue-property plots

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

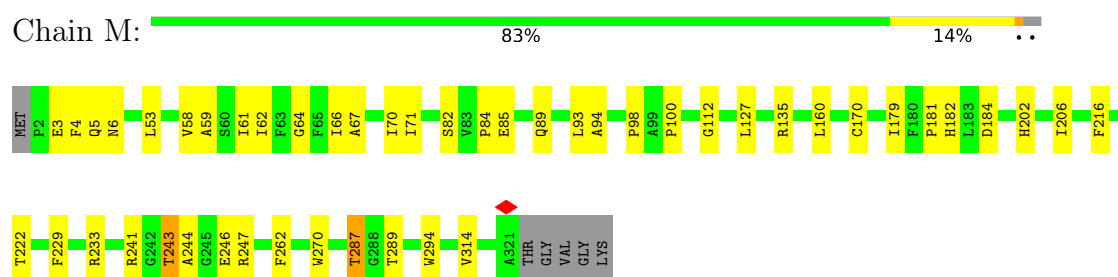
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



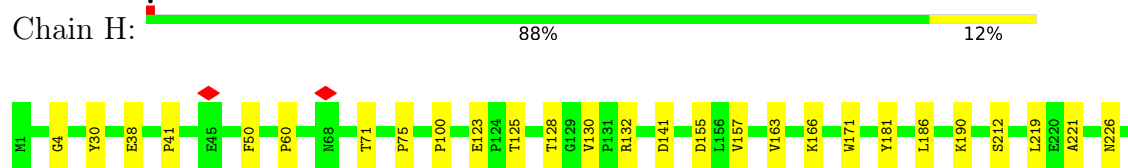
- Molecule 2: Reaction center protein L chain

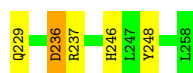


- Molecule 3: Reaction center protein M chain



- Molecule 4: Photosynthetic reaction center H subunit

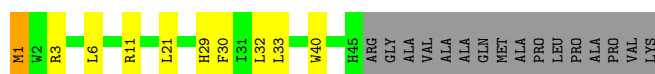




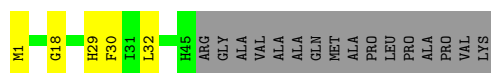
- Molecule 5: Light-harvesting protein



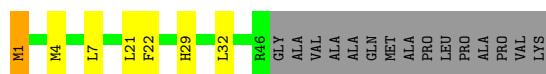
- Molecule 5: Light-harvesting protein



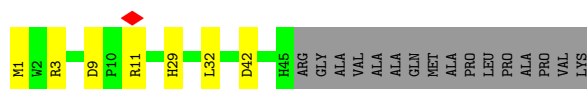
- Molecule 5: Light-harvesting protein



- Molecule 5: Light-harvesting protein



- Molecule 5: Light-harvesting protein

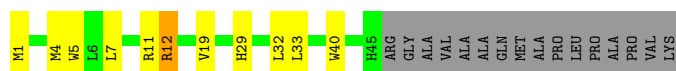


- Molecule 5: Light-harvesting protein

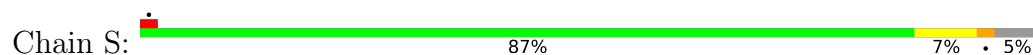


- Molecule 5: Light-harvesting protein

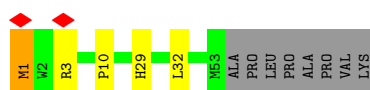
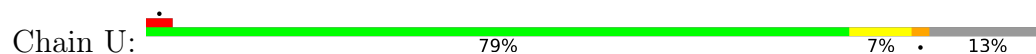




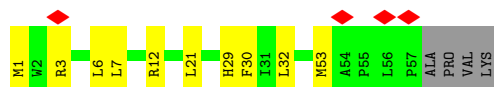
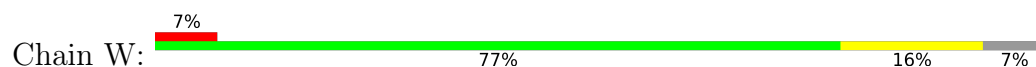
- Molecule 5: Light-harvesting protein



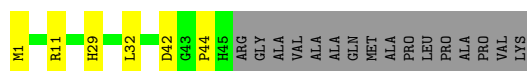
- Molecule 5: Light-harvesting protein



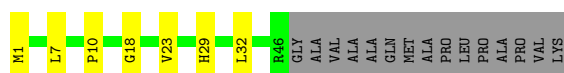
- Molecule 5: Light-harvesting protein



- Molecule 5: Light-harvesting protein



- Molecule 5: Light-harvesting protein

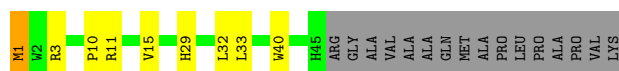


- Molecule 5: Light-harvesting protein

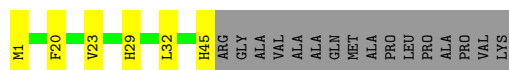


- Molecule 5: Light-harvesting protein

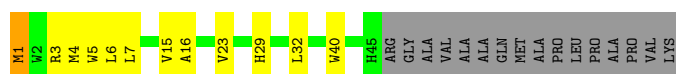




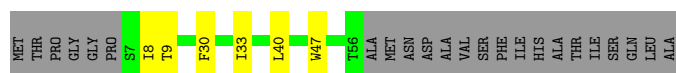
- Molecule 5: Light-harvesting protein



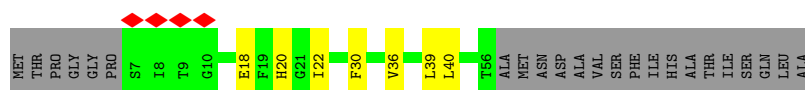
- Molecule 5: Light-harvesting protein



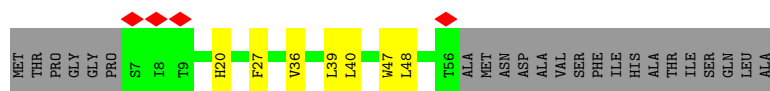
- Molecule 6: Light-harvesting protein



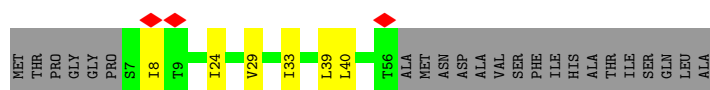
- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein

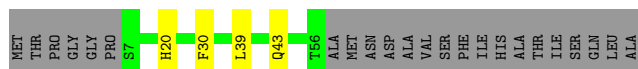


- Molecule 6: Light-harvesting protein





- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein



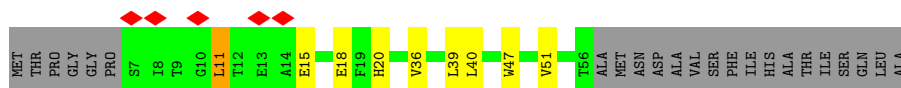
- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein



- Molecule 6: Light-harvesting protein



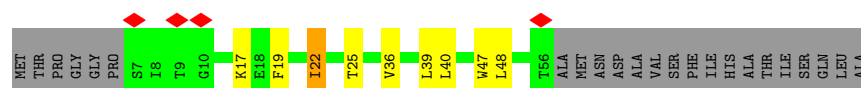
- Molecule 6: Light-harvesting protein



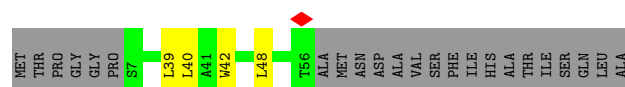
- Molecule 6: Light-harvesting protein



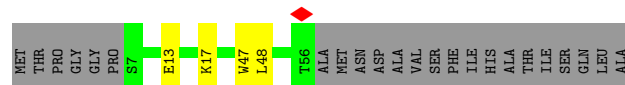
- Molecule 6: Light-harvesting protein



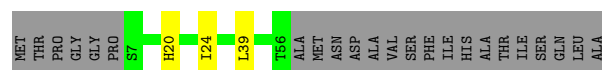
- Molecule 6: Light-harvesting protein



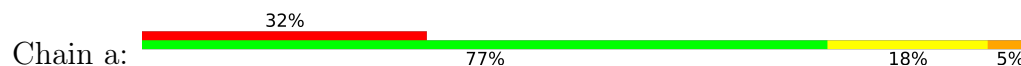
- Molecule 6: Light-harvesting protein



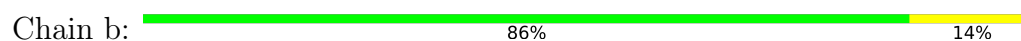
- Molecule 6: Light-harvesting protein



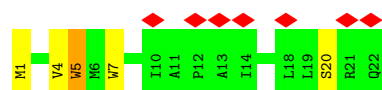
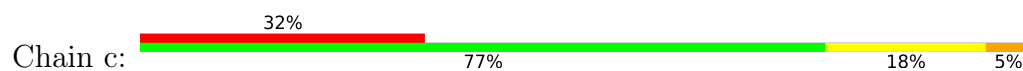
- Molecule 7: Light-harvesting protein LH1 Gamma-like



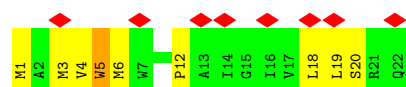
- Molecule 7: Light-harvesting protein LH1 Gamma-like



• Molecule 7: Light-harvesting protein LH1 Gamma-like



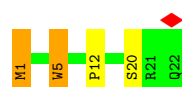
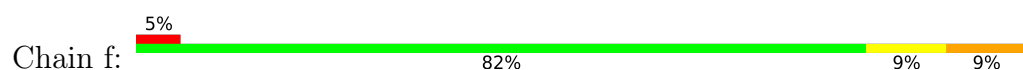
• Molecule 7: Light-harvesting protein LH1 Gamma-like



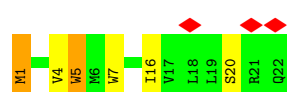
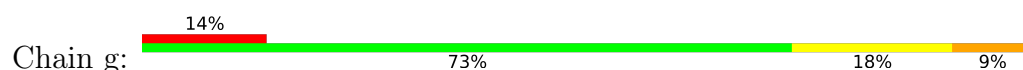
• Molecule 7: Light-harvesting protein LH1 Gamma-like



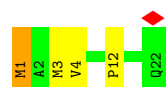
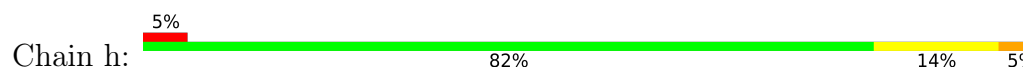
• Molecule 7: Light-harvesting protein LH1 Gamma-like



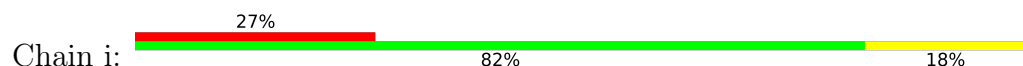
• Molecule 7: Light-harvesting protein LH1 Gamma-like

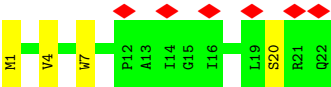


• Molecule 7: Light-harvesting protein LH1 Gamma-like

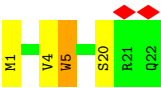
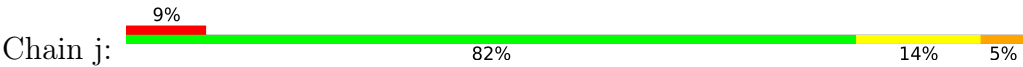


• Molecule 7: Light-harvesting protein LH1 Gamma-like





• Molecule 7: Light-harvesting protein LH1 Gamma-like



• Molecule 7: Light-harvesting protein LH1 Gamma-like



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128119	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.316	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, I7D, MQ9, LMT, CDL, FE, U10, PGV, FME, BCL, BPH, HEC

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	C	0.14	0/2730	0.28	0/3730
2	L	0.14	0/2266	0.30	0/3102
3	M	0.14	0/2652	0.29	0/3624
4	H	0.12	0/2053	0.27	0/2800
5	1	0.11	0/398	0.25	0/542
5	3	0.13	0/478	0.26	0/651
5	5	0.12	0/393	0.21	0/536
5	7	0.11	0/393	0.25	0/536
5	9	0.13	0/395	0.25	0/539
5	A	0.13	0/387	0.26	0/528
5	D	0.12	0/387	0.26	0/528
5	F	0.12	0/387	0.22	0/528
5	I	0.11	0/398	0.22	0/543
5	K	0.11	0/387	0.24	0/528
5	O	0.12	0/393	0.22	0/536
5	Q	0.13	0/393	0.25	0/536
5	S	0.12	0/481	0.24	0/657
5	U	0.13	0/447	0.28	0/608
5	W	0.11	0/476	0.24	0/650
5	Y	0.12	0/387	0.26	0/528
6	0	0.11	0/410	0.22	0/563
6	2	0.10	0/410	0.21	0/563
6	4	0.10	0/410	0.21	0/563
6	6	0.12	0/410	0.23	0/563
6	8	0.10	0/410	0.21	0/563
6	B	0.10	0/410	0.19	0/563
6	E	0.11	0/410	0.20	0/563
6	G	0.11	0/410	0.20	0/563
6	J	0.11	0/410	0.20	0/563
6	N	0.11	0/410	0.22	0/563
6	P	0.12	0/410	0.22	0/563
6	R	0.11	0/410	0.20	0/563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	T	0.11	0/410	0.22	0/563
6	V	0.10	0/410	0.21	0/563
6	X	0.12	0/410	0.24	0/563
6	Z	0.11	0/410	0.22	0/563
7	a	0.10	0/171	0.25	0/232
7	b	0.11	0/171	0.27	0/232
7	c	0.10	0/171	0.28	0/232
7	d	0.11	0/171	0.28	0/232
7	e	0.11	0/171	0.27	0/232
7	f	0.12	0/171	0.25	0/232
7	g	0.11	0/171	0.25	0/232
7	h	0.10	0/171	0.26	0/232
7	i	0.11	0/171	0.28	0/232
7	j	0.10	0/171	0.25	0/232
7	k	0.12	0/171	0.32	0/232
All	All	0.12	0/24722	0.26	0/33790

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2655	0	2591	26	0
2	L	2177	0	2130	34	0
3	M	2550	0	2503	38	0
4	H	2000	0	1985	20	0
5	1	395	0	409	6	0
5	3	472	0	491	12	0
5	5	389	0	401	7	0
5	7	389	0	401	7	0
5	9	392	0	406	10	0
5	A	384	0	396	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	384	0	396	10	0
5	F	384	0	396	4	0
5	I	394	0	403	8	0
5	K	384	0	396	6	0
5	O	389	0	401	9	0
5	Q	389	0	401	7	0
5	S	475	0	493	5	0
5	U	443	0	458	6	0
5	W	470	0	488	8	0
5	Y	384	0	396	4	0
6	0	396	0	394	3	0
6	2	396	0	394	9	0
6	4	396	0	394	7	0
6	6	396	0	394	4	0
6	8	396	0	394	4	0
6	B	396	0	394	7	0
6	E	396	0	394	8	0
6	G	396	0	394	9	0
6	J	396	0	394	7	0
6	N	396	0	394	11	0
6	P	396	0	394	6	0
6	R	396	0	394	3	0
6	T	396	0	394	5	0
6	V	396	0	394	4	0
6	X	396	0	394	8	0
6	Z	396	0	394	7	0
7	a	177	0	194	6	0
7	b	177	0	194	2	0
7	c	177	0	194	7	0
7	d	177	0	194	10	0
7	e	177	0	194	7	0
7	f	177	0	194	4	0
7	g	177	0	194	9	0
7	h	177	0	194	4	0
7	i	177	0	194	3	0
7	j	177	0	194	4	0
7	k	177	0	194	9	0
8	C	172	0	120	9	0
9	5	111	0	132	6	0
9	C	124	0	155	7	0
9	D	33	0	36	1	0
9	F	39	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	72	0	83	2	0
9	K	39	0	48	1	0
9	L	191	0	241	15	0
9	M	84	0	112	4	0
10	0	66	0	74	4	0
10	1	66	0	74	1	0
10	2	66	0	74	3	0
10	3	66	0	74	3	0
10	4	66	0	74	4	0
10	5	66	0	74	3	0
10	6	66	0	74	2	0
10	7	66	0	74	0	0
10	8	66	0	74	4	0
10	9	66	0	74	4	0
10	A	66	0	74	3	0
10	B	66	0	74	5	0
10	D	66	0	74	3	0
10	E	66	0	74	5	0
10	F	66	0	74	2	0
10	G	66	0	74	10	0
10	I	66	0	74	3	0
10	J	66	0	74	4	0
10	K	66	0	74	3	0
10	L	132	0	148	3	0
10	M	132	0	148	5	0
10	N	66	0	74	7	0
10	O	66	0	74	1	0
10	P	66	0	74	7	0
10	Q	66	0	74	1	0
10	R	66	0	74	6	0
10	S	66	0	74	1	0
10	T	66	0	74	3	0
10	U	66	0	74	1	0
10	V	66	0	74	3	0
10	W	66	0	74	1	0
10	X	66	0	74	6	0
10	Y	66	0	74	2	0
10	Z	66	0	74	5	0
11	L	65	0	76	4	0
11	M	65	0	76	9	0
12	7	63	0	90	9	0
12	L	86	0	98	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	35	0	46	1	0
13	3	31	0	35	8	0
13	I	33	0	39	3	0
13	L	65	0	79	4	0
14	M	1	0	0	0	0
15	M	39	0	47	3	0
16	1	45	0	0	0	0
16	3	45	0	0	0	0
16	4	45	0	0	0	0
16	6	45	0	0	1	0
16	8	45	0	0	0	0
16	A	45	0	0	0	0
16	D	45	0	0	0	0
16	E	45	0	0	0	0
16	I	45	0	0	0	0
16	K	45	0	0	0	0
16	M	45	0	0	0	0
16	N	45	0	0	0	0
16	Q	45	0	0	0	0
16	R	45	0	0	0	0
16	T	45	0	0	0	0
16	V	45	0	0	0	0
16	X	45	0	0	0	0
17	0	63	0	70	3	0
17	2	72	0	88	4	0
17	6	132	0	152	9	0
17	A	58	0	60	1	0
17	H	72	0	88	4	0
17	M	104	0	102	7	0
17	T	72	0	88	4	0
18	M	44	0	62	3	0
19	0	1	0	0	0	0
19	1	2	0	0	0	0
19	2	4	0	0	0	0
19	3	7	0	0	0	0
19	4	7	0	0	0	0
19	5	3	0	0	0	0
19	6	4	0	0	0	0
19	7	7	0	0	0	0
19	8	2	0	0	0	0
19	9	7	0	0	0	0
19	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	7	0	0	0	0
19	C	136	0	0	0	0
19	D	3	0	0	0	0
19	E	3	0	0	0	0
19	F	4	0	0	0	0
19	G	2	0	0	0	0
19	H	81	0	0	1	0
19	I	6	0	0	0	0
19	J	3	0	0	0	0
19	K	3	0	0	0	0
19	L	65	0	0	0	0
19	M	81	0	0	0	0
19	N	4	0	0	0	0
19	O	7	0	0	0	0
19	P	5	0	0	0	0
19	Q	9	0	0	0	0
19	R	12	0	0	0	0
19	S	16	0	0	0	0
19	T	6	0	0	0	0
19	U	8	0	0	0	0
19	V	5	0	0	0	0
19	W	11	0	0	0	0
19	X	3	0	0	0	0
19	Y	6	0	0	0	0
19	Z	3	0	0	0	0
19	b	1	0	0	0	0
All	All	29826	0	29312	395	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 7.

All (395) 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)
1:C:162:CYS:SG	8:C:402:HEC:CAC	2.01	1.46
1:C:114:CYS:SG	8:C:401:HEC:CAC	2.04	1.45
1:C:259:CYS:SG	8:C:403:HEC:CAC	2.04	1.45
2:L:2:ALA:N	9:L:311:PGV:H1	1.58	1.00
3:M:287:THR:HB	3:M:294:TRP:HE1	1.45	0.80
1:C:248:PHE:HZ	1:C:282:ILE:HD11	1.55	0.72
1:C:114:CYS:SG	8:C:401:HEC:C3C	2.78	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:CYS:SG	8:C:402:HEC:C3C	2.78	0.70
9:L:311:PGV:H012	5:A:15:VAL:HG21	1.73	0.69
9:M:410:PGV:H22	5:O:33:LEU:HD23	1.76	0.68
6:O:20:HIS:HE2	7:a:20:SER:HB3	1.57	0.68
1:C:259:CYS:SG	8:C:403:HEC:C3C	2.79	0.68
6:P:20:HIS:HE2	7:g:20:SER:HB3	1.59	0.68
6:E:20:HIS:HE2	7:c:20:SER:HB2	1.59	0.68
2:L:131:THR:HA	2:L:135:PHE:HB2	1.76	0.67
6:2:40:LEU:HB3	17:2:101:CDL:H532	1.76	0.67
4:H:190:LYS:NZ	4:H:221:ALA:O	2.28	0.66
2:L:62:ILE:HD11	9:L:304:PGV:H251	1.79	0.65
3:M:289:THR:HB	9:K:103:PGV:H241	1.77	0.65
3:M:243:THR:HG22	3:M:247:ARG:HE	1.61	0.65
6:G:20:HIS:HE2	7:d:20:SER:HB3	1.61	0.65
5:I:7:LEU:O	5:K:11:ARG:NH1	2.30	0.65
10:G:101:BCL:H91	10:G:101:BCL:H142	1.79	0.63
3:M:61:ILE:HG23	11:M:404:BPH:H102	1.81	0.63
5:3:31:ILE:HG12	9:5:103:PGV:H231	1.80	0.63
4:H:4:GLY:H	13:I:103:LMT:H2B	1.62	0.63
5:D:1:FME:HB3	7:c:20:SER:HA	1.81	0.62
5:I:1:FME:HE3	10:J:101:BCL:H18	1.81	0.62
3:M:243:THR:OG1	4:H:236:ASP:OD2	2.14	0.62
3:M:135:ARG:NH1	18:M:409:PEE:O2P	2.32	0.62
2:L:217:PHE:HA	2:L:220:VAL:HG22	1.81	0.61
17:6:101:CDL:H171	17:6:101:CDL:H352	1.82	0.61
9:C:407:PGV:H52	13:3:103:LMT:H21	1.81	0.61
13:I:103:LMT:O6B	5:K:42:ASP:OD2	2.17	0.61
9:C:405:PGV:H261	5:1:23:VAL:HG13	1.81	0.61
10:L:301:BCL:H2	11:L:302:BPH:HBB3	1.83	0.61
9:L:312:PGV:H41	9:L:312:PGV:H232	1.83	0.60
3:M:53:LEU:O	5:Q:12:ARG:NH2	2.34	0.60
11:M:404:BPH:HHC	11:M:404:BPH:HBB3	1.82	0.60
9:C:407:PGV:H271	9:C:407:PGV:H82	1.82	0.60
5:9:1:FME:HB2	7:a:20:SER:HA	1.82	0.60
4:H:155:ASP:OD1	4:H:166:LYS:NZ	2.35	0.60
10:R:102:BCL:H41	7:h:12:PRO:HB2	1.85	0.59
6:X:20:HIS:HE2	7:j:20:SER:HB2	1.67	0.59
1:C:21:GLY:HA2	13:1:103:LMT:H41	1.84	0.59
1:C:112:GLY:O	1:C:125:LYS:NZ	2.35	0.59
5:D:32:LEU:HD11	10:E:102:BCL:HHD	1.85	0.59
5:A:18:GLY:HA3	10:A:102:BCL:H121	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1:FME:HE3	10:E:102:BCL:H191	1.85	0.58
5:O:32:LEU:HD11	10:P:101:BCL:HHD	1.86	0.58
10:2:102:BCL:H172	7:k:16:ILE:HG12	1.85	0.58
1:C:203:SER:OG	3:M:184:ASP:OD2	2.18	0.58
3:M:4:PHE:HE1	17:M:407:CDL:HA21	1.69	0.58
1:C:162:CYS:SG	8:C:402:HEC:CBC	2.84	0.58
5:W:3:ARG:HG3	5:W:6:LEU:HD12	1.86	0.58
2:L:41:PHE:CE2	12:7:401:U10:H361	2.39	0.58
5:K:32:LEU:HD11	10:N:102:BCL:HHD	1.85	0.58
4:H:125:THR:OG1	4:H:128:THR:O	2.18	0.57
11:L:302:BPH:HBB3	11:L:302:BPH:HHC	1.85	0.57
13:3:103:LMT:H51	9:5:103:PGV:H261	1.85	0.57
2:L:275:HIS:NE2	3:M:85:GLU:OE2	2.32	0.57
5:O:7:LEU:HG	5:Q:11:ARG:HG2	1.86	0.57
5:7:32:LEU:HD11	10:8:102:BCL:HHD	1.87	0.57
1:C:3:THR:OG1	5:W:12:ARG:NH2	2.38	0.57
5:S:32:LEU:HD11	10:T:102:BCL:HHD	1.87	0.56
6:X:40:LEU:HD13	7:i:4:VAL:HA	1.88	0.56
7:h:1:FME:HCN	7:h:3:MET:HE1	1.87	0.56
5:F:29:HIS:CE1	10:G:101:BCL:HMD3	2.40	0.56
6:N:33:ILE:HG21	7:e:12:PRO:HG3	1.86	0.56
1:C:248:PHE:CZ	1:C:282:ILE:HD11	2.37	0.56
5:7:20:PHE:CD1	12:7:401:U10:H28	2.41	0.56
9:L:311:PGV:H31	17:H:303:CDL:HA61	1.88	0.55
10:N:102:BCL:H61	7:f:12:PRO:HB2	1.89	0.55
6:Z:40:LEU:HB3	7:j:4:VAL:HG22	1.88	0.55
6:E:20:HIS:NE2	7:c:20:SER:HB2	2.20	0.55
5:F:32:LEU:HD11	10:G:101:BCL:HHD	1.88	0.55
10:P:101:BCL:H111	6:R:30:PHE:HD1	1.72	0.55
6:J:33:ILE:HG21	7:d:12:PRO:HG3	1.87	0.55
10:M:403:BCL:H141	11:M:404:BPH:H2	1.89	0.55
5:Y:32:LEU:HD11	10:Z:101:BCL:HHD	1.87	0.55
5:1:7:LEU:HD12	6:2:8:ILE:HD11	1.88	0.55
13:L:308:LMT:H5B	13:L:308:LMT:H6D	1.88	0.55
3:M:3:GLU:O	3:M:5:GLN:NE2	2.40	0.55
3:M:241:ARG:NH1	4:H:38:GLU:OE1	2.38	0.54
17:6:101:CDL:H742	17:6:101:CDL:H322	1.90	0.54
3:M:85:GLU:OE1	3:M:89:GLN:NE2	2.38	0.54
3:M:64:GLY:HA3	11:M:404:BPH:H5C1	1.90	0.54
18:M:409:PEE:H5	5:O:11:ARG:HH12	1.55	0.54
10:R:102:BCL:H111	6:T:30:PHE:HD1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:21:LEU:HB3	10:S:101:BCL:H12	1.90	0.53
2:L:25:PHE:HZ	5:9:15:VAL:HG21	1.73	0.53
11:M:404:BPH:H202	5:S:19:VAL:HG13	1.89	0.53
5:5:32:LEU:HD11	10:6:103:BCL:HHD	1.89	0.53
2:L:200:ASN:HB3	17:M:408:CDL:HB22	1.91	0.53
5:A:29:HIS:CE1	10:B:101:BCL:HMD3	2.44	0.53
17:A:101:CDL:HB21	5:D:11:ARG:HD2	1.90	0.53
6:6:40:LEU:HB3	17:6:101:CDL:H542	1.91	0.53
6:N:39:LEU:HD23	7:f:5:TRP:HH2	1.74	0.52
3:M:67:ALA:O	3:M:71:ILE:HG12	2.09	0.52
2:L:73:SER:H	5:3:61:LYS:HZ1	1.56	0.52
5:3:7:LEU:HD21	5:5:10:PRO:HG2	1.91	0.52
5:3:32:LEU:HD11	10:4:102:BCL:HHD	1.92	0.52
5:7:29:HIS:CE1	10:8:102:BCL:HMD3	2.45	0.52
12:L:307:U10:H101	12:L:307:U10:H13	1.92	0.51
5:W:32:LEU:HD11	10:X:102:BCL:HHD	1.92	0.51
10:B:101:BCL:H142	6:E:30:PHE:HB2	1.92	0.51
6:2:44:TRP:HB2	17:2:101:CDL:H521	1.92	0.51
5:A:7:LEU:HD12	6:B:8:ILE:HD11	1.92	0.51
6:E:36:VAL:HA	6:E:39:LEU:HD12	1.92	0.51
6:8:13:GLU:OE2	6:8:17:LYS:NZ	2.30	0.51
2:L:38:THR:HA	12:7:401:U10:H301	1.93	0.51
6:6:42:TRP:CZ2	17:6:104:CDL:HA32	2.45	0.51
1:C:245:MET:HB3	8:C:403:HEC:C4B	2.41	0.51
6:8:48:LEU:HD13	17:0:101:CDL:H511	1.94	0.51
12:L:307:U10:H262	12:L:307:U10:H211	1.91	0.50
10:G:101:BCL:H41	7:d:12:PRO:HB2	1.93	0.50
11:M:404:BPH:HBC3	11:M:404:BPH:HHD	1.92	0.50
10:P:101:BCL:H121	7:g:16:ILE:HD11	1.93	0.50
2:L:10:TYR:OH	3:M:246:GLU:OE1	2.23	0.50
2:L:133:VAL:HG23	2:L:134:VAL:HG12	1.94	0.50
6:R:40:LEU:HD13	7:g:4:VAL:HA	1.93	0.50
2:L:240:SER:HB3	12:L:306:U10:H4M3	1.94	0.50
4:H:226:ASN:HD21	4:H:229:GLN:HG2	1.76	0.50
5:O:29:HIS:CE1	10:P:101:BCL:HMD1	2.46	0.50
5:U:3:ARG:NH1	6:X:18:GLU:OE2	2.44	0.50
6:Z:40:LEU:HD13	7:j:4:VAL:HA	1.93	0.50
5:7:20:PHE:HD1	12:7:401:U10:H28	1.77	0.50
5:1:32:LEU:HD11	10:2:102:BCL:HHD	1.94	0.50
5:D:3:ARG:HG3	5:D:6:LEU:HD12	1.94	0.49
5:Q:4:MET:HE3	5:Q:5:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:0:101:CDL:HA62	17:0:101:CDL:H121	1.93	0.49
17:M:408:CDL:H332	17:M:408:CDL:H731	1.93	0.49
7:k:11:ALA:HA	7:k:14:ILE:HG12	1.93	0.49
1:C:146:LYS:HB2	1:C:150:MET:HB2	1.95	0.49
9:C:407:PGV:H92	13:3:103:LMT:H62	1.94	0.49
2:L:2:ALA:N	9:L:311:PGV:O05	2.36	0.49
6:4:40:LEU:HD13	7:k:4:VAL:HA	1.95	0.49
6:6:48:LEU:HD13	17:6:104:CDL:H511	1.94	0.49
6:P:39:LEU:HD23	7:g:5:TRP:HH2	1.77	0.49
6:B:30:PHE:HB2	10:0:102:BCL:H142	1.95	0.49
5:Q:32:LEU:HD11	10:R:102:BCL:HHD	1.94	0.49
1:C:177:PRO:HB3	5:W:53:MET:HA	1.94	0.49
2:L:170:TYR:HA	2:L:175:MET:HE3	1.95	0.49
6:N:20:HIS:CE1	7:f:20:SER:HB3	2.48	0.49
5:7:20:PHE:HD1	12:7:401:U10:H33	1.77	0.49
3:M:58[B]:VAL:HG23	9:M:411:PGV:H252	1.95	0.49
6:X:39:LEU:HD23	7:j:5:TRP:HH2	1.77	0.49
10:X:102:BCL:H122	6:Z:30:PHE:HD1	1.78	0.49
13:3:103:LMT:H22	9:5:103:PGV:H261	1.95	0.49
7:k:6:MET:HG3	7:k:10:ILE:HD12	1.94	0.49
18:M:409:PEE:H54	5:O:19:VAL:HG11	1.95	0.48
2:L:174:HIS:CE1	2:L:178:ILE:HD11	2.48	0.48
3:M:94:ALA:HB2	3:M:181:PRO:HG2	1.94	0.48
6:T:27:PHE:HZ	10:T:102:BCL:H43	1.79	0.48
6:N:9:THR:HG22	6:N:11:LEU:HD13	1.94	0.48
10:4:102:BCL:H71	10:5:102:BCL:HMA2	1.96	0.48
2:L:130:PHE:O	2:L:134:VAL:HG13	2.13	0.48
10:P:101:BCL:H101	10:Q:102:BCL:H43	1.96	0.48
6:0:39:LEU:HD23	7:a:5:TRP:HH2	1.79	0.48
6:J:24:ILE:HG23	7:e:17:VAL:HG12	1.96	0.48
6:2:39:LEU:HD23	7:k:5:TRP:HH2	1.79	0.48
11:L:302:BPH:HHC	11:L:302:BPH:CBB	2.43	0.48
6:J:29:VAL:HG21	7:d:19:LEU:HD11	1.96	0.48
6:J:40:LEU:HD13	7:d:4:VAL:HA	1.96	0.48
10:X:102:BCL:H101	10:Y:101:BCL:H43	1.94	0.48
9:L:311:PGV:H31	17:H:303:CDL:HA31	1.95	0.48
3:M:233:ARG:NH2	4:H:123:GLU:OE1	2.41	0.48
6:J:8:ILE:HG21	5:K:11:ARG:HH22	1.79	0.48
10:G:101:BCL:H162	10:G:101:BCL:H192	1.67	0.47
5:3:29:HIS:CE1	10:4:102:BCL:HMD1	2.49	0.47
6:4:47:TRP:CE2	10:4:102:BCL:H2C	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:40:LEU:HD13	7:e:4:VAL:HA	1.96	0.47
5:A:11:ARG:HG2	5:9:7:LEU:HG	1.97	0.47
5:W:7:LEU:HG	5:Y:11:ARG:HG2	1.95	0.47
5:9:32:LEU:HD11	10:0:102:BCL:HHD	1.95	0.47
10:Z:101:BCL:H192	10:Z:101:BCL:H161	1.77	0.47
6:J:39:LEU:HD23	7:e:5:TRP:HH2	1.80	0.47
5:K:9:ASP:HA	6:N:9:THR:HG23	1.97	0.47
3:M:62:ILE:HG12	11:M:404:BPH:H193	1.97	0.47
10:N:102:BCL:H111	6:P:30:PHE:HD1	1.80	0.47
5:7:23:VAL:HG12	12:7:401:U10:H371	1.97	0.47
4:H:123:GLU:OE2	4:H:132:ARG:NH1	2.46	0.47
6:B:40:LEU:HB3	7:a:4:VAL:HG22	1.97	0.47
5:5:29:HIS:CE1	10:6:103:BCL:HMD1	2.49	0.47
5:7:20:PHE:CD1	12:7:401:U10:H33	2.50	0.47
1:C:264:LEU:HD23	1:C:267:SER:HB2	1.96	0.46
9:L:311:PGV:H252	5:9:16:ALA:HB2	1.97	0.46
5:D:33:LEU:HG	5:D:40:TRP:CH2	2.50	0.46
6:N:33:ILE:HD13	7:e:12:PRO:HA	1.97	0.46
6:4:22:ILE:HA	6:4:25:THR:HG22	1.97	0.46
4:H:60:PRO:HA	4:H:75:PRO:HD2	1.96	0.46
10:B:101:BCL:H152	7:b:16:ILE:HG12	1.96	0.46
10:X:102:BCL:H122	6:Z:30:PHE:CD1	2.51	0.46
5:U:1:FME:HB2	7:i:20:SER:HA	1.97	0.46
1:C:287:ASP:OD1	1:C:291:ASN:ND2	2.37	0.46
9:C:405:PGV:H131	2:L:250:ILE:HG21	1.97	0.46
13:L:308:LMT:H52	13:3:103:LMT:H31	1.97	0.46
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.97	0.46
5:I:21:LEU:HB3	10:I:102:BCL:H12	1.96	0.46
10:K:102:BCL:H61	10:K:102:BCL:H41	1.58	0.46
6:4:48:LEU:HD13	17:6:101:CDL:H531	1.96	0.46
6:6:39:LEU:HD23	17:6:104:CDL:H141	1.97	0.46
7:d:3:MET:HA	7:d:6:MET:HB2	1.98	0.46
6:N:29:VAL:HG21	7:e:19:LEU:HD21	1.96	0.46
6:G:39:LEU:HD23	7:d:5:TRP:HH2	1.81	0.46
5:U:29:HIS:CE1	10:V:102:BCL:HMD1	2.51	0.46
10:M:402:BCL:H13	10:M:402:BCL:H172	1.70	0.46
10:M:403:BCL:HAA2	10:M:403:BCL:HBD	1.98	0.46
5:S:1:FME:HB3	6:T:20:HIS:CE1	2.51	0.46
5:5:1:FME:O1	5:5:3:ARG:NH1	2.49	0.46
12:7:401:U10:H122	12:7:401:U10:H101	1.64	0.46
6:G:40:LEU:HD13	7:c:4:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:101:CDL:H311	17:6:101:CDL:H532	1.98	0.46
15:M:405:MQ9:H23	17:H:303:CDL:H751	1.98	0.45
5:U:32:LEU:HD11	10:V:102:BCL:HHD	1.98	0.45
6:X:11:LEU:HG	6:X:15:GLU:HG3	1.97	0.45
2:L:60:TRP:HB3	9:L:304:PGV:H212	1.98	0.45
13:I:103:LMT:H41	13:I:103:LMT:H72	1.66	0.45
6:B:33:ILE:HG21	7:a:12:PRO:HG3	1.99	0.45
10:P:101:BCL:H203	7:g:16:ILE:HG13	1.99	0.45
10:R:102:BCL:H112	7:h:12:PRO:HB3	1.97	0.45
2:L:194:LEU:HD22	2:L:217:PHE:CE2	2.51	0.45
17:M:408:CDL:H762	9:H:301:PGV:H231	1.99	0.45
2:L:131:THR:HG23	2:L:250:ILE:HD13	1.99	0.45
4:H:186:LEU:HD13	4:H:219:LEU:HA	1.97	0.45
6:E:39:LEU:HD23	7:c:5:TRP:HH2	1.80	0.45
5:I:29:HIS:CE1	10:J:101:BCL:HMD1	2.52	0.45
10:A:102:BCL:H61	10:A:102:BCL:H41	1.53	0.45
6:B:47:TRP:CE2	10:B:101:BCL:H2C	2.52	0.45
10:Z:101:BCL:H112	6:2:30:PHE:HD1	1.81	0.45
3:M:243:THR:CG2	3:M:247:ARG:HE	2.29	0.45
17:2:101:CDL:H182	17:2:101:CDL:H352	1.99	0.45
17:2:101:CDL:HA62	17:2:101:CDL:CB7	2.47	0.45
4:H:100:PRO:HG3	4:H:248:TYR:CZ	2.52	0.45
5:K:29:HIS:CE1	10:N:102:BCL:HMD1	2.52	0.45
5:Q:29:HIS:CE1	10:R:102:BCL:HMD1	2.52	0.45
1:C:62:VAL:HG23	1:C:330:LYS:HE2	1.99	0.45
5:S:29:HIS:CE1	10:T:102:BCL:HMD1	2.52	0.45
17:T:103:CDL:H521	6:V:44:TRP:HB2	1.99	0.44
4:H:157:VAL:HG22	4:H:163:VAL:HG22	2.00	0.44
6:G:36:VAL:HB	7:c:7:TRP:NE1	2.32	0.44
3:M:98:PRO:HA	3:M:112:GLY:HA3	2.00	0.44
6:E:40:LEU:HD13	7:b:4:VAL:HA	1.98	0.44
9:L:305:PGV:H52	9:5:101:PGV:H202	1.99	0.44
4:H:41:PRO:HB2	4:H:50:PHE:HB3	2.00	0.44
3:M:127:LEU:HD12	9:M:410:PGV:H183	2.00	0.44
3:M:206:ILE:HD13	10:M:402:BCL:HMD2	1.99	0.44
5:F:30:PHE:CE1	9:F:102:PGV:H31	2.53	0.44
10:K:102:BCL:H8	10:K:102:BCL:H122	1.80	0.44
3:M:179:ILE:O	3:M:182:HIS:ND1	2.44	0.44
6:Z:22:ILE:HA	6:Z:25:THR:HG22	2.00	0.44
1:C:258:TYR:OH	8:C:404:HEC:O1A	2.29	0.44
6:2:20:HIS:NE2	7:k:20:SER:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:PRO:HB2	13:3:103:LMT:H41	1.98	0.44
10:L:309:BCL:H151	10:L:309:BCL:H18	1.86	0.44
4:H:237:ARG:NH1	19:H:405:HOH:O	2.42	0.44
5:F:18:GLY:HA2	10:F:101:BCL:H61	1.99	0.43
6:P:20:HIS:NE2	7:g:20:SER:HB3	2.29	0.43
5:W:21:LEU:HB3	10:W:101:BCL:H12	1.99	0.43
3:M:160:LEU:HD21	10:M:403:BCL:OBD	2.18	0.43
5:A:1:FME:HE1	6:E:22:ILE:HG23	2.00	0.43
1:C:155:THR:HA	1:C:331:SER:HB2	1.99	0.43
5:3:22:PHE:HB2	10:3:102:BCL:H191	2.00	0.43
9:C:407:PGV:H72	13:3:103:LMT:H42	2.00	0.43
2:L:73:SER:N	5:3:61:LYS:HZ1	2.16	0.43
9:L:305:PGV:H71	9:5:101:PGV:H222	2.01	0.43
6:G:47:TRP:CE2	10:G:101:BCL:H2C	2.52	0.43
6:J:33:ILE:HD13	7:d:12:PRO:HA	1.99	0.43
5:U:1:FME:O1	5:U:3:ARG:NH1	2.52	0.43
7:g:1:FME:HB3	7:g:1:FME:HCN	1.79	0.43
12:L:307:U10:H102	12:L:307:U10:H1M1	2.01	0.43
6:N:47:TRP:CE2	10:N:102:BCL:H2C	2.54	0.43
5:3:10:PRO:HB3	6:4:19:PHE:CE1	2.54	0.43
5:9:40:TRP:CE3	10:9:101:BCL:HBC3	2.54	0.43
9:L:311:PGV:H262	17:H:303:CDL:H141	2.00	0.43
5:W:29:HIS:CE1	10:X:102:BCL:HMD1	2.54	0.43
5:3:53:MET:HE3	5:3:53:MET:HA	2.00	0.43
9:C:407:PGV:H202	9:C:407:PGV:H231	1.81	0.43
2:L:62:ILE:HD13	9:L:304:PGV:H52	2.01	0.43
10:G:101:BCL:H143	10:I:102:BCL:H51	2.00	0.43
6:T:40:LEU:HD13	7:h:4:VAL:HA	1.99	0.43
2:L:266:TRP:HA	13:L:313:LMT:H6'2	2.00	0.42
10:Y:101:BCL:H41	10:Y:101:BCL:H71	2.01	0.42
10:Z:101:BCL:H192	6:2:26:SER:HA	2.01	0.42
2:L:182:PHE:HB3	11:M:404:BPH:HBB2	2.00	0.42
11:L:302:BPH:HED1	15:M:405:MQ9:H18	2.01	0.42
15:M:405:MQ9:H312	15:M:405:MQ9:H272	1.89	0.42
12:7:401:U10:H351	12:7:401:U10:H372	1.61	0.42
10:8:102:BCL:H41	10:8:102:BCL:H61	1.55	0.42
5:9:4:MET:HE3	5:9:5:TRP:CZ2	2.54	0.42
10:O:101:BCL:H61	10:O:101:BCL:H41	1.65	0.42
5:1:29:HIS:CE1	10:2:102:BCL:HMD1	2.54	0.42
6:4:36:VAL:HB	7:k:7:TRP:NE1	2.34	0.42
9:M:410:PGV:H21	5:O:30:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:307:U10:H4M1	10:L:309:BCL:H191	2.01	0.42
3:M:89:GLN:O	3:M:93:LEU:HG	2.19	0.42
4:H:128:THR:C	4:H:130:VAL:H	2.28	0.42
6:Z:47:TRP:HD1	6:Z:48:LEU:HG	1.84	0.42
2:L:118:ILE:HD11	3:M:222:THR:HA	2.01	0.42
6:G:40:LEU:HB3	7:c:4:VAL:HG22	2.00	0.42
5:5:15:VAL:HA	10:5:102:BCL:H161	2.01	0.42
10:9:101:BCL:H3C	17:0:101:CDL:H561	2.01	0.42
9:L:312:PGV:H51	5:D:30:PHE:HD2	1.85	0.42
5:D:29:HIS:CE1	10:E:102:BCL:HMD1	2.54	0.42
5:D:33:LEU:HD23	5:D:33:LEU:HA	1.88	0.42
6:G:27:PHE:HZ	10:G:101:BCL:H43	1.84	0.42
17:T:103:CDL:H762	17:T:103:CDL:H362	2.01	0.42
5:1:10:PRO:HB3	6:2:19:PHE:CZ	2.55	0.42
6:2:28:ILE:HD11	7:k:17:VAL:CG2	2.49	0.42
2:L:172:PRO:HG2	12:L:307:U10:H202	2.02	0.42
5:A:32:LEU:HD11	10:B:101:BCL:HHD	2.01	0.42
5:O:1:FME:HB2	7:g:20:SER:HA	2.01	0.42
5:O:24:LEU:HD23	10:P:101:BCL:HED3	2.02	0.42
6:X:51:VAL:O	5:Y:44:PRO:HG3	2.20	0.42
5:3:7:LEU:O	5:5:11:ARG:HD2	2.20	0.42
6:4:39:LEU:HD23	17:6:101:CDL:H161	2.01	0.42
5:D:21:LEU:HD13	10:D:102:BCL:H42	2.02	0.42
10:R:102:BCL:H161	10:R:102:BCL:H122	1.73	0.42
5:1:18:GLY:HA3	10:1:102:BCL:H161	2.01	0.42
1:C:200:ASN:N	1:C:250:GLN:OE1	2.52	0.41
6:8:47:TRP:HD1	6:8:48:LEU:HG	1.85	0.41
10:D:102:BCL:H92	10:D:102:BCL:H61	1.82	0.41
3:M:100:PRO:HA	3:M:170:CYS:SG	2.60	0.41
5:I:32:LEU:HD11	10:J:101:BCL:HHD	2.02	0.41
10:K:102:BCL:H202	10:K:102:BCL:H162	1.74	0.41
5:Q:33:LEU:HG	5:Q:40:TRP:CH2	2.55	0.41
6:Z:11:LEU:HB3	6:Z:15:GLU:HG3	2.02	0.41
2:L:186:LEU:HD13	11:M:404:BPH:ND	2.36	0.41
2:L:194:LEU:HD22	2:L:217:PHE:HE2	1.85	0.41
3:M:270:TRP:HH2	17:M:408:CDL:H322	1.85	0.41
6:G:47:TRP:HD1	6:G:48:LEU:HG	1.84	0.41
5:I:4:MET:HE3	5:I:4:MET:HB2	1.89	0.41
10:N:102:BCL:H162	10:N:102:BCL:H192	1.75	0.41
1:C:31:PRO:HD3	13:3:103:LMT:H2'	2.03	0.41
4:H:141:ASP:OD1	4:H:141:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:40:LEU:HD13	7:a:4:VAL:HA	2.03	0.41
10:N:102:BCL:H111	6:P:30:PHE:CD1	2.55	0.41
6:P:43:GLN:HE21	7:f:1:FME:HE2	1.86	0.41
6:0:24:ILE:HD13	6:0:24:ILE:HA	1.88	0.41
7:d:18:LEU:HD23	7:d:18:LEU:HA	1.91	0.41
7:k:6:MET:HE2	7:k:6:MET:HB2	1.92	0.41
4:H:212:SER:HB3	4:H:246:HIS:CE1	2.56	0.41
10:G:101:BCL:H52	7:d:12:PRO:HB2	2.02	0.41
10:U:101:BCL:HBC3	10:U:101:BCL:H2C	1.89	0.41
6:X:47:TRP:CE2	10:X:102:BCL:H2C	2.56	0.41
10:3:102:BCL:H202	10:3:102:BCL:H162	1.78	0.41
1:C:283:ARG:HD2	1:C:283:ARG:N	2.36	0.41
2:L:129:TYR:O	2:L:133:VAL:HG22	2.20	0.41
2:L:271:PRO:HD3	13:L:313:LMT:H2'	2.03	0.41
3:M:4:PHE:CZ	3:M:6:ASN:HA	2.56	0.41
17:M:408:CDL:H511	4:H:30:TYR:CE2	2.56	0.41
5:A:3:ARG:NH2	6:E:18:GLU:OE2	2.47	0.41
5:9:29:HIS:CE1	10:0:102:BCL:HMD1	2.54	0.41
10:0:102:BCL:H162	10:0:102:BCL:H192	1.78	0.41
9:L:305:PGV:H012	3:M:5:GLN:OE1	2.20	0.41
9:D:103:PGV:H251	9:D:103:PGV:H222	1.95	0.41
5:I:21:LEU:HD22	10:J:101:BCL:HED1	2.03	0.41
5:U:10:PRO:HG2	6:V:11:LEU:HD11	2.03	0.41
5:5:33:LEU:HG	5:5:40:TRP:CH2	2.55	0.41
10:9:101:BCL:HAC2	10:9:101:BCL:HHD	1.87	0.41
2:L:136:ARG:HB3	2:L:137:PRO:HD3	2.03	0.41
2:L:217:PHE:O	2:L:221:ILE:HG22	2.20	0.41
3:M:66:ILE:O	3:M:70:ILE:HG12	2.21	0.41
10:G:101:BCL:H162	10:G:101:BCL:H122	1.86	0.41
5:I:22:PHE:HA	10:I:102:BCL:H11	2.02	0.41
6:N:36:VAL:HB	7:e:7:TRP:NE1	2.36	0.41
5:3:4:MET:HB3	16:6:102:I7D:C34	2.50	0.41
5:3:15:VAL:HG22	10:3:102:BCL:H141	2.03	0.41
6:8:48:LEU:HD21	10:9:101:BCL:HMC1	2.03	0.41
1:C:258:TYR:CE2	1:C:274:GLN:HG2	2.56	0.41
17:M:408:CDL:H572	9:H:301:PGV:H31	2.03	0.41
6:N:15:GLU:HA	6:N:18:GLU:HB2	2.03	0.41
10:8:102:BCL:H102	10:8:102:BCL:H13	1.84	0.41
2:L:44:ILE:HG22	5:9:23:VAL:HG11	2.03	0.40
3:M:84:PRO:HG3	5:W:30:PHE:CE1	2.56	0.40
5:Y:29:HIS:CE1	10:Z:101:BCL:HMD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5:101:PGV:H251	9:5:101:PGV:H62	2.04	0.40
3:M:59:ALA:HA	5:Q:19:VAL:HG11	2.03	0.40
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.03	0.40
10:E:102:BCL:H8	10:E:102:BCL:H51	1.76	0.40
6:X:36:VAL:HB	7:i:7:TRP:NE1	2.37	0.40
5:9:1:FME:O1	5:9:3:ARG:NH1	2.55	0.40
10:D:102:BCL:H8	10:D:102:BCL:H121	1.83	0.40
6:R:36:VAL:HB	7:g:7:TRP:NE1	2.37	0.40
6:T:42:TRP:CZ3	17:T:103:CDL:H332	2.57	0.40
10:E:102:BCL:H143	10:E:102:BCL:H111	1.84	0.40
6:G:47:TRP:CD1	6:G:48:LEU:HG	2.55	0.40
6:V:47:TRP:CE2	10:V:102:BCL:H2C	2.57	0.40
10:5:102:BCL:H2C	10:5:102:BCL:HBC3	1.86	0.40
3:M:82:SER:HB3	3:M:85:GLU:HB2	2.04	0.40
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.57	0.40
5:A:9:ASP:HA	6:B:9:THR:HG23	2.03	0.40
5:A:40:TRP:CE3	10:A:102:BCL:HBC3	2.56	0.40
10:F:101:BCL:HAC2	10:F:101:BCL:HHD	1.84	0.40
17:T:103:CDL:H572	6:V:37:ALA:HB1	2.03	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	C	341/344 (99%)	332 (97%)	9 (3%)	0	100	100
2	L	272/275 (99%)	268 (98%)	4 (2%)	0	100	100
3	M	319/326 (98%)	313 (98%)	6 (2%)	0	100	100
4	H	256/258 (99%)	248 (97%)	8 (3%)	0	100	100
5	1	44/61 (72%)	43 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	3	53/61 (87%)	52 (98%)	1 (2%)	0	100	100
5	5	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	7	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	9	44/61 (72%)	43 (98%)	1 (2%)	0	100	100
5	A	43/61 (70%)	41 (95%)	2 (5%)	0	100	100
5	D	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	F	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	I	44/61 (72%)	43 (98%)	1 (2%)	0	100	100
5	K	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	O	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	Q	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
5	S	56/61 (92%)	55 (98%)	1 (2%)	0	100	100
5	U	51/61 (84%)	49 (96%)	2 (4%)	0	100	100
5	W	55/61 (90%)	53 (96%)	2 (4%)	0	100	100
5	Y	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
6	0	48/73 (66%)	45 (94%)	3 (6%)	0	100	100
6	2	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	4	48/73 (66%)	45 (94%)	3 (6%)	0	100	100
6	6	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	8	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	B	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	E	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	G	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	J	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	N	48/73 (66%)	45 (94%)	3 (6%)	0	100	100
6	P	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	R	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	T	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	V	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	X	48/73 (66%)	46 (96%)	2 (4%)	0	100	100
6	Z	48/73 (66%)	46 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	a	20/22 (91%)	20 (100%)	0	0	100	100
7	b	20/22 (91%)	20 (100%)	0	0	100	100
7	c	20/22 (91%)	20 (100%)	0	0	100	100
7	d	20/22 (91%)	19 (95%)	1 (5%)	0	100	100
7	e	20/22 (91%)	20 (100%)	0	0	100	100
7	f	20/22 (91%)	20 (100%)	0	0	100	100
7	g	20/22 (91%)	20 (100%)	0	0	100	100
7	h	20/22 (91%)	19 (95%)	1 (5%)	0	100	100
7	i	20/22 (91%)	20 (100%)	0	0	100	100
7	j	20/22 (91%)	20 (100%)	0	0	100	100
7	k	20/22 (91%)	20 (100%)	0	0	100	100
All	All	2910/3589 (81%)	2827 (97%)	83 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	C	283/284 (100%)	283 (100%)	0	100	100
2	L	214/215 (100%)	209 (98%)	5 (2%)	44	53
3	M	251/254 (99%)	246 (98%)	5 (2%)	48	58
4	H	212/212 (100%)	210 (99%)	2 (1%)	70	78
5	1	40/50 (80%)	40 (100%)	0	100	100
5	3	48/50 (96%)	48 (100%)	0	100	100
5	5	40/50 (80%)	40 (100%)	0	100	100
5	7	40/50 (80%)	39 (98%)	1 (2%)	42	50
5	9	40/50 (80%)	38 (95%)	2 (5%)	22	22
5	A	39/50 (78%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	39/50 (78%)	39 (100%)	0	100	100
5	F	39/50 (78%)	39 (100%)	0	100	100
5	I	40/50 (80%)	40 (100%)	0	100	100
5	K	39/50 (78%)	38 (97%)	1 (3%)	40	48
5	O	40/50 (80%)	39 (98%)	1 (2%)	42	50
5	Q	40/50 (80%)	38 (95%)	2 (5%)	22	22
5	S	47/50 (94%)	47 (100%)	0	100	100
5	U	44/50 (88%)	44 (100%)	0	100	100
5	W	47/50 (94%)	47 (100%)	0	100	100
5	Y	39/50 (78%)	38 (97%)	1 (3%)	40	48
6	0	40/57 (70%)	40 (100%)	0	100	100
6	2	40/57 (70%)	40 (100%)	0	100	100
6	4	40/57 (70%)	38 (95%)	2 (5%)	22	22
6	6	40/57 (70%)	40 (100%)	0	100	100
6	8	40/57 (70%)	40 (100%)	0	100	100
6	B	40/57 (70%)	40 (100%)	0	100	100
6	E	40/57 (70%)	40 (100%)	0	100	100
6	G	40/57 (70%)	40 (100%)	0	100	100
6	J	40/57 (70%)	40 (100%)	0	100	100
6	N	40/57 (70%)	40 (100%)	0	100	100
6	P	40/57 (70%)	40 (100%)	0	100	100
6	R	40/57 (70%)	40 (100%)	0	100	100
6	T	40/57 (70%)	40 (100%)	0	100	100
6	V	40/57 (70%)	40 (100%)	0	100	100
6	X	40/57 (70%)	39 (98%)	1 (2%)	42	50
6	Z	40/57 (70%)	39 (98%)	1 (2%)	42	50
7	a	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	b	17/17 (100%)	17 (100%)	0	100	100
7	c	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	d	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	e	17/17 (100%)	16 (94%)	1 (6%)	18	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	f	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	g	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	h	17/17 (100%)	17 (100%)	0	100	100
7	i	17/17 (100%)	17 (100%)	0	100	100
7	j	17/17 (100%)	16 (94%)	1 (6%)	18	16
7	k	17/17 (100%)	15 (88%)	2 (12%)	5	2
All	All	2448/2864 (86%)	2415 (99%)	33 (1%)	59	71

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	48	LEU
2	L	62	ILE
2	L	134	VAL
2	L	166	LEU
2	L	248	CYS
3	M	216	PHE
3	M	243	THR
3	M	262	PHE
3	M	287	THR
3	M	314	VAL
4	H	71	THR
4	H	236	ASP
5	K	3	ARG
5	O	45	HIS
5	Q	7	LEU
5	Q	12	ARG
6	X	11	LEU
5	Y	42	ASP
6	Z	56	THR
6	4	17	LYS
6	4	22	ILE
5	7	45	HIS
5	9	6[A]	LEU
5	9	6[B]	LEU
7	a	5	TRP
7	c	5	TRP
7	d	5	TRP
7	e	5	TRP
7	f	5	TRP

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Mol	Chain	Res	Type
7	g	5	TRP
7	j	5	TRP
7	k	3	MET
7	k	5	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	321	ASN
2	L	214	ASN
4	H	69	GLN
4	H	229	GLN
4	H	246	HIS
4	H	251	GLN
6	G	43	GLN
6	J	43	GLN
6	N	20	HIS
6	N	43	GLN
6	P	43	GLN
6	R	43	GLN
6	Z	20	HIS
6	Z	43	GLN
6	8	43	GLN
7	c	22	GLN
7	g	22	GLN
7	h	22	GLN
7	k	22	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

27 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	$\# Z > 2$
5	FME	D	1	5	8,9,10	0.50	0	7,9,11	1.19	1 (14%)
7	FME	i	1	7	8,9,10	0.51	0	7,9,11	1.08	1 (14%)
7	FME	f	1	7	8,9,10	0.50	0	7,9,11	0.96	1 (14%)
5	FME	K	1	5	8,9,10	0.50	0	7,9,11	1.11	1 (14%)
5	FME	S	1	5	8,9,10	0.49	0	7,9,11	0.97	1 (14%)
5	FME	O	1	5	8,9,10	0.53	0	7,9,11	0.98	1 (14%)
7	FME	e	1	7	8,9,10	0.53	0	7,9,11	0.99	1 (14%)
5	FME	7	1	5	8,9,10	0.51	0	7,9,11	1.09	1 (14%)
7	FME	b	1	7	8,9,10	0.52	0	7,9,11	0.93	1 (14%)
5	FME	5	1	5	8,9,10	0.52	0	7,9,11	0.91	1 (14%)
7	FME	k	1	7	8,9,10	0.53	0	7,9,11	0.95	1 (14%)
5	FME	Q	1	5	8,9,10	0.46	0	7,9,11	1.22	1 (14%)
5	FME	3	1	5	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
7	FME	a	1	7	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
5	FME	A	1	5	8,9,10	0.49	0	7,9,11	0.98	1 (14%)
7	FME	c	1	7	8,9,10	0.52	0	7,9,11	1.18	1 (14%)
5	FME	Y	1	5	8,9,10	0.53	0	7,9,11	0.91	1 (14%)
7	FME	d	1	7	8,9,10	0.52	0	7,9,11	0.93	1 (14%)
7	FME	h	1	7	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
7	FME	j	1	7	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
5	FME	I	1	5	8,9,10	0.51	0	7,9,11	1.16	1 (14%)
5	FME	W	1	5	8,9,10	0.51	0	7,9,11	0.92	1 (14%)
7	FME	g	1	7	8,9,10	0.51	0	7,9,11	0.95	1 (14%)
5	FME	U	1	5	8,9,10	0.53	0	7,9,11	0.93	1 (14%)
5	FME	9	1	5	8,9,10	0.49	0	7,9,11	0.94	1 (14%)
5	FME	F	1	5	8,9,10	0.52	0	7,9,11	0.97	1 (14%)
5	FME	1	1	5	8,9,10	0.50	0	7,9,11	1.08	1 (14%)

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
5	FME	D	1	5	-	1/7/9/11	-
7	FME	i	1	7	-	0/7/9/11	-
7	FME	f	1	7	-	1/7/9/11	-
5	FME	K	1	5	-	3/7/9/11	-
5	FME	S	1	5	-	1/7/9/11	-
5	FME	O	1	5	-	0/7/9/11	-
7	FME	e	1	7	-	1/7/9/11	-
5	FME	7	1	5	-	4/7/9/11	-
7	FME	b	1	7	-	3/7/9/11	-
5	FME	5	1	5	-	3/7/9/11	-
7	FME	k	1	7	-	0/7/9/11	-
5	FME	Q	1	5	-	1/7/9/11	-
5	FME	3	1	5	-	0/7/9/11	-
7	FME	a	1	7	-	3/7/9/11	-
5	FME	A	1	5	-	1/7/9/11	-
7	FME	c	1	7	-	2/7/9/11	-
5	FME	Y	1	5	-	2/7/9/11	-
7	FME	d	1	7	-	2/7/9/11	-
7	FME	h	1	7	-	2/7/9/11	-
7	FME	j	1	7	-	1/7/9/11	-
5	FME	I	1	5	-	0/7/9/11	-
5	FME	W	1	5	-	2/7/9/11	-
7	FME	g	1	7	-	4/7/9/11	-
5	FME	U	1	5	-	1/7/9/11	-
5	FME	9	1	5	-	1/7/9/11	-
5	FME	F	1	5	-	1/7/9/11	-
5	FME	1	1	5	-	2/7/9/11	-

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	1	FME	O-C-CA	-2.84	117.33	124.78
5	D	1	FME	O-C-CA	-2.76	117.54	124.78
5	I	1	FME	O-C-CA	-2.75	117.58	124.78
5	K	1	FME	O-C-CA	-2.67	117.79	124.78
5	1	1	FME	O-C-CA	-2.64	117.86	124.78
5	7	1	FME	O-C-CA	-2.63	117.88	124.78
7	i	1	FME	O-C-CA	-2.60	117.95	124.78
7	j	1	FME	O-C-CA	-2.58	118.02	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	1	FME	O-C-CA	-2.50	118.24	124.78
5	3	1	FME	O-C-CA	-2.49	118.24	124.78
7	h	1	FME	O-C-CA	-2.49	118.25	124.78
5	O	1	FME	O-C-CA	-2.49	118.25	124.78
5	A	1	FME	O-C-CA	-2.48	118.28	124.78
7	e	1	FME	O-C-CA	-2.45	118.36	124.78
5	F	1	FME	O-C-CA	-2.45	118.36	124.78
7	g	1	FME	O-C-CA	-2.44	118.38	124.78
5	S	1	FME	O-C-CA	-2.43	118.42	124.78
7	d	1	FME	O-C-CA	-2.41	118.47	124.78
5	9	1	FME	O-C-CA	-2.39	118.51	124.78
5	U	1	FME	O-C-CA	-2.38	118.54	124.78
7	k	1	FME	O-C-CA	-2.37	118.56	124.78
7	b	1	FME	O-C-CA	-2.36	118.59	124.78
7	f	1	FME	O-C-CA	-2.35	118.62	124.78
5	W	1	FME	O-C-CA	-2.34	118.64	124.78
7	c	1	FME	O-C-CA	-2.32	118.69	124.78
5	Y	1	FME	O-C-CA	-2.32	118.69	124.78
5	5	1	FME	O-C-CA	-2.23	118.93	124.78

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	FME	O1-CN-N-CA
5	K	1	FME	CB-CA-N-CN
5	U	1	FME	O1-CN-N-CA
5	Y	1	FME	O1-CN-N-CA
5	Y	1	FME	CB-CA-N-CN
5	1	1	FME	O1-CN-N-CA
5	1	1	FME	CB-CA-N-CN
5	5	1	FME	O1-CN-N-CA
5	7	1	FME	O1-CN-N-CA
5	7	1	FME	C-CA-CB-CG
5	9	1	FME	O1-CN-N-CA
7	a	1	FME	O1-CN-N-CA
7	a	1	FME	CB-CA-N-CN
7	a	1	FME	C-CA-CB-CG
7	b	1	FME	O1-CN-N-CA
7	b	1	FME	CB-CA-N-CN
7	c	1	FME	CB-CA-N-CN
7	d	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
7	d	1	FME	O-C-CA-CB
7	e	1	FME	O1-CN-N-CA
7	f	1	FME	O1-CN-N-CA
7	g	1	FME	O1-CN-N-CA
7	g	1	FME	CB-CA-N-CN
7	g	1	FME	O-C-CA-CB
7	h	1	FME	O1-CN-N-CA
7	h	1	FME	O-C-CA-CB
5	5	1	FME	N-CA-CB-CG
5	D	1	FME	C-CA-CB-CG
5	Q	1	FME	C-CA-CB-CG
5	W	1	FME	N-CA-CB-CG
5	5	1	FME	CB-CG-SD-CE
5	S	1	FME	N-CA-CB-CG
7	b	1	FME	N-CA-CB-CG
5	F	1	FME	N-CA-CB-CG
5	K	1	FME	C-CA-CB-CG
5	7	1	FME	N-CA-CB-CG
7	c	1	FME	N-CA-CB-CG
7	g	1	FME	C-CA-CB-CG
5	A	1	FME	CA-CB-CG-SD
5	W	1	FME	CB-CA-N-CN
5	7	1	FME	CB-CA-N-CN
7	j	1	FME	CB-CA-N-CN

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1	FME	2	0
7	f	1	FME	1	0
5	S	1	FME	1	0
5	O	1	FME	1	0
5	5	1	FME	1	0
5	A	1	FME	1	0
7	h	1	FME	1	0
5	I	1	FME	1	0
7	g	1	FME	1	0
5	U	1	FME	2	0
5	9	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 98 ligands modelled in this entry, 1 is monoatomic - leaving 97 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
9	PGV	L	304	-	42,42,50	0.96	2 (4%)	45,48,56	1.14	4 (8%)
10	BCL	E	102	6	69,74,74	1.78	17 (24%)	83,115,115	2.50	24 (28%)
12	U10	L	307	-	35,35,63	0.79	2 (5%)	42,45,79	0.71	0
13	LMT	L	308	-	31,31,36	0.38	0	42,42,47	0.68	0
10	BCL	U	101	5	69,74,74	1.79	17 (24%)	83,115,115	2.51	25 (30%)
16	I7D	M	406	-	43,44,44	1.95	11 (25%)	51,56,56	1.74	8 (15%)
16	I7D	K	101	-	43,44,44	1.97	10 (23%)	51,56,56	1.85	11 (21%)
9	PGV	H	301	-	35,35,50	1.10	2 (5%)	38,41,56	1.17	3 (7%)
16	I7D	V	101	-	43,44,44	1.98	10 (23%)	51,56,56	1.84	11 (21%)
17	CDL	T	103	-	71,71,99	1.08	4 (5%)	77,83,111	1.15	6 (7%)
10	BCL	L	309	3	69,74,74	1.77	17 (24%)	83,115,115	2.50	26 (31%)
8	HEC	C	404	1	50,50,50	1.76	10 (20%)	68,82,82	1.77	16 (23%)
9	PGV	H	302	-	35,35,50	1.08	2 (5%)	38,41,56	1.18	4 (10%)
10	BCL	6	103	6	69,74,74	1.79	18 (26%)	83,115,115	2.46	24 (28%)
10	BCL	9	101	5	69,74,74	1.79	18 (26%)	83,115,115	2.52	25 (30%)
9	PGV	M	410	-	50,50,50	0.90	2 (4%)	53,56,56	1.06	3 (5%)
10	BCL	W	101	5	69,74,74	1.79	18 (26%)	83,115,115	2.56	25 (30%)
16	I7D	6	102	-	43,44,44	2.04	10 (23%)	51,56,56	2.00	13 (25%)
9	PGV	C	405	-	43,43,50	1.00	2 (4%)	45,49,56	1.12	3 (6%)
10	BCL	5	102	5	69,74,74	1.80	17 (24%)	83,115,115	2.54	25 (30%)
10	BCL	0	102	6	69,74,74	1.78	18 (26%)	83,115,115	2.43	25 (30%)
16	I7D	R	101	-	43,44,44	1.99	10 (23%)	51,56,56	1.86	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PGV	M	411	-	32,32,50	1.14	2 (6%)	35,38,56	1.22	3 (8%)
13	LMT	I	103	-	34,34,36	0.38	0	45,45,47	0.74	1 (2%)
16	I7D	X	101	-	43,44,44	2.03	10 (23%)	51,56,56	1.94	11 (21%)
13	LMT	L	313	-	36,36,36	0.36	0	47,47,47	0.74	2 (4%)
17	CDL	0	101	-	62,62,99	1.16	4 (6%)	68,74,111	1.18	6 (8%)
10	BCL	Z	101	6	69,74,74	1.78	18 (26%)	83,115,115	2.46	24 (28%)
10	BCL	L	301	2	69,74,74	1.78	16 (23%)	83,115,115	2.51	26 (31%)
16	I7D	Q	101	-	43,44,44	1.97	10 (23%)	51,56,56	1.84	11 (21%)
16	I7D	A	103	-	43,44,44	1.97	10 (23%)	51,56,56	1.89	11 (21%)
9	PGV	C	406	-	41,41,50	1.02	2 (4%)	44,47,56	1.20	3 (6%)
15	MQ9	M	405	-	40,40,59	0.40	0	49,52,75	0.38	0
10	BCL	V	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.45	25 (30%)
16	I7D	N	101	-	43,44,44	1.98	10 (23%)	51,56,56	1.90	13 (25%)
12	U10	L	303	-	36,36,63	0.77	2 (5%)	43,46,79	0.58	0
17	CDL	H	303	-	71,71,99	1.08	4 (5%)	77,83,111	1.08	5 (6%)
10	BCL	R	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.50	26 (31%)
16	I7D	3	101	-	43,44,44	1.98	10 (23%)	51,56,56	1.86	11 (21%)
10	BCL	M	402	2	69,74,74	1.79	18 (26%)	83,115,115	2.46	24 (28%)
10	BCL	P	101	6	69,74,74	1.76	18 (26%)	83,115,115	2.46	25 (30%)
9	PGV	5	104	-	36,36,50	1.08	2 (5%)	39,42,56	1.01	2 (5%)
16	I7D	D	101	-	43,44,44	1.96	11 (25%)	51,56,56	1.84	11 (21%)
17	CDL	A	101	-	57,57,99	1.12	4 (7%)	63,69,111	1.27	7 (11%)
10	BCL	N	102	6	69,74,74	1.78	17 (24%)	83,115,115	2.50	25 (30%)
18	PEE	M	409	-	43,43,50	0.78	2 (4%)	46,48,55	0.57	0
9	PGV	L	310	-	36,36,50	1.07	2 (5%)	39,42,56	1.12	3 (7%)
10	BCL	S	101	5	69,74,74	1.80	17 (24%)	83,115,115	2.58	25 (30%)
9	PGV	D	103	-	32,32,50	1.13	2 (6%)	35,38,56	1.20	3 (8%)
16	I7D	8	101	-	43,44,44	2.01	10 (23%)	51,56,56	2.27	14 (27%)
9	PGV	5	103	-	36,36,50	1.07	2 (5%)	39,41,56	1.10	3 (7%)
9	PGV	C	407	-	37,37,50	1.09	2 (5%)	41,42,56	1.22	4 (9%)
10	BCL	G	101	6	69,74,74	1.77	17 (24%)	83,115,115	2.46	25 (30%)
10	BCL	O	101	5	69,74,74	1.79	17 (24%)	83,115,115	2.63	27 (32%)
10	BCL	8	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.45	26 (31%)
10	BCL	K	102	5	69,74,74	1.79	18 (26%)	83,115,115	2.57	26 (31%)
8	HEC	C	402	1	50,50,50	1.75	11 (22%)	68,82,82	1.78	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	I7D	4	101	-	43,44,44	1.99	10 (23%)	51,56,56	1.85	12 (23%)
10	BCL	Q	102	5	69,74,74	1.78	18 (26%)	83,115,115	2.55	24 (28%)
10	BCL	Y	101	5	69,74,74	1.80	16 (23%)	83,115,115	2.55	24 (28%)
8	HEC	C	403	1	50,50,50	1.78	10 (20%)	68,82,82	1.77	17 (25%)
10	BCL	4	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.50	26 (31%)
10	BCL	1	102	5	69,74,74	1.77	17 (24%)	83,115,115	2.59	28 (33%)
10	BCL	B	101	6	69,74,74	1.78	18 (26%)	83,115,115	2.47	24 (28%)
16	I7D	I	101	-	43,44,44	2.01	10 (23%)	51,56,56	1.87	11 (21%)
10	BCL	7	402	5	69,74,74	1.78	17 (24%)	83,115,115	2.51	24 (28%)
9	PGV	F	102	-	38,38,50	1.05	2 (5%)	41,43,56	1.01	2 (4%)
10	BCL	A	102	5	69,74,74	1.80	16 (23%)	83,115,115	2.52	24 (28%)
9	PGV	5	101	-	36,36,50	1.08	2 (5%)	39,41,56	1.18	4 (10%)
10	BCL	F	101	5	69,74,74	1.78	18 (26%)	83,115,115	2.59	26 (31%)
10	BCL	M	403	3	69,74,74	1.78	17 (24%)	83,115,115	2.56	25 (30%)
10	BCL	D	102	5	69,74,74	1.80	17 (24%)	83,115,115	2.55	25 (30%)
11	BPH	M	404	-	59,70,70	0.76	3 (5%)	61,101,101	0.93	2 (3%)
13	LMT	1	103	-	36,36,36	0.37	0	47,47,47	0.74	1 (2%)
10	BCL	I	102	5	69,74,74	1.79	18 (26%)	83,115,115	2.57	26 (31%)
10	BCL	2	102	6	69,74,74	1.77	17 (24%)	83,115,115	2.47	25 (30%)
10	BCL	J	101	6	69,74,74	1.77	18 (26%)	83,115,115	2.44	24 (28%)
17	CDL	6	104	-	62,62,99	1.16	4 (6%)	68,74,111	1.26	6 (8%)
11	BPH	L	302	-	59,70,70	0.77	2 (3%)	61,101,101	0.91	2 (3%)
16	I7D	1	101	-	43,44,44	2.03	10 (23%)	51,56,56	1.89	12 (23%)
17	CDL	2	101	-	71,71,99	1.10	4 (5%)	77,83,111	1.08	5 (6%)
9	PGV	K	103	-	38,38,50	1.06	2 (5%)	41,44,56	1.04	2 (4%)
10	BCL	3	102	5	69,74,74	1.79	18 (26%)	83,115,115	2.51	27 (32%)
8	HEC	C	401	1	50,50,50	1.77	11 (22%)	68,82,82	1.81	21 (30%)
12	U10	7	401	-	63,63,63	0.59	2 (3%)	76,79,79	0.54	0
17	CDL	M	407	-	34,34,99	1.42	3 (8%)	39,45,111	1.49	5 (12%)
13	LMT	3	103	-	32,32,36	0.40	0	43,43,47	0.85	1 (2%)
16	I7D	T	101	-	43,44,44	1.99	11 (25%)	51,56,56	1.91	12 (23%)
10	BCL	X	102	6	69,74,74	1.78	17 (24%)	83,115,115	2.48	24 (28%)
10	BCL	T	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.45	24 (28%)
12	U10	L	306	-	15,15,63	1.15	2 (13%)	19,21,79	0.87	0
9	PGV	L	311	-	32,32,50	1.15	2 (6%)	35,38,56	1.27	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PGV	L	312	-	33,33,50	1.11	2 (6%)	36,39,56	1.22	3 (8%)
17	CDL	6	101	-	68,68,99	1.12	4 (5%)	74,80,111	1.11	5 (6%)
9	PGV	L	305	-	43,43,50	0.97	2 (4%)	46,49,56	1.01	2 (4%)
16	I7D	E	101	-	43,44,44	2.00	10 (23%)	51,56,56	1.88	11 (21%)
17	CDL	M	408	-	68,68,99	1.10	4 (5%)	74,80,111	1.09	4 (5%)

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
9	PGV	L	304	-	-	15/47/47/55	-
10	BCL	E	102	6	-	17/41/137/137	-
12	U10	L	307	-	-	3/30/54/87	0/1/1/1
13	LMT	L	308	-	-	4/16/56/61	0/2/2/2
10	BCL	U	101	5	-	10/41/137/137	-
16	I7D	M	406	-	-	3/54/54/54	-
16	I7D	K	101	-	-	6/54/54/54	-
9	PGV	H	301	-	-	10/40/40/55	-
16	I7D	V	101	-	-	6/54/54/54	-
17	CDL	T	103	-	-	25/82/82/110	-
10	BCL	L	309	3	-	15/41/137/137	-
8	HEC	C	404	1	1/1/3/7	6/14/54/54	-
9	PGV	H	302	-	-	13/40/40/55	-
10	BCL	6	103	6	-	8/41/137/137	-
10	BCL	9	101	5	-	13/41/137/137	-
9	PGV	M	410	-	-	15/55/55/55	-
10	BCL	W	101	5	-	10/41/137/137	-
16	I7D	6	102	-	-	2/54/54/54	-
9	PGV	C	405	-	-	6/48/48/55	-
10	BCL	5	102	5	-	12/41/137/137	-
10	BCL	0	102	6	-	17/41/137/137	-
16	I7D	R	101	-	-	1/54/54/54	-
9	PGV	M	411	-	-	11/37/37/55	-
13	LMT	I	103	-	-	9/19/59/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	I7D	X	101	-	-	5/54/54/54	-
13	LMT	L	313	-	-	4/21/61/61	0/2/2/2
17	CDL	0	101	-	-	32/73/73/110	-
10	BCL	Z	101	6	-	15/41/137/137	-
10	BCL	L	301	2	-	9/41/137/137	-
16	I7D	Q	101	-	-	4/54/54/54	-
16	I7D	A	103	-	-	4/54/54/54	-
9	PGV	C	406	-	-	14/46/46/55	-
15	MQ9	M	405	-	-	0/31/51/73	0/2/2/2
10	BCL	V	102	6	-	13/41/137/137	-
16	I7D	N	101	-	-	8/54/54/54	-
12	U10	L	303	-	-	5/31/55/87	0/1/1/1
17	CDL	H	303	-	-	31/82/82/110	-
10	BCL	R	102	6	-	13/41/137/137	-
16	I7D	3	101	-	-	5/54/54/54	-
10	BCL	M	402	2	-	6/41/137/137	-
10	BCL	P	101	6	-	12/41/137/137	-
9	PGV	5	104	-	-	11/41/41/55	-
16	I7D	D	101	-	-	3/54/54/54	-
17	CDL	A	101	-	-	19/67/67/110	-
10	BCL	N	102	6	-	14/41/137/137	-
18	PEE	M	409	-	-	9/47/47/54	-
9	PGV	L	310	-	-	8/41/41/55	-
10	BCL	S	101	5	-	11/41/137/137	-
9	PGV	D	103	-	-	10/37/37/55	-
16	I7D	8	101	-	-	10/54/54/54	-
9	PGV	5	103	-	-	11/40/40/55	-
9	PGV	C	407	-	-	7/39/39/55	-
10	BCL	G	101	6	-	14/41/137/137	-
10	BCL	O	101	5	-	15/41/137/137	-
10	BCL	8	102	6	-	16/41/137/137	-
10	BCL	K	102	5	-	8/41/137/137	-
8	HEC	C	402	1	1/1/3/7	6/14/54/54	-
16	I7D	4	101	-	-	5/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCL	Q	102	5	-	8/41/137/137	-
10	BCL	Y	101	5	-	13/41/137/137	-
8	HEC	C	403	1	1/1/3/7	4/14/54/54	-
10	BCL	4	102	6	-	17/41/137/137	-
10	BCL	1	102	5	-	4/41/137/137	-
10	BCL	B	101	6	-	10/41/137/137	-
16	I7D	I	101	-	-	5/54/54/54	-
10	BCL	7	402	5	-	10/41/137/137	-
9	PGV	F	102	-	-	6/42/42/55	-
10	BCL	A	102	5	-	14/41/137/137	-
9	PGV	5	101	-	-	13/40/40/55	-
10	BCL	F	101	5	-	14/41/137/137	-
10	BCL	M	403	3	-	5/41/137/137	-
10	BCL	D	102	5	-	13/41/137/137	-
11	BPH	M	404	-	-	1/37/105/105	0/5/6/6
13	LMT	1	103	-	-	2/21/61/61	0/2/2/2
10	BCL	I	102	5	-	11/41/137/137	-
10	BCL	2	102	6	-	15/41/137/137	-
10	BCL	J	101	6	-	15/41/137/137	-
17	CDL	6	104	-	-	28/73/73/110	-
11	BPH	L	302	-	-	4/37/105/105	0/5/6/6
16	I7D	1	101	-	-	4/54/54/54	-
17	CDL	2	101	-	-	22/82/82/110	-
9	PGV	K	103	-	-	7/43/43/55	-
10	BCL	3	102	5	-	9/41/137/137	-
8	HEC	C	401	1	1/1/3/7	6/14/54/54	-
12	U10	7	401	-	-	15/63/87/87	0/1/1/1
17	CDL	M	407	-	-	12/43/43/110	-
13	LMT	3	103	-	-	4/17/57/61	0/2/2/2
16	I7D	T	101	-	-	5/54/54/54	-
10	BCL	X	102	6	-	13/41/137/137	-
10	BCL	T	102	6	-	8/41/137/137	-
12	U10	L	306	-	-	1/6/30/87	0/1/1/1
9	PGV	L	311	-	-	12/37/37/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PGV	L	312	-	-	12/38/38/55	-
17	CDL	6	101	-	-	29/79/79/110	-
9	PGV	L	305	-	-	10/48/48/55	-
16	I7D	E	101	-	-	3/54/54/54	-
17	CDL	M	408	-	-	25/79/79/110	-

All (929) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	101	I7D	C35-C36	7.06	1.50	1.32
16	6	102	I7D	C35-C36	7.02	1.50	1.32
16	8	101	I7D	C35-C36	6.94	1.50	1.32
16	I	101	I7D	C35-C36	6.92	1.50	1.32
16	E	101	I7D	C35-C36	6.91	1.50	1.32
16	1	101	I7D	C35-C36	6.91	1.50	1.32
16	3	101	I7D	C35-C36	6.90	1.50	1.32
16	N	101	I7D	C35-C36	6.90	1.50	1.32
16	R	101	I7D	C35-C36	6.88	1.50	1.32
16	4	101	I7D	C35-C36	6.86	1.49	1.32
16	K	101	I7D	C35-C36	6.84	1.49	1.32
16	A	103	I7D	C35-C36	6.84	1.49	1.32
16	T	101	I7D	C35-C36	6.83	1.49	1.32
16	Q	101	I7D	C35-C36	6.82	1.49	1.32
16	V	101	I7D	C35-C36	6.77	1.49	1.32
16	D	101	I7D	C35-C36	6.73	1.49	1.32
16	M	406	I7D	C35-C36	6.72	1.49	1.32
8	C	404	HEC	FE-NB	5.31	2.11	1.94
8	C	403	HEC	FE-NB	5.27	2.11	1.94
8	C	402	HEC	FE-NB	5.23	2.11	1.94
10	L	301	BCL	O2D-CGD	5.22	1.45	1.33
8	C	401	HEC	FE-NB	5.21	2.11	1.94
10	M	403	BCL	O2D-CGD	5.20	1.45	1.33
10	1	102	BCL	O2D-CGD	5.13	1.45	1.33
10	9	101	BCL	O2D-CGD	5.12	1.45	1.33
10	3	102	BCL	O2D-CGD	5.11	1.45	1.33
10	0	102	BCL	O2D-CGD	5.11	1.45	1.33
10	6	103	BCL	O2D-CGD	5.10	1.45	1.33
10	O	101	BCL	O2D-CGD	5.08	1.45	1.33
10	W	101	BCL	O2D-CGD	5.08	1.45	1.33
10	T	102	BCL	O2D-CGD	5.08	1.45	1.33
10	A	102	BCL	O2D-CGD	5.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	8	102	BCL	O2D-CGD	5.07	1.45	1.33
10	5	102	BCL	O2D-CGD	5.07	1.45	1.33
10	B	101	BCL	O2D-CGD	5.06	1.45	1.33
10	K	102	BCL	O2D-CGD	5.06	1.45	1.33
10	V	102	BCL	O2D-CGD	5.06	1.45	1.33
10	Y	101	BCL	O2D-CGD	5.06	1.45	1.33
10	X	102	BCL	O2D-CGD	5.05	1.45	1.33
10	E	102	BCL	O2D-CGD	5.05	1.45	1.33
10	7	402	BCL	O2D-CGD	5.05	1.45	1.33
10	2	102	BCL	O2D-CGD	5.05	1.45	1.33
10	I	102	BCL	O2D-CGD	5.04	1.45	1.33
10	G	101	BCL	O2D-CGD	5.04	1.45	1.33
10	S	101	BCL	O2D-CGD	5.04	1.45	1.33
10	R	102	BCL	O2D-CGD	5.03	1.45	1.33
10	M	402	BCL	O2D-CGD	5.02	1.45	1.33
10	U	101	BCL	O2D-CGD	5.02	1.45	1.33
10	Z	101	BCL	O2D-CGD	5.02	1.45	1.33
10	4	102	BCL	O2D-CGD	5.00	1.45	1.33
10	D	102	BCL	O2D-CGD	5.00	1.45	1.33
10	N	102	BCL	O2D-CGD	4.99	1.45	1.33
10	P	101	BCL	O2D-CGD	4.99	1.45	1.33
10	Q	102	BCL	O2D-CGD	4.99	1.45	1.33
10	F	101	BCL	O2D-CGD	4.98	1.45	1.33
10	J	101	BCL	O2D-CGD	4.96	1.45	1.33
10	L	309	BCL	O2D-CGD	4.85	1.45	1.33
17	M	407	CDL	OB6-CB5	4.76	1.46	1.35
10	O	101	BCL	C3D-C4D	-4.68	1.33	1.44
10	M	402	BCL	C3D-C4D	-4.68	1.33	1.44
10	L	309	BCL	C3D-C4D	-4.68	1.33	1.44
10	L	301	BCL	C3D-C4D	-4.67	1.33	1.44
10	A	102	BCL	C3D-C4D	-4.64	1.33	1.44
10	2	102	BCL	C3D-C4D	-4.64	1.33	1.44
10	M	403	BCL	C3D-C4D	-4.64	1.33	1.44
10	E	102	BCL	C3D-C4D	-4.64	1.33	1.44
10	D	102	BCL	C3D-C4D	-4.63	1.33	1.44
10	5	102	BCL	C3D-C4D	-4.63	1.33	1.44
10	Y	101	BCL	C3D-C4D	-4.62	1.33	1.44
10	Q	102	BCL	C3D-C4D	-4.61	1.33	1.44
10	4	102	BCL	C3D-C4D	-4.61	1.33	1.44
10	R	102	BCL	C3D-C4D	-4.61	1.33	1.44
10	N	102	BCL	C3D-C4D	-4.61	1.33	1.44
10	V	102	BCL	C3D-C4D	-4.61	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	6	103	BCL	C3D-C4D	-4.60	1.33	1.44
10	7	402	BCL	C3D-C4D	-4.60	1.33	1.44
10	J	101	BCL	C3D-C4D	-4.59	1.33	1.44
10	W	101	BCL	C3D-C4D	-4.58	1.33	1.44
10	S	101	BCL	C3D-C4D	-4.58	1.33	1.44
10	T	102	BCL	C3D-C4D	-4.58	1.33	1.44
10	B	101	BCL	C3D-C4D	-4.58	1.33	1.44
10	X	102	BCL	C3D-C4D	-4.58	1.33	1.44
10	G	101	BCL	C3D-C4D	-4.57	1.33	1.44
10	8	102	BCL	C3D-C4D	-4.57	1.33	1.44
10	3	102	BCL	C3D-C4D	-4.57	1.33	1.44
10	9	101	BCL	C3D-C4D	-4.57	1.33	1.44
10	U	101	BCL	C3D-C4D	-4.57	1.33	1.44
10	1	102	BCL	C3D-C4D	-4.57	1.33	1.44
10	P	101	BCL	C3D-C4D	-4.57	1.33	1.44
10	K	102	BCL	C3D-C4D	-4.56	1.33	1.44
10	I	102	BCL	C3D-C4D	-4.55	1.33	1.44
10	Z	101	BCL	C3D-C4D	-4.55	1.33	1.44
10	0	102	BCL	C3D-C4D	-4.53	1.33	1.44
10	F	101	BCL	C3D-C4D	-4.52	1.34	1.44
10	S	101	BCL	C3B-C4B	4.42	1.49	1.41
17	M	408	CDL	OA6-CA5	4.39	1.46	1.34
17	2	101	CDL	OA6-CA5	4.38	1.46	1.34
10	N	102	BCL	C3B-C4B	4.36	1.49	1.41
10	Y	101	BCL	C3B-C4B	4.35	1.49	1.41
10	9	101	BCL	C3B-C4B	4.34	1.49	1.41
10	W	101	BCL	C3B-C4B	4.33	1.49	1.41
17	H	303	CDL	OA8-CA7	4.33	1.46	1.33
10	A	102	BCL	O2A-CGA	4.33	1.46	1.33
10	A	102	BCL	C3B-C4B	4.33	1.49	1.41
9	L	311	PGV	O03-C19	4.32	1.46	1.33
10	M	402	BCL	O2A-CGA	4.32	1.46	1.33
10	D	102	BCL	C3B-C4B	4.32	1.49	1.41
10	B	101	BCL	O2A-CGA	4.32	1.46	1.33
10	U	101	BCL	C3B-C4B	4.32	1.49	1.41
10	8	102	BCL	O2A-CGA	4.32	1.46	1.33
10	J	101	BCL	O2A-CGA	4.31	1.45	1.33
10	I	102	BCL	C3B-C4B	4.31	1.49	1.41
17	6	101	CDL	OA6-CA5	4.31	1.46	1.34
9	C	405	PGV	O03-C19	4.30	1.45	1.33
10	Y	101	BCL	O2A-CGA	4.30	1.45	1.33
9	5	104	PGV	O01-C1	4.30	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	102	BCL	O2A-CGA	4.29	1.45	1.33
10	D	102	BCL	O2A-CGA	4.29	1.45	1.33
10	Z	101	BCL	O2A-CGA	4.28	1.45	1.33
17	0	101	CDL	OA8-CA7	4.28	1.45	1.33
10	7	402	BCL	C3B-C4B	4.28	1.49	1.41
10	F	101	BCL	C3B-C4B	4.27	1.49	1.41
9	C	406	PGV	O01-C1	4.27	1.46	1.34
10	F	101	BCL	O2A-CGA	4.27	1.45	1.33
10	M	403	BCL	C3B-C4B	4.27	1.49	1.41
10	6	103	BCL	O2A-CGA	4.26	1.45	1.33
10	2	102	BCL	C3B-C4B	4.26	1.49	1.41
9	C	407	PGV	O03-C19	4.26	1.45	1.33
9	5	101	PGV	O03-C19	4.26	1.45	1.33
17	6	101	CDL	OA8-CA7	4.26	1.45	1.33
10	X	102	BCL	C3B-C4B	4.26	1.49	1.41
9	H	301	PGV	O03-C19	4.25	1.45	1.33
10	K	102	BCL	O2A-CGA	4.25	1.45	1.33
17	6	104	CDL	OA8-CA7	4.25	1.45	1.33
17	T	103	CDL	OA8-CA7	4.25	1.45	1.33
10	O	101	BCL	C3B-C4B	4.24	1.49	1.41
17	2	101	CDL	OA8-CA7	4.24	1.45	1.33
9	L	312	PGV	O03-C19	4.24	1.45	1.33
17	0	101	CDL	OB8-CB7	4.24	1.45	1.33
17	6	104	CDL	OB8-CB7	4.24	1.45	1.33
10	9	101	BCL	O2A-CGA	4.23	1.45	1.33
9	5	103	PGV	O03-C19	4.23	1.45	1.33
17	6	101	CDL	OB8-CB7	4.23	1.45	1.33
17	T	103	CDL	OB8-CB7	4.23	1.45	1.33
17	2	101	CDL	OB8-CB7	4.23	1.45	1.33
17	H	303	CDL	OB8-CB7	4.23	1.45	1.33
10	L	301	BCL	C3B-C4B	4.22	1.49	1.41
10	B	101	BCL	C3B-C4B	4.22	1.48	1.41
10	O	101	BCL	O2A-CGA	4.22	1.45	1.33
9	M	411	PGV	O03-C19	4.22	1.45	1.33
9	K	103	PGV	O03-C19	4.22	1.45	1.33
10	U	101	BCL	O2A-CGA	4.22	1.45	1.33
17	A	101	CDL	OB8-CB7	4.21	1.45	1.33
9	L	310	PGV	O03-C19	4.21	1.45	1.33
10	7	402	BCL	O2A-CGA	4.21	1.45	1.33
10	R	102	BCL	C3B-C4B	4.21	1.48	1.41
10	T	102	BCL	O2A-CGA	4.21	1.45	1.33
9	H	302	PGV	O03-C19	4.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	102	BCL	C3B-C4B	4.21	1.48	1.41
8	C	403	HEC	FE-NC	4.20	2.09	1.95
17	6	104	CDL	OA6-CA5	4.20	1.46	1.34
10	E	102	BCL	C3B-C4B	4.20	1.48	1.41
9	K	103	PGV	O01-C1	4.20	1.46	1.34
10	W	101	BCL	O2A-CGA	4.20	1.45	1.33
10	G	101	BCL	C3B-C4B	4.20	1.48	1.41
10	1	102	BCL	O2A-CGA	4.20	1.45	1.33
16	1	101	I7D	C19-C17	4.20	1.41	1.35
17	0	101	CDL	OA6-CA5	4.19	1.46	1.34
10	2	102	BCL	O2A-CGA	4.19	1.45	1.33
9	5	104	PGV	O03-C19	4.19	1.45	1.33
16	6	102	I7D	C19-C17	4.19	1.41	1.35
17	2	101	CDL	OB6-CB5	4.18	1.46	1.34
17	H	303	CDL	OA6-CA5	4.18	1.46	1.34
9	D	103	PGV	O03-C19	4.18	1.45	1.33
17	6	101	CDL	OB6-CB5	4.18	1.46	1.34
16	8	101	I7D	C14-C12	4.18	1.41	1.35
10	0	102	BCL	O2A-CGA	4.17	1.45	1.33
9	F	102	PGV	O03-C19	4.17	1.45	1.33
10	Q	102	BCL	O2A-CGA	4.17	1.45	1.33
10	J	101	BCL	C3B-C4B	4.17	1.48	1.41
17	M	407	CDL	OA8-CA7	4.17	1.45	1.33
16	6	102	I7D	C22-C23	4.17	1.41	1.35
9	C	406	PGV	O03-C19	4.17	1.45	1.33
9	L	311	PGV	O01-C1	4.17	1.46	1.34
17	M	407	CDL	OA6-CA5	4.17	1.46	1.34
16	X	101	I7D	C19-C17	4.16	1.41	1.35
9	H	301	PGV	O01-C1	4.16	1.46	1.34
17	M	408	CDL	OA8-CA7	4.16	1.45	1.33
10	L	301	BCL	O2A-CGA	4.16	1.45	1.33
9	M	410	PGV	O03-C19	4.16	1.45	1.33
17	A	101	CDL	OA6-CA5	4.15	1.46	1.34
10	L	309	BCL	C3B-C4B	4.15	1.48	1.41
10	L	309	BCL	O2A-CGA	4.14	1.45	1.33
16	8	101	I7D	C19-C17	4.14	1.41	1.35
10	P	101	BCL	C3B-C4B	4.14	1.48	1.41
10	5	102	BCL	C3B-C4B	4.14	1.48	1.41
10	5	102	BCL	O2A-CGA	4.14	1.45	1.33
9	5	103	PGV	O01-C1	4.14	1.46	1.34
10	N	102	BCL	O2A-CGA	4.14	1.45	1.33
8	C	404	HEC	FE-NC	4.14	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	V	102	BCL	O2A-CGA	4.14	1.45	1.33
10	3	102	BCL	C3B-C4B	4.14	1.48	1.41
10	0	102	BCL	C3B-C4B	4.14	1.48	1.41
16	1	101	I7D	C22-C23	4.13	1.41	1.35
9	F	102	PGV	O01-C1	4.13	1.45	1.34
9	M	411	PGV	O01-C1	4.12	1.45	1.34
17	6	104	CDL	OB6-CB5	4.12	1.45	1.34
10	3	102	BCL	O2A-CGA	4.12	1.45	1.33
10	M	403	BCL	O2A-CGA	4.12	1.45	1.33
8	C	401	HEC	FE-NC	4.12	2.09	1.95
9	C	405	PGV	O01-C1	4.12	1.45	1.34
17	T	103	CDL	OA6-CA5	4.12	1.45	1.34
10	4	102	BCL	O2A-CGA	4.11	1.45	1.33
8	C	402	HEC	FE-NC	4.11	2.09	1.95
17	M	408	CDL	OB6-CB5	4.11	1.45	1.34
17	0	101	CDL	OB6-CB5	4.10	1.45	1.34
17	T	103	CDL	OB6-CB5	4.10	1.45	1.34
9	C	407	PGV	O01-C1	4.10	1.45	1.34
9	D	103	PGV	O01-C1	4.10	1.45	1.34
10	G	101	BCL	O2A-CGA	4.10	1.45	1.33
10	6	103	BCL	C3B-C4B	4.10	1.48	1.41
8	C	404	HEC	CBC-CAC	-4.10	1.33	1.51
16	6	102	I7D	C27-C28	4.10	1.41	1.35
17	M	408	CDL	OB8-CB7	4.09	1.45	1.33
9	L	305	PGV	O03-C19	4.09	1.45	1.33
10	E	102	BCL	O2A-CGA	4.08	1.45	1.33
8	C	401	HEC	CBC-CAC	-4.08	1.33	1.51
8	C	404	HEC	CBB-CAB	-4.08	1.33	1.51
10	V	102	BCL	C3B-C4B	4.08	1.48	1.41
8	C	403	HEC	CBC-CAC	-4.08	1.33	1.51
10	K	102	BCL	C3B-C4B	4.08	1.48	1.41
8	C	403	HEC	CBB-CAB	-4.08	1.33	1.51
10	1	102	BCL	C3B-C4B	4.08	1.48	1.41
8	C	402	HEC	CBC-CAC	-4.07	1.33	1.51
9	5	101	PGV	O01-C1	4.07	1.45	1.34
10	P	101	BCL	O2A-CGA	4.07	1.45	1.33
8	C	401	HEC	CBB-CAB	-4.06	1.33	1.51
10	Z	101	BCL	C3B-C4B	4.06	1.48	1.41
8	C	402	HEC	CBB-CAB	-4.06	1.33	1.51
10	I	102	BCL	O2A-CGA	4.06	1.45	1.33
10	S	101	BCL	O2A-CGA	4.06	1.45	1.33
16	1	101	I7D	C27-C28	4.06	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	102	BCL	C3B-C4B	4.06	1.48	1.41
9	L	310	PGV	O01-C1	4.05	1.45	1.34
16	X	101	I7D	C22-C23	4.04	1.41	1.35
10	M	402	BCL	C3B-C4B	4.04	1.48	1.41
17	A	101	CDL	OB6-CB5	4.04	1.45	1.34
16	X	101	I7D	C27-C28	4.04	1.41	1.35
10	T	102	BCL	C3B-C4B	4.03	1.48	1.41
10	R	102	BCL	O2A-CGA	4.03	1.45	1.33
9	L	312	PGV	O01-C1	4.02	1.45	1.34
9	L	304	PGV	O03-C19	4.02	1.45	1.33
17	H	303	CDL	OB6-CB5	3.99	1.45	1.34
9	L	304	PGV	O01-C1	3.99	1.45	1.34
9	L	305	PGV	O01-C1	3.99	1.45	1.34
16	X	101	I7D	C14-C12	3.98	1.41	1.35
16	6	102	I7D	C14-C12	3.98	1.41	1.35
16	E	101	I7D	C27-C28	3.98	1.41	1.35
16	E	101	I7D	C19-C17	3.98	1.41	1.35
16	I	101	I7D	C19-C17	3.96	1.41	1.35
16	1	101	I7D	C14-C12	3.95	1.41	1.35
10	8	102	BCL	C3B-C4B	3.95	1.48	1.41
16	4	101	I7D	C19-C17	3.95	1.41	1.35
9	M	410	PGV	O01-C1	3.94	1.45	1.34
16	I	101	I7D	C22-C23	3.94	1.41	1.35
16	I	101	I7D	C14-C12	3.93	1.41	1.35
16	8	101	I7D	C27-C28	3.93	1.41	1.35
16	T	101	I7D	C19-C17	3.93	1.41	1.35
16	V	101	I7D	C22-C23	3.93	1.41	1.35
9	H	302	PGV	O01-C1	3.92	1.45	1.34
16	8	101	I7D	C22-C23	3.92	1.41	1.35
16	E	101	I7D	C22-C23	3.91	1.41	1.35
16	4	101	I7D	C22-C23	3.90	1.41	1.35
16	T	101	I7D	C22-C23	3.90	1.41	1.35
16	N	101	I7D	C19-C17	3.90	1.41	1.35
16	R	101	I7D	C22-C23	3.89	1.40	1.35
16	M	406	I7D	C14-C12	3.89	1.40	1.35
16	T	101	I7D	C27-C28	3.88	1.40	1.35
16	R	101	I7D	C14-C12	3.88	1.40	1.35
16	N	101	I7D	C22-C23	3.84	1.40	1.35
16	R	101	I7D	C19-C17	3.83	1.40	1.35
16	V	101	I7D	C14-C12	3.83	1.40	1.35
16	V	101	I7D	C19-C17	3.83	1.40	1.35
16	A	103	I7D	C19-C17	3.83	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	R	101	I7D	C27-C28	3.81	1.40	1.35
16	N	101	I7D	C27-C28	3.81	1.40	1.35
16	4	101	I7D	C27-C28	3.81	1.40	1.35
16	I	101	I7D	C27-C28	3.80	1.40	1.35
16	V	101	I7D	C27-C28	3.80	1.40	1.35
10	K	102	BCL	CHB-C1B	3.78	1.47	1.39
16	A	103	I7D	C27-C28	3.78	1.40	1.35
16	Q	101	I7D	C19-C17	3.76	1.40	1.35
16	K	101	I7D	C22-C23	3.74	1.40	1.35
16	K	101	I7D	C27-C28	3.73	1.40	1.35
10	F	101	BCL	CHB-C1B	3.72	1.47	1.39
16	3	101	I7D	C22-C23	3.71	1.40	1.35
10	S	101	BCL	CHB-C1B	3.71	1.47	1.39
16	Q	101	I7D	C27-C28	3.71	1.40	1.35
16	4	101	I7D	C14-C12	3.71	1.40	1.35
16	E	101	I7D	C14-C12	3.70	1.40	1.35
16	A	103	I7D	C22-C23	3.69	1.40	1.35
16	K	101	I7D	C19-C17	3.69	1.40	1.35
16	A	103	I7D	C14-C12	3.68	1.40	1.35
16	3	101	I7D	C19-C17	3.68	1.40	1.35
16	3	101	I7D	C27-C28	3.68	1.40	1.35
16	3	101	I7D	C14-C12	3.68	1.40	1.35
16	T	101	I7D	C14-C12	3.67	1.40	1.35
10	L	301	BCL	CHD-C1D	3.66	1.45	1.38
16	D	101	I7D	C27-C28	3.66	1.40	1.35
16	N	101	I7D	C14-C12	3.63	1.40	1.35
10	Q	102	BCL	CHB-C1B	3.63	1.47	1.39
10	7	402	BCL	CHD-C1D	3.63	1.45	1.38
10	2	102	BCL	OBD-CAD	3.62	1.28	1.22
10	M	402	BCL	CHD-C1D	3.62	1.45	1.38
16	Q	101	I7D	C14-C12	3.62	1.40	1.35
10	Y	101	BCL	CHB-C1B	3.62	1.47	1.39
10	0	102	BCL	OBD-CAD	3.61	1.28	1.22
10	5	102	BCL	CHD-C1D	3.61	1.45	1.38
10	5	102	BCL	OBD-CAD	3.61	1.28	1.22
16	M	406	I7D	C19-C17	3.60	1.40	1.35
10	4	102	BCL	CHD-C1D	3.59	1.45	1.38
16	D	101	I7D	C22-C23	3.59	1.40	1.35
10	D	102	BCL	CHB-C1B	3.59	1.47	1.39
10	O	101	BCL	CHB-C1B	3.59	1.47	1.39
10	X	102	BCL	OBD-CAD	3.58	1.28	1.22
10	A	102	BCL	CHB-C1B	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	102	BCL	OBD-CAD	3.58	1.28	1.22
10	U	101	BCL	CHD-C1D	3.58	1.45	1.38
10	V	102	BCL	OBD-CAD	3.58	1.28	1.22
10	9	101	BCL	OBD-CAD	3.58	1.28	1.22
10	9	101	BCL	CHB-C1B	3.58	1.47	1.39
16	Q	101	I7D	C22-C23	3.57	1.40	1.35
10	E	102	BCL	CHD-C1D	3.57	1.45	1.38
10	I	102	BCL	OBD-CAD	3.57	1.28	1.22
16	K	101	I7D	C14-C12	3.57	1.40	1.35
10	B	101	BCL	OBD-CAD	3.56	1.28	1.22
10	9	101	BCL	CHD-C1D	3.55	1.45	1.38
10	W	101	BCL	CHD-C1D	3.55	1.45	1.38
10	A	102	BCL	CHD-C1D	3.54	1.45	1.38
10	O	101	BCL	OBD-CAD	3.54	1.28	1.22
10	4	102	BCL	OBD-CAD	3.53	1.28	1.22
10	W	101	BCL	CHB-C1B	3.53	1.47	1.39
16	D	101	I7D	C19-C17	3.53	1.40	1.35
10	E	102	BCL	OBD-CAD	3.53	1.28	1.22
10	R	102	BCL	OBD-CAD	3.53	1.28	1.22
10	6	103	BCL	CHD-C1D	3.53	1.45	1.38
10	Y	101	BCL	OBD-CAD	3.53	1.28	1.22
10	Y	101	BCL	CHD-C1D	3.53	1.45	1.38
10	I	102	BCL	CHD-C1D	3.52	1.45	1.38
10	6	103	BCL	OBD-CAD	3.52	1.28	1.22
10	A	102	BCL	OBD-CAD	3.52	1.28	1.22
16	D	101	I7D	C14-C12	3.52	1.40	1.35
10	Z	101	BCL	OBD-CAD	3.52	1.28	1.22
10	1	102	BCL	OBD-CAD	3.52	1.28	1.22
10	1	102	BCL	CHB-C1B	3.51	1.47	1.39
10	M	402	BCL	OBD-CAD	3.51	1.28	1.22
10	J	101	BCL	OBD-CAD	3.51	1.28	1.22
10	T	102	BCL	OBD-CAD	3.50	1.28	1.22
8	C	403	HEC	C4B-NB	-3.50	1.34	1.40
10	L	309	BCL	CHD-C1D	3.50	1.45	1.38
10	S	101	BCL	OBD-CAD	3.50	1.28	1.22
10	F	101	BCL	OBD-CAD	3.50	1.28	1.22
10	7	402	BCL	CHB-C1B	3.50	1.47	1.39
10	U	101	BCL	CHB-C1B	3.49	1.47	1.39
10	P	101	BCL	OBD-CAD	3.49	1.28	1.22
16	M	406	I7D	C22-C23	3.49	1.40	1.35
10	7	402	BCL	OBD-CAD	3.49	1.28	1.22
10	D	102	BCL	OBD-CAD	3.49	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	102	BCL	OBD-CAD	3.49	1.28	1.22
10	J	101	BCL	CHD-C1D	3.49	1.45	1.38
10	N	102	BCL	OBD-CAD	3.49	1.28	1.22
10	0	102	BCL	CHD-C1D	3.48	1.45	1.38
10	3	102	BCL	CHD-C1D	3.48	1.45	1.38
10	8	102	BCL	OBD-CAD	3.48	1.28	1.22
10	T	102	BCL	CHD-C1D	3.48	1.45	1.38
16	M	406	I7D	C27-C28	3.48	1.40	1.35
10	U	101	BCL	OBD-CAD	3.48	1.28	1.22
10	O	101	BCL	CHD-C1D	3.47	1.45	1.38
10	6	103	BCL	CHB-C1B	3.47	1.47	1.39
10	5	102	BCL	CHB-C1B	3.47	1.47	1.39
10	Z	101	BCL	CHB-C1B	3.47	1.47	1.39
10	G	101	BCL	OBD-CAD	3.47	1.28	1.22
10	W	101	BCL	OBD-CAD	3.47	1.28	1.22
10	N	102	BCL	CHD-C1D	3.46	1.45	1.38
10	L	301	BCL	OBD-CAD	3.46	1.28	1.22
10	B	101	BCL	CHD-C1D	3.46	1.45	1.38
10	F	101	BCL	CHD-C1D	3.45	1.45	1.38
10	M	403	BCL	CHD-C1D	3.45	1.45	1.38
10	L	309	BCL	OBD-CAD	3.45	1.28	1.22
10	D	102	BCL	CHD-C1D	3.44	1.45	1.38
10	2	102	BCL	CHD-C1D	3.44	1.45	1.38
10	Q	102	BCL	OBD-CAD	3.44	1.28	1.22
10	M	402	BCL	CHB-C1B	3.43	1.47	1.39
10	G	101	BCL	CHD-C1D	3.43	1.45	1.38
10	X	102	BCL	CHD-C1D	3.43	1.45	1.38
10	L	309	BCL	CHB-C1B	3.42	1.47	1.39
10	8	102	BCL	CHD-C1D	3.41	1.45	1.38
10	3	102	BCL	CHB-C1B	3.40	1.47	1.39
10	S	101	BCL	CHD-C1D	3.40	1.45	1.38
10	1	102	BCL	CHD-C1D	3.40	1.45	1.38
10	R	102	BCL	CHD-C1D	3.40	1.45	1.38
10	V	102	BCL	CHB-C1B	3.39	1.47	1.39
10	P	101	BCL	CHD-C1D	3.38	1.45	1.38
10	L	301	BCL	CHB-C1B	3.38	1.47	1.39
10	I	102	BCL	CHB-C1B	3.37	1.47	1.39
10	Z	101	BCL	CHD-C1D	3.36	1.44	1.38
10	G	101	BCL	CHB-C1B	3.36	1.46	1.39
10	T	102	BCL	CHB-C1B	3.36	1.46	1.39
8	C	401	HEC	C4B-NB	-3.36	1.34	1.40
18	M	409	PEE	C39-C38	3.35	1.51	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	V	102	BCL	CHD-C1D	3.35	1.44	1.38
10	8	102	BCL	CHB-C1B	3.34	1.46	1.39
10	U	101	BCL	CHC-C4B	3.34	1.46	1.39
10	4	102	BCL	CHB-C1B	3.34	1.46	1.39
10	M	403	BCL	CHC-C4B	3.33	1.46	1.39
10	J	101	BCL	CHB-C1B	3.33	1.46	1.39
10	M	403	BCL	CHB-C1B	3.32	1.46	1.39
10	N	102	BCL	CHB-C1B	3.32	1.46	1.39
10	N	102	BCL	CHC-C4B	3.32	1.46	1.39
18	M	409	PEE	C18-C19	3.32	1.51	1.31
10	2	102	BCL	CHB-C1B	3.31	1.46	1.39
10	P	101	BCL	CHC-C4B	3.31	1.46	1.39
10	P	101	BCL	CHB-C1B	3.31	1.46	1.39
10	X	102	BCL	CHC-C4B	3.30	1.46	1.39
10	B	101	BCL	CHB-C1B	3.30	1.46	1.39
10	R	102	BCL	CHC-C4B	3.30	1.46	1.39
10	0	102	BCL	CHB-C1B	3.29	1.46	1.39
10	G	101	BCL	CHC-C4B	3.29	1.46	1.39
10	A	102	BCL	CHC-C4B	3.29	1.46	1.39
10	Q	102	BCL	CHD-C1D	3.29	1.44	1.38
10	5	102	BCL	CHC-C4B	3.28	1.46	1.39
10	Z	101	BCL	CHC-C4B	3.28	1.46	1.39
10	K	102	BCL	CHD-C1D	3.28	1.44	1.38
10	R	102	BCL	CHB-C1B	3.28	1.46	1.39
8	C	402	HEC	C4B-NB	-3.28	1.34	1.40
10	E	102	BCL	CHB-C1B	3.27	1.46	1.39
8	C	403	HEC	C1D-ND	-3.26	1.34	1.40
10	9	101	BCL	CHC-C4B	3.26	1.46	1.39
10	X	102	BCL	CHB-C1B	3.25	1.46	1.39
10	2	102	BCL	CHC-C4B	3.25	1.46	1.39
10	M	403	BCL	OBD-CAD	3.25	1.28	1.22
10	7	402	BCL	CHC-C4B	3.25	1.46	1.39
10	I	102	BCL	CHC-C4B	3.24	1.46	1.39
10	3	102	BCL	CHC-C4B	3.23	1.46	1.39
10	S	101	BCL	CHC-C4B	3.23	1.46	1.39
10	6	103	BCL	CHC-C4B	3.23	1.46	1.39
8	C	404	HEC	C4B-NB	-3.23	1.34	1.40
10	E	102	BCL	CHC-C4B	3.23	1.46	1.39
10	J	101	BCL	CHC-C4B	3.22	1.46	1.39
10	8	102	BCL	CHC-C4B	3.22	1.46	1.39
8	C	401	HEC	C1D-ND	-3.22	1.34	1.40
10	L	301	BCL	CHC-C4B	3.21	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	0	102	BCL	CHC-C4B	3.20	1.46	1.39
8	C	404	HEC	C1D-ND	-3.20	1.34	1.40
10	T	102	BCL	CHC-C4B	3.20	1.46	1.39
10	4	102	BCL	CHC-C4B	3.18	1.46	1.39
8	C	402	HEC	C1D-ND	-3.18	1.34	1.40
11	M	404	BPH	C4D-CHA	3.17	1.44	1.39
10	V	102	BCL	CHC-C4B	3.17	1.46	1.39
10	K	102	BCL	C4B-NB	-3.17	1.33	1.37
10	Y	101	BCL	CHC-C4B	3.17	1.46	1.39
10	L	309	BCL	CHC-C4B	3.17	1.46	1.39
10	W	101	BCL	CHC-C4B	3.16	1.46	1.39
10	1	102	BCL	CHC-C4B	3.16	1.46	1.39
10	B	101	BCL	CHC-C4B	3.15	1.46	1.39
10	S	101	BCL	C4B-NB	-3.14	1.33	1.37
10	D	102	BCL	CHC-C4B	3.13	1.46	1.39
10	M	402	BCL	CHC-C4B	3.12	1.46	1.39
10	V	102	BCL	C1D-ND	-3.10	1.34	1.37
10	Q	102	BCL	CHC-C4B	3.08	1.46	1.39
10	F	101	BCL	CHC-C4B	3.07	1.46	1.39
10	0	102	BCL	C1D-ND	-3.07	1.34	1.37
10	0	102	BCL	C3D-C2D	3.07	1.47	1.39
10	O	101	BCL	CHC-C4B	3.06	1.46	1.39
10	M	402	BCL	C3D-C2D	3.06	1.47	1.39
10	P	101	BCL	C1D-ND	-3.04	1.34	1.37
10	N	102	BCL	C1D-ND	-3.03	1.34	1.37
11	L	302	BPH	C4D-CHA	3.02	1.44	1.39
10	K	102	BCL	CHC-C4B	3.01	1.46	1.39
10	R	102	BCL	C3D-C2D	3.00	1.47	1.39
10	Q	102	BCL	C4B-NB	-3.00	1.34	1.37
10	X	102	BCL	C3D-C2D	2.99	1.47	1.39
10	6	103	BCL	C1D-ND	-2.99	1.34	1.37
10	L	309	BCL	C3D-C2D	2.98	1.47	1.39
10	F	101	BCL	C4B-NB	-2.98	1.34	1.37
10	J	101	BCL	C1D-ND	-2.97	1.34	1.37
10	P	101	BCL	C3D-C2D	2.97	1.47	1.39
10	V	102	BCL	C3D-C2D	2.96	1.47	1.39
10	6	103	BCL	C3D-C2D	2.96	1.47	1.39
10	J	101	BCL	C3D-C2D	2.96	1.47	1.39
10	X	102	BCL	C1D-ND	-2.96	1.34	1.37
10	N	102	BCL	C3D-C2D	2.96	1.47	1.39
10	U	101	BCL	C3D-C2D	2.96	1.47	1.39
10	2	102	BCL	C3D-C2D	2.96	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	T	102	BCL	C3D-C2D	2.96	1.47	1.39
10	5	102	BCL	C4B-NB	-2.95	1.34	1.37
10	Y	101	BCL	C3D-C2D	2.95	1.47	1.39
10	E	102	BCL	C1D-ND	-2.95	1.34	1.37
10	O	101	BCL	C4B-NB	-2.95	1.34	1.37
10	W	101	BCL	C4B-NB	-2.94	1.34	1.37
10	5	102	BCL	C3D-C2D	2.94	1.47	1.39
10	T	102	BCL	C1D-ND	-2.94	1.34	1.37
10	D	102	BCL	C4B-NB	-2.94	1.34	1.37
10	3	102	BCL	C4B-NB	-2.94	1.34	1.37
10	B	101	BCL	C1D-ND	-2.93	1.34	1.37
10	L	309	BCL	C4B-NB	-2.93	1.34	1.37
10	Z	101	BCL	C1D-ND	-2.93	1.34	1.37
10	G	101	BCL	C1D-ND	-2.93	1.34	1.37
10	E	102	BCL	C3D-C2D	2.93	1.47	1.39
10	8	102	BCL	C1D-ND	-2.92	1.34	1.37
10	Z	101	BCL	C3D-C2D	2.92	1.47	1.39
10	R	102	BCL	C1D-ND	-2.92	1.34	1.37
10	7	402	BCL	C3D-C2D	2.91	1.47	1.39
10	B	101	BCL	C3D-C2D	2.91	1.47	1.39
10	G	101	BCL	C3D-C2D	2.91	1.47	1.39
10	K	102	BCL	C3D-C2D	2.91	1.47	1.39
10	D	102	BCL	C3D-C2D	2.91	1.47	1.39
10	3	102	BCL	C3D-C2D	2.91	1.47	1.39
10	8	102	BCL	C3D-C2D	2.91	1.47	1.39
10	F	101	BCL	C3D-C2D	2.91	1.47	1.39
10	Q	102	BCL	C3D-C2D	2.91	1.47	1.39
10	I	102	BCL	C4B-NB	-2.91	1.34	1.37
10	9	101	BCL	C3D-C2D	2.90	1.47	1.39
10	U	101	BCL	C4B-NB	-2.90	1.34	1.37
10	I	102	BCL	C3D-C2D	2.90	1.47	1.39
10	M	402	BCL	C4B-NB	-2.90	1.34	1.37
10	A	102	BCL	C4B-NB	-2.88	1.34	1.37
10	W	101	BCL	C3D-C2D	2.88	1.47	1.39
10	A	102	BCL	C3D-C2D	2.87	1.47	1.39
10	4	102	BCL	C3D-C2D	2.87	1.47	1.39
10	Y	101	BCL	C1D-ND	-2.87	1.34	1.37
10	M	402	BCL	C1D-ND	-2.87	1.34	1.37
10	S	101	BCL	C3D-C2D	2.86	1.46	1.39
10	E	102	BCL	C4B-NB	-2.85	1.34	1.37
10	L	309	BCL	C1D-ND	-2.85	1.34	1.37
10	2	102	BCL	C1D-ND	-2.85	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	101	BCL	C3D-C2D	2.83	1.46	1.39
10	R	102	BCL	C4B-NB	-2.82	1.34	1.37
10	1	102	BCL	C4B-NB	-2.82	1.34	1.37
10	7	402	BCL	CHD-C4C	2.81	1.47	1.39
10	M	403	BCL	C3D-C2D	2.81	1.46	1.39
10	Q	102	BCL	C1D-ND	-2.81	1.34	1.37
10	G	101	BCL	C4B-NB	-2.81	1.34	1.37
10	9	101	BCL	C4B-NB	-2.80	1.34	1.37
10	1	102	BCL	C3D-C2D	2.80	1.46	1.39
10	4	102	BCL	C4B-NB	-2.80	1.34	1.37
10	M	403	BCL	C4B-NB	-2.80	1.34	1.37
10	0	102	BCL	C4B-NB	-2.80	1.34	1.37
10	T	102	BCL	C4B-NB	-2.79	1.34	1.37
10	L	301	BCL	C3D-C2D	2.79	1.46	1.39
10	3	102	BCL	C1D-ND	-2.78	1.34	1.37
10	D	102	BCL	C1D-ND	-2.78	1.34	1.37
10	K	102	BCL	C1D-ND	-2.78	1.34	1.37
10	A	102	BCL	CHD-C4C	2.78	1.47	1.39
10	Z	101	BCL	C4B-NB	-2.78	1.34	1.37
10	Y	101	BCL	C4B-NB	-2.77	1.34	1.37
10	U	101	BCL	CHD-C4C	2.76	1.47	1.39
10	5	102	BCL	CHD-C4C	2.76	1.47	1.39
10	7	402	BCL	C1D-C2D	2.75	1.50	1.45
10	W	101	BCL	CHD-C4C	2.75	1.47	1.39
10	Y	101	BCL	CHD-C4C	2.75	1.47	1.39
10	P	101	BCL	C4B-NB	-2.75	1.34	1.37
10	1	102	BCL	C1D-ND	-2.74	1.34	1.37
10	K	102	BCL	MG-NA	-2.74	1.99	2.06
10	L	301	BCL	C4B-NB	-2.74	1.34	1.37
10	I	102	BCL	C1D-C2D	2.74	1.50	1.45
10	6	103	BCL	C4B-NB	-2.74	1.34	1.37
10	8	102	BCL	C4B-NB	-2.73	1.34	1.37
10	L	301	BCL	CHD-C4C	2.73	1.46	1.39
10	9	101	BCL	CHD-C4C	2.73	1.46	1.39
10	X	102	BCL	C4B-NB	-2.73	1.34	1.37
10	3	102	BCL	CHD-C4C	2.73	1.46	1.39
10	5	102	BCL	C1D-ND	-2.72	1.34	1.37
10	O	101	BCL	C1D-C2D	2.72	1.50	1.45
10	J	101	BCL	C4B-NB	-2.72	1.34	1.37
10	D	102	BCL	CHD-C4C	2.72	1.46	1.39
10	B	101	BCL	C4B-NB	-2.71	1.34	1.37
10	L	309	BCL	CHD-C4C	2.71	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	102	BCL	C1D-ND	-2.71	1.34	1.37
10	4	102	BCL	C1D-ND	-2.70	1.34	1.37
10	S	101	BCL	C1D-C2D	2.70	1.50	1.45
10	S	101	BCL	C1D-ND	-2.70	1.34	1.37
10	I	102	BCL	C1D-ND	-2.69	1.34	1.37
12	L	307	U10	C3-C2	-2.69	1.41	1.48
10	K	102	BCL	CHD-C4C	2.69	1.46	1.39
10	O	101	BCL	CHD-C4C	2.69	1.46	1.39
10	5	102	BCL	C1D-C2D	2.68	1.50	1.45
10	L	301	BCL	C1D-ND	-2.68	1.34	1.37
10	N	102	BCL	C4B-NB	-2.68	1.34	1.37
10	W	101	BCL	C1D-C2D	2.68	1.50	1.45
10	M	403	BCL	C1D-ND	-2.67	1.34	1.37
10	1	102	BCL	CHD-C4C	2.67	1.46	1.39
10	I	102	BCL	CHD-C4C	2.67	1.46	1.39
10	M	403	BCL	C1D-C2D	2.66	1.50	1.45
10	V	102	BCL	C4B-NB	-2.66	1.34	1.37
10	2	102	BCL	C4B-NB	-2.66	1.34	1.37
10	M	402	BCL	CHD-C4C	2.65	1.46	1.39
12	L	306	U10	C4-C5	-2.65	1.41	1.48
10	1	102	BCL	C1D-C2D	2.65	1.50	1.45
10	3	102	BCL	C1D-C2D	2.65	1.50	1.45
10	S	101	BCL	CHD-C4C	2.65	1.46	1.39
10	N	102	BCL	CHD-C4C	2.64	1.46	1.39
10	Q	102	BCL	CHD-C4C	2.64	1.46	1.39
10	S	101	BCL	MG-NA	-2.64	2.00	2.06
10	7	402	BCL	C4B-NB	-2.63	1.34	1.37
10	F	101	BCL	C1D-ND	-2.63	1.34	1.37
10	E	102	BCL	CHD-C4C	2.63	1.46	1.39
10	O	101	BCL	C1D-ND	-2.63	1.34	1.37
16	M	406	I7D	C25-C23	-2.62	1.40	1.45
10	A	102	BCL	C1D-C2D	2.62	1.50	1.45
10	4	102	BCL	CHD-C4C	2.62	1.46	1.39
10	W	101	BCL	C1D-ND	-2.62	1.34	1.37
10	6	103	BCL	CHD-C4C	2.61	1.46	1.39
10	F	101	BCL	CHD-C4C	2.61	1.46	1.39
10	U	101	BCL	C1D-ND	-2.61	1.34	1.37
12	L	303	U10	C4-C5	-2.61	1.41	1.48
10	K	102	BCL	C1D-C2D	2.60	1.50	1.45
10	D	102	BCL	C1D-C2D	2.60	1.50	1.45
10	9	101	BCL	C1D-ND	-2.60	1.34	1.37
10	L	301	BCL	C1D-C2D	2.59	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	101	I7D	C25-C23	-2.59	1.40	1.45
12	7	401	U10	C3-C2	-2.59	1.41	1.48
10	M	403	BCL	CHD-C4C	2.59	1.46	1.39
10	U	101	BCL	C1D-C2D	2.58	1.50	1.45
10	8	102	BCL	CHD-C4C	2.57	1.46	1.39
10	X	102	BCL	CHD-C4C	2.57	1.46	1.39
10	R	102	BCL	CHD-C4C	2.56	1.46	1.39
10	Q	102	BCL	C1D-C2D	2.56	1.50	1.45
16	D	101	I7D	C25-C23	-2.56	1.40	1.45
10	F	101	BCL	C1B-C2B	2.56	1.49	1.43
16	K	101	I7D	C16-C17	-2.56	1.40	1.45
10	B	101	BCL	C1B-NB	-2.56	1.34	1.37
10	2	102	BCL	CHD-C4C	2.55	1.46	1.39
10	Y	101	BCL	C1D-C2D	2.55	1.50	1.45
17	A	101	CDL	OA8-CA7	2.55	1.46	1.33
10	9	101	BCL	C1D-C2D	2.55	1.50	1.45
16	D	101	I7D	C11-C12	-2.55	1.40	1.45
10	G	101	BCL	CHD-C4C	2.55	1.46	1.39
10	4	102	BCL	C1D-C2D	2.54	1.50	1.45
10	7	402	BCL	C1D-ND	-2.54	1.34	1.37
10	B	101	BCL	CHD-C4C	2.54	1.46	1.39
10	D	102	BCL	MG-NA	-2.52	2.00	2.06
16	K	101	I7D	C11-C12	-2.52	1.40	1.45
10	0	102	BCL	CHD-C4C	2.52	1.46	1.39
10	R	102	BCL	C1B-NB	-2.52	1.34	1.37
16	D	101	I7D	C16-C17	-2.52	1.40	1.45
10	Z	101	BCL	C1B-C2B	2.51	1.49	1.43
10	K	102	BCL	C1B-C2B	2.51	1.49	1.43
10	M	403	BCL	C1B-NB	-2.51	1.34	1.37
10	3	102	BCL	C1B-C2B	2.51	1.49	1.43
10	6	103	BCL	C1B-C2B	2.51	1.49	1.43
10	Q	102	BCL	MG-NA	-2.51	2.00	2.06
10	F	101	BCL	C1D-C2D	2.50	1.50	1.45
10	O	101	BCL	MG-NA	-2.50	2.00	2.06
10	T	102	BCL	CHD-C4C	2.50	1.46	1.39
10	V	102	BCL	CHD-C4C	2.50	1.46	1.39
16	3	101	I7D	C11-C12	-2.49	1.40	1.45
10	6	103	BCL	C1B-NB	-2.49	1.34	1.37
10	O	101	BCL	C1B-C2B	2.49	1.49	1.43
16	M	406	I7D	C30-C28	-2.49	1.40	1.45
10	J	101	BCL	CHD-C4C	2.49	1.46	1.39
10	A	102	BCL	MG-NA	-2.48	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	101	I7D	C30-C28	-2.48	1.40	1.45
10	1	102	BCL	C1B-C2B	2.48	1.49	1.43
16	Q	101	I7D	C30-C28	-2.48	1.40	1.45
16	Q	101	I7D	C16-C17	-2.48	1.40	1.45
10	Z	101	BCL	CHD-C4C	2.48	1.46	1.39
16	3	101	I7D	C16-C17	-2.47	1.40	1.45
10	L	309	BCL	C1D-C2D	2.47	1.50	1.45
10	P	101	BCL	CHD-C4C	2.47	1.46	1.39
10	L	301	BCL	C1B-C2B	2.47	1.49	1.43
16	6	102	I7D	C35-C33	2.46	1.51	1.45
12	L	307	U10	C4-C5	-2.46	1.41	1.48
10	I	102	BCL	C1B-C2B	2.46	1.49	1.43
10	W	101	BCL	MG-NA	-2.46	2.00	2.06
16	K	101	I7D	C25-C23	-2.46	1.40	1.45
10	5	102	BCL	MG-NA	-2.46	2.00	2.06
16	3	101	I7D	C25-C23	-2.45	1.40	1.45
16	X	101	I7D	C35-C33	2.45	1.51	1.45
16	A	103	I7D	C25-C23	-2.44	1.40	1.45
16	3	101	I7D	C35-C33	2.44	1.51	1.45
16	T	101	I7D	C16-C17	-2.44	1.40	1.45
10	E	102	BCL	C1B-NB	-2.44	1.34	1.37
10	0	102	BCL	C1B-NB	-2.43	1.34	1.37
10	D	102	BCL	C1B-C2B	2.43	1.49	1.43
10	W	101	BCL	C1B-C2B	2.43	1.49	1.43
10	Q	102	BCL	C1B-C2B	2.43	1.49	1.43
10	A	102	BCL	C1B-C2B	2.43	1.49	1.43
10	8	102	BCL	C1B-C2B	2.43	1.49	1.43
10	M	402	BCL	C1B-NB	-2.43	1.34	1.37
10	M	402	BCL	C1D-C2D	2.43	1.50	1.45
16	M	406	I7D	C35-C33	2.42	1.51	1.45
16	8	101	I7D	C35-C33	2.42	1.51	1.45
10	2	102	BCL	C1B-NB	-2.42	1.34	1.37
10	U	101	BCL	MG-NA	-2.42	2.00	2.06
10	7	402	BCL	C1B-C2B	2.41	1.48	1.43
16	4	101	I7D	C35-C33	2.41	1.51	1.45
16	I	101	I7D	C35-C33	2.41	1.51	1.45
16	K	101	I7D	C35-C33	2.41	1.51	1.45
16	V	101	I7D	C25-C23	-2.41	1.40	1.45
16	N	101	I7D	C35-C33	2.41	1.51	1.45
16	1	101	I7D	C35-C33	2.41	1.51	1.45
16	T	101	I7D	C35-C33	2.41	1.51	1.45
16	E	101	I7D	C35-C33	2.41	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	5	102	BCL	C1B-C2B	2.41	1.48	1.43
16	N	101	I7D	C16-C17	-2.40	1.40	1.45
10	1	102	BCL	MG-NA	-2.40	2.00	2.06
10	X	102	BCL	C1B-NB	-2.40	1.34	1.37
16	V	101	I7D	C30-C28	-2.40	1.40	1.45
10	V	102	BCL	C1B-C2B	2.40	1.48	1.43
16	R	101	I7D	C35-C33	2.40	1.51	1.45
16	T	101	I7D	C11-C12	-2.40	1.40	1.45
16	Q	101	I7D	C35-C33	2.40	1.51	1.45
10	N	102	BCL	C1D-C2D	2.40	1.50	1.45
10	9	101	BCL	C1B-C2B	2.40	1.48	1.43
10	T	102	BCL	C1B-C2B	2.40	1.48	1.43
16	I	101	I7D	C16-C17	-2.40	1.40	1.45
16	4	101	I7D	C16-C17	-2.39	1.40	1.45
16	Q	101	I7D	C11-C12	-2.39	1.40	1.45
10	3	102	BCL	MG-NA	-2.39	2.00	2.06
10	4	102	BCL	C1B-NB	-2.39	1.34	1.37
16	D	101	I7D	C35-C33	2.39	1.51	1.45
16	M	406	I7D	C16-C17	-2.39	1.40	1.45
16	R	101	I7D	C30-C28	-2.39	1.40	1.45
16	4	101	I7D	C11-C12	-2.39	1.40	1.45
16	I	101	I7D	C25-C23	-2.38	1.40	1.45
16	A	103	I7D	C30-C28	-2.38	1.40	1.45
10	Y	101	BCL	C1B-C2B	2.38	1.48	1.43
16	X	101	I7D	C16-C17	-2.38	1.40	1.45
10	P	101	BCL	C1B-C2B	2.38	1.48	1.43
10	4	102	BCL	C1B-C2B	2.37	1.48	1.43
16	A	103	I7D	C35-C33	2.37	1.51	1.45
10	U	101	BCL	C1B-C2B	2.37	1.48	1.43
10	Y	101	BCL	MG-NA	-2.37	2.00	2.06
10	F	101	BCL	MG-NA	-2.36	2.00	2.06
16	V	101	I7D	C35-C33	2.36	1.51	1.45
10	S	101	BCL	C1B-C2B	2.36	1.48	1.43
10	Z	101	BCL	C1B-NB	-2.36	1.34	1.37
16	M	406	I7D	C11-C12	-2.36	1.40	1.45
16	R	101	I7D	C25-C23	-2.36	1.40	1.45
16	4	101	I7D	C25-C23	-2.36	1.40	1.45
10	5	102	BCL	C1B-NB	-2.36	1.34	1.37
10	J	101	BCL	C1B-NB	-2.36	1.34	1.37
10	E	102	BCL	C1B-C2B	2.36	1.48	1.43
10	L	309	BCL	C1B-C2B	2.36	1.48	1.43
10	I	102	BCL	MG-NA	-2.35	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	102	BCL	C1B-C2B	2.35	1.48	1.43
16	N	101	I7D	C25-C23	-2.35	1.40	1.45
10	M	402	BCL	C1B-C2B	2.35	1.48	1.43
8	C	403	HEC	FE-ND	-2.35	1.87	1.94
8	C	403	HEC	C4A-C3A	-2.35	1.40	1.45
16	E	101	I7D	C16-C17	-2.35	1.40	1.45
16	E	101	I7D	C11-C12	-2.35	1.40	1.45
16	K	101	I7D	C30-C28	-2.35	1.40	1.45
10	I	102	BCL	C1B-NB	-2.35	1.34	1.37
8	C	401	HEC	C4A-C3A	-2.35	1.40	1.45
10	T	102	BCL	C1B-NB	-2.34	1.34	1.37
10	G	101	BCL	C1D-C2D	2.34	1.49	1.45
16	R	101	I7D	C16-C17	-2.34	1.40	1.45
10	N	102	BCL	C1B-NB	-2.34	1.34	1.37
16	A	103	I7D	C16-C17	-2.34	1.40	1.45
10	E	102	BCL	C1D-C2D	2.34	1.49	1.45
16	N	101	I7D	C11-C12	-2.34	1.40	1.45
10	T	102	BCL	C1D-C2D	2.34	1.49	1.45
8	C	401	HEC	FE-ND	-2.34	1.87	1.94
8	C	404	HEC	C4A-C3A	-2.33	1.40	1.45
8	C	402	HEC	FE-ND	-2.33	1.87	1.94
16	I	101	I7D	C11-C12	-2.33	1.40	1.45
10	V	102	BCL	C1B-NB	-2.33	1.34	1.37
10	X	102	BCL	C1B-C2B	2.33	1.48	1.43
10	W	101	BCL	C1B-NB	-2.31	1.34	1.37
16	V	101	I7D	C16-C17	-2.31	1.41	1.45
10	8	102	BCL	C1D-C2D	2.31	1.49	1.45
10	3	102	BCL	C1B-NB	-2.31	1.34	1.37
16	E	101	I7D	C25-C23	-2.31	1.41	1.45
16	E	101	I7D	C30-C28	-2.31	1.41	1.45
16	I	101	I7D	C30-C28	-2.31	1.41	1.45
16	T	101	I7D	C30-C28	-2.31	1.41	1.45
8	C	404	HEC	FE-ND	-2.31	1.87	1.94
8	C	402	HEC	C1A-C2A	-2.31	1.41	1.45
10	L	309	BCL	C1B-NB	-2.30	1.35	1.37
10	Z	101	BCL	C1D-C2D	2.30	1.49	1.45
10	8	102	BCL	C1B-NB	-2.30	1.35	1.37
10	B	101	BCL	C1B-C2B	2.30	1.48	1.43
16	A	103	I7D	C11-C12	-2.30	1.41	1.45
10	6	103	BCL	C1D-C2D	2.30	1.49	1.45
10	J	101	BCL	C1B-C2B	2.30	1.48	1.43
10	9	101	BCL	C1B-NB	-2.29	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	403	BCL	C1B-C2B	2.29	1.48	1.43
16	1	101	I7D	C16-C17	-2.29	1.41	1.45
10	P	101	BCL	C1B-NB	-2.28	1.35	1.37
8	C	404	HEC	C1A-C2A	-2.28	1.41	1.45
10	9	101	BCL	MG-NA	-2.28	2.00	2.06
10	0	102	BCL	C1B-C2B	2.28	1.48	1.43
10	G	101	BCL	C1B-C2B	2.28	1.48	1.43
10	Q	102	BCL	C1B-NB	-2.27	1.35	1.37
8	C	403	HEC	C1A-C2A	-2.27	1.41	1.45
10	G	101	BCL	C1B-NB	-2.27	1.35	1.37
16	V	101	I7D	C11-C12	-2.27	1.41	1.45
16	X	101	I7D	C11-C12	-2.27	1.41	1.45
10	R	102	BCL	C1B-C2B	2.27	1.48	1.43
16	3	101	I7D	C30-C28	-2.27	1.41	1.45
10	1	102	BCL	C1B-NB	-2.26	1.35	1.37
16	1	101	I7D	C11-C12	-2.26	1.41	1.45
10	X	102	BCL	C1D-C2D	2.26	1.49	1.45
16	1	101	I7D	C25-C23	-2.26	1.41	1.45
10	2	102	BCL	C1D-C2D	2.26	1.49	1.45
16	6	102	I7D	C30-C28	-2.26	1.41	1.45
10	2	102	BCL	C1B-C2B	2.25	1.48	1.43
16	6	102	I7D	C11-C12	-2.25	1.41	1.45
10	Y	101	BCL	C1B-NB	-2.25	1.35	1.37
10	0	102	BCL	C1D-C2D	2.25	1.49	1.45
16	8	101	I7D	C11-C12	-2.25	1.41	1.45
12	7	401	U10	C4-C5	-2.25	1.42	1.48
8	C	402	HEC	C4A-C3A	-2.25	1.40	1.45
10	A	102	BCL	C1B-NB	-2.25	1.35	1.37
16	T	101	I7D	C25-C23	-2.25	1.41	1.45
12	L	306	U10	C3-C2	-2.25	1.42	1.48
10	7	402	BCL	C1B-NB	-2.24	1.35	1.37
16	N	101	I7D	C30-C28	-2.23	1.41	1.45
10	B	101	BCL	C1D-C2D	2.23	1.49	1.45
11	M	404	BPH	C3A-C2A	-2.23	1.52	1.54
10	U	101	BCL	C1B-NB	-2.22	1.35	1.37
16	6	102	I7D	C16-C17	-2.22	1.41	1.45
10	R	102	BCL	C1D-C2D	2.22	1.49	1.45
10	M	402	BCL	MG-NA	-2.22	2.01	2.06
10	L	309	BCL	MG-NA	-2.22	2.01	2.06
16	R	101	I7D	C11-C12	-2.21	1.41	1.45
12	L	303	U10	C3-C2	-2.21	1.42	1.48
16	6	102	I7D	C25-C23	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	404	HEC	C1B-NB	-2.21	1.34	1.38
10	V	102	BCL	C1D-C2D	2.20	1.49	1.45
8	C	401	HEC	C1A-C2A	-2.20	1.41	1.45
10	Z	101	BCL	MG-NC	-2.20	2.01	2.06
10	7	402	BCL	MG-NC	-2.19	2.01	2.06
10	Q	102	BCL	CHC-C1C	-2.18	1.32	1.37
10	P	101	BCL	C1D-C2D	2.18	1.49	1.45
10	7	402	BCL	MG-NA	-2.18	2.01	2.06
10	O	101	BCL	C1B-NB	-2.17	1.35	1.37
16	4	101	I7D	C30-C28	-2.17	1.41	1.45
10	J	101	BCL	C1D-C2D	2.17	1.49	1.45
10	K	102	BCL	C1B-NB	-2.17	1.35	1.37
16	X	101	I7D	C25-C23	-2.16	1.41	1.45
16	8	101	I7D	C25-C23	-2.16	1.41	1.45
10	U	101	BCL	MG-NC	-2.16	2.01	2.06
10	K	102	BCL	CHC-C1C	-2.15	1.32	1.37
10	6	103	BCL	CHC-C1C	-2.15	1.32	1.37
10	G	101	BCL	MG-NC	-2.15	2.01	2.06
10	X	102	BCL	MG-NC	-2.14	2.01	2.06
10	M	402	BCL	CHC-C1C	-2.14	1.32	1.37
8	C	402	HEC	C1B-NB	-2.13	1.34	1.38
10	E	102	BCL	MG-NC	-2.13	2.01	2.06
10	F	101	BCL	C1B-NB	-2.13	1.35	1.37
10	L	301	BCL	C1B-NB	-2.13	1.35	1.37
10	D	102	BCL	C1B-NB	-2.13	1.35	1.37
11	L	302	BPH	C1B-C2B	2.12	1.41	1.39
8	C	401	HEC	C1B-NB	-2.12	1.34	1.38
16	8	101	I7D	C30-C28	-2.12	1.41	1.45
10	6	103	BCL	MG-NA	-2.12	2.01	2.06
10	T	102	BCL	CHC-C1C	-2.12	1.32	1.37
10	S	101	BCL	C1B-NB	-2.12	1.35	1.37
10	V	102	BCL	MG-NC	-2.12	2.01	2.06
10	6	103	BCL	MG-NC	-2.11	2.01	2.06
10	Z	101	BCL	MG-NA	-2.11	2.01	2.06
10	N	102	BCL	MG-NC	-2.11	2.01	2.06
10	4	102	BCL	MG-NC	-2.11	2.01	2.06
10	3	102	BCL	MG-NC	-2.11	2.01	2.06
10	X	102	BCL	MG-NA	-2.11	2.01	2.06
16	8	101	I7D	C16-C17	-2.10	1.41	1.45
10	B	101	BCL	MG-NC	-2.10	2.01	2.06
10	5	102	BCL	MG-NC	-2.10	2.01	2.06
10	F	101	BCL	CHC-C1C	-2.10	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	R	102	BCL	MG-NA	-2.10	2.01	2.06
10	2	102	BCL	MG-NC	-2.09	2.01	2.06
10	T	102	BCL	MG-NA	-2.09	2.01	2.06
10	8	102	BCL	MG-NC	-2.09	2.01	2.06
10	V	102	BCL	CHC-C1C	-2.09	1.32	1.37
10	P	101	BCL	MG-NC	-2.09	2.01	2.06
10	O	101	BCL	CHC-C1C	-2.09	1.32	1.37
10	9	101	BCL	MG-NC	-2.08	2.01	2.06
10	4	102	BCL	MG-NA	-2.08	2.01	2.06
10	T	102	BCL	MG-NC	-2.08	2.01	2.06
10	8	102	BCL	CHC-C1C	-2.08	1.32	1.37
10	F	101	BCL	C4D-CHA	2.08	1.45	1.38
10	B	101	BCL	CHC-C1C	-2.08	1.32	1.37
10	E	102	BCL	MG-NA	-2.07	2.01	2.06
10	L	301	BCL	MG-NC	-2.07	2.01	2.06
8	C	403	HEC	C1B-NB	-2.07	1.34	1.38
10	P	101	BCL	CHC-C1C	-2.07	1.32	1.37
10	J	101	BCL	MG-NC	-2.07	2.01	2.06
10	0	102	BCL	MG-NC	-2.06	2.01	2.06
10	N	102	BCL	MG-NA	-2.06	2.01	2.06
10	M	403	BCL	MG-NC	-2.06	2.01	2.06
10	D	102	BCL	CHC-C1C	-2.06	1.32	1.37
10	M	403	BCL	MG-NA	-2.06	2.01	2.06
10	2	102	BCL	MG-NA	-2.06	2.01	2.06
10	8	102	BCL	MG-NA	-2.06	2.01	2.06
10	I	102	BCL	MG-NC	-2.06	2.01	2.06
10	R	102	BCL	MG-NC	-2.06	2.01	2.06
16	X	101	I7D	C30-C28	-2.05	1.41	1.45
10	I	102	BCL	CHC-C1C	-2.05	1.32	1.37
10	0	102	BCL	CHC-C1C	-2.05	1.32	1.37
10	J	101	BCL	MG-NA	-2.05	2.01	2.06
10	B	101	BCL	MG-NA	-2.04	2.01	2.06
11	M	404	BPH	C1B-C2B	2.04	1.41	1.39
10	V	102	BCL	MG-NA	-2.04	2.01	2.06
10	M	402	BCL	MG-NC	-2.04	2.01	2.06
10	1	102	BCL	CHC-C1C	-2.03	1.32	1.37
8	C	402	HEC	C4D-ND	-2.03	1.34	1.38
10	P	101	BCL	MG-NA	-2.03	2.01	2.06
10	0	102	BCL	MG-NA	-2.03	2.01	2.06
10	R	102	BCL	CHC-C1C	-2.03	1.32	1.37
10	W	101	BCL	CHC-C1C	-2.03	1.32	1.37
10	K	102	BCL	C4D-CHA	2.02	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	102	BCL	CHC-C1C	-2.02	1.32	1.37
16	1	101	I7D	C30-C28	-2.02	1.41	1.45
10	G	101	BCL	MG-NA	-2.02	2.01	2.06
16	M	406	I7D	C32-C33	-2.02	1.33	1.35
10	4	102	BCL	CHC-C1C	-2.01	1.32	1.37
10	L	309	BCL	MG-NC	-2.01	2.01	2.06
10	Z	101	BCL	CHC-C1C	-2.01	1.32	1.37
8	C	401	HEC	C4D-ND	-2.01	1.34	1.38
10	Q	102	BCL	MG-NC	-2.01	2.01	2.06
10	W	101	BCL	MG-NC	-2.01	2.01	2.06
10	S	101	BCL	CHC-C1C	-2.01	1.32	1.37
16	T	101	I7D	C32-C33	-2.00	1.33	1.35
10	J	101	BCL	CHC-C1C	-2.00	1.32	1.37
16	D	101	I7D	C32-C33	-2.00	1.33	1.35
10	9	101	BCL	CHC-C1C	-2.00	1.32	1.37

All (1280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	R	102	BCL	C2B-C1B-NB	10.38	117.19	110.23
10	X	102	BCL	C2B-C1B-NB	10.37	117.19	110.23
10	4	102	BCL	C2B-C1B-NB	10.26	117.11	110.23
10	2	102	BCL	C2B-C1B-NB	10.25	117.10	110.23
10	I	102	BCL	C2B-C1B-NB	10.22	117.08	110.23
10	B	101	BCL	C2B-C1B-NB	10.22	117.08	110.23
10	N	102	BCL	C2B-C1B-NB	10.20	117.07	110.23
10	E	102	BCL	C2B-C1B-NB	10.18	117.06	110.23
10	M	403	BCL	C2B-C1B-NB	10.11	117.01	110.23
10	L	301	BCL	C2B-C1B-NB	10.07	116.98	110.23
10	J	101	BCL	C2B-C1B-NB	10.03	116.96	110.23
10	G	101	BCL	C2B-C1B-NB	10.03	116.96	110.23
10	T	102	BCL	C2B-C1B-NB	10.00	116.94	110.23
10	W	101	BCL	C2B-C1B-NB	10.00	116.94	110.23
10	0	102	BCL	C2B-C1B-NB	10.00	116.93	110.23
10	7	402	BCL	C2B-C1B-NB	9.93	116.89	110.23
10	8	102	BCL	C2B-C1B-NB	9.93	116.89	110.23
10	U	101	BCL	C2B-C1B-NB	9.93	116.89	110.23
10	O	101	BCL	C2B-C1B-NB	9.92	116.88	110.23
10	9	101	BCL	C2B-C1B-NB	9.90	116.87	110.23
10	A	102	BCL	C2B-C1B-NB	9.88	116.86	110.23
10	Z	101	BCL	C2B-C1B-NB	9.83	116.82	110.23
10	D	102	BCL	C2B-C1B-NB	9.83	116.82	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Y	101	BCL	C2B-C1B-NB	9.83	116.82	110.23
10	L	309	BCL	C2B-C1B-NB	9.82	116.81	110.23
10	5	102	BCL	C2B-C1B-NB	9.79	116.80	110.23
10	P	101	BCL	C2B-C1B-NB	9.78	116.79	110.23
10	1	102	BCL	C2B-C1B-NB	9.78	116.79	110.23
10	V	102	BCL	C2B-C1B-NB	9.76	116.78	110.23
10	S	101	BCL	C2B-C1B-NB	9.71	116.74	110.23
10	F	101	BCL	C2B-C1B-NB	9.70	116.74	110.23
10	Q	102	BCL	C2B-C1B-NB	9.69	116.73	110.23
10	M	402	BCL	C2B-C1B-NB	9.64	116.69	110.23
10	6	103	BCL	C2B-C1B-NB	9.64	116.69	110.23
10	3	102	BCL	C2B-C1B-NB	9.58	116.65	110.23
10	K	102	BCL	C2B-C1B-NB	9.20	116.40	110.23
10	S	101	BCL	CHD-C1D-ND	-9.09	116.11	124.45
10	5	102	BCL	CHD-C1D-ND	-8.98	116.20	124.45
16	8	101	I7D	C36-C35-C33	-8.98	112.33	125.89
10	W	101	BCL	CHD-C1D-ND	-8.81	116.36	124.45
10	D	102	BCL	CHD-C1D-ND	-8.80	116.37	124.45
10	K	102	BCL	CHD-C1D-ND	-8.79	116.38	124.45
10	O	101	BCL	CHD-C1D-ND	-8.76	116.41	124.45
10	I	102	BCL	CHD-C1D-ND	-8.71	116.45	124.45
10	1	102	BCL	CHD-C1D-ND	-8.66	116.49	124.45
10	3	102	BCL	CHD-C1D-ND	-8.63	116.53	124.45
10	U	101	BCL	CHD-C1D-ND	-8.61	116.54	124.45
10	F	101	BCL	CHD-C1D-ND	-8.60	116.56	124.45
10	7	402	BCL	CHD-C1D-ND	-8.59	116.56	124.45
16	T	101	I7D	C36-C35-C33	-8.58	112.92	125.89
10	A	102	BCL	CHD-C1D-ND	-8.54	116.61	124.45
10	Y	101	BCL	CHD-C1D-ND	-8.52	116.62	124.45
10	Q	102	BCL	CHD-C1D-ND	-8.51	116.63	124.45
10	9	101	BCL	CHD-C1D-ND	-8.45	116.69	124.45
10	M	403	BCL	CHD-C1D-ND	-8.44	116.70	124.45
10	L	309	BCL	CHD-C1D-ND	-8.39	116.74	124.45
16	K	101	I7D	C36-C35-C33	-8.39	113.22	125.89
16	6	102	I7D	C36-C35-C33	-8.35	113.27	125.89
16	3	101	I7D	C36-C35-C33	-8.35	113.28	125.89
16	Q	101	I7D	C36-C35-C33	-8.34	113.29	125.89
16	D	101	I7D	C36-C35-C33	-8.33	113.31	125.89
10	L	301	BCL	CHD-C1D-ND	-8.33	116.80	124.45
10	O	101	BCL	CMD-C2D-C1D	8.30	139.35	124.71
16	A	103	I7D	C36-C35-C33	-8.30	113.36	125.89
10	L	301	BCL	CMD-C2D-C1D	8.25	139.24	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	E	101	I7D	C36-C35-C33	-8.22	113.47	125.89
10	W	101	BCL	CMD-C2D-C1D	8.20	139.16	124.71
10	M	403	BCL	CMD-C2D-C1D	8.19	139.15	124.71
16	X	101	I7D	C36-C35-C33	-8.17	113.55	125.89
10	S	101	BCL	CMD-C2D-C1D	8.15	139.08	124.71
10	1	102	BCL	CMD-C2D-C1D	8.14	139.06	124.71
16	V	101	I7D	C36-C35-C33	-8.14	113.60	125.89
16	4	101	I7D	C36-C35-C33	-8.11	113.64	125.89
10	M	402	BCL	CHD-C1D-ND	-8.10	117.01	124.45
16	I	101	I7D	C36-C35-C33	-8.10	113.66	125.89
10	5	102	BCL	CMD-C2D-C1D	8.06	138.92	124.71
10	7	402	BCL	CMD-C2D-C1D	8.03	138.87	124.71
10	3	102	BCL	CMD-C2D-C1D	8.01	138.83	124.71
10	I	102	BCL	CMD-C2D-C1D	8.00	138.81	124.71
10	A	102	BCL	CMD-C2D-C1D	7.99	138.79	124.71
10	D	102	BCL	CMD-C2D-C1D	7.98	138.78	124.71
16	1	101	I7D	C36-C35-C33	-7.98	113.84	125.89
10	9	101	BCL	CMD-C2D-C1D	7.96	138.74	124.71
10	Y	101	BCL	CMD-C2D-C1D	7.92	138.68	124.71
10	K	102	BCL	CMD-C2D-C1D	7.91	138.66	124.71
10	F	101	BCL	CMD-C2D-C1D	7.86	138.56	124.71
10	U	101	BCL	CMD-C2D-C1D	7.85	138.55	124.71
10	Q	102	BCL	CMD-C2D-C1D	7.83	138.50	124.71
10	4	102	BCL	CHD-C1D-ND	-7.82	117.27	124.45
10	E	102	BCL	CHD-C1D-ND	-7.81	117.28	124.45
10	N	102	BCL	CHD-C1D-ND	-7.80	117.29	124.45
16	N	101	I7D	C36-C35-C33	-7.70	114.25	125.89
10	6	103	BCL	CHD-C1D-ND	-7.69	117.38	124.45
16	R	101	I7D	C36-C35-C33	-7.65	114.34	125.89
10	X	102	BCL	CHD-C1D-ND	-7.64	117.43	124.45
16	M	406	I7D	C36-C35-C33	-7.62	114.37	125.89
10	8	102	BCL	CHD-C1D-ND	-7.58	117.49	124.45
10	L	309	BCL	CMD-C2D-C1D	7.58	138.06	124.71
10	P	101	BCL	CHD-C1D-ND	-7.57	117.49	124.45
10	2	102	BCL	CHD-C1D-ND	-7.56	117.51	124.45
10	Z	101	BCL	CHD-C1D-ND	-7.55	117.51	124.45
10	T	102	BCL	CHD-C1D-ND	-7.54	117.53	124.45
10	G	101	BCL	CHD-C1D-ND	-7.51	117.55	124.45
10	B	101	BCL	CHD-C1D-ND	-7.50	117.56	124.45
10	4	102	BCL	CMD-C2D-C1D	7.50	137.93	124.71
10	R	102	BCL	CHD-C1D-ND	-7.47	117.59	124.45
10	V	102	BCL	CHD-C1D-ND	-7.35	117.70	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	0	102	BCL	CHD-C1D-ND	-7.34	117.71	124.45
10	J	101	BCL	CHD-C1D-ND	-7.22	117.82	124.45
10	M	402	BCL	CMD-C2D-C1D	7.20	137.40	124.71
10	E	102	BCL	CMD-C2D-C1D	7.16	137.34	124.71
10	N	102	BCL	CMD-C2D-C1D	7.12	137.27	124.71
10	T	102	BCL	CMD-C2D-C1D	7.09	137.21	124.71
10	B	101	BCL	CMD-C2D-C1D	7.08	137.19	124.71
10	8	102	BCL	CMD-C2D-C1D	7.06	137.16	124.71
10	G	101	BCL	CMD-C2D-C1D	7.04	137.13	124.71
10	6	103	BCL	CMD-C2D-C1D	7.03	137.10	124.71
10	X	102	BCL	CMD-C2D-C1D	7.03	137.10	124.71
10	Z	101	BCL	CMD-C2D-C1D	7.02	137.09	124.71
10	2	102	BCL	CMD-C2D-C1D	6.95	136.96	124.71
10	J	101	BCL	CMD-C2D-C1D	6.91	136.89	124.71
10	R	102	BCL	CMD-C2D-C1D	6.78	136.66	124.71
10	P	101	BCL	CMD-C2D-C1D	6.77	136.64	124.71
10	V	102	BCL	CMD-C2D-C1D	6.70	136.51	124.71
10	0	102	BCL	CMD-C2D-C1D	6.60	136.35	124.71
10	L	309	BCL	O2D-CGD-CBD	5.80	121.57	111.27
10	P	101	BCL	C2D-C1D-ND	5.47	114.13	110.10
10	R	102	BCL	C2D-C1D-ND	5.35	114.05	110.10
10	V	102	BCL	C2D-C1D-ND	5.35	114.05	110.10
10	1	102	BCL	C2D-C1D-ND	5.34	114.04	110.10
10	N	102	BCL	C2D-C1D-ND	5.33	114.03	110.10
10	Z	101	BCL	C2D-C1D-ND	5.31	114.02	110.10
10	X	102	BCL	C2D-C1D-ND	5.30	114.01	110.10
10	M	403	BCL	C2D-C1D-ND	5.29	114.00	110.10
10	M	402	BCL	O2D-CGD-CBD	5.29	120.67	111.27
10	G	101	BCL	C2D-C1D-ND	5.27	113.99	110.10
10	0	102	BCL	C2D-C1D-ND	5.26	113.98	110.10
10	Q	102	BCL	C2D-C1D-ND	5.24	113.97	110.10
10	8	102	BCL	C2D-C1D-ND	5.21	113.94	110.10
10	M	403	BCL	C3D-C2D-C1D	-5.20	98.73	105.83
10	F	101	BCL	C2D-C1D-ND	5.19	113.93	110.10
10	6	103	BCL	C2D-C1D-ND	5.17	113.91	110.10
10	I	102	BCL	C2D-C1D-ND	5.16	113.91	110.10
10	3	102	BCL	C2D-C1D-ND	5.16	113.91	110.10
10	T	102	BCL	C2D-C1D-ND	5.13	113.89	110.10
10	J	101	BCL	C2D-C1D-ND	5.11	113.87	110.10
10	D	102	BCL	C2D-C1D-ND	5.11	113.87	110.10
10	E	102	BCL	C2D-C1D-ND	5.10	113.86	110.10
10	O	101	BCL	C2D-C1D-ND	5.10	113.86	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	101	BCL	C2D-C1D-ND	5.08	113.85	110.10
10	2	102	BCL	C2D-C1D-ND	5.08	113.85	110.10
10	D	102	BCL	O2D-CGD-CBD	5.06	120.27	111.27
10	S	101	BCL	C2D-C1D-ND	5.06	113.83	110.10
10	U	101	BCL	O2D-CGD-CBD	5.06	120.25	111.27
10	1	102	BCL	C3D-C2D-C1D	-5.04	98.95	105.83
10	5	102	BCL	C2D-C1D-ND	5.04	113.82	110.10
10	L	309	BCL	C2D-C1D-ND	5.04	113.82	110.10
10	K	102	BCL	C2D-C1D-ND	5.04	113.82	110.10
10	Q	102	BCL	C3D-C2D-C1D	-5.04	98.96	105.83
10	S	101	BCL	C3D-C2D-C1D	-5.01	98.99	105.83
10	Y	101	BCL	C2D-C1D-ND	5.01	113.80	110.10
10	7	402	BCL	C2D-C1D-ND	5.00	113.79	110.10
10	F	101	BCL	C4A-NA-C1A	5.00	108.95	106.71
10	D	102	BCL	C3D-C2D-C1D	-5.00	99.01	105.83
10	W	101	BCL	C2D-C1D-ND	5.00	113.79	110.10
10	7	402	BCL	C3D-C2D-C1D	-5.00	99.01	105.83
10	4	102	BCL	C2D-C1D-ND	4.98	113.78	110.10
10	9	101	BCL	C2D-C1D-ND	4.96	113.76	110.10
10	F	101	BCL	C3D-C2D-C1D	-4.96	99.06	105.83
9	C	406	PGV	O01-C1-C2	4.95	122.18	111.50
10	3	102	BCL	C3D-C2D-C1D	-4.95	99.07	105.83
10	I	102	BCL	C3D-C2D-C1D	-4.95	99.07	105.83
10	9	101	BCL	C3D-C2D-C1D	-4.95	99.08	105.83
17	M	407	CDL	OB6-CB5-C51	4.94	120.18	111.09
8	C	403	HEC	CHC-C4B-NB	4.93	130.45	124.37
10	5	102	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
10	W	101	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
10	O	101	BCL	C3D-C2D-C1D	-4.91	99.13	105.83
10	L	301	BCL	C2D-C1D-ND	4.91	113.72	110.10
10	U	101	BCL	C3D-C2D-C1D	-4.91	99.13	105.83
10	L	301	BCL	C3D-C2D-C1D	-4.90	99.14	105.83
10	L	309	BCL	C3D-C2D-C1D	-4.90	99.15	105.83
10	U	101	BCL	C2D-C1D-ND	4.89	113.71	110.10
10	A	102	BCL	C2D-C1D-ND	4.89	113.71	110.10
10	S	101	BCL	O2D-CGD-CBD	4.88	119.95	111.27
10	Y	101	BCL	C3D-C2D-C1D	-4.88	99.18	105.83
10	O	101	BCL	O2D-CGD-CBD	4.87	119.92	111.27
10	A	102	BCL	C3D-C2D-C1D	-4.87	99.19	105.83
10	M	402	BCL	C2D-C1D-ND	4.87	113.69	110.10
10	Q	102	BCL	O2D-CGD-CBD	4.87	119.91	111.27
10	K	102	BCL	C3D-C2D-C1D	-4.86	99.19	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	102	BCL	C4A-NA-C1A	4.86	108.89	106.71
10	J	101	BCL	O2D-CGD-CBD	4.81	119.81	111.27
8	C	404	HEC	CHC-C4B-NB	4.80	130.30	124.37
10	F	101	BCL	O2D-CGD-CBD	4.80	119.79	111.27
10	7	402	BCL	O2D-CGD-CBD	4.79	119.78	111.27
10	N	102	BCL	C3D-C2D-C1D	-4.76	99.33	105.83
10	Z	101	BCL	C3D-C2D-C1D	-4.76	99.33	105.83
8	C	401	HEC	CHC-C4B-NB	4.76	130.24	124.37
10	T	102	BCL	C3D-C2D-C1D	-4.75	99.35	105.83
10	G	101	BCL	C3D-C2D-C1D	-4.75	99.35	105.83
10	W	101	BCL	O2D-CGD-CBD	4.75	119.71	111.27
10	X	102	BCL	C3D-C2D-C1D	-4.75	99.35	105.83
10	8	102	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
10	P	101	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
10	R	102	BCL	C3D-C2D-C1D	-4.73	99.38	105.83
10	6	103	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
10	M	402	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
10	4	102	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
10	2	102	BCL	C3D-C2D-C1D	-4.71	99.40	105.83
10	O	101	BCL	CHD-C4C-NC	4.70	130.30	125.08
10	J	101	BCL	C3D-C2D-C1D	-4.69	99.42	105.83
9	L	312	PGV	O01-C1-C2	4.68	121.59	111.50
10	2	102	BCL	O2D-CGD-CBD	4.67	119.56	111.27
8	C	402	HEC	CHC-C4B-NB	4.67	130.13	124.37
10	0	102	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
10	V	102	BCL	C3D-C2D-C1D	-4.65	99.48	105.83
10	Y	101	BCL	O2D-CGD-CBD	4.65	119.53	111.27
10	5	102	BCL	O2D-CGD-CBD	4.65	119.53	111.27
10	E	102	BCL	C3D-C2D-C1D	-4.64	99.50	105.83
10	B	101	BCL	C3D-C2D-C1D	-4.63	99.51	105.83
10	A	102	BCL	O2D-CGD-CBD	4.61	119.46	111.27
10	M	403	BCL	CHD-C4C-NC	4.59	130.18	125.08
10	1	102	BCL	CHD-C4C-NC	4.59	130.17	125.08
10	B	101	BCL	CHD-C4C-NC	4.56	130.15	125.08
10	9	101	BCL	O2D-CGD-CBD	4.56	119.38	111.27
10	S	101	BCL	CHC-C4B-NB	-4.54	119.45	124.26
10	6	103	BCL	O2D-CGD-CBD	4.52	119.30	111.27
10	K	102	BCL	CHD-C4C-NC	4.52	130.10	125.08
10	E	102	BCL	O2D-CGD-CBD	4.51	119.28	111.27
10	Z	101	BCL	O2D-CGD-CBD	4.51	119.28	111.27
10	X	102	BCL	O2D-CGD-CBD	4.50	119.26	111.27
10	Z	101	BCL	CHD-C4C-NC	4.49	130.06	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	102	BCL	O2D-CGD-CBD	4.48	119.23	111.27
10	P	101	BCL	CHD-C4C-NC	4.48	130.05	125.08
10	O	101	BCL	C3C-C4C-CHD	-4.48	113.83	123.39
10	V	102	BCL	C3C-C4C-CHD	-4.47	113.85	123.39
10	P	101	BCL	C3C-C4C-CHD	-4.47	113.85	123.39
10	R	102	BCL	CHD-C4C-NC	4.46	130.03	125.08
10	N	102	BCL	CHD-C4C-NC	4.45	130.02	125.08
10	F	101	BCL	C1C-NC-C4C	-4.44	104.71	106.71
10	N	102	BCL	C1D-ND-C4D	-4.44	103.18	106.33
10	B	101	BCL	C3C-C4C-CHD	-4.44	113.91	123.39
9	L	304	PGV	O01-C1-C2	4.44	121.06	111.50
10	6	103	BCL	CHD-C4C-NC	4.43	130.00	125.08
10	V	102	BCL	C1D-ND-C4D	-4.43	103.19	106.33
10	W	101	BCL	CHC-C4B-NB	-4.43	119.57	124.26
10	M	403	BCL	C3C-C4C-CHD	-4.43	113.93	123.39
9	L	311	PGV	O01-C1-C2	4.43	121.04	111.50
10	P	101	BCL	O2D-CGD-CBD	4.42	119.13	111.27
10	A	102	BCL	CHC-C4B-NB	-4.42	119.58	124.26
10	Z	101	BCL	C3C-C4C-CHD	-4.41	113.97	123.39
10	8	102	BCL	CHD-C4C-NC	4.41	129.97	125.08
10	P	101	BCL	C1D-ND-C4D	-4.41	103.20	106.33
10	M	402	BCL	CHD-C4C-NC	4.40	129.97	125.08
10	V	102	BCL	CHD-C4C-NC	4.40	129.96	125.08
10	2	102	BCL	CHD-C4C-NC	4.39	129.95	125.08
10	K	102	BCL	O2D-CGD-CBD	4.38	119.05	111.27
10	R	102	BCL	C1D-ND-C4D	-4.38	103.22	106.33
17	6	104	CDL	OA6-CA5-C11	4.38	120.94	111.50
10	R	102	BCL	C3C-C4C-CHD	-4.37	114.06	123.39
10	3	102	BCL	O2D-CGD-CBD	4.37	119.03	111.27
10	4	102	BCL	O2D-CGD-CBD	4.37	119.03	111.27
10	Y	101	BCL	CHC-C4B-NB	-4.37	119.63	124.26
10	0	102	BCL	C3C-C4C-CHD	-4.36	114.07	123.39
10	J	101	BCL	C3C-C4C-CHD	-4.36	114.07	123.39
10	B	101	BCL	O2D-CGD-CBD	4.36	119.01	111.27
10	N	102	BCL	C3C-C4C-CHD	-4.36	114.08	123.39
10	O	101	BCL	C1D-ND-C4D	-4.36	103.24	106.33
17	A	101	CDL	OA6-CA5-C11	4.36	120.89	111.50
10	8	102	BCL	C3C-C4C-CHD	-4.35	114.10	123.39
10	L	309	BCL	CHD-C4C-NC	4.34	129.90	125.08
10	6	103	BCL	C3C-C4C-CHD	-4.34	114.13	123.39
10	J	101	BCL	CHD-C4C-NC	4.33	129.89	125.08
10	G	101	BCL	C3C-C4C-CHD	-4.33	114.14	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	R	102	BCL	O2D-CGD-CBD	4.33	118.95	111.27
10	4	102	BCL	C1D-ND-C4D	-4.32	103.27	106.33
10	G	101	BCL	C1D-ND-C4D	-4.32	103.27	106.33
10	8	102	BCL	O2D-CGD-CBD	4.32	118.94	111.27
10	T	102	BCL	CHD-C4C-NC	4.31	129.86	125.08
10	Y	101	BCL	CHD-C4C-NC	4.31	129.86	125.08
10	E	102	BCL	C1D-ND-C4D	-4.30	103.28	106.33
11	M	404	BPH	C4D-CHA-CBD	-4.30	106.57	108.52
10	4	102	BCL	CHD-C4C-NC	4.30	129.85	125.08
10	T	102	BCL	C3C-C4C-CHD	-4.30	114.21	123.39
10	S	101	BCL	C4A-NA-C1A	4.30	108.64	106.71
10	X	102	BCL	CHD-C4C-NC	4.29	129.84	125.08
10	X	102	BCL	C3C-C4C-CHD	-4.28	114.24	123.39
10	T	102	BCL	O2D-CGD-CBD	4.28	118.87	111.27
8	C	402	HEC	CHA-C4D-ND	4.28	129.07	124.42
17	6	104	CDL	OB6-CB5-C51	4.27	120.71	111.50
10	G	101	BCL	CHD-C4C-NC	4.27	129.82	125.08
10	0	102	BCL	CHD-C4C-NC	4.27	129.82	125.08
10	E	102	BCL	CHD-C4C-NC	4.26	129.81	125.08
10	5	102	BCL	CHC-C4B-NB	-4.26	119.75	124.26
17	M	408	CDL	OB6-CB5-C51	4.26	120.68	111.50
10	N	102	BCL	O2D-CGD-CBD	4.26	118.83	111.27
10	2	102	BCL	C3C-C4C-CHD	-4.26	114.30	123.39
10	I	102	BCL	CHC-C4B-NB	-4.26	119.75	124.26
10	Z	101	BCL	C1D-ND-C4D	-4.25	103.31	106.33
10	V	102	BCL	O2D-CGD-CBD	4.25	118.81	111.27
17	A	101	CDL	OB6-CB5-C51	4.25	120.65	111.50
10	1	102	BCL	C1D-ND-C4D	-4.24	103.32	106.33
10	I	102	BCL	CHD-C4C-NC	4.24	129.78	125.08
9	C	405	PGV	O01-C1-C2	4.24	120.63	111.50
10	M	403	BCL	C1D-ND-C4D	-4.24	103.33	106.33
10	D	102	BCL	CHC-C4B-NB	-4.23	119.78	124.26
10	U	101	BCL	CHC-C4B-NB	-4.23	119.78	124.26
9	H	301	PGV	O01-C1-C2	4.22	120.59	111.50
10	I	102	BCL	C1D-ND-C4D	-4.21	103.34	106.33
10	K	102	BCL	C1C-NC-C4C	-4.21	104.81	106.71
10	E	102	BCL	C3C-C4C-CHD	-4.20	114.42	123.39
9	H	302	PGV	O01-C1-C2	4.20	120.54	111.50
10	X	102	BCL	C1D-ND-C4D	-4.19	103.36	106.33
10	1	102	BCL	O2D-CGD-CBD	4.19	118.72	111.27
10	F	101	BCL	CHC-C4B-NB	-4.19	119.82	124.26
11	L	302	BPH	C4D-CHA-CBD	-4.19	106.62	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	301	BCL	CHD-C4C-NC	4.19	129.73	125.08
10	M	402	BCL	C3C-C4C-CHD	-4.18	114.45	123.39
10	Q	102	BCL	CHC-C4B-NB	-4.18	119.84	124.26
9	M	411	PGV	O01-C1-C2	4.17	120.48	111.50
17	T	103	CDL	OB6-CB5-C51	4.17	120.48	111.50
10	L	301	BCL	C3C-C4C-CHD	-4.16	114.49	123.39
10	4	102	BCL	C3C-C4C-CHD	-4.16	114.50	123.39
10	9	101	BCL	CHC-C4B-NB	-4.16	119.85	124.26
10	8	102	BCL	C1D-ND-C4D	-4.15	103.38	106.33
10	5	102	BCL	CHD-C4C-NC	4.15	129.69	125.08
10	0	102	BCL	O2D-CGD-CBD	4.15	118.64	111.27
10	3	102	BCL	CHD-C4C-NC	4.15	129.68	125.08
8	C	401	HEC	CHA-C4D-ND	4.15	128.92	124.42
9	L	310	PGV	O01-C1-C2	4.14	120.43	111.50
9	C	407	PGV	O01-C1-C2	4.14	120.43	111.50
10	G	101	BCL	O2D-CGD-CBD	4.13	118.60	111.27
10	K	102	BCL	CHC-C4B-NB	-4.12	119.89	124.26
17	0	101	CDL	OA6-CA5-C11	4.12	120.39	111.50
10	6	103	BCL	C1D-ND-C4D	-4.12	103.41	106.33
16	1	101	I7D	C21-C20-C19	4.12	131.91	123.47
10	W	101	BCL	CHD-C4C-NC	4.11	129.65	125.08
16	I	101	I7D	C21-C20-C19	4.11	131.90	123.47
10	2	102	BCL	C1-C2-C3	-4.11	118.94	126.04
10	0	102	BCL	C1D-ND-C4D	-4.11	103.42	106.33
10	B	101	BCL	C1D-ND-C4D	-4.10	103.42	106.33
10	2	102	BCL	C1D-ND-C4D	-4.09	103.43	106.33
10	O	101	BCL	CHC-C4B-NB	-4.09	119.93	124.26
17	T	103	CDL	OA6-CA5-C11	4.09	120.31	111.50
8	C	404	HEC	CHA-C4D-ND	4.08	128.86	124.42
10	T	102	BCL	C1D-ND-C4D	-4.08	103.44	106.33
10	3	102	BCL	C1D-ND-C4D	-4.08	103.44	106.33
10	K	102	BCL	C3C-C4C-CHD	-4.06	114.72	123.39
10	E	102	BCL	C1-C2-C3	-4.06	119.02	126.04
10	7	402	BCL	CHD-C4C-NC	4.05	129.57	125.08
17	0	101	CDL	OB6-CB5-C51	4.05	120.22	111.50
9	M	410	PGV	O01-C1-C2	4.04	120.21	111.50
9	5	101	PGV	O01-C1-C2	4.04	120.21	111.50
10	7	402	BCL	C1D-ND-C4D	-4.04	103.47	106.33
10	Q	102	BCL	C4A-NA-C1A	4.04	108.52	106.71
10	L	309	BCL	C3C-C4C-CHD	-4.04	114.77	123.39
16	R	101	I7D	C21-C20-C19	4.03	131.73	123.47
10	5	102	BCL	C1D-ND-C4D	-4.03	103.47	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	303	CDL	OB6-CB5-C51	4.02	120.17	111.50
10	D	102	BCL	CHD-C4C-NC	4.02	129.54	125.08
10	W	101	BCL	C1D-ND-C4D	-4.01	103.48	106.33
10	M	403	BCL	O2D-CGD-CBD	4.00	118.38	111.27
9	5	103	PGV	O01-C1-C2	3.99	120.11	111.50
10	Q	102	BCL	C1D-ND-C4D	-3.99	103.50	106.33
8	C	401	HEC	CHD-C1D-ND	3.99	129.29	124.37
8	C	403	HEC	C4B-NB-C1B	3.98	109.19	105.07
10	L	301	BCL	C1D-ND-C4D	-3.98	103.51	106.33
10	L	309	BCL	C1D-ND-C4D	-3.98	103.51	106.33
10	J	101	BCL	C1D-ND-C4D	-3.97	103.51	106.33
17	2	101	CDL	OB6-CB5-C51	3.97	120.06	111.50
10	Q	102	BCL	CHD-C4C-NC	3.97	129.48	125.08
10	3	102	BCL	CHC-C4B-NB	-3.97	120.06	124.26
10	1	102	BCL	C3C-C4C-CHD	-3.96	114.94	123.39
10	M	402	BCL	C1D-ND-C4D	-3.95	103.53	106.33
16	8	101	I7D	C21-C20-C19	3.94	131.56	123.47
8	C	404	HEC	CHD-C1D-ND	3.94	129.23	124.37
8	C	403	HEC	CHA-C4D-ND	3.93	128.68	124.42
10	D	102	BCL	C1D-ND-C4D	-3.92	103.55	106.33
10	S	101	BCL	C1D-ND-C4D	-3.92	103.55	106.33
8	C	402	HEC	C4B-NB-C1B	3.92	109.12	105.07
10	F	101	BCL	CHD-C4C-NC	3.92	129.43	125.08
10	S	101	BCL	CHD-C4C-NC	3.91	129.42	125.08
10	X	102	BCL	C1-C2-C3	-3.90	119.29	126.04
10	A	102	BCL	C1D-ND-C4D	-3.90	103.57	106.33
10	9	101	BCL	CHD-C4C-NC	3.90	129.41	125.08
10	V	102	BCL	C1-C2-C3	-3.90	119.31	126.04
9	D	103	PGV	O01-C1-C2	3.89	119.89	111.50
16	8	101	I7D	C25-C23-C22	3.88	124.90	118.94
10	Y	101	BCL	C3C-C4C-CHD	-3.88	115.11	123.39
10	Z	101	BCL	C1-C2-C3	-3.88	119.34	126.04
8	C	403	HEC	CHD-C1D-ND	3.87	129.15	124.37
17	6	101	CDL	OA6-CA5-C11	3.87	119.83	111.50
16	8	101	I7D	C30-C28-C27	3.86	124.86	118.94
16	8	101	I7D	C29-C28-C27	-3.85	117.53	122.92
10	K	102	BCL	C1D-ND-C4D	-3.84	103.61	106.33
9	K	103	PGV	O01-C1-C2	3.84	119.77	111.50
10	U	101	BCL	CHD-C4C-NC	3.83	129.33	125.08
10	F	101	BCL	C1D-ND-C4D	-3.83	103.61	106.33
10	Y	101	BCL	C1D-ND-C4D	-3.83	103.61	106.33
10	1	102	BCL	C1-C2-C3	-3.83	119.42	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1	102	BCL	CHC-C4B-NB	-3.82	120.21	124.26
10	9	101	BCL	C1D-ND-C4D	-3.79	103.64	106.33
10	A	102	BCL	CHD-C4C-NC	3.78	129.28	125.08
10	L	301	BCL	O2D-CGD-CBD	3.78	117.99	111.27
16	8	101	I7D	C24-C23-C22	-3.78	117.62	122.92
16	K	101	I7D	C21-C20-C19	3.78	131.21	123.47
10	M	403	BCL	CHC-C4B-NB	-3.76	120.27	124.26
8	C	404	HEC	C4B-NB-C1B	3.76	108.96	105.07
16	A	103	I7D	C21-C20-C19	3.75	131.16	123.47
8	C	402	HEC	CHD-C1D-ND	3.75	129.00	124.37
16	D	101	I7D	C21-C20-C19	3.75	131.15	123.47
10	I	102	BCL	C3C-C4C-CHD	-3.75	115.39	123.39
16	X	101	I7D	C21-C20-C19	3.74	131.14	123.47
16	8	101	I7D	C20-C21-C22	3.73	131.12	123.47
10	U	101	BCL	C1D-ND-C4D	-3.72	103.69	106.33
17	2	101	CDL	OA6-CA5-C11	3.71	119.50	111.50
10	R	102	BCL	C1-C2-C3	-3.69	119.65	126.04
16	4	101	I7D	C21-C20-C19	3.69	131.03	123.47
10	R	102	BCL	CHC-C4B-NB	-3.69	120.35	124.26
16	6	102	I7D	C21-C20-C19	3.69	131.03	123.47
16	3	101	I7D	C21-C20-C19	3.69	131.03	123.47
9	5	104	PGV	O01-C1-C2	3.68	119.44	111.50
16	N	101	I7D	C21-C20-C19	3.67	130.99	123.47
17	6	101	CDL	OB6-CB5-C51	3.66	119.39	111.50
8	C	401	HEC	CHB-C1B-NB	3.64	128.38	124.42
10	B	101	BCL	CHC-C4B-NB	-3.64	120.40	124.26
10	N	102	BCL	CHC-C4B-NB	-3.63	120.41	124.26
17	M	408	CDL	OA6-CA5-C11	3.63	119.32	111.50
8	C	401	HEC	C4B-NB-C1B	3.62	108.81	105.07
10	3	102	BCL	C3C-C4C-CHD	-3.62	115.65	123.39
10	W	101	BCL	C3C-C4C-CHD	-3.62	115.66	123.39
8	C	402	HEC	CHB-C1B-NB	3.61	128.34	124.42
10	Y	101	BCL	C4-C3-C5	3.61	121.34	115.27
10	Q	102	BCL	C3C-C4C-CHD	-3.60	115.70	123.39
10	5	102	BCL	C3C-C4C-CHD	-3.59	115.72	123.39
10	X	102	BCL	CHC-C4B-NB	-3.59	120.45	124.26
10	N	102	BCL	C3D-C4D-ND	3.59	116.04	110.24
10	V	102	BCL	C3D-C4D-ND	3.58	116.04	110.24
10	F	101	BCL	C3C-C4C-CHD	-3.58	115.75	123.39
10	D	102	BCL	C3C-C4C-CHD	-3.57	115.76	123.39
10	L	309	BCL	CHC-C4B-NB	-3.57	120.48	124.26
16	V	101	I7D	C21-C20-C19	3.56	130.78	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	102	BCL	C1C-NC-C4C	-3.56	105.11	106.71
10	2	102	BCL	CHC-C4B-NB	-3.55	120.50	124.26
10	0	102	BCL	C1-C2-C3	-3.53	119.93	126.04
10	U	101	BCL	C1-C2-C3	-3.52	119.95	126.04
17	H	303	CDL	OA6-CA5-C11	3.51	119.08	111.50
10	4	102	BCL	C3D-C4D-ND	3.51	115.92	110.24
10	E	102	BCL	C3D-C4D-ND	3.51	115.92	110.24
10	P	101	BCL	C1-C2-C3	-3.50	119.98	126.04
10	7	402	BCL	CHC-C4B-NB	-3.50	120.55	124.26
10	L	301	BCL	CHC-C4B-NB	-3.50	120.56	124.26
10	7	402	BCL	C3C-C4C-CHD	-3.50	115.92	123.39
8	C	402	HEC	C4C-NC-C1C	3.49	108.77	105.35
10	6	103	BCL	CHC-C4B-NB	-3.49	120.56	124.26
10	G	101	BCL	CHC-C4B-NB	-3.49	120.57	124.26
10	M	402	BCL	C3D-C4D-ND	3.49	115.88	110.24
10	L	309	BCL	C1-C2-C3	-3.48	120.03	126.04
16	8	101	I7D	C18-C17-C19	-3.48	118.06	122.92
16	T	101	I7D	C21-C20-C19	3.47	130.59	123.47
10	P	101	BCL	C3D-C4D-ND	3.47	115.85	110.24
10	R	102	BCL	C3D-C4D-ND	3.47	115.85	110.24
10	6	103	BCL	CHB-C1B-NB	-3.45	120.60	124.26
17	M	407	CDL	OA6-CA5-C11	3.45	120.43	110.80
10	G	101	BCL	C3D-C4D-ND	3.45	115.81	110.24
10	0	102	BCL	CHC-C4B-NB	-3.44	120.62	124.26
8	C	402	HEC	CBC-CAC-C3C	3.44	121.91	112.43
10	S	101	BCL	C3C-C4C-CHD	-3.43	116.07	123.39
9	L	305	PGV	O01-C1-C2	3.42	118.88	111.50
10	A	102	BCL	C1-C2-C3	-3.42	120.13	126.04
16	X	101	I7D	C29-C28-C27	-3.42	118.14	122.92
10	6	103	BCL	C1-C2-C3	-3.42	120.14	126.04
10	0	102	BCL	C3D-C4D-ND	3.41	115.76	110.24
10	I	102	BCL	C1-C2-C3	-3.41	120.15	126.04
10	T	102	BCL	C3D-C4D-ND	3.41	115.75	110.24
10	J	101	BCL	CHC-C4B-NB	-3.41	120.65	124.26
8	C	404	HEC	CHB-C1B-NB	3.40	128.12	124.42
10	9	101	BCL	C3C-C4C-CHD	-3.40	116.13	123.39
10	2	102	BCL	C3D-C4D-ND	3.39	115.73	110.24
10	Z	101	BCL	C3D-C4D-ND	3.39	115.72	110.24
10	4	102	BCL	C1-C2-C3	-3.39	120.18	126.04
10	6	103	BCL	C3D-C4D-ND	3.39	115.72	110.24
8	C	403	HEC	CHB-C1B-NB	3.39	128.10	124.42
16	E	101	I7D	C20-C21-C22	3.39	130.41	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	102	BCL	CHC-C4B-NB	-3.38	120.67	124.26
9	F	102	PGV	O01-C1-C2	3.38	118.79	111.50
10	L	309	BCL	C3D-C4D-ND	3.38	115.70	110.24
10	X	102	BCL	C3D-C4D-ND	3.38	115.70	110.24
10	4	102	BCL	CHC-C4B-NB	-3.37	120.69	124.26
10	B	101	BCL	C3D-C4D-ND	3.37	115.68	110.24
17	M	407	CDL	OA8-CA7-C31	3.36	120.19	111.38
10	M	402	BCL	CHC-C4B-NB	-3.36	120.70	124.26
10	O	101	BCL	C3D-C4D-ND	3.36	115.67	110.24
16	8	101	I7D	C13-C12-C14	-3.36	118.22	122.92
16	Q	101	I7D	C21-C20-C19	3.35	130.34	123.47
10	M	403	BCL	C3D-C4D-ND	3.35	115.65	110.24
16	8	101	I7D	C31-C32-C33	-3.35	122.53	127.31
16	N	101	I7D	C29-C28-C27	-3.34	118.24	122.92
10	I	102	BCL	C3D-C4D-ND	3.34	115.64	110.24
10	8	102	BCL	C3D-C4D-ND	3.34	115.64	110.24
16	6	102	I7D	C20-C21-C22	3.34	130.31	123.47
9	M	410	PGV	C02-O01-C1	-3.32	109.61	117.79
10	J	101	BCL	C3D-C4D-ND	3.32	115.61	110.24
16	M	406	I7D	C13-C12-C14	-3.32	118.28	122.92
10	D	102	BCL	C4A-NA-C1A	3.31	108.20	106.71
8	C	401	HEC	C4C-NC-C1C	3.31	108.59	105.35
10	S	101	BCL	C1C-NC-C4C	-3.31	105.22	106.71
10	A	102	BCL	C4A-NA-C1A	3.31	108.19	106.71
16	E	101	I7D	C21-C20-C19	3.31	130.25	123.47
10	I	102	BCL	CHB-C1B-NB	-3.30	120.76	124.26
10	5	102	BCL	CHB-C1B-NB	-3.30	120.77	124.26
10	7	402	BCL	C3D-C4D-ND	3.29	115.57	110.24
10	M	402	BCL	C1-C2-C3	-3.29	120.35	126.04
10	5	102	BCL	C3D-C4D-ND	3.29	115.56	110.24
8	C	403	HEC	C4C-NC-C1C	3.29	108.56	105.35
8	C	404	HEC	C4C-NC-C1C	3.29	108.56	105.35
10	P	101	BCL	CHC-C4B-NB	-3.28	120.78	124.26
10	K	102	BCL	C1-C2-C3	-3.27	120.38	126.04
16	X	101	I7D	C20-C21-C22	3.27	130.17	123.47
10	3	102	BCL	C3D-C4D-ND	3.27	115.53	110.24
16	R	101	I7D	C18-C17-C19	-3.27	118.34	122.92
10	V	102	BCL	CHC-C4B-NB	-3.27	120.80	124.26
10	3	102	BCL	CHB-C1B-NB	-3.26	120.80	124.26
16	1	101	I7D	C18-C17-C19	-3.26	118.36	122.92
10	Z	101	BCL	CHC-C4B-NB	-3.25	120.81	124.26
10	A	102	BCL	C3C-C4C-CHD	-3.25	116.44	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	101	I7D	C18-C17-C19	-3.24	118.38	122.92
10	O	101	BCL	C1-C2-C3	-3.24	120.44	126.04
10	L	301	BCL	C3D-C4D-ND	3.24	115.48	110.24
16	D	101	I7D	C18-C17-C19	-3.23	118.39	122.92
16	A	103	I7D	C29-C28-C27	-3.23	118.40	122.92
16	6	102	I7D	C13-C12-C14	-3.23	118.40	122.92
8	C	401	HEC	CBC-CAC-C3C	3.23	121.33	112.43
10	T	102	BCL	CHC-C4B-NB	-3.23	120.84	124.26
10	W	101	BCL	C3D-C4D-ND	3.22	115.45	110.24
10	3	102	BCL	C1-C2-C3	-3.22	120.48	126.04
8	C	403	HEC	CBC-CAC-C3C	3.22	121.30	112.43
10	G	101	BCL	C1-C2-C3	-3.21	120.49	126.04
16	K	101	I7D	C18-C17-C19	-3.21	118.43	122.92
10	1	102	BCL	C3D-C4D-ND	3.20	115.42	110.24
16	E	101	I7D	C29-C28-C27	-3.20	118.44	122.92
10	J	101	BCL	C1-C2-C3	-3.20	120.51	126.04
16	R	101	I7D	C13-C12-C14	-3.20	118.44	122.92
16	X	101	I7D	C24-C23-C22	-3.20	118.44	122.92
16	X	101	I7D	C18-C17-C19	-3.20	118.45	122.92
11	M	404	BPH	C2B-C1B-NB	-3.20	107.32	109.53
10	A	102	BCL	C3D-C4D-ND	3.19	115.40	110.24
10	Y	101	BCL	C3D-C4D-ND	3.19	115.40	110.24
10	Q	102	BCL	C1-C2-C3	-3.19	120.53	126.04
16	8	101	I7D	C16-C17-C19	3.18	123.82	118.94
10	D	102	BCL	C3D-C4D-ND	3.18	115.38	110.24
16	6	102	I7D	C24-C23-C22	-3.18	118.47	122.92
10	S	101	BCL	C3D-C4D-ND	3.18	115.38	110.24
10	U	101	BCL	C3C-C4C-CHD	-3.18	116.60	123.39
10	F	101	BCL	O2A-CGA-CBA	3.18	121.88	111.91
10	Q	102	BCL	C3D-C4D-ND	3.17	115.37	110.24
16	M	406	I7D	C18-C17-C19	-3.17	118.48	122.92
10	9	101	BCL	C1-C2-C3	-3.17	120.56	126.04
10	N	102	BCL	C1-C2-C3	-3.16	120.57	126.04
16	Q	101	I7D	C18-C17-C19	-3.16	118.50	122.92
16	N	101	I7D	C18-C17-C19	-3.16	118.50	122.92
10	8	102	BCL	CHC-C4B-NB	-3.16	120.92	124.26
16	3	101	I7D	C18-C17-C19	-3.15	118.51	122.92
10	1	102	BCL	CHB-C1B-NB	-3.15	120.92	124.26
10	K	102	BCL	C3D-C4D-ND	3.15	115.33	110.24
16	V	101	I7D	C13-C12-C14	-3.15	118.52	122.92
16	N	101	I7D	C13-C12-C14	-3.14	118.52	122.92
16	A	103	I7D	C18-C17-C19	-3.14	118.52	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	101	I7D	C13-C12-C14	-3.14	118.53	122.92
8	C	404	HEC	CBC-CAC-C3C	3.13	121.07	112.43
16	6	102	I7D	C18-C17-C19	-3.13	118.54	122.92
10	U	101	BCL	C3D-C4D-ND	3.13	115.29	110.24
16	V	101	I7D	C18-C17-C19	-3.12	118.55	122.92
10	B	101	BCL	C1-C2-C3	-3.11	120.66	126.04
10	9	101	BCL	C3D-C4D-ND	3.11	115.27	110.24
16	I	101	I7D	C13-C12-C14	-3.10	118.58	122.92
10	Z	101	BCL	CHB-C1B-NB	-3.10	120.98	124.26
16	X	101	I7D	C13-C12-C14	-3.09	118.59	122.92
16	E	101	I7D	C24-C23-C22	-3.09	118.59	122.92
16	4	101	I7D	C18-C17-C19	-3.09	118.59	122.92
10	Y	101	BCL	C4A-NA-C1A	3.09	108.09	106.71
16	A	103	I7D	C13-C12-C14	-3.09	118.60	122.92
10	9	101	BCL	C4A-NA-C1A	3.08	108.09	106.71
10	L	301	BCL	O2A-CGA-CBA	3.08	121.57	111.91
16	T	101	I7D	C18-C17-C19	-3.08	118.61	122.92
10	8	102	BCL	C4-C3-C5	3.08	120.45	115.27
10	T	102	BCL	O2A-CGA-CBA	3.07	121.55	111.91
10	D	102	BCL	C1-C2-C3	-3.07	120.73	126.04
10	M	403	BCL	CHB-C1B-NB	-3.07	121.01	124.26
16	T	101	I7D	C20-C21-C22	3.07	129.76	123.47
10	E	102	BCL	O2A-CGA-CBA	3.07	121.53	111.91
16	T	101	I7D	C24-C23-C22	-3.06	118.63	122.92
16	3	101	I7D	C29-C28-C27	-3.06	118.63	122.92
17	A	101	CDL	CB4-OB6-CB5	-3.06	110.25	117.79
10	O	101	BCL	C4A-NA-C1A	3.06	108.08	106.71
10	8	102	BCL	CHB-C1B-NB	-3.06	121.02	124.26
16	A	103	I7D	C24-C23-C22	-3.05	118.65	122.92
17	M	407	CDL	CB4-OB6-CB5	-3.04	112.23	117.90
10	F	101	BCL	CHB-C1B-NB	-3.04	121.04	124.26
10	Q	102	BCL	CHB-C1B-NB	-3.04	121.04	124.26
16	1	101	I7D	C13-C12-C14	-3.03	118.67	122.92
10	7	402	BCL	CHB-C1B-NB	-3.03	121.05	124.26
16	D	101	I7D	C13-C12-C14	-3.03	118.68	122.92
10	F	101	BCL	C1D-CHD-C4C	-3.03	119.32	126.62
10	7	402	BCL	C1-C2-C3	-3.00	120.85	126.04
10	F	101	BCL	C1-C2-C3	-3.00	120.85	126.04
9	L	311	PGV	O03-C19-C20	3.00	121.32	111.91
16	Q	101	I7D	C24-C23-C22	-3.00	118.72	122.92
10	6	103	BCL	C4-C3-C5	3.00	120.31	115.27
16	E	101	I7D	C18-C17-C19	-3.00	118.73	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	101	I7D	C13-C12-C14	-2.99	118.74	122.92
11	L	302	BPH	C2B-C1B-NB	-2.99	107.46	109.53
16	8	101	I7D	C32-C31-C30	2.98	132.53	123.22
10	Y	101	BCL	C4B-C3B-C2B	-2.98	103.56	108.36
10	B	101	BCL	C4B-C3B-C2B	-2.98	103.57	108.36
16	1	101	I7D	C24-C23-C22	-2.98	118.75	122.92
10	O	101	BCL	CHB-C1B-NB	-2.98	121.11	124.26
10	V	102	BCL	O2A-CGA-CBA	2.97	121.24	111.91
10	O	101	BCL	CHC-C1C-NC	2.97	128.62	124.51
10	F	101	BCL	C3D-C4D-ND	2.97	115.04	110.24
9	5	101	PGV	O03-C19-C20	2.97	121.22	111.91
16	N	101	I7D	C24-C23-C22	-2.96	118.77	122.92
10	O	101	BCL	C4B-C3B-C2B	-2.96	103.59	108.36
10	N	102	BCL	O2A-CGA-CBA	2.96	121.20	111.91
16	6	102	I7D	C29-C28-C27	-2.96	118.78	122.92
10	T	102	BCL	CHB-C1B-NB	-2.96	121.13	124.26
10	N	102	BCL	C4-C3-C5	2.96	120.24	115.27
16	4	101	I7D	C29-C28-C27	-2.95	118.78	122.92
10	L	301	BCL	CHB-C1B-NB	-2.95	121.13	124.26
16	R	101	I7D	C24-C23-C22	-2.95	118.78	122.92
10	W	101	BCL	CHB-C1B-NB	-2.95	121.13	124.26
10	2	102	BCL	O2A-CGA-CBA	2.95	121.17	111.91
10	B	101	BCL	O2A-CGA-CBA	2.95	121.16	111.91
16	1	101	I7D	C29-C28-C27	-2.95	118.80	122.92
10	9	101	BCL	O2A-CGA-CBA	2.95	121.15	111.91
16	X	101	I7D	C30-C28-C27	2.94	123.46	118.94
10	4	102	BCL	O2A-CGA-CBA	2.94	121.14	111.91
10	N	102	BCL	C2A-C1A-CHA	-2.94	118.71	123.86
16	8	101	I7D	C11-C12-C14	2.94	123.46	118.94
10	X	102	BCL	O2A-CGA-CBA	2.94	121.14	111.91
16	I	101	I7D	C24-C23-C22	-2.94	118.80	122.92
10	8	102	BCL	C1-C2-C3	-2.93	120.97	126.04
10	S	101	BCL	C1D-CHD-C4C	-2.93	119.55	126.62
16	3	101	I7D	C13-C12-C14	-2.93	118.82	122.92
16	3	101	I7D	C24-C23-C22	-2.93	118.82	122.92
9	D	103	PGV	C02-O01-C1	-2.93	110.59	117.79
16	D	101	I7D	C24-C23-C22	-2.93	118.83	122.92
10	K	102	BCL	CHB-C1B-NB	-2.93	121.16	124.26
17	0	101	CDL	OA8-CA7-C31	2.93	121.09	111.91
16	M	406	I7D	C11-C12-C14	2.92	123.43	118.94
16	K	101	I7D	C13-C12-C14	-2.92	118.83	122.92
17	6	104	CDL	CA6-CA4-CA3	-2.92	104.89	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4	101	I7D	C24-C23-C22	-2.91	118.84	122.92
10	9	101	BCL	C4-C3-C5	2.91	120.17	115.27
10	V	102	BCL	CHB-C1B-NB	-2.91	121.17	124.26
10	7	402	BCL	C4-C3-C5	2.91	120.17	115.27
10	J	101	BCL	CHB-C1B-NB	-2.91	121.18	124.26
16	T	101	I7D	C29-C28-C27	-2.90	118.86	122.92
10	T	102	BCL	C4-C3-C5	2.90	120.15	115.27
10	W	101	BCL	C4B-C3B-C2B	-2.90	103.70	108.36
16	D	101	I7D	C29-C28-C27	-2.90	118.86	122.92
10	9	101	BCL	CHB-C1B-NB	-2.89	121.20	124.26
16	4	101	I7D	C13-C12-C14	-2.89	118.87	122.92
10	P	101	BCL	O2A-CGA-CBA	2.89	120.98	111.91
10	Y	101	BCL	C1-C2-C3	-2.89	121.05	126.04
10	6	103	BCL	C4B-C3B-C2B	-2.89	103.71	108.36
10	W	101	BCL	C1-C2-C3	-2.89	121.05	126.04
10	L	309	BCL	O2A-CGA-CBA	2.89	120.97	111.91
10	1	102	BCL	C4A-NA-C1A	2.88	108.00	106.71
10	X	102	BCL	CHB-C1B-NB	-2.88	121.20	124.26
16	N	101	I7D	C30-C28-C27	2.88	123.36	118.94
10	G	101	BCL	O2A-CGA-CBA	2.88	120.95	111.91
16	V	101	I7D	C24-C23-C22	-2.88	118.89	122.92
10	R	102	BCL	O2A-CGA-CBA	2.88	120.94	111.91
16	N	101	I7D	C20-C21-C22	2.88	129.37	123.47
10	J	101	BCL	O2A-CGA-CBA	2.87	120.93	111.91
16	Q	101	I7D	C29-C28-C27	-2.87	118.90	122.92
10	4	102	BCL	CHB-C1B-NB	-2.87	121.22	124.26
9	L	312	PGV	O03-C19-C20	2.87	120.90	111.91
16	K	101	I7D	C29-C28-C27	-2.86	118.91	122.92
10	2	102	BCL	CHB-C1B-NB	-2.86	121.23	124.26
10	V	102	BCL	C4-C3-C5	2.86	120.08	115.27
16	E	101	I7D	C13-C12-C14	-2.85	118.92	122.92
16	V	101	I7D	C29-C28-C27	-2.85	118.93	122.92
10	V	102	BCL	C2A-C1A-CHA	-2.84	118.89	123.86
8	C	403	HEC	CHA-C1A-NA	2.84	127.52	124.44
17	H	303	CDL	OA8-CA7-C31	2.84	120.83	111.91
10	Z	101	BCL	O2A-CGA-CBA	2.84	120.83	111.91
13	I	103	LMT	C1B-O1B-C4'	-2.84	110.94	117.96
8	C	401	HEC	CHA-C1A-NA	2.84	127.51	124.44
10	Y	101	BCL	C1C-NC-C4C	-2.84	105.43	106.71
10	R	102	BCL	CHB-C1B-NB	-2.84	121.25	124.26
9	C	405	PGV	O03-C19-C20	2.84	120.81	111.91
10	F	101	BCL	C4B-C3B-C2B	-2.84	103.80	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	301	BCL	C4B-C3B-C2B	-2.83	103.80	108.36
10	0	102	BCL	C4B-C3B-C2B	-2.83	103.80	108.36
10	D	102	BCL	C1C-NC-C4C	-2.83	105.43	106.71
10	1	102	BCL	CHB-C4A-NA	2.83	128.43	124.51
17	6	101	CDL	OA8-CA7-C31	2.83	120.79	111.91
10	K	102	BCL	C1D-CHD-C4C	-2.83	119.80	126.62
10	Q	102	BCL	C4B-C3B-C2B	-2.83	103.81	108.36
10	2	102	BCL	C4-C3-C5	2.83	120.02	115.27
10	P	101	BCL	CHB-C1B-NB	-2.83	121.27	124.26
9	L	305	PGV	O03-C19-C20	2.82	120.76	111.91
10	E	102	BCL	C2A-C1A-CHA	-2.82	118.93	123.86
10	8	102	BCL	O2A-CGA-CBA	2.82	120.75	111.91
10	P	101	BCL	C4-C3-C5	2.82	120.01	115.27
10	6	103	BCL	O2A-CGA-CBA	2.82	120.75	111.91
16	K	101	I7D	C24-C23-C22	-2.81	118.98	122.92
8	C	402	HEC	CHA-C1A-NA	2.81	127.48	124.44
10	E	102	BCL	CHB-C1B-NB	-2.81	121.28	124.26
10	R	102	BCL	CHB-C4A-NA	2.81	128.40	124.51
10	D	102	BCL	C4B-C3B-C2B	-2.81	103.84	108.36
10	U	101	BCL	C4A-NA-C1A	2.81	107.97	106.71
16	4	101	I7D	C20-C21-C22	2.81	129.23	123.47
10	I	102	BCL	C4B-C3B-C2B	-2.81	103.84	108.36
10	G	101	BCL	C2A-C1A-CHA	-2.81	118.95	123.86
10	9	101	BCL	C4B-C3B-C2B	-2.80	103.86	108.36
10	0	102	BCL	C4-C3-C5	2.79	119.97	115.27
16	I	101	I7D	C16-C17-C19	2.79	123.23	118.94
10	Z	101	BCL	CHB-C4A-NA	2.79	128.38	124.51
16	I	101	I7D	C29-C28-C27	-2.79	119.01	122.92
10	W	101	BCL	C4A-NA-C1A	2.79	107.96	106.71
10	T	102	BCL	C1-C2-C3	-2.79	121.22	126.04
16	M	406	I7D	C29-C28-C27	-2.79	119.02	122.92
10	R	102	BCL	C4-C3-C5	2.79	119.96	115.27
10	D	102	BCL	CHB-C1B-NB	-2.79	121.31	124.26
8	C	402	HEC	CBB-CAB-C3B	2.78	120.10	112.43
10	M	402	BCL	C4B-C3B-C2B	-2.78	103.88	108.36
8	C	404	HEC	CBB-CAB-C3B	2.78	120.10	112.43
13	3	103	LMT	C1B-O1B-C4'	-2.78	111.09	117.96
10	B	101	BCL	CHB-C1B-NB	-2.78	121.32	124.26
10	S	101	BCL	C1-C2-C3	-2.78	121.24	126.04
16	8	101	I7D	C27-C26-C25	2.78	131.88	123.22
16	6	102	I7D	C11-C12-C14	2.77	123.20	118.94
10	4	102	BCL	C4-C3-C5	2.77	119.94	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	102	BCL	C4B-C3B-C2B	-2.77	103.90	108.36
16	1	101	I7D	C16-C17-C19	2.77	123.19	118.94
10	G	101	BCL	C4-C3-C5	2.77	119.93	115.27
16	A	103	I7D	C30-C28-C27	2.77	123.19	118.94
10	0	102	BCL	CHB-C1B-NB	-2.77	121.33	124.26
10	4	102	BCL	C2A-C1A-CHA	-2.76	119.03	123.86
16	Q	101	I7D	C20-C21-C22	2.76	129.14	123.47
10	N	102	BCL	C4B-C3B-C2B	-2.76	103.92	108.36
10	2	102	BCL	C4B-C3B-C2B	-2.76	103.92	108.36
10	B	101	BCL	C4-C3-C5	2.76	119.92	115.27
10	S	101	BCL	C4B-C3B-C2B	-2.76	103.92	108.36
10	0	102	BCL	O2A-CGA-CBA	2.76	120.56	111.91
10	4	102	BCL	CHB-C4A-NA	2.76	128.32	124.51
10	K	102	BCL	C4B-C3B-C2B	-2.76	103.93	108.36
17	A	101	CDL	CA4-OA6-CA5	-2.75	111.01	117.79
16	E	101	I7D	C30-C28-C27	2.75	123.17	118.94
10	U	101	BCL	O2A-CGA-CBA	2.75	120.55	111.91
10	M	403	BCL	CMB-C2B-C3B	2.75	133.37	125.93
16	R	101	I7D	C29-C28-C27	-2.75	119.07	122.92
10	M	403	BCL	C4B-C3B-C2B	-2.75	103.93	108.36
10	A	102	BCL	O2A-CGA-CBA	2.75	120.54	111.91
10	T	102	BCL	CHB-C4A-NA	2.75	128.32	124.51
10	M	403	BCL	CED-O2D-CGD	2.75	122.15	115.94
8	C	402	HEC	CHA-C4D-C3D	-2.75	120.80	124.84
8	C	404	HEC	CHA-C1A-NA	2.75	127.41	124.44
10	A	102	BCL	C4B-C3B-C2B	-2.74	103.95	108.36
10	G	101	BCL	CHB-C1B-NB	-2.74	121.35	124.26
9	M	411	PGV	C02-O01-C1	-2.74	111.05	117.79
10	B	101	BCL	CMB-C2B-C3B	2.74	133.32	125.93
10	I	102	BCL	CHB-C4A-NA	2.73	128.29	124.51
10	R	102	BCL	C4B-C3B-C2B	-2.73	103.96	108.36
10	L	301	BCL	CED-O2D-CGD	2.73	122.12	115.94
10	5	102	BCL	C1-C2-C3	-2.73	121.32	126.04
10	M	403	BCL	O2A-CGA-CBA	2.73	120.48	111.91
10	4	102	BCL	CHC-C1C-NC	2.73	128.28	124.51
10	P	101	BCL	C2A-C1A-CHA	-2.73	119.09	123.86
10	P	101	BCL	C4B-C3B-C2B	-2.72	103.98	108.36
10	7	402	BCL	C4B-C3B-C2B	-2.72	103.98	108.36
9	D	103	PGV	O03-C19-C20	2.72	120.44	111.91
10	G	101	BCL	C4B-C3B-C2B	-2.72	103.99	108.36
10	X	102	BCL	C4B-C3B-C2B	-2.72	103.99	108.36
10	U	101	BCL	C1D-CHD-C4C	-2.72	120.07	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	309	BCL	CHB-C1B-NB	-2.71	121.38	124.26
16	D	101	I7D	C16-C17-C19	2.71	123.11	118.94
10	L	301	BCL	C4-C3-C5	2.71	119.83	115.27
10	B	101	BCL	CHC-C1C-NC	2.71	128.26	124.51
10	5	102	BCL	C4B-C3B-C2B	-2.71	104.00	108.36
10	A	102	BCL	CHB-C1B-NB	-2.71	121.39	124.26
9	L	311	PGV	C02-O01-C1	-2.70	111.14	117.79
10	Y	101	BCL	CHC-C1C-NC	2.70	128.25	124.51
10	A	102	BCL	C1C-NC-C4C	-2.70	105.49	106.71
10	T	102	BCL	C4B-C3B-C2B	-2.70	104.02	108.36
10	8	102	BCL	CHB-C4A-NA	2.70	128.25	124.51
16	R	101	I7D	C16-C17-C19	2.70	123.08	118.94
10	Z	101	BCL	C4B-C3B-C2B	-2.70	104.02	108.36
10	1	102	BCL	C4B-C3B-C2B	-2.70	104.02	108.36
10	A	102	BCL	C1D-CHD-C4C	-2.70	120.11	126.62
9	M	411	PGV	O03-C19-C20	2.70	120.37	111.91
10	D	102	BCL	C1D-CHD-C4C	-2.70	120.12	126.62
10	J	101	BCL	C4B-C3B-C2B	-2.70	104.02	108.36
10	U	101	BCL	C4B-C3B-C2B	-2.69	104.03	108.36
10	U	101	BCL	CHB-C1B-NB	-2.69	121.41	124.26
10	B	101	BCL	CHB-C4A-NA	2.69	128.23	124.51
10	E	102	BCL	CHB-C4A-NA	2.69	128.23	124.51
16	K	101	I7D	C16-C17-C19	2.69	123.06	118.94
10	Y	101	BCL	O2A-CGA-CBA	2.68	120.31	111.91
16	6	102	I7D	C25-C23-C22	2.68	123.05	118.94
10	E	102	BCL	C4-C3-C5	2.68	119.77	115.27
17	A	101	CDL	OB8-CB7-C71	2.68	120.31	111.91
10	J	101	BCL	CHB-C4A-NA	2.68	128.21	124.51
16	1	101	I7D	C20-C21-C22	2.67	128.95	123.47
10	L	309	BCL	O2D-CGD-O1D	-2.67	118.61	123.84
10	M	402	BCL	O2D-CGD-O1D	-2.67	118.62	123.84
10	M	402	BCL	CMB-C2B-C3B	2.67	133.14	125.93
16	V	101	I7D	C20-C21-C22	2.67	128.94	123.47
10	O	101	BCL	C1C-NC-C4C	-2.67	105.51	106.71
10	3	102	BCL	C4B-C3B-C2B	-2.67	104.07	108.36
10	9	101	BCL	C1D-CHD-C4C	-2.67	120.19	126.62
9	H	301	PGV	O03-C19-C20	2.67	120.28	111.91
10	E	102	BCL	C4B-C3B-C2B	-2.66	104.07	108.36
9	L	310	PGV	C02-O01-C1	-2.66	111.23	117.79
10	S	101	BCL	CMB-C2B-C3B	2.66	133.12	125.93
10	5	102	BCL	C4-C3-C5	2.66	119.75	115.27
10	M	402	BCL	CHC-C1C-NC	2.66	128.19	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	102	BCL	C1D-CHD-C4C	-2.66	120.21	126.62
10	D	102	BCL	CHC-C1C-NC	2.66	128.19	124.51
10	N	102	BCL	CHC-C1C-NC	2.65	128.18	124.51
10	E	102	BCL	CHC-C1C-NC	2.65	128.18	124.51
10	L	309	BCL	CHC-C1C-NC	2.65	128.18	124.51
10	D	102	BCL	C4-C3-C5	2.65	119.73	115.27
10	O	101	BCL	CMD-C2D-C3D	-2.65	121.53	127.61
10	2	102	BCL	CMB-C2B-C3B	2.65	133.07	125.93
16	X	101	I7D	C25-C23-C22	2.65	123.00	118.94
10	R	102	BCL	C2A-C1A-CHA	-2.64	119.23	123.86
10	Y	101	BCL	CMB-C2B-C3B	2.64	133.06	125.93
10	L	301	BCL	CHC-C1C-NC	2.64	128.16	124.51
9	H	302	PGV	C02-O01-C1	-2.64	111.29	117.79
10	I	102	BCL	C4-C3-C5	2.64	119.71	115.27
10	T	102	BCL	C2A-C1A-CHA	-2.64	119.25	123.86
10	X	102	BCL	CHB-C4A-NA	2.64	128.16	124.51
10	4	102	BCL	C4B-C3B-C2B	-2.64	104.12	108.36
16	M	406	I7D	C16-C17-C19	2.64	122.99	118.94
16	6	102	I7D	C16-C17-C19	2.63	122.98	118.94
10	N	102	BCL	CHB-C1B-NB	-2.63	121.47	124.26
8	C	401	HEC	CBB-CAB-C3B	2.63	119.68	112.43
10	X	102	BCL	CHC-C1C-NC	2.63	128.15	124.51
10	U	101	BCL	CMB-C2B-C3B	2.63	133.02	125.93
10	0	102	BCL	C2A-C1A-CHA	-2.62	119.27	123.86
10	0	102	BCL	CHC-C1C-NC	2.62	128.14	124.51
9	C	406	PGV	O03-C19-C20	2.62	120.12	111.91
10	8	102	BCL	C4B-C3B-C2B	-2.61	104.15	108.36
10	1	102	BCL	O2A-CGA-CBA	2.61	120.11	111.91
17	2	101	CDL	OB8-CB7-C71	2.61	120.11	111.91
10	F	101	BCL	CHC-C1C-NC	2.61	128.12	124.51
16	N	101	I7D	C31-C32-C33	-2.61	123.58	127.31
10	M	402	BCL	C4-C3-C5	2.61	119.66	115.27
10	J	101	BCL	CMB-C2B-C3B	2.61	132.98	125.93
10	L	301	BCL	CMD-C2D-C3D	-2.61	121.61	127.61
10	U	101	BCL	O2D-CGD-O1D	-2.60	118.75	123.84
10	M	402	BCL	C1D-CHD-C4C	-2.60	120.34	126.62
10	5	102	BCL	C4A-NA-C1A	2.60	107.88	106.71
10	M	403	BCL	CAA-C2A-C3A	-2.60	105.66	112.78
10	D	102	BCL	CMB-C2B-C3B	2.60	132.95	125.93
10	O	101	BCL	CHB-C4A-NA	2.60	128.10	124.51
10	3	102	BCL	C1D-CHD-C4C	-2.60	120.36	126.62
10	0	102	BCL	CHB-C4A-NA	2.60	128.10	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	102	BCL	C1C-NC-C4C	-2.60	105.54	106.71
10	D	102	BCL	O2A-CGA-CBA	2.59	120.05	111.91
10	Q	102	BCL	O2A-CGA-CBA	2.59	120.05	111.91
10	D	102	BCL	O2D-CGD-O1D	-2.59	118.77	123.84
10	L	301	BCL	CMB-C2B-C3B	2.59	132.92	125.93
10	2	102	BCL	CHC-C1C-NC	2.59	128.09	124.51
10	W	101	BCL	CMB-C2B-C3B	2.59	132.92	125.93
10	G	101	BCL	CHC-C1C-NC	2.59	128.09	124.51
10	E	102	BCL	CMB-C2B-C3B	2.59	132.92	125.93
10	J	101	BCL	C4-C3-C5	2.59	119.62	115.27
10	Z	101	BCL	C4-C3-C5	2.58	119.62	115.27
10	S	101	BCL	CHB-C1B-NB	-2.58	121.52	124.26
10	X	102	BCL	CMB-C2B-C3B	2.58	132.91	125.93
10	V	102	BCL	CHB-C4A-NA	2.58	128.08	124.51
10	9	101	BCL	CMB-C2B-C3B	2.58	132.90	125.93
10	6	103	BCL	CHB-C4A-NA	2.58	128.08	124.51
10	J	101	BCL	CHC-C1C-NC	2.58	128.08	124.51
10	T	102	BCL	CHC-C1C-NC	2.58	128.08	124.51
10	W	101	BCL	O2A-CGA-CBA	2.58	119.99	111.91
10	P	101	BCL	CMB-C2B-C3B	2.57	132.88	125.93
10	M	403	BCL	C1-C2-C3	-2.57	121.59	126.04
10	9	101	BCL	C1C-NC-C4C	-2.57	105.55	106.71
10	W	101	BCL	CHC-C1C-NC	2.57	128.07	124.51
16	X	101	I7D	C16-C17-C19	2.57	122.88	118.94
17	6	101	CDL	OB8-CB7-C71	2.57	119.97	111.91
9	L	304	PGV	C02-O01-C1	-2.57	111.47	117.79
16	3	101	I7D	C20-C21-C22	2.57	128.73	123.47
10	N	102	BCL	CHB-C4A-NA	2.57	128.06	124.51
10	0	102	BCL	CMB-C2B-C3B	2.56	132.86	125.93
16	N	101	I7D	C16-C17-C19	2.56	122.88	118.94
10	Z	101	BCL	C2A-C1A-CHA	-2.56	119.38	123.86
10	J	101	BCL	C1C-NC-C4C	-2.56	105.55	106.71
17	2	101	CDL	OA8-CA7-C31	2.56	119.95	111.91
10	R	102	BCL	CMB-C2B-C3B	2.56	132.85	125.93
10	W	101	BCL	CMD-C2D-C3D	-2.56	121.73	127.61
10	J	101	BCL	O2D-CGD-O1D	-2.56	118.84	123.84
10	7	402	BCL	O2A-CGA-CBA	2.56	119.93	111.91
16	R	101	I7D	C20-C21-C22	2.56	128.71	123.47
10	G	101	BCL	CHB-C4A-NA	2.55	128.04	124.51
10	7	402	BCL	CHC-C1C-NC	2.55	128.04	124.51
10	8	102	BCL	CHC-C1C-NC	2.55	128.04	124.51
9	C	407	PGV	C02-O01-C1	-2.55	111.50	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	103	I7D	C16-C17-C19	2.55	122.86	118.94
10	2	102	BCL	C2A-C1A-CHA	-2.55	119.40	123.86
10	Y	101	BCL	CHB-C1B-NB	-2.55	121.56	124.26
16	M	406	I7D	C24-C23-C22	-2.55	119.35	122.92
10	N	102	BCL	CMB-C2B-C3B	2.55	132.81	125.93
10	1	102	BCL	C1C-NC-C4C	-2.55	105.56	106.71
10	G	101	BCL	CMB-C2B-C3B	2.55	132.81	125.93
17	2	101	CDL	CB4-OB6-CB5	-2.55	111.52	117.79
10	3	102	BCL	CHB-C4A-NA	2.54	128.03	124.51
9	L	310	PGV	O03-C19-C20	2.54	119.88	111.91
16	Q	101	I7D	C11-C12-C14	2.54	122.84	118.94
8	C	401	HEC	CBD-CAD-C3D	-2.54	105.57	112.63
17	6	104	CDL	CB4-OB6-CB5	-2.54	111.54	117.79
10	1	102	BCL	C1D-CHD-C4C	-2.54	120.50	126.62
10	I	102	BCL	O2A-CGA-CBA	2.54	119.87	111.91
10	Y	101	BCL	C1D-CHD-C4C	-2.54	120.50	126.62
10	3	102	BCL	C4A-NA-C1A	2.54	107.85	106.71
10	X	102	BCL	C2A-C1A-CHA	-2.53	119.43	123.86
10	A	102	BCL	CMB-C2B-C3B	2.53	132.77	125.93
8	C	401	HEC	CHA-C4D-C3D	-2.53	121.12	124.84
10	S	101	BCL	O2A-CGA-CBA	2.53	119.85	111.91
10	Q	102	BCL	O2D-CGD-O1D	-2.53	118.89	123.84
10	O	101	BCL	C4-C3-C5	2.53	119.52	115.27
10	F	101	BCL	CHB-C4A-NA	2.53	128.00	124.51
16	A	103	I7D	C20-C21-C22	2.53	128.65	123.47
16	I	101	I7D	C20-C21-C22	2.53	128.65	123.47
16	3	101	I7D	C16-C17-C19	2.52	122.81	118.94
10	Q	102	BCL	C4-C3-C5	2.52	119.51	115.27
16	V	101	I7D	C16-C17-C19	2.52	122.81	118.94
16	4	101	I7D	C16-C17-C19	2.52	122.80	118.94
10	8	102	BCL	C2A-C1A-CHA	-2.52	119.46	123.86
10	1	102	BCL	CHC-C1C-NC	2.52	127.99	124.51
10	W	101	BCL	C1D-CHD-C4C	-2.51	120.56	126.62
10	M	403	BCL	C4-C3-C5	2.51	119.50	115.27
10	V	102	BCL	CHC-C1C-NC	2.51	127.99	124.51
16	R	101	I7D	C11-C12-C14	2.51	122.80	118.94
10	O	101	BCL	O2D-CGD-O1D	-2.51	118.93	123.84
10	5	102	BCL	C1D-CHD-C4C	-2.51	120.57	126.62
10	K	102	BCL	C4-C3-C5	2.51	119.49	115.27
16	T	101	I7D	C16-C17-C19	2.51	122.79	118.94
10	2	102	BCL	CHB-C4A-NA	2.51	127.98	124.51
9	5	101	PGV	C02-O01-C1	-2.50	111.64	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	302	PGV	O03-C19-C20	2.50	119.75	111.91
10	X	102	BCL	C4-C3-C5	2.50	119.47	115.27
10	B	101	BCL	C2A-C1A-CHA	-2.50	119.50	123.86
17	0	101	CDL	OB8-CB7-C71	2.49	119.74	111.91
17	M	408	CDL	OA8-CA7-C31	2.49	119.73	111.91
10	4	102	BCL	CMB-C2B-C3B	2.49	132.66	125.93
16	Q	101	I7D	C16-C17-C19	2.49	122.76	118.94
8	C	404	HEC	CHA-C4D-C3D	-2.49	121.18	124.84
10	M	403	BCL	CHC-C1C-NC	2.49	127.95	124.51
10	K	102	BCL	CHC-C1C-NC	2.49	127.95	124.51
16	V	101	I7D	C11-C12-C14	2.48	122.75	118.94
10	A	102	BCL	CHC-C1C-NC	2.48	127.95	124.51
10	Q	102	BCL	CHC-C1C-NC	2.48	127.94	124.51
10	M	402	BCL	CHB-C1B-NB	-2.48	121.63	124.26
8	C	403	HEC	C1D-ND-C4D	2.48	107.64	105.07
10	N	102	BCL	O2D-CGD-O1D	-2.48	118.99	123.84
9	5	104	PGV	O03-C19-C20	2.48	119.69	111.91
10	P	101	BCL	CHB-C4A-NA	2.48	127.94	124.51
10	Z	101	BCL	CHC-C1C-NC	2.48	127.94	124.51
10	6	103	BCL	CHC-C1C-NC	2.48	127.94	124.51
10	F	101	BCL	O2D-CGD-O1D	-2.48	119.00	123.84
10	Q	102	BCL	CMB-C2B-C3B	2.48	132.62	125.93
10	K	102	BCL	O2A-CGA-CBA	2.48	119.68	111.91
16	D	101	I7D	C20-C21-C22	2.47	128.54	123.47
17	T	103	CDL	OA8-CA7-C31	2.47	119.66	111.91
10	S	101	BCL	CMD-C2D-C3D	-2.47	121.93	127.61
16	K	101	I7D	C20-C21-C22	2.47	128.53	123.47
8	C	401	HEC	CBA-CAA-C2A	-2.46	105.78	112.63
17	6	104	CDL	OA8-CA7-C31	2.46	119.62	111.91
10	V	102	BCL	CMB-C2B-C3B	2.46	132.57	125.93
10	I	102	BCL	CMB-C2B-C3B	2.46	132.57	125.93
10	L	301	BCL	C2A-C1A-CHA	-2.46	119.56	123.86
16	X	101	I7D	C11-C12-C14	2.46	122.71	118.94
10	P	101	BCL	CHC-C1C-NC	2.46	127.91	124.51
10	0	102	BCL	C1C-NC-C4C	-2.46	105.60	106.71
10	Z	101	BCL	CMB-C2B-C3B	2.46	132.56	125.93
16	E	101	I7D	C25-C23-C22	2.45	122.71	118.94
10	O	101	BCL	CMB-C2B-C3B	2.45	132.55	125.93
10	M	402	BCL	O2A-CGA-CBA	2.45	119.60	111.91
10	5	102	BCL	CMD-C2D-C3D	-2.45	121.98	127.61
10	S	101	BCL	O2D-CGD-O1D	-2.45	119.05	123.84
10	1	102	BCL	CMD-C2D-C3D	-2.44	121.99	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1	102	BCL	C4-C3-C5	2.44	119.38	115.27
10	L	309	BCL	C4B-C3B-C2B	-2.44	104.44	108.36
16	A	103	I7D	C25-C23-C22	2.43	122.67	118.94
17	6	104	CDL	OB8-CB7-C71	2.43	119.54	111.91
10	A	102	BCL	CMD-C2D-C3D	-2.43	122.02	127.61
10	T	102	BCL	CMB-C2B-C3B	2.43	132.49	125.93
10	7	402	BCL	CMB-C2B-C3B	2.43	132.48	125.93
10	O	101	BCL	O2A-CGA-CBA	2.43	119.52	111.91
10	9	101	BCL	CHB-C4A-NA	2.43	127.87	124.51
8	C	401	HEC	CHB-C1B-C2B	-2.42	121.20	124.98
10	I	102	BCL	C1D-CHD-C4C	-2.42	120.79	126.62
10	E	102	BCL	O2D-CGD-O1D	-2.42	119.11	123.84
10	B	101	BCL	O2D-CGD-O1D	-2.42	119.11	123.84
10	5	102	BCL	CMB-C2B-C3B	2.42	132.46	125.93
10	L	301	BCL	CHB-C4A-NA	2.42	127.85	124.51
10	4	102	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
10	Z	101	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
17	T	103	CDL	OB8-CB7-C71	2.41	119.47	111.91
17	T	103	CDL	CB4-OB6-CB5	-2.41	111.86	117.79
10	6	103	BCL	O2D-CGD-O1D	-2.41	119.13	123.84
16	E	101	I7D	C16-C17-C19	2.41	122.64	118.94
16	I	101	I7D	C11-C12-C14	2.40	122.63	118.94
10	8	102	BCL	CMB-C2B-C3B	2.40	132.42	125.93
10	R	102	BCL	CHC-C1C-NC	2.40	127.83	124.51
10	L	309	BCL	C4-C3-C5	2.40	119.31	115.27
10	3	102	BCL	CMD-C2D-C3D	-2.40	122.10	127.61
16	N	101	I7D	C11-C12-C14	2.40	122.62	118.94
10	L	301	BCL	C1-C2-C3	-2.39	121.90	126.04
16	A	103	I7D	C11-C12-C14	2.39	122.61	118.94
10	I	102	BCL	CMD-C2D-C3D	-2.39	122.11	127.61
10	X	102	BCL	O2D-CGD-O1D	-2.39	119.16	123.84
10	M	403	BCL	CMD-C2D-C3D	-2.39	122.12	127.61
8	C	403	HEC	C3B-C4B-NB	-2.39	107.51	110.17
10	7	402	BCL	CMD-C2D-C3D	-2.39	122.12	127.61
10	M	403	BCL	CHB-C4A-NA	2.39	127.81	124.51
10	6	103	BCL	C2A-C1A-CHA	-2.39	119.68	123.86
10	U	101	BCL	CHC-C1C-NC	2.39	127.81	124.51
9	F	102	PGV	O03-C19-C20	2.39	119.40	111.91
9	5	103	PGV	O03-C19-C20	2.39	119.39	111.91
10	2	102	BCL	O2D-CGD-O1D	-2.38	119.18	123.84
10	7	402	BCL	O2D-CGD-O1D	-2.38	119.18	123.84
8	C	402	HEC	C1A-CHA-C4D	-2.38	120.92	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	8	102	BCL	O2D-CGD-O1D	-2.38	119.18	123.84
10	P	101	BCL	O2D-CGD-O1D	-2.38	119.19	123.84
10	Y	101	BCL	CMD-C2D-C3D	-2.38	122.15	127.61
10	K	102	BCL	CMD-C2D-C3D	-2.38	122.15	127.61
10	J	101	BCL	C2A-C1A-CHA	-2.37	119.71	123.86
8	C	404	HEC	C1A-CHA-C4D	-2.37	120.94	126.06
10	V	102	BCL	O2D-CGD-O1D	-2.37	119.20	123.84
10	T	102	BCL	O2D-CGD-O1D	-2.37	119.21	123.84
13	1	103	LMT	C1-O1'-C1'	-2.36	109.92	113.84
10	M	402	BCL	C1C-NC-C4C	-2.36	105.64	106.71
10	9	101	BCL	CHC-C1C-NC	2.36	127.78	124.51
9	L	304	PGV	O03-C19-C20	2.36	119.33	111.91
10	9	101	BCL	CMD-C2D-C3D	-2.36	122.18	127.61
10	D	102	BCL	CHB-C4A-NA	2.36	127.78	124.51
10	Q	102	BCL	CHB-C4A-NA	2.36	127.78	124.51
16	D	101	I7D	C11-C12-C14	2.36	122.56	118.94
10	W	101	BCL	CHB-C4A-NA	2.36	127.78	124.51
10	5	102	BCL	CHB-C4A-NA	2.36	127.77	124.51
10	R	102	BCL	O2D-CGD-O1D	-2.36	119.23	123.84
10	B	101	BCL	C1C-NC-C4C	-2.36	105.65	106.71
16	1	101	I7D	C11-C12-C14	2.35	122.55	118.94
10	U	101	BCL	CHB-C4A-NA	2.35	127.77	124.51
10	D	102	BCL	CMD-C2D-C3D	-2.35	122.21	127.61
10	F	101	BCL	CMB-C2B-C3B	2.35	132.27	125.93
10	K	102	BCL	CHB-C4A-NA	2.35	127.76	124.51
10	3	102	BCL	O2A-CGA-CBA	2.35	119.27	111.91
16	3	101	I7D	C30-C28-C27	2.35	122.54	118.94
10	I	102	BCL	O2D-CGD-O1D	-2.34	119.26	123.84
16	6	102	I7D	C30-C28-C27	2.34	122.54	118.94
16	T	101	I7D	C25-C23-C22	2.34	122.53	118.94
17	0	101	CDL	CB4-OB6-CB5	-2.34	112.03	117.79
10	J	101	BCL	C1D-CHD-C4C	-2.34	120.98	126.62
10	A	102	BCL	O2D-CGD-O1D	-2.34	119.27	123.84
9	C	407	PGV	O14-P-O13	2.34	119.83	110.68
8	C	401	HEC	C1A-CHA-C4D	-2.33	121.03	126.06
10	I	102	BCL	CHC-C1C-NC	2.33	127.74	124.51
10	9	101	BCL	O2D-CGD-O1D	-2.33	119.28	123.84
16	T	101	I7D	C11-C12-C14	2.32	122.51	118.94
17	T	103	CDL	CA4-OA6-CA5	-2.32	112.08	117.79
9	K	103	PGV	O03-C19-C20	2.32	119.19	111.91
8	C	401	HEC	C1D-ND-C4D	2.32	107.47	105.07
17	H	303	CDL	OB8-CB7-C71	2.31	119.17	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	309	BCL	CMB-C2B-C3B	2.31	132.17	125.93
10	6	103	BCL	CMB-C2B-C3B	2.31	132.17	125.93
10	Y	101	BCL	CHB-C4A-NA	2.31	127.70	124.51
10	Y	101	BCL	O2D-CGD-O1D	-2.31	119.33	123.84
10	U	101	BCL	CMD-C2D-C3D	-2.30	122.32	127.61
13	L	313	LMT	C1B-O1B-C4'	-2.30	112.27	117.96
10	S	101	BCL	C4-C3-C5	2.30	119.14	115.27
10	Z	101	BCL	C1D-CHD-C4C	-2.30	121.07	126.62
10	O	101	BCL	C1D-CHD-C4C	-2.30	121.07	126.62
8	C	404	HEC	C1D-ND-C4D	2.30	107.45	105.07
10	A	102	BCL	CHB-C4A-NA	2.30	127.69	124.51
10	5	102	BCL	O2D-CGD-O1D	-2.29	119.35	123.84
10	0	102	BCL	O2D-CGD-O1D	-2.29	119.36	123.84
10	B	101	BCL	C1D-CHD-C4C	-2.29	121.10	126.62
10	W	101	BCL	C4-C3-C5	2.29	119.12	115.27
8	C	402	HEC	C1D-ND-C4D	2.29	107.43	105.07
10	T	102	BCL	CHC-C4B-C3B	-2.29	124.22	132.35
10	8	102	BCL	CHC-C4B-C3B	-2.28	124.22	132.35
10	P	101	BCL	C1C-NC-C4C	-2.28	105.68	106.71
10	3	102	BCL	O2D-CGD-O1D	-2.28	119.38	123.84
10	L	309	BCL	O1D-CGD-CBD	-2.28	119.82	124.48
10	W	101	BCL	O2D-CGD-O1D	-2.28	119.39	123.84
10	F	101	BCL	CMD-C2D-C3D	-2.28	122.38	127.61
10	Z	101	BCL	CHC-C4B-C3B	-2.27	124.27	132.35
10	3	102	BCL	CMB-C2B-C3B	2.27	132.06	125.93
10	L	301	BCL	CHC-C4B-C3B	-2.27	124.28	132.35
10	1	102	BCL	CMB-C2B-C3B	2.27	132.05	125.93
10	8	102	BCL	C1C-NC-C4C	-2.27	105.69	106.71
10	1	102	BCL	O2D-CGD-O1D	-2.27	119.41	123.84
16	6	102	I7D	O6-C6-C5	-2.27	116.19	121.20
10	G	101	BCL	O2D-CGD-O1D	-2.26	119.41	123.84
16	1	101	I7D	C30-C28-C27	2.26	122.41	118.94
10	S	101	BCL	CHC-C1C-NC	2.26	127.64	124.51
16	K	101	I7D	C11-C12-C14	2.26	122.41	118.94
16	1	101	I7D	C25-C23-C22	2.26	122.41	118.94
10	I	102	BCL	C4A-NA-C1A	2.26	107.72	106.71
10	A	102	BCL	C4-C3-C5	2.26	119.07	115.27
10	0	102	BCL	CED-O2D-CGD	2.26	121.04	115.94
10	V	102	BCL	CHC-C4B-C3B	-2.25	124.33	132.35
10	I	102	BCL	C2A-C1A-CHA	-2.25	119.92	123.86
16	6	102	I7D	C9-C10-C11	2.25	130.24	123.22
10	K	102	BCL	CMB-C2B-C3B	2.25	132.00	125.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	301	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
8	C	403	HEC	CBB-CAB-C3B	2.25	118.62	112.43
10	2	102	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
10	6	103	BCL	CHC-C4B-C3B	-2.24	124.37	132.35
10	1	102	BCL	CED-O2D-CGD	2.24	121.01	115.94
10	L	301	BCL	O2A-CGA-O1A	-2.24	117.94	123.59
10	R	102	BCL	C6-C5-C3	-2.24	107.58	113.45
10	5	102	BCL	O2A-CGA-CBA	2.24	118.93	111.91
9	5	103	PGV	C02-O01-C1	-2.24	112.28	117.79
10	X	102	BCL	C1D-CHD-C4C	-2.24	121.22	126.62
10	Z	101	BCL	C1C-NC-C4C	-2.24	105.70	106.71
10	S	101	BCL	CHB-C4A-NA	2.24	127.61	124.51
9	L	312	PGV	O01-C1-O02	-2.24	118.30	123.70
16	3	101	I7D	C11-C12-C14	2.24	122.37	118.94
16	4	101	I7D	C25-C23-C22	2.23	122.36	118.94
8	C	401	HEC	CHB-C4A-NA	2.23	126.85	124.44
10	M	403	BCL	C1C-NC-C4C	-2.23	105.70	106.71
8	C	403	HEC	CHA-C4D-C3D	-2.23	121.57	124.84
8	C	403	HEC	C1A-CHA-C4D	-2.23	121.25	126.06
10	G	101	BCL	C1D-CHD-C4C	-2.23	121.25	126.62
10	4	102	BCL	CHC-C4B-C3B	-2.22	124.44	132.35
10	P	101	BCL	CHC-C4B-C3B	-2.22	124.45	132.35
17	M	408	CDL	OB8-CB7-C71	2.22	118.87	111.91
10	0	102	BCL	C1D-CHD-C4C	-2.22	121.27	126.62
10	F	101	BCL	O2A-CGA-O1A	-2.22	118.00	123.59
10	W	101	BCL	C1C-NC-C4C	-2.22	105.71	106.71
16	4	101	I7D	C30-C28-C27	2.22	122.34	118.94
16	T	101	I7D	C30-C28-C27	2.22	122.34	118.94
10	K	102	BCL	O2D-CGD-O1D	-2.22	119.51	123.84
10	3	102	BCL	C2A-C1A-CHA	-2.21	119.99	123.86
10	L	309	BCL	CHB-C4A-NA	2.21	127.57	124.51
10	0	102	BCL	CHC-C4B-C3B	-2.21	124.48	132.35
10	V	102	BCL	C1D-CHD-C4C	-2.21	121.29	126.62
10	M	402	BCL	CHC-C4B-C3B	-2.21	124.49	132.35
10	Q	102	BCL	CMD-C2D-C3D	-2.21	122.53	127.61
10	R	102	BCL	C1D-CHD-C4C	-2.21	121.29	126.62
10	7	402	BCL	C1D-CHD-C4C	-2.21	121.30	126.62
10	7	402	BCL	CHB-C4A-NA	2.21	127.56	124.51
10	B	101	BCL	CHC-C4B-C3B	-2.21	124.50	132.35
10	M	403	BCL	C1D-CHD-C4C	-2.20	121.30	126.62
16	N	101	I7D	C25-C23-C22	2.20	122.32	118.94
10	L	309	BCL	O2A-CGA-O1A	-2.20	118.04	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	407	PGV	O03-C19-C20	2.19	118.79	111.91
16	I	101	I7D	C25-C23-C22	2.19	122.30	118.94
13	L	313	LMT	C1-O1'-C1'	-2.19	110.21	113.84
16	Q	101	I7D	C25-C23-C22	2.19	122.30	118.94
16	R	101	I7D	C26-C27-C28	2.19	130.43	127.31
16	N	101	I7D	C32-C31-C30	2.18	130.03	123.22
10	1	102	BCL	C2A-C1A-CHA	-2.18	120.04	123.86
10	O	101	BCL	C2A-C1A-CHA	-2.18	120.04	123.86
10	U	101	BCL	C4-C3-C5	2.18	118.94	115.27
10	S	101	BCL	CHD-C1D-C2D	2.18	130.05	125.48
10	3	102	BCL	CBA-CAA-C2A	-2.18	107.43	113.86
8	C	401	HEC	C3B-C4B-NB	-2.18	107.74	110.17
10	P	101	BCL	C1D-CHD-C4C	-2.18	121.37	126.62
10	E	102	BCL	CHC-C4B-C3B	-2.17	124.62	132.35
8	C	404	HEC	CAD-CBD-CGD	-2.17	108.93	113.60
10	8	102	BCL	C1D-CHD-C4C	-2.17	121.39	126.62
10	9	101	BCL	O2A-CGA-O1A	-2.17	118.12	123.59
10	L	301	BCL	C4D-CHA-C1A	-2.17	118.61	121.25
8	C	403	HEC	C4A-NA-C1A	2.17	107.47	105.35
16	V	101	I7D	C25-C23-C22	2.16	122.26	118.94
10	J	101	BCL	CHC-C4B-C3B	-2.16	124.66	132.35
16	I	101	I7D	C26-C27-C28	2.16	130.40	127.31
9	M	410	PGV	O03-C19-C20	2.16	118.69	111.91
10	T	102	BCL	C1C-NC-C4C	-2.16	105.73	106.71
10	2	102	BCL	C1C-NC-C4C	-2.16	105.73	106.71
17	H	303	CDL	CB4-OB6-CB5	-2.16	112.47	117.79
8	C	402	HEC	C3B-C4B-NB	-2.16	107.76	110.17
10	G	101	BCL	CHC-C4B-C3B	-2.15	124.69	132.35
10	4	102	BCL	C1D-CHD-C4C	-2.15	121.43	126.62
10	M	402	BCL	C2A-C1A-CHA	-2.15	120.10	123.86
10	7	402	BCL	CHC-C4B-C3B	-2.15	124.72	132.35
16	M	406	I7D	C21-C22-C23	2.14	130.37	127.31
10	4	102	BCL	CMD-C2D-C3D	-2.14	122.68	127.61
10	M	402	BCL	CHB-C4A-NA	2.14	127.48	124.51
16	4	101	I7D	C11-C12-C14	2.14	122.23	118.94
10	3	102	BCL	CHC-C1C-NC	2.14	127.47	124.51
10	1	102	BCL	C6-C5-C3	-2.14	107.84	113.45
10	5	102	BCL	CHD-C1D-C2D	2.14	129.97	125.48
10	E	102	BCL	C1D-CHD-C4C	-2.14	121.46	126.62
8	C	403	HEC	C2A-C1A-NA	-2.14	108.24	110.32
10	L	309	BCL	C2A-C1A-CHA	-2.14	120.12	123.86
10	T	102	BCL	C1D-CHD-C4C	-2.14	121.47	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	101	BCL	CHC-C4B-C3B	-2.13	124.76	132.35
10	2	102	BCL	CHC-C4B-C3B	-2.13	124.76	132.35
8	C	402	HEC	CHB-C1B-C2B	-2.13	121.65	124.98
10	5	102	BCL	CHC-C1C-NC	2.13	127.46	124.51
10	N	102	BCL	C1D-CHD-C4C	-2.13	121.48	126.62
10	X	102	BCL	CHC-C4B-C3B	-2.13	124.77	132.35
16	R	101	I7D	C25-C23-C22	2.13	122.21	118.94
16	3	101	I7D	C25-C23-C22	2.13	122.21	118.94
16	V	101	I7D	C30-C28-C27	2.13	122.21	118.94
10	3	102	BCL	C6-C5-C3	-2.13	107.88	113.45
10	6	103	BCL	C1D-CHD-C4C	-2.13	121.49	126.62
8	C	404	HEC	CHD-C1D-C2D	-2.12	120.83	126.73
10	N	102	BCL	CHC-C4B-C3B	-2.12	124.81	132.35
16	K	101	I7D	C30-C28-C27	2.12	122.19	118.94
16	Q	101	I7D	C30-C28-C27	2.11	122.18	118.94
10	6	103	BCL	C4D-CHA-C1A	-2.11	118.68	121.25
9	C	405	PGV	C02-O01-C1	-2.11	112.60	117.79
10	4	102	BCL	C4D-CHA-C1A	-2.11	118.68	121.25
10	L	309	BCL	C1D-CHD-C4C	-2.11	121.54	126.62
10	R	102	BCL	CHC-C4B-C3B	-2.10	124.87	132.35
16	D	101	I7D	C25-C23-C22	2.10	122.17	118.94
8	C	401	HEC	CHD-C1D-C2D	-2.10	120.89	126.73
10	L	309	BCL	CMD-C2D-C3D	-2.10	122.79	127.61
10	1	102	BCL	CHC-C4B-C3B	-2.10	124.89	132.35
16	E	101	I7D	C11-C12-C14	2.10	122.16	118.94
9	C	406	PGV	C3-C2-C1	-2.09	106.00	113.62
16	D	101	I7D	C30-C28-C27	2.09	122.16	118.94
9	H	301	PGV	C02-O01-C1	-2.09	112.64	117.79
8	C	401	HEC	C3C-C4C-NC	-2.09	107.81	110.15
9	5	101	PGV	O03-C19-O04	-2.09	118.32	123.59
8	C	402	HEC	C3C-C4C-NC	-2.09	107.81	110.15
9	L	311	PGV	O01-C1-O02	-2.09	118.66	123.70
10	I	102	BCL	CBA-CAA-C2A	-2.08	107.73	113.86
9	L	304	PGV	O01-C1-O02	-2.07	118.69	123.70
10	8	102	BCL	C4D-CHA-C1A	-2.07	118.72	121.25
10	W	101	BCL	CHD-C1D-C2D	2.07	129.83	125.48
17	6	101	CDL	CB4-OB6-CB5	-2.07	112.69	117.79
10	U	101	BCL	C6-C5-C3	-2.07	108.02	113.45
9	H	302	PGV	O01-C1-O02	-2.07	118.70	123.70
16	1	101	I7D	C26-C27-C28	2.07	130.26	127.31
16	R	101	I7D	C31-C32-C33	2.06	130.26	127.31
10	E	102	BCL	O2A-CGA-O1A	-2.06	118.39	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	102	BCL	CHD-C1D-C2D	2.06	129.81	125.48
10	R	102	BCL	C4D-CHA-C1A	-2.06	118.74	121.25
10	2	102	BCL	O2A-CGA-O1A	-2.06	118.39	123.59
10	7	402	BCL	C2A-C1A-CHA	-2.05	120.27	123.86
10	F	101	BCL	C6-C5-C3	-2.05	108.08	113.45
17	A	101	CDL	OA6-CA5-OA7	-2.05	118.75	123.70
10	8	102	BCL	CED-O2D-CGD	2.05	120.56	115.94
10	N	102	BCL	CHB-C1B-C2B	-2.05	121.46	127.24
10	F	101	BCL	CHC-C4B-C3B	-2.04	125.08	132.35
10	G	101	BCL	C1C-NC-C4C	-2.04	105.79	106.71
10	N	102	BCL	C6-C7-C8	-2.04	109.32	115.92
16	K	101	I7D	C25-C23-C22	2.04	122.07	118.94
8	C	401	HEC	O2D-CGD-CBD	2.04	120.58	114.03
10	M	403	BCL	CHC-C4B-C3B	-2.04	125.11	132.35
10	D	102	BCL	CHD-C1D-C2D	2.04	129.75	125.48
17	M	407	CDL	CA4-OA6-CA5	-2.04	112.78	117.79
10	3	102	BCL	C4-C3-C5	2.04	118.69	115.27
10	4	102	BCL	O2A-CGA-O1A	-2.03	118.46	123.59
10	X	102	BCL	O2A-CGA-O1A	-2.03	118.46	123.59
17	0	101	CDL	OA8-CA7-OA9	-2.03	118.47	123.59
8	C	403	HEC	CHB-C1B-C2B	-2.03	121.81	124.98
10	U	101	BCL	CHD-C1D-C2D	2.02	129.72	125.48
8	C	403	HEC	CHD-C1D-C2D	-2.02	121.11	126.73
10	G	101	BCL	C4D-CHA-C1A	-2.02	118.79	121.25
10	O	101	BCL	CHD-C1D-C2D	2.02	129.72	125.48
17	A	101	CDL	OB6-CB5-OB7	-2.02	118.82	123.70
8	C	404	HEC	CHB-C1B-C2B	-2.02	121.83	124.98
10	V	102	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
10	R	102	BCL	CHB-C1B-C2B	-2.02	121.55	127.24
10	5	102	BCL	CED-O2D-CGD	2.01	120.49	115.94
16	T	101	I7D	C26-C27-C28	2.01	130.18	127.31
16	4	101	I7D	C26-C27-C28	2.01	130.18	127.31
10	K	102	BCL	CHC-C4B-C3B	-2.01	125.19	132.35
10	L	309	BCL	CHC-C4B-C3B	-2.01	125.20	132.35
8	C	401	HEC	C2A-C1A-NA	-2.01	108.37	110.32
10	3	102	BCL	CHC-C4B-C3B	-2.01	125.21	132.35
8	C	404	HEC	O2A-CGA-CBA	2.00	120.46	114.03
10	P	101	BCL	C6-C5-C3	-2.00	108.21	113.45
10	I	102	BCL	CHC-C4B-C3B	-2.00	125.23	132.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	401	HEC	NA
8	C	402	HEC	NA
8	C	403	HEC	NA
8	C	404	HEC	NA

All (1003) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	405	PGV	C03-O11-P-O14
9	C	406	PGV	C2-C1-O01-C02
9	L	304	PGV	C03-O11-P-O12
9	L	304	PGV	C03-O11-P-O14
9	L	304	PGV	C04-O12-P-O11
9	L	304	PGV	C04-O12-P-O13
9	L	310	PGV	C03-O11-P-O14
9	L	312	PGV	C03-O11-P-O14
9	L	312	PGV	C2-C1-O01-C02
9	M	410	PGV	C04-O12-P-O14
9	H	301	PGV	C04-O12-P-O13
9	H	302	PGV	C03-O11-P-O13
9	H	302	PGV	C04-O12-P-O13
9	D	103	PGV	C2-C1-O01-C02
9	5	101	PGV	C2-C1-O01-C02
9	5	101	PGV	O04-C19-O03-C01
9	5	101	PGV	C20-C19-O03-C01
9	5	103	PGV	C03-O11-P-O13
9	5	104	PGV	C03-O11-P-O14
10	A	102	BCL	C2-C3-C5-C6
10	A	102	BCL	C4-C3-C5-C6
10	B	101	BCL	C2C-C3C-CAC-CBC
10	B	101	BCL	C4C-C3C-CAC-CBC
10	G	101	BCL	C2C-C3C-CAC-CBC
10	G	101	BCL	C4C-C3C-CAC-CBC
10	G	101	BCL	C11-C10-C8-C9
10	K	102	BCL	C2-C3-C5-C6
10	K	102	BCL	C4-C3-C5-C6
10	N	102	BCL	C2C-C3C-CAC-CBC
10	N	102	BCL	C4C-C3C-CAC-CBC
10	N	102	BCL	C2-C3-C5-C6
10	N	102	BCL	C4-C3-C5-C6
10	O	101	BCL	C2C-C3C-CAC-CBC
10	O	101	BCL	C4C-C3C-CAC-CBC
10	O	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	T	102	BCL	C4C-C3C-CAC-CBC
10	V	102	BCL	C2C-C3C-CAC-CBC
10	V	102	BCL	C4C-C3C-CAC-CBC
10	X	102	BCL	C2C-C3C-CAC-CBC
10	X	102	BCL	C4C-C3C-CAC-CBC
10	Z	101	BCL	C2C-C3C-CAC-CBC
10	Z	101	BCL	C4C-C3C-CAC-CBC
10	Z	101	BCL	C11-C10-C8-C9
10	4	102	BCL	C2C-C3C-CAC-CBC
10	4	102	BCL	C4C-C3C-CAC-CBC
10	5	102	BCL	C1A-C2A-CAA-CBA
10	5	102	BCL	C3A-C2A-CAA-CBA
10	8	102	BCL	C2C-C3C-CAC-CBC
10	8	102	BCL	C4C-C3C-CAC-CBC
10	8	102	BCL	C4-C3-C5-C6
10	8	102	BCL	C11-C10-C8-C9
10	0	102	BCL	C4C-C3C-CAC-CBC
10	0	102	BCL	C2-C3-C5-C6
10	0	102	BCL	C4-C3-C5-C6
12	7	401	U10	C12-C11-C9-C8
12	7	401	U10	C12-C11-C9-C10
12	7	401	U10	C22-C23-C24-C25
12	7	401	U10	C22-C23-C24-C26
13	L	308	LMT	C2-C1-O1'-C1'
16	M	406	I7D	C35-C36-C37-C38
16	A	103	I7D	C35-C36-C37-C38
16	D	101	I7D	C35-C36-C37-C38
16	E	101	I7D	C35-C36-C37-C38
16	I	101	I7D	C35-C36-C37-C38
16	K	101	I7D	C35-C36-C37-C38
16	N	101	I7D	C32-C33-C35-C36
16	N	101	I7D	C34-C33-C35-C36
16	N	101	I7D	C33-C35-C36-C37
16	Q	101	I7D	C35-C36-C37-C38
16	T	101	I7D	C2-C1-C4-C5
16	T	101	I7D	C3-C1-C4-C5
16	T	101	I7D	C34-C33-C35-C36
16	T	101	I7D	C35-C36-C37-C38
16	V	101	I7D	C35-C36-C37-C38
16	X	101	I7D	C35-C36-C37-C38
16	1	101	I7D	C35-C36-C37-C38
16	3	101	I7D	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
16	3	101	I7D	C34-C33-C35-C36
16	3	101	I7D	C35-C36-C37-C38
16	4	101	I7D	C35-C36-C37-C38
16	8	101	I7D	C35-C36-C37-C38
17	M	407	CDL	O1-C1-CB2-OB2
17	M	407	CDL	CA2-OA2-PA1-OA3
17	M	407	CDL	CA2-OA2-PA1-OA5
17	M	408	CDL	CA2-OA2-PA1-OA5
17	M	408	CDL	CA3-OA5-PA1-OA3
17	M	408	CDL	CB3-OB5-PB2-OB4
17	M	408	CDL	C51-CB5-OB6-CB4
17	H	303	CDL	CB2-OB2-PB2-OB3
17	H	303	CDL	CB2-OB2-PB2-OB4
17	H	303	CDL	CB2-OB2-PB2-OB5
17	A	101	CDL	CA2-OA2-PA1-OA5
17	A	101	CDL	CA3-OA5-PA1-OA3
17	A	101	CDL	CA3-OA5-PA1-OA4
17	A	101	CDL	CB2-OB2-PB2-OB3
17	A	101	CDL	CB3-OB5-PB2-OB3
17	T	103	CDL	CA2-OA2-PA1-OA4
17	T	103	CDL	CB2-OB2-PB2-OB3
17	2	101	CDL	CA2-C1-CB2-OB2
17	2	101	CDL	C11-CA5-OA6-CA4
17	6	101	CDL	CA2-OA2-PA1-OA5
17	6	101	CDL	CA3-OA5-PA1-OA3
17	6	101	CDL	CB3-OB5-PB2-OB3
17	6	104	CDL	CA2-OA2-PA1-OA3
17	6	104	CDL	CA2-OA2-PA1-OA4
17	6	104	CDL	CA2-OA2-PA1-OA5
17	6	104	CDL	CA3-OA5-PA1-OA2
17	6	104	CDL	CA3-OA5-PA1-OA3
17	6	104	CDL	CA3-OA5-PA1-OA4
17	6	104	CDL	CB2-OB2-PB2-OB3
17	6	104	CDL	OB7-CB5-OB6-CB4
17	6	104	CDL	C51-CB5-OB6-CB4
17	0	101	CDL	CA2-OA2-PA1-OA3
17	0	101	CDL	CA2-OA2-PA1-OA5
17	0	101	CDL	CA3-OA5-PA1-OA2
17	0	101	CDL	CA3-OA5-PA1-OA3
17	0	101	CDL	CB3-OB5-PB2-OB4
10	L	301	BCL	CBD-CGD-O2D-CED
9	C	406	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
9	L	312	PGV	O02-C1-O01-C02
9	D	103	PGV	O02-C1-O01-C02
9	5	101	PGV	O02-C1-O01-C02
17	M	408	CDL	OB7-CB5-OB6-CB4
17	2	101	CDL	OA7-CA5-OA6-CA4
17	6	101	CDL	OA7-CA5-OA6-CA4
10	G	101	BCL	C3-C5-C6-C7
10	S	101	BCL	C3-C5-C6-C7
10	8	102	BCL	C3-C5-C6-C7
17	6	101	CDL	C11-CA5-OA6-CA4
17	6	104	CDL	C11-CA5-OA6-CA4
10	O	101	BCL	C8-C10-C11-C12
10	O	101	BCL	C2-C3-C5-C6
10	8	102	BCL	C2-C3-C5-C6
10	W	101	BCL	C3-C5-C6-C7
12	L	307	U10	C22-C23-C24-C25
12	L	307	U10	C22-C23-C24-C26
10	Z	101	BCL	C5-C6-C7-C8
9	L	305	PGV	O12-C04-C05-O05
9	M	410	PGV	O12-C04-C05-O05
17	H	303	CDL	O1-C1-CB2-OB2
17	2	101	CDL	O1-C1-CB2-OB2
17	0	101	CDL	O1-C1-CA2-OA2
10	F	101	BCL	C3-C5-C6-C7
10	I	102	BCL	C3-C5-C6-C7
10	Q	102	BCL	C3-C5-C6-C7
10	V	102	BCL	C3-C5-C6-C7
10	1	102	BCL	C3-C5-C6-C7
13	L	313	LMT	O5'-C5'-C6'-O6'
10	E	102	BCL	C5-C6-C7-C8
17	6	104	CDL	OA7-CA5-OA6-CA4
10	D	102	BCL	C4-C3-C5-C6
10	6	103	BCL	C4-C3-C5-C6
10	9	101	BCL	C4-C3-C5-C6
12	7	401	U10	C15-C14-C16-C17
12	7	401	U10	C35-C34-C36-C37
10	D	102	BCL	C2-C3-C5-C6
10	6	103	BCL	C2-C3-C5-C6
10	9	101	BCL	C2-C3-C5-C6
12	7	401	U10	C13-C14-C16-C17
12	7	401	U10	C33-C34-C36-C37
10	R	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	7	401	U10	C39-C41-C42-C43
9	M	410	PGV	O12-C04-C05-C06
17	A	101	CDL	CB2-C1-CA2-OA2
13	I	103	LMT	C4'-C5'-C6'-O6'
10	E	102	BCL	C3-C5-C6-C7
10	3	102	BCL	C3-C5-C6-C7
10	5	102	BCL	C3-C5-C6-C7
17	6	101	CDL	C31-CA7-OA8-CA6
17	0	101	CDL	C31-CA7-OA8-CA6
10	2	102	BCL	C5-C6-C7-C8
10	3	102	BCL	C13-C15-C16-C17
17	A	101	CDL	O1-C1-CA2-OA2
17	0	101	CDL	OA9-CA7-OA8-CA6
10	L	309	BCL	C6-C7-C8-C9
10	T	102	BCL	C11-C10-C8-C9
10	V	102	BCL	C11-C10-C8-C9
10	4	102	BCL	C14-C13-C15-C16
10	6	103	BCL	C11-C10-C8-C9
10	7	402	BCL	C11-C10-C8-C9
10	9	101	BCL	C6-C7-C8-C9
10	9	101	BCL	C11-C12-C13-C14
10	8	102	BCL	C2A-CAA-CBA-CGA
10	0	102	BCL	C2A-CAA-CBA-CGA
16	A	103	I7D	C34-C33-C35-C36
16	K	101	I7D	C34-C33-C35-C36
16	V	101	I7D	C34-C33-C35-C36
16	6	102	I7D	C34-C33-C35-C36
16	8	101	I7D	C34-C33-C35-C36
16	A	103	I7D	C32-C33-C35-C36
16	T	101	I7D	C32-C33-C35-C36
16	6	102	I7D	C32-C33-C35-C36
16	8	101	I7D	C32-C33-C35-C36
13	I	103	LMT	O5B-C5B-C6B-O6B
17	H	303	CDL	CB5-C51-C52-C53
17	A	101	CDL	CB5-C51-C52-C53
17	6	101	CDL	OA9-CA7-OA8-CA6
10	N	102	BCL	C15-C16-C17-C18
10	X	102	BCL	C15-C16-C17-C18
17	H	303	CDL	C71-CB7-OB8-CB6
10	E	102	BCL	C15-C16-C17-C18
9	D	103	PGV	C1-C2-C3-C4
10	J	101	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
10	T	102	BCL	C5-C6-C7-C8
10	2	102	BCL	C10-C11-C12-C13
10	2	102	BCL	C13-C15-C16-C17
9	L	304	PGV	C19-C20-C21-C22
9	M	410	PGV	C1-C2-C3-C4
17	6	101	CDL	CB5-C51-C52-C53
10	E	102	BCL	CBD-CGD-O2D-CED
10	4	102	BCL	C12-C13-C15-C16
10	B	101	BCL	C2A-CAA-CBA-CGA
10	L	301	BCL	O1D-CGD-O2D-CED
10	Q	102	BCL	C15-C16-C17-C18
10	S	101	BCL	C15-C16-C17-C18
10	V	102	BCL	C5-C6-C7-C8
10	X	102	BCL	C5-C6-C7-C8
13	L	313	LMT	C4'-C5'-C6'-O6'
13	3	103	LMT	O5'-C1'-O1'-C1
10	R	102	BCL	C10-C11-C12-C13
10	R	102	BCL	C13-C15-C16-C17
10	X	102	BCL	C13-C15-C16-C17
16	8	101	I7D	C23-C25-C26-C27
10	G	101	BCL	C13-C15-C16-C17
10	T	102	BCL	C15-C16-C17-C18
10	4	102	BCL	C10-C11-C12-C13
10	5	102	BCL	C13-C15-C16-C17
10	N	102	BCL	C13-C15-C16-C17
10	P	101	BCL	C15-C16-C17-C18
13	I	103	LMT	O5'-C5'-C6'-O6'
9	5	104	PGV	C2-C1-O01-C02
17	H	303	CDL	C11-CA5-OA6-CA4
10	B	101	BCL	C8-C10-C11-C12
10	0	102	BCL	C8-C10-C11-C12
9	C	406	PGV	C03-O11-P-O12
9	L	310	PGV	C03-O11-P-O12
9	L	311	PGV	C03-O11-P-O12
9	H	302	PGV	C03-O11-P-O12
9	K	103	PGV	C03-O11-P-O12
9	5	104	PGV	C03-O11-P-O12
17	M	407	CDL	CA3-OA5-PA1-OA2
17	M	408	CDL	CB3-OB5-PB2-OB2
17	A	101	CDL	CA3-OA5-PA1-OA2
17	T	103	CDL	CA2-OA2-PA1-OA5
17	T	103	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
17	2	101	CDL	CB2-OB2-PB2-OB5
17	2	101	CDL	CB3-OB5-PB2-OB2
17	6	104	CDL	CB2-OB2-PB2-OB5
17	6	104	CDL	CB3-OB5-PB2-OB2
17	0	101	CDL	CB3-OB5-PB2-OB2
9	C	407	PGV	C1-C2-C3-C4
10	Z	101	BCL	CBA-CGA-O2A-C1
10	E	102	BCL	C8-C10-C11-C12
10	Q	102	BCL	C13-C15-C16-C17
10	4	102	BCL	C15-C16-C17-C18
17	M	407	CDL	CA2-C1-CB2-OB2
9	5	104	PGV	O02-C1-O01-C02
17	H	303	CDL	OA7-CA5-OA6-CA4
10	B	101	BCL	C15-C16-C17-C18
10	R	102	BCL	C5-C6-C7-C8
10	G	101	BCL	C2A-CAA-CBA-CGA
10	N	102	BCL	C2A-CAA-CBA-CGA
10	P	101	BCL	C2A-CAA-CBA-CGA
10	T	102	BCL	C2A-CAA-CBA-CGA
10	V	102	BCL	C2A-CAA-CBA-CGA
10	Y	101	BCL	C16-C17-C18-C19
9	H	302	PGV	C1-C2-C3-C4
17	0	101	CDL	C11-CA5-OA6-CA4
16	N	101	I7D	C31-C32-C33-C34
16	8	101	I7D	C26-C27-C28-C29
9	L	312	PGV	C21-C22-C23-C24
17	2	101	CDL	CA6-CA4-OA6-CA5
17	0	101	CDL	OA7-CA5-OA6-CA4
9	C	406	PGV	C20-C21-C22-C23
17	M	408	CDL	C51-C52-C53-C54
9	M	411	PGV	C20-C21-C22-C23
10	M	403	BCL	C5-C6-C7-C8
17	H	303	CDL	C51-C52-C53-C54
17	T	103	CDL	C35-C36-C37-C38
17	6	101	CDL	CA5-C11-C12-C13
13	3	103	LMT	C2'-C1'-O1'-C1
16	N	101	I7D	C31-C32-C33-C35
16	8	101	I7D	C26-C27-C28-C30
9	L	305	PGV	C6-C7-C8-C9
10	L	309	BCL	C16-C17-C18-C19
9	L	311	PGV	C21-C22-C23-C24
10	L	301	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	D	102	BCL	C11-C10-C8-C9
10	I	102	BCL	C14-C13-C15-C16
10	S	101	BCL	C14-C13-C15-C16
10	U	101	BCL	C14-C13-C15-C16
10	9	101	BCL	C14-C13-C15-C16
10	6	103	BCL	C2A-CAA-CBA-CGA
10	Z	101	BCL	O1A-CGA-O2A-C1
17	H	303	CDL	OB9-CB7-OB8-CB6
16	D	101	I7D	C34-C33-C35-C36
16	E	101	I7D	C34-C33-C35-C36
16	I	101	I7D	C34-C33-C35-C36
16	Q	101	I7D	C34-C33-C35-C36
16	X	101	I7D	C34-C33-C35-C36
16	1	101	I7D	C34-C33-C35-C36
16	4	101	I7D	C34-C33-C35-C36
9	L	304	PGV	C04-C05-C06-O06
9	L	312	PGV	C04-C05-C06-O06
16	D	101	I7D	C32-C33-C35-C36
16	E	101	I7D	C32-C33-C35-C36
16	I	101	I7D	C32-C33-C35-C36
16	K	101	I7D	C32-C33-C35-C36
16	Q	101	I7D	C32-C33-C35-C36
16	V	101	I7D	C32-C33-C35-C36
16	X	101	I7D	C32-C33-C35-C36
16	1	101	I7D	C32-C33-C35-C36
16	4	101	I7D	C32-C33-C35-C36
17	T	103	CDL	C11-CA5-OA6-CA4
9	C	406	PGV	C22-C23-C24-C25
9	M	411	PGV	C23-C24-C25-C26
9	F	102	PGV	C19-C20-C21-C22
17	T	103	CDL	CA5-C11-C12-C13
9	D	103	PGV	C21-C22-C23-C24
17	T	103	CDL	C33-C34-C35-C36
9	L	305	PGV	C29-C30-C31-C32
9	5	101	PGV	C1-C2-C3-C4
17	T	103	CDL	CB5-C51-C52-C53
17	6	104	CDL	CB7-C71-C72-C73
9	5	101	PGV	C12-C13-C14-C15
10	Z	101	BCL	C3-C5-C6-C7
10	X	102	BCL	CBA-CGA-O2A-C1
10	A	102	BCL	C3A-C2A-CAA-CBA
10	8	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	C	405	PGV	O03-C01-C02-C03
10	W	101	BCL	C15-C16-C17-C18
9	L	312	PGV	O05-C05-C06-O06
9	L	305	PGV	C5-C6-C7-C8
9	5	103	PGV	C26-C27-C28-C29
17	T	103	CDL	C51-C52-C53-C54
9	5	101	PGV	C11-C10-C9-C8
9	K	103	PGV	O12-C04-C05-O05
10	Y	101	BCL	C3-C5-C6-C7
9	L	304	PGV	O12-C04-C05-C06
17	H	303	CDL	CA2-C1-CB2-OB2
17	0	101	CDL	CB2-C1-CA2-OA2
17	T	103	CDL	OA7-CA5-OA6-CA4
13	L	313	LMT	C1-C2-C3-C4
9	5	103	PGV	C3-C4-C5-C6
17	H	303	CDL	C12-C13-C14-C15
10	G	101	BCL	C8-C10-C11-C12
10	X	102	BCL	O1A-CGA-O2A-C1
10	A	102	BCL	C13-C15-C16-C17
17	0	101	CDL	C51-CB5-OB6-CB4
10	L	301	BCL	C11-C10-C8-C7
10	D	102	BCL	C12-C13-C15-C16
10	S	101	BCL	C12-C13-C15-C16
10	W	101	BCL	C12-C13-C15-C16
10	7	402	BCL	C11-C10-C8-C7
10	9	101	BCL	C11-C12-C13-C15
10	9	101	BCL	C12-C13-C15-C16
10	0	102	BCL	C12-C13-C15-C16
10	7	402	BCL	C3-C5-C6-C7
17	6	104	CDL	C51-C52-C53-C54
10	J	101	BCL	C13-C15-C16-C17
17	2	101	CDL	OB7-CB5-OB6-CB4
9	5	104	PGV	C19-C20-C21-C22
10	B	101	BCL	CBA-CGA-O2A-C1
10	V	102	BCL	CBA-CGA-O2A-C1
10	2	102	BCL	CBA-CGA-O2A-C1
10	0	102	BCL	CBA-CGA-O2A-C1
10	E	102	BCL	C2A-CAA-CBA-CGA
10	X	102	BCL	C2A-CAA-CBA-CGA
10	Z	101	BCL	C2A-CAA-CBA-CGA
10	2	102	BCL	C2A-CAA-CBA-CGA
9	L	305	PGV	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
10	N	102	BCL	C10-C11-C12-C13
10	2	102	BCL	C3-C5-C6-C7
10	P	101	BCL	C16-C17-C18-C19
10	D	102	BCL	C10-C11-C12-C13
10	I	102	BCL	C15-C16-C17-C18
13	1	103	LMT	C3-C4-C5-C6
17	2	101	CDL	C51-CB5-OB6-CB4
9	M	410	PGV	C20-C21-C22-C23
9	5	104	PGV	C24-C25-C26-C27
17	H	303	CDL	OB6-CB4-CB6-OB8
10	L	309	BCL	C16-C17-C18-C20
10	D	102	BCL	C14-C13-C15-C16
10	N	102	BCL	C11-C10-C8-C9
10	W	101	BCL	C14-C13-C15-C16
10	X	102	BCL	C11-C10-C8-C9
10	4	102	BCL	C6-C7-C8-C9
10	0	102	BCL	C14-C13-C15-C16
13	L	308	LMT	O1'-C1-C2-C3
10	D	102	BCL	C15-C16-C17-C18
10	B	101	BCL	O1A-CGA-O2A-C1
10	V	102	BCL	O1A-CGA-O2A-C1
10	8	102	BCL	C1A-C2A-CAA-CBA
10	P	101	BCL	C16-C17-C18-C20
10	8	102	BCL	C16-C17-C18-C19
17	0	101	CDL	OB7-CB5-OB6-CB4
17	H	303	CDL	C72-C73-C74-C75
10	G	101	BCL	C15-C16-C17-C18
10	U	101	BCL	C15-C16-C17-C18
9	C	405	PGV	C03-O11-P-O12
9	M	410	PGV	C04-O12-P-O11
9	H	301	PGV	C04-O12-P-O11
17	0	101	CDL	CB2-OB2-PB2-OB5
10	Z	101	BCL	C15-C16-C17-C18
9	H	302	PGV	C01-C02-C03-O11
9	F	102	PGV	C01-C02-C03-O11
17	2	101	CDL	OA5-CA3-CA4-CA6
17	6	104	CDL	OA5-CA3-CA4-CA6
10	5	102	BCL	C8-C10-C11-C12
10	7	402	BCL	C8-C10-C11-C12
10	Y	101	BCL	C16-C17-C18-C20
10	T	102	BCL	C2C-C3C-CAC-CBC
10	0	102	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	I	103	LMT	C3-C4-C5-C6
9	D	103	PGV	C20-C21-C22-C23
9	F	102	PGV	C2-C1-O01-C02
10	2	102	BCL	O1A-CGA-O2A-C1
10	0	102	BCL	O1A-CGA-O2A-C1
10	F	101	BCL	C15-C16-C17-C18
13	3	103	LMT	O5'-C5'-C6'-O6'
9	L	312	PGV	O03-C01-C02-C03
17	M	408	CDL	CB3-CB4-CB6-OB8
17	6	101	CDL	CA3-CA4-CA6-OA8
8	C	403	HEC	C2C-C3C-CAC-CBC
10	U	101	BCL	C13-C15-C16-C17
10	8	102	BCL	C15-C16-C17-C18
13	L	313	LMT	O5B-C5B-C6B-O6B
17	6	104	CDL	C37-C38-C39-C40
8	C	402	HEC	C2C-C3C-CAC-CBC
17	0	101	CDL	C55-C56-C57-C58
10	7	402	BCL	C4-C3-C5-C6
12	L	303	U10	C15-C14-C16-C17
10	7	402	BCL	C2-C3-C5-C6
9	C	406	PGV	C19-C20-C21-C22
9	M	411	PGV	C1-C2-C3-C4
17	M	408	CDL	CB7-C71-C72-C73
9	M	411	PGV	C25-C26-C27-C28
17	H	303	CDL	C55-C56-C57-C58
9	L	312	PGV	C01-C02-O01-C1
17	6	101	CDL	CA6-CA4-OA6-CA5
10	X	102	BCL	C3-C5-C6-C7
9	L	311	PGV	C20-C21-C22-C23
17	M	408	CDL	OA5-CA3-CA4-OA6
17	T	103	CDL	OA5-CA3-CA4-OA6
10	8	102	BCL	C16-C17-C18-C20
9	M	411	PGV	C19-C20-C21-C22
17	2	101	CDL	C54-C55-C56-C57
9	L	304	PGV	O12-C04-C05-O05
10	E	102	BCL	O1D-CGD-O2D-CED
17	A	101	CDL	CA5-C11-C12-C13
17	6	104	CDL	CB5-C51-C52-C53
17	M	407	CDL	OA6-CA4-CA6-OA8
16	X	101	I7D	C36-C37-C38-C40
10	4	102	BCL	C4-C3-C5-C6
10	L	309	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
10	M	403	BCL	C12-C13-C15-C16
10	I	102	BCL	C12-C13-C15-C16
10	N	102	BCL	C11-C10-C8-C7
10	P	101	BCL	C6-C7-C8-C10
10	P	101	BCL	C11-C10-C8-C7
10	R	102	BCL	C11-C10-C8-C7
10	S	101	BCL	C11-C10-C8-C7
10	T	102	BCL	C11-C10-C8-C7
10	U	101	BCL	C12-C13-C15-C16
10	V	102	BCL	C6-C7-C8-C10
10	X	102	BCL	C11-C10-C8-C7
10	Y	101	BCL	C6-C7-C8-C10
10	Z	101	BCL	C6-C7-C8-C10
10	1	102	BCL	C6-C7-C8-C10
10	2	102	BCL	C11-C10-C8-C7
10	2	102	BCL	C12-C13-C15-C16
10	3	102	BCL	C11-C10-C8-C7
10	4	102	BCL	C2-C3-C5-C6
10	4	102	BCL	C6-C7-C8-C10
10	5	102	BCL	C6-C7-C8-C10
10	9	101	BCL	C6-C7-C8-C10
10	9	101	BCL	C11-C10-C8-C7
12	L	303	U10	C13-C14-C16-C17
10	U	101	BCL	C3-C5-C6-C7
10	M	403	BCL	C14-C13-C15-C16
10	B	101	BCL	C6-C7-C8-C9
10	I	102	BCL	C11-C10-C8-C9
10	O	101	BCL	C11-C10-C8-C9
10	P	101	BCL	C11-C10-C8-C9
10	Q	102	BCL	C11-C10-C8-C9
10	R	102	BCL	C11-C10-C8-C9
10	S	101	BCL	C11-C10-C8-C9
10	V	102	BCL	C6-C7-C8-C9
10	W	101	BCL	C11-C10-C8-C9
10	Y	101	BCL	C6-C7-C8-C9
10	2	102	BCL	C11-C10-C8-C9
10	3	102	BCL	C11-C10-C8-C9
10	5	102	BCL	C11-C10-C8-C9
10	7	402	BCL	C6-C7-C8-C9
10	9	101	BCL	C11-C10-C8-C9
17	6	104	CDL	CA7-C31-C32-C33
10	L	309	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	0	101	CDL	C54-C55-C56-C57
9	H	301	PGV	C04-C05-C06-O06
9	L	305	PGV	O12-C04-C05-C06
10	K	102	BCL	C15-C16-C17-C18
9	L	304	PGV	C2-C1-O01-C02
9	M	410	PGV	C2-C1-O01-C02
10	P	101	BCL	C10-C11-C12-C13
10	S	101	BCL	C13-C15-C16-C17
9	L	304	PGV	C01-C02-C03-O11
9	L	305	PGV	C01-C02-C03-O11
17	T	103	CDL	C55-C56-C57-C58
9	5	104	PGV	C20-C19-O03-C01
10	2	102	BCL	C4-C3-C5-C6
10	2	102	BCL	C2-C3-C5-C6
10	F	101	BCL	CBA-CGA-O2A-C1
9	F	102	PGV	C5-C6-C7-C8
10	9	101	BCL	C8-C10-C11-C12
16	A	103	I7D	C2-C1-C4-C5
16	I	101	I7D	C3-C1-C4-C5
16	K	101	I7D	C2-C1-C4-C5
16	K	101	I7D	C3-C1-C4-C5
16	N	101	I7D	C2-C1-C4-C5
16	Q	101	I7D	C2-C1-C4-C5
16	R	101	I7D	C2-C1-C4-C5
16	1	101	I7D	C2-C1-C4-C5
16	3	101	I7D	C2-C1-C4-C5
16	4	101	I7D	C2-C1-C4-C5
17	H	303	CDL	CA3-CA4-CA6-OA8
17	H	303	CDL	CB3-CB4-CB6-OB8
17	0	101	CDL	CA3-CA4-CA6-OA8
9	F	102	PGV	O02-C1-O01-C02
9	L	312	PGV	C03-O11-P-O12
9	M	410	PGV	C03-O11-P-O12
9	H	302	PGV	C04-O12-P-O11
17	6	101	CDL	CB3-OB5-PB2-OB2
10	J	101	BCL	C2A-CAA-CBA-CGA
9	H	302	PGV	O01-C02-C03-O11
17	H	303	CDL	OA5-CA3-CA4-OA6
17	6	104	CDL	OA5-CA3-CA4-OA6
9	M	411	PGV	C20-C19-O03-C01
10	F	101	BCL	C16-C17-C18-C19
10	L	309	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
10	L	309	BCL	O1A-CGA-O2A-C1
9	D	103	PGV	O03-C01-C02-O01
17	H	303	CDL	OA6-CA4-CA6-OA8
12	7	401	U10	C34-C36-C37-C38
17	6	101	CDL	CA2-C1-CB2-OB2
9	L	304	PGV	O02-C1-O01-C02
10	E	102	BCL	C2-C1-O2A-CGA
10	G	101	BCL	C5-C6-C7-C8
10	M	402	BCL	C11-C10-C8-C9
10	M	403	BCL	C11-C10-C8-C9
10	D	102	BCL	C6-C7-C8-C9
10	F	101	BCL	C11-C10-C8-C9
10	K	102	BCL	C11-C10-C8-C9
10	U	101	BCL	C11-C10-C8-C9
10	1	102	BCL	C6-C7-C8-C9
10	4	102	BCL	C11-C10-C8-C9
10	L	309	BCL	C15-C16-C17-C18
10	I	102	BCL	C13-C15-C16-C17
9	H	302	PGV	C02-C03-O11-P
13	1	103	LMT	C1-C2-C3-C4
18	M	409	PEE	C18-C19-C20-C21
9	M	410	PGV	O02-C1-O01-C02
9	C	407	PGV	C2-C1-O01-C02
17	A	101	CDL	C11-CA5-OA6-CA4
17	M	408	CDL	OA5-CA3-CA4-CA6
17	6	101	CDL	OA5-CA3-CA4-CA6
17	0	101	CDL	OB5-CB3-CB4-CB6
13	3	103	LMT	C2-C3-C4-C5
10	B	101	BCL	C6-C7-C8-C10
10	D	102	BCL	C11-C10-C8-C7
10	G	101	BCL	C11-C10-C8-C7
10	I	102	BCL	C6-C7-C8-C10
10	I	102	BCL	C11-C10-C8-C7
10	J	101	BCL	C6-C7-C8-C10
10	J	101	BCL	C11-C10-C8-C7
10	K	102	BCL	C11-C10-C8-C7
10	N	102	BCL	C6-C7-C8-C10
10	O	101	BCL	C11-C10-C8-C7
10	Q	102	BCL	C6-C7-C8-C10
10	Q	102	BCL	C11-C10-C8-C7
10	U	101	BCL	C11-C10-C8-C7
10	W	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
10	Y	101	BCL	C11-C10-C8-C7
10	5	102	BCL	C11-C10-C8-C7
10	7	402	BCL	C6-C7-C8-C10
10	8	102	BCL	C11-C10-C8-C7
10	0	102	BCL	C11-C10-C8-C7
9	L	311	PGV	C22-C23-C24-C25
17	6	101	CDL	C72-C73-C74-C75
10	J	101	BCL	C16-C17-C18-C19
10	5	102	BCL	C2A-CAA-CBA-CGA
10	T	102	BCL	C3-C5-C6-C7
10	P	101	BCL	CBA-CGA-O2A-C1
10	4	102	BCL	C13-C15-C16-C17
9	5	104	PGV	C01-C02-O01-C1
10	L	301	BCL	CAD-CBD-CGD-O2D
10	L	309	BCL	CAD-CBD-CGD-O2D
17	6	104	CDL	CA6-CA4-OA6-CA5
10	3	102	BCL	C10-C11-C12-C13
9	C	407	PGV	C20-C19-O03-C01
12	L	303	U10	C12-C11-C9-C10
10	J	101	BCL	C8-C10-C11-C12
10	W	101	BCL	C13-C15-C16-C17
17	6	104	CDL	C1-CA2-OA2-PA1
9	H	301	PGV	O01-C02-C03-O11
17	M	408	CDL	OB5-CB3-CB4-OB6
17	6	101	CDL	OA5-CA3-CA4-OA6
17	0	101	CDL	OB5-CB3-CB4-OB6
8	C	403	HEC	C4C-C3C-CAC-CBC
10	R	102	BCL	CBA-CGA-O2A-C1
9	C	407	PGV	O02-C1-O01-C02
17	A	101	CDL	OA7-CA5-OA6-CA4
10	M	403	BCL	CHA-CBD-CGD-O1D
8	C	402	HEC	C4C-C3C-CAC-CBC
10	F	101	BCL	O1A-CGA-O2A-C1
10	1	102	BCL	C15-C16-C17-C18
9	C	407	PGV	O03-C01-C02-O01
9	L	312	PGV	O03-C01-C02-O01
17	M	408	CDL	OB6-CB4-CB6-OB8
17	2	101	CDL	OA6-CA4-CA6-OA8
17	0	101	CDL	OA6-CA4-CA6-OA8
10	J	101	BCL	C5-C6-C7-C8
9	5	104	PGV	O04-C19-O03-C01
9	D	103	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
17	2	101	CDL	CA7-C31-C32-C33
10	J	101	BCL	C6-C7-C8-C9
10	J	101	BCL	C11-C10-C8-C9
10	N	102	BCL	C6-C7-C8-C9
9	C	406	PGV	C21-C22-C23-C24
17	H	303	CDL	C15-C16-C17-C18
10	P	101	BCL	O1A-CGA-O2A-C1
17	6	104	CDL	C11-C12-C13-C14
17	T	103	CDL	C71-C72-C73-C74
10	A	102	BCL	C1A-C2A-CAA-CBA
10	K	102	BCL	C1A-C2A-CAA-CBA
10	M	402	BCL	C13-C15-C16-C17
9	5	103	PGV	C25-C26-C27-C28
9	5	103	PGV	C03-O11-P-O12
17	A	101	CDL	CB3-OB5-PB2-OB2
17	T	103	CDL	CA3-OA5-PA1-OA2
17	T	103	CDL	CB2-OB2-PB2-OB5
17	6	101	CDL	CA3-OA5-PA1-OA2
17	M	408	CDL	C14-C15-C16-C17
17	T	103	CDL	C72-C73-C74-C75
9	C	405	PGV	C03-O11-P-O13
9	C	406	PGV	C03-O11-P-O13
9	L	304	PGV	C03-O11-P-O13
9	L	310	PGV	C03-O11-P-O13
9	L	311	PGV	C03-O11-P-O13
9	L	311	PGV	C03-O11-P-O14
9	L	312	PGV	C03-O11-P-O13
9	M	410	PGV	C04-O12-P-O13
9	H	302	PGV	C03-O11-P-O14
9	K	103	PGV	C03-O11-P-O13
17	M	407	CDL	CA3-OA5-PA1-OA3
17	M	408	CDL	CA2-OA2-PA1-OA4
17	A	101	CDL	CA2-OA2-PA1-OA4
17	T	103	CDL	CB3-OB5-PB2-OB3
17	2	101	CDL	CB2-OB2-PB2-OB3
17	2	101	CDL	CB3-OB5-PB2-OB3
17	6	101	CDL	CA2-OA2-PA1-OA4
17	6	104	CDL	CB2-OB2-PB2-OB4
17	6	104	CDL	CB3-OB5-PB2-OB3
17	0	101	CDL	CB2-OB2-PB2-OB4
10	6	103	BCL	C10-C11-C12-C13
10	E	102	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	L	310	PGV	C01-C02-C03-O11
9	H	301	PGV	C01-C02-C03-O11
17	M	408	CDL	OB5-CB3-CB4-CB6
17	A	101	CDL	OB5-CB3-CB4-CB6
10	J	101	BCL	C3-C5-C6-C7
17	0	101	CDL	C56-C57-C58-C59
9	M	411	PGV	O04-C19-O03-C01
10	D	102	BCL	C16-C17-C18-C19
10	7	402	BCL	C5-C6-C7-C8
9	5	103	PGV	C1-C2-C3-C4
9	L	305	PGV	O01-C02-C03-O11
9	L	310	PGV	O01-C02-C03-O11
9	M	410	PGV	O01-C02-C03-O11
9	F	102	PGV	O01-C02-C03-O11
10	M	402	BCL	C6-C7-C8-C10
10	E	102	BCL	C11-C10-C8-C7
10	F	101	BCL	C2C-C3C-CAC-CBC
10	O	101	BCL	C11-C12-C13-C15
10	S	101	BCL	C6-C7-C8-C10
10	W	101	BCL	C6-C7-C8-C10
10	3	102	BCL	C6-C7-C8-C10
10	4	102	BCL	C3A-C2A-CAA-CBA
10	0	102	BCL	C6-C7-C8-C10
17	A	101	CDL	OB5-CB3-CB4-OB6
17	2	101	CDL	OA5-CA3-CA4-OA6
10	Y	101	BCL	C13-C15-C16-C17
10	R	102	BCL	O1A-CGA-O2A-C1
17	M	407	CDL	CA3-CA4-CA6-OA8
17	2	101	CDL	CA3-CA4-CA6-OA8
9	C	405	PGV	O03-C01-C02-O01
17	6	101	CDL	OA6-CA4-CA6-OA8
11	L	302	BPH	O2A-C1-C2-C3
9	H	302	PGV	C7-C8-C9-C10
10	L	301	BCL	C3-C5-C6-C7
10	A	102	BCL	C3-C5-C6-C7
9	C	407	PGV	O04-C19-O03-C01
10	7	402	BCL	C10-C11-C12-C13
10	N	102	BCL	CBA-CGA-O2A-C1
10	A	102	BCL	C11-C10-C8-C9
10	A	102	BCL	C11-C12-C13-C14
10	Q	102	BCL	C6-C7-C8-C9
10	Y	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	0	102	BCL	C11-C10-C8-C9
10	E	102	BCL	O1A-CGA-O2A-C1
9	L	312	PGV	C5-C6-C7-C8
17	M	408	CDL	CA5-C11-C12-C13
16	V	101	I7D	C4-C5-C6-C7
17	6	101	CDL	C52-C53-C54-C55
13	I	103	LMT	C6-C7-C8-C9
10	N	102	BCL	O1A-CGA-O2A-C1
12	L	303	U10	C12-C11-C9-C8
9	L	305	PGV	C23-C24-C25-C26
9	C	407	PGV	C2-C3-C4-C5
17	H	303	CDL	CA6-CA4-OA6-CA5
17	0	101	CDL	CA6-CA4-OA6-CA5
9	M	410	PGV	C01-C02-C03-O11
17	T	103	CDL	OA5-CA3-CA4-CA6
17	6	101	CDL	OB7-CB5-OB6-CB4
10	D	102	BCL	C2-C1-O2A-CGA
10	O	101	BCL	C2-C1-O2A-CGA
10	V	102	BCL	C2-C1-O2A-CGA
10	8	102	BCL	C2-C1-O2A-CGA
9	L	304	PGV	O01-C02-C03-O11
9	D	103	PGV	O01-C02-C03-O11
10	R	102	BCL	C16-C17-C18-C19
17	6	101	CDL	C51-CB5-OB6-CB4
18	M	409	PEE	C16-C17-C18-C19
16	8	101	I7D	C16-C17-C19-C20
9	C	406	PGV	C04-O12-P-O11
9	H	301	PGV	C03-O11-P-O12
9	5	101	PGV	C03-O11-P-O12
9	5	104	PGV	C04-O12-P-O11
17	M	407	CDL	CB2-OB2-PB2-OB5
17	M	407	CDL	CB3-OB5-PB2-OB2
17	M	408	CDL	CB2-OB2-PB2-OB5
17	H	303	CDL	CA2-OA2-PA1-OA5
17	H	303	CDL	CA3-OA5-PA1-OA2
17	H	303	CDL	CB3-OB5-PB2-OB2
17	A	101	CDL	CB2-OB2-PB2-OB5
17	2	101	CDL	CA2-OA2-PA1-OA5
17	2	101	CDL	CA3-OA5-PA1-OA2
18	M	409	PEE	C4-O4P-P-O3P
9	5	103	PGV	C04-O12-P-O13
10	L	301	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	L	302	BPH	CHA-CBD-CGD-O2D
9	C	406	PGV	O03-C01-C02-C03
9	D	103	PGV	O03-C01-C02-C03
17	T	103	CDL	C54-C55-C56-C57
10	F	101	BCL	C11-C10-C8-C7
10	6	103	BCL	C11-C10-C8-C7
10	M	402	BCL	C6-C7-C8-C9
10	E	102	BCL	C11-C10-C8-C9
10	I	102	BCL	C6-C7-C8-C9
10	P	101	BCL	C6-C7-C8-C9
10	S	101	BCL	C6-C7-C8-C9
10	Z	101	BCL	C6-C7-C8-C9
10	5	102	BCL	C6-C7-C8-C9
10	0	102	BCL	C6-C7-C8-C9
17	T	103	CDL	C31-CA7-OA8-CA6
10	Z	101	BCL	C8-C10-C11-C12
12	L	306	U10	C5-C4-O4-C4M
17	6	104	CDL	C35-C36-C37-C38
13	I	103	LMT	O1'-C1-C2-C3
17	T	103	CDL	OA9-CA7-OA8-CA6
11	L	302	BPH	C16-C17-C18-C20
10	J	101	BCL	CBA-CGA-O2A-C1
17	0	101	CDL	CB4-CB3-OB5-PB2
9	K	103	PGV	O03-C19-C20-C21
18	M	409	PEE	C36-C37-C38-C39
18	M	409	PEE	C38-C39-C40-C41
10	L	309	BCL	C10-C11-C12-C13
10	A	102	BCL	C15-C16-C17-C18
10	0	102	BCL	C15-C16-C17-C18
11	M	404	BPH	C3-C5-C6-C7
17	M	408	CDL	CB2-C1-CA2-OA2
10	A	102	BCL	C16-C17-C18-C19
8	C	401	HEC	C2C-C3C-CAC-CBC
17	2	101	CDL	C55-C56-C57-C58
10	D	102	BCL	C5-C6-C7-C8
10	D	102	BCL	C16-C17-C18-C20
17	6	104	CDL	C71-C72-C73-C74
9	L	304	PGV	C22-C23-C24-C25
9	H	301	PGV	C4-C5-C6-C7
9	5	103	PGV	C21-C22-C23-C24
17	H	303	CDL	C13-C14-C15-C16
9	K	103	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
9	5	103	PGV	C5-C6-C7-C8
10	J	101	BCL	O1A-CGA-O2A-C1
17	6	101	CDL	C32-C33-C34-C35
10	Y	101	BCL	C2-C1-O2A-CGA
10	0	102	BCL	C2-C1-O2A-CGA
9	L	310	PGV	C28-C29-C30-C31
10	F	101	BCL	C16-C17-C18-C20
10	K	102	BCL	C3A-C2A-CAA-CBA
8	C	401	HEC	CAA-CBA-CGA-O1A
8	C	402	HEC	CAA-CBA-CGA-O1A
8	C	404	HEC	CAD-CBD-CGD-O1D
9	5	101	PGV	C2-C3-C4-C5
16	I	101	I7D	C2-C1-C4-C5
17	0	101	CDL	CA2-C1-CB2-OB2
9	K	103	PGV	C20-C21-C22-C23
17	M	408	CDL	O1-C1-CA2-OA2
17	0	101	CDL	C53-C54-C55-C56
10	2	102	BCL	C8-C10-C11-C12
8	C	401	HEC	CAA-CBA-CGA-O2A
17	M	408	CDL	CA6-CA4-OA6-CA5
17	T	103	CDL	CA6-CA4-OA6-CA5
18	M	409	PEE	C3-C2-O2-C10
10	G	101	BCL	C1A-C2A-CAA-CBA
10	O	101	BCL	C1A-C2A-CAA-CBA
10	4	102	BCL	C1A-C2A-CAA-CBA
10	A	102	BCL	C11-C10-C8-C7
10	O	101	BCL	C5-C6-C7-C8
8	C	404	HEC	CAD-CBD-CGD-O2D
9	L	305	PGV	C30-C31-C32-C33
9	C	406	PGV	C1-C2-C3-C4
9	L	311	PGV	C02-C03-O11-P
9	M	411	PGV	C22-C23-C24-C25
9	5	101	PGV	O01-C02-C03-O11
9	D	103	PGV	C01-C02-C03-O11
17	H	303	CDL	OA5-CA3-CA4-CA6
16	M	406	I7D	C4-C5-C6-O6
16	V	101	I7D	C4-C5-C6-O6
8	C	402	HEC	CAA-CBA-CGA-O2A
17	6	101	CDL	C12-C13-C14-C15
10	4	102	BCL	C3-C5-C6-C7
9	L	311	PGV	O02-C1-O01-C02
16	N	101	I7D	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
9	5	103	PGV	C4-C5-C6-C7
18	M	409	PEE	C17-C18-C19-C20
12	L	307	U10	C9-C11-C12-C13
10	J	101	BCL	C2-C1-O2A-CGA
10	U	101	BCL	C2-C1-O2A-CGA
10	6	103	BCL	C2-C1-O2A-CGA
10	9	101	BCL	C2-C1-O2A-CGA
10	2	102	BCL	C2C-C3C-CAC-CBC
10	L	309	BCL	C11-C12-C13-C14
10	E	102	BCL	C11-C12-C13-C14
10	O	101	BCL	C6-C7-C8-C9
17	6	104	CDL	C32-C33-C34-C35
10	F	101	BCL	CAA-CBA-CGA-O2A
13	I	103	LMT	C4-C5-C6-C7
17	0	101	CDL	C36-C37-C38-C39
10	M	402	BCL	C15-C16-C17-C18
9	M	410	PGV	C14-C15-C16-C17
17	0	101	CDL	C51-C52-C53-C54
10	E	102	BCL	C4-C3-C5-C6
10	R	102	BCL	C4-C3-C5-C6
16	8	101	I7D	C27-C28-C30-C31
10	A	102	BCL	C8-C10-C11-C12
10	G	101	BCL	C16-C17-C18-C19
10	R	102	BCL	C16-C17-C18-C20
8	C	401	HEC	C4C-C3C-CAC-CBC
10	F	101	BCL	C13-C15-C16-C17
10	F	101	BCL	C2A-CAA-CBA-CGA
12	L	303	U10	C5-C4-O4-C4M
8	C	404	HEC	C2B-C3B-CAB-CBB
9	H	301	PGV	C21-C22-C23-C24
9	H	302	PGV	C3-C4-C5-C6
10	X	102	BCL	C4-C3-C5-C6
17	6	101	CDL	C31-C32-C33-C34
9	L	310	PGV	C31-C32-C33-C34
17	6	101	CDL	C73-C74-C75-C76
9	L	311	PGV	O03-C01-C02-O01
17	T	103	CDL	OA6-CA4-CA6-OA8
13	L	308	LMT	C1-C2-C3-C4
10	K	102	BCL	C8-C10-C11-C12
10	8	102	BCL	CAA-CBA-CGA-O2A
16	V	101	I7D	C31-C32-C33-C34
16	8	101	I7D	C18-C17-C19-C20

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Mol	Chain	Res	Type	Atoms
10	P	101	BCL	C4-C3-C5-C6
10	V	102	BCL	C4-C3-C5-C6
10	E	102	BCL	C2-C3-C5-C6
10	O	101	BCL	C11-C12-C13-C14
10	W	101	BCL	C6-C7-C8-C9
10	3	102	BCL	C6-C7-C8-C9
10	G	101	BCL	C3A-C2A-CAA-CBA
17	6	101	CDL	C72-C71-CB7-OB8
10	M	402	BCL	CAD-CBD-CGD-O2D
10	9	101	BCL	C15-C16-C17-C18
9	C	405	PGV	C4-C5-C6-C7
8	C	404	HEC	C2C-C3C-CAC-CBC
10	G	101	BCL	C4-C3-C5-C6
10	Y	101	BCL	C4-C3-C5-C6
10	Z	101	BCL	C4-C3-C5-C6
12	7	401	U10	C30-C29-C31-C32
9	5	101	PGV	O03-C19-C20-C21
10	L	309	BCL	CAA-CBA-CGA-O2A
17	0	101	CDL	C12-C11-CA5-OA6
8	C	402	HEC	CAD-CBD-CGD-O2D
10	Y	101	BCL	C5-C6-C7-C8
10	S	101	BCL	O2A-C1-C2-C3
10	W	101	BCL	O2A-C1-C2-C3
10	3	102	BCL	O2A-C1-C2-C3
10	5	102	BCL	O2A-C1-C2-C3
9	H	301	PGV	C5-C6-C7-C8
10	O	101	BCL	O1D-CGD-O2D-CED
10	L	301	BCL	C16-C17-C18-C19
10	4	102	BCL	C16-C17-C18-C19
17	6	101	CDL	O1-C1-CB2-OB2
10	X	102	BCL	C2-C3-C5-C6
16	M	406	I7D	C3-C1-O1-C1M
8	C	402	HEC	CAD-CBD-CGD-O1D
9	L	310	PGV	C30-C31-C32-C33
9	M	411	PGV	O03-C19-C20-C21
9	H	302	PGV	O03-C01-C02-O01
9	5	103	PGV	C2-C3-C4-C5
17	H	303	CDL	C18-C19-C20-C21
10	L	301	BCL	C2A-CAA-CBA-CGA
9	L	304	PGV	O05-C05-C06-O06
9	H	301	PGV	O05-C05-C06-O06
16	X	101	I7D	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
9	L	311	PGV	C20-C19-O03-C01
12	7	401	U10	C40-C39-C41-C42
8	C	404	HEC	C4B-C3B-CAB-CBB
10	L	309	BCL	C11-C12-C13-C15
10	F	101	BCL	C6-C7-C8-C10
10	Y	101	BCL	C12-C13-C15-C16
10	Z	101	BCL	C11-C10-C8-C7
10	A	102	BCL	C16-C17-C18-C20
17	H	303	CDL	C32-C31-CA7-OA8
8	C	403	HEC	CAA-CBA-CGA-O2A
16	K	101	I7D	C1-C4-C5-C6
16	N	101	I7D	C1-C4-C5-C6
16	3	101	I7D	C1-C4-C5-C6
16	4	101	I7D	C1-C4-C5-C6
17	H	303	CDL	OA9-CA7-OA8-CA6
9	L	311	PGV	C2-C1-O01-C02
12	7	401	U10	C31-C32-C33-C34
9	M	411	PGV	C2-C3-C4-C5
17	H	303	CDL	C31-CA7-OA8-CA6
8	C	404	HEC	C4C-C3C-CAC-CBC
16	8	101	I7D	C29-C28-C30-C31
10	Q	102	BCL	C8-C10-C11-C12
13	L	308	LMT	C4'-C5'-C6'-O6'
10	F	101	BCL	C1A-C2A-CAA-CBA
10	R	102	BCL	C1A-C2A-CAA-CBA
10	U	101	BCL	C1A-C2A-CAA-CBA
10	L	309	BCL	CAA-CBA-CGA-O1A
10	8	102	BCL	CAA-CBA-CGA-O1A
17	0	101	CDL	C12-C11-CA5-OA7
18	M	409	PEE	O2-C10-C11-C12
10	4	102	BCL	C2A-CAA-CBA-CGA
17	M	408	CDL	CA3-OA5-PA1-OA2
10	J	101	BCL	C16-C17-C18-C20
17	6	101	CDL	C72-C71-CB7-OB9
10	0	102	BCL	C13-C15-C16-C17
9	M	411	PGV	O04-C19-C20-C21
9	5	101	PGV	O04-C19-C20-C21
9	M	410	PGV	C03-O11-P-O13
17	M	407	CDL	CB2-OB2-PB2-OB3
17	M	407	CDL	CB3-OB5-PB2-OB3
17	M	408	CDL	CB2-OB2-PB2-OB3
17	2	101	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
17	2	101	CDL	CA3-OA5-PA1-OA3
9	5	101	PGV	C01-C02-C03-O11
10	V	102	BCL	C8-C10-C11-C12
9	K	103	PGV	O02-C1-O01-C02
17	M	408	CDL	C53-C54-C55-C56
10	E	102	BCL	C13-C15-C16-C17
8	C	401	HEC	CAD-CBD-CGD-O2D
12	7	401	U10	C45-C44-C46-C47
12	7	401	U10	C2-C3-O3-C3M
10	R	102	BCL	C2-C3-C5-C6
17	A	101	CDL	C53-C54-C55-C56
9	C	406	PGV	C01-C02-O01-C1
9	C	406	PGV	C03-C02-O01-C1
10	E	102	BCL	CAD-CBD-CGD-O1D
10	U	101	BCL	CAD-CBD-CGD-O1D
10	2	102	BCL	CAD-CBD-CGD-O1D
17	T	103	CDL	C34-C35-C36-C37
17	0	101	CDL	O1-C1-CB2-OB2
10	L	309	BCL	C11-C10-C8-C9
10	Y	101	BCL	C14-C13-C15-C16
10	3	102	BCL	C11-C12-C13-C14
10	5	102	BCL	C14-C13-C15-C16
8	C	401	HEC	CAD-CBD-CGD-O1D
9	L	311	PGV	O04-C19-O03-C01
8	C	403	HEC	CAA-CBA-CGA-O1A
10	A	102	BCL	C11-C12-C13-C15
10	B	101	BCL	C11-C10-C8-C7
10	O	101	BCL	C3A-C2A-CAA-CBA
10	S	101	BCL	C2C-C3C-CAC-CBC
10	Z	101	BCL	C11-C12-C13-C15
10	6	103	BCL	C2C-C3C-CAC-CBC
11	L	302	BPH	C11-C12-C13-C15
18	M	409	PEE	O4-C10-C11-C12
9	M	410	PGV	C25-C26-C27-C28
9	H	302	PGV	O01-C1-C2-C3
10	I	102	BCL	CAA-CBA-CGA-O2A
9	C	406	PGV	C23-C24-C25-C26
13	I	103	LMT	C2-C3-C4-C5
9	5	104	PGV	O03-C19-C20-C21
17	H	303	CDL	C32-C31-CA7-OA9
17	M	408	CDL	O1-C1-CB2-OB2
13	I	103	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
17	A	101	CDL	C75-C76-C77-C78
10	I	102	BCL	CAA-CBA-CGA-O1A

There are no ring outliers.

75 monomers are involved in 224 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	304	PGV	3	0
10	E	102	BCL	5	0
12	L	307	U10	5	0
13	L	308	LMT	2	0
10	U	101	BCL	1	0
9	H	301	PGV	2	0
17	T	103	CDL	4	0
10	L	309	BCL	2	0
8	C	404	HEC	1	0
10	6	103	BCL	2	0
10	9	101	BCL	4	0
9	M	410	PGV	3	0
10	W	101	BCL	1	0
16	6	102	I7D	1	0
9	C	405	PGV	2	0
10	5	102	BCL	3	0
10	0	102	BCL	4	0
9	M	411	PGV	1	0
13	I	103	LMT	3	0
13	L	313	LMT	2	0
17	0	101	CDL	3	0
10	Z	101	BCL	5	0
10	L	301	BCL	1	0
15	M	405	MQ9	3	0
10	V	102	BCL	3	0
17	H	303	CDL	4	0
10	R	102	BCL	6	0
10	M	402	BCL	2	0
10	P	101	BCL	7	0
17	A	101	CDL	1	0
10	N	102	BCL	7	0
18	M	409	PEE	3	0
10	S	101	BCL	1	0
9	D	103	PGV	1	0
9	5	103	PGV	3	0

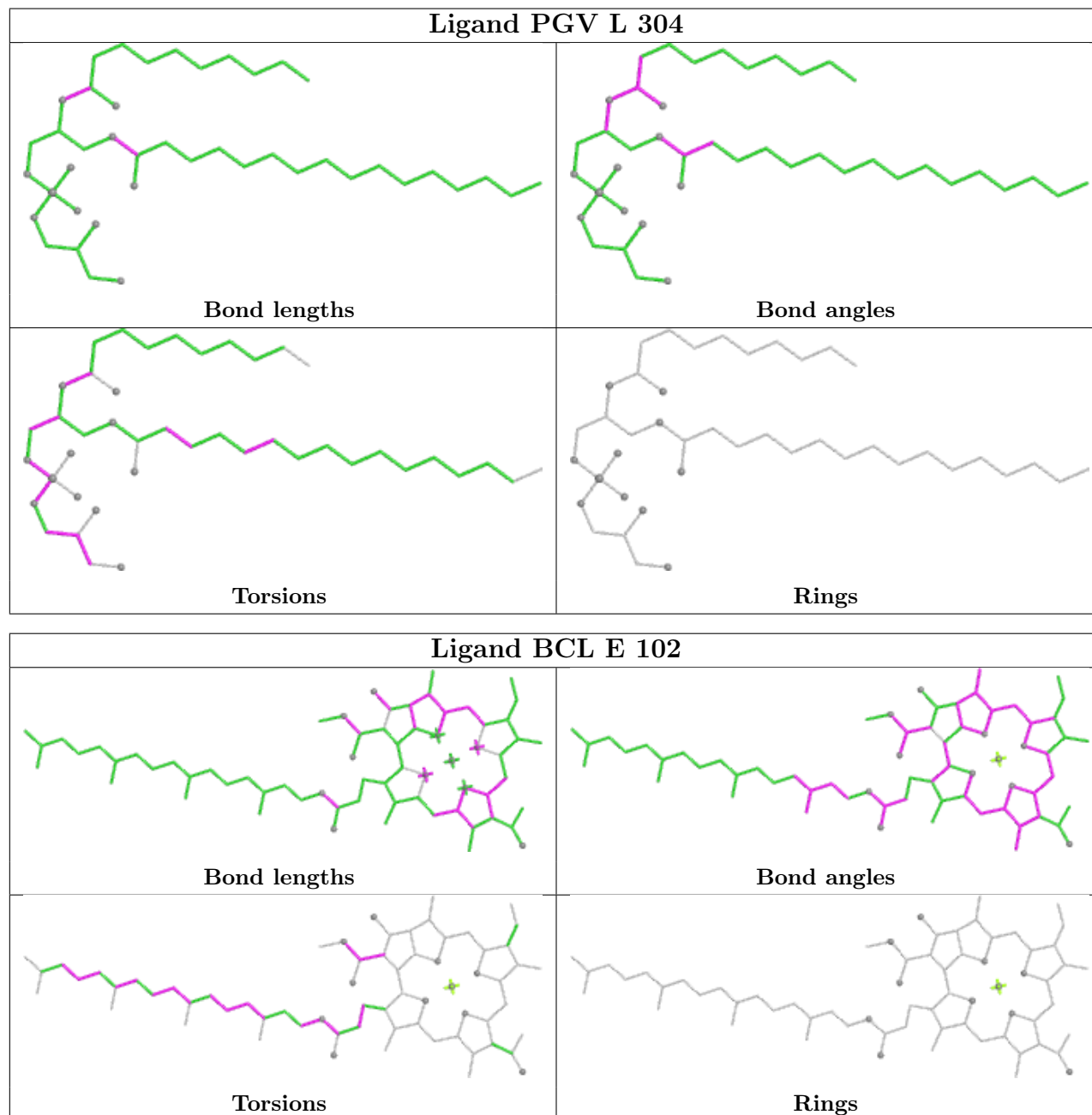
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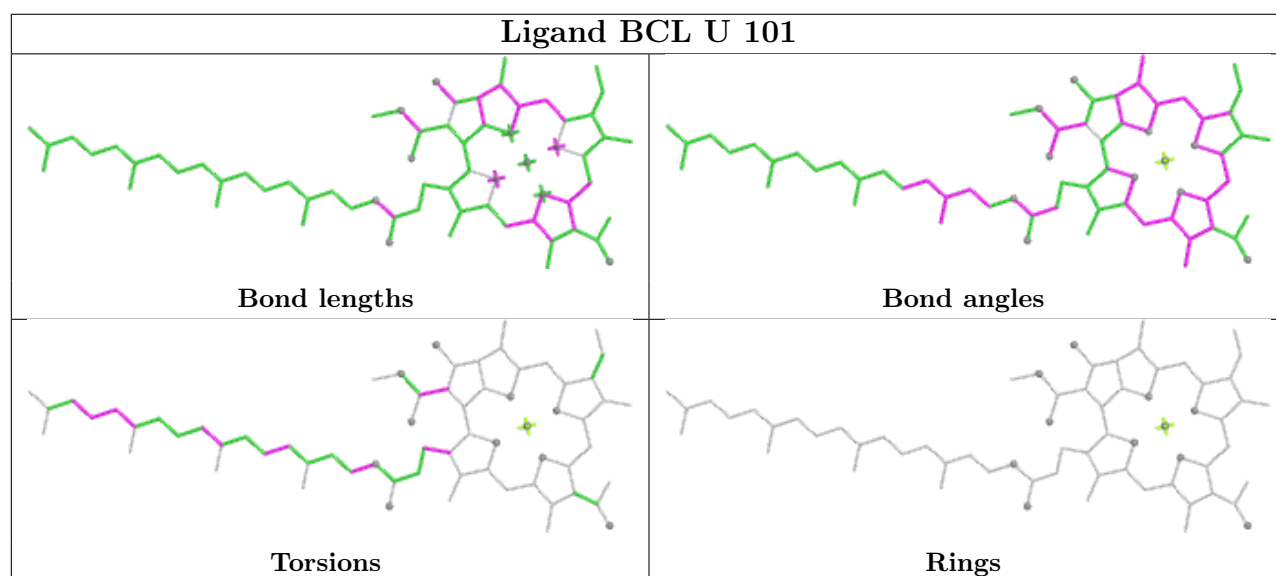
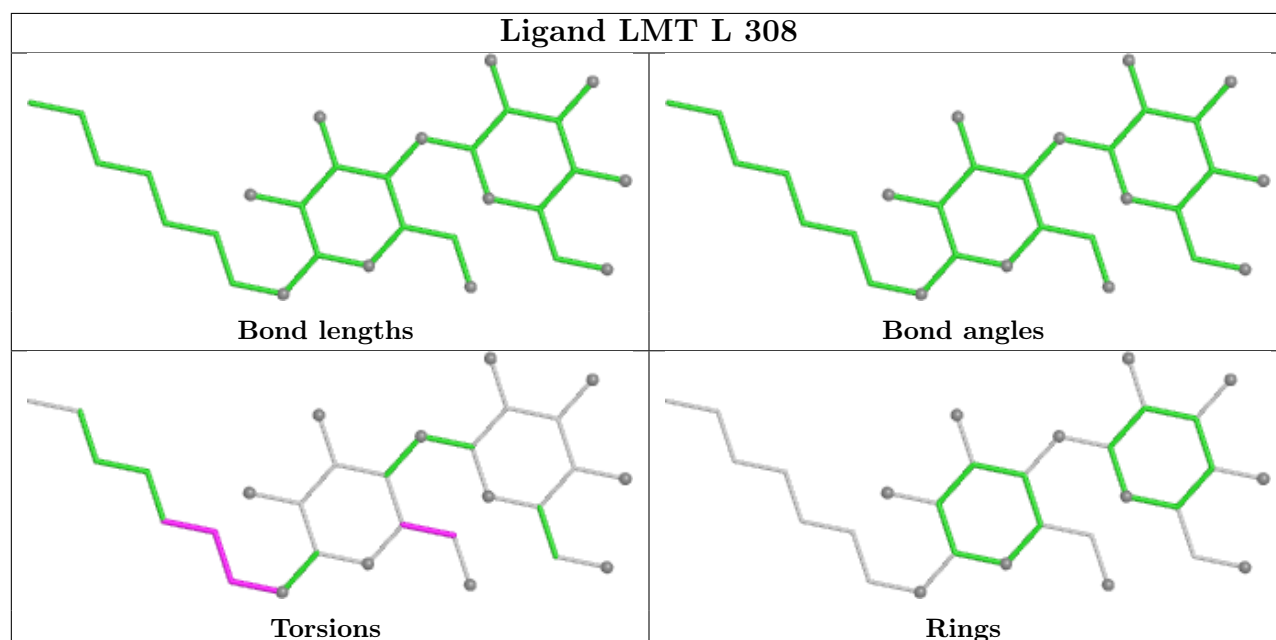
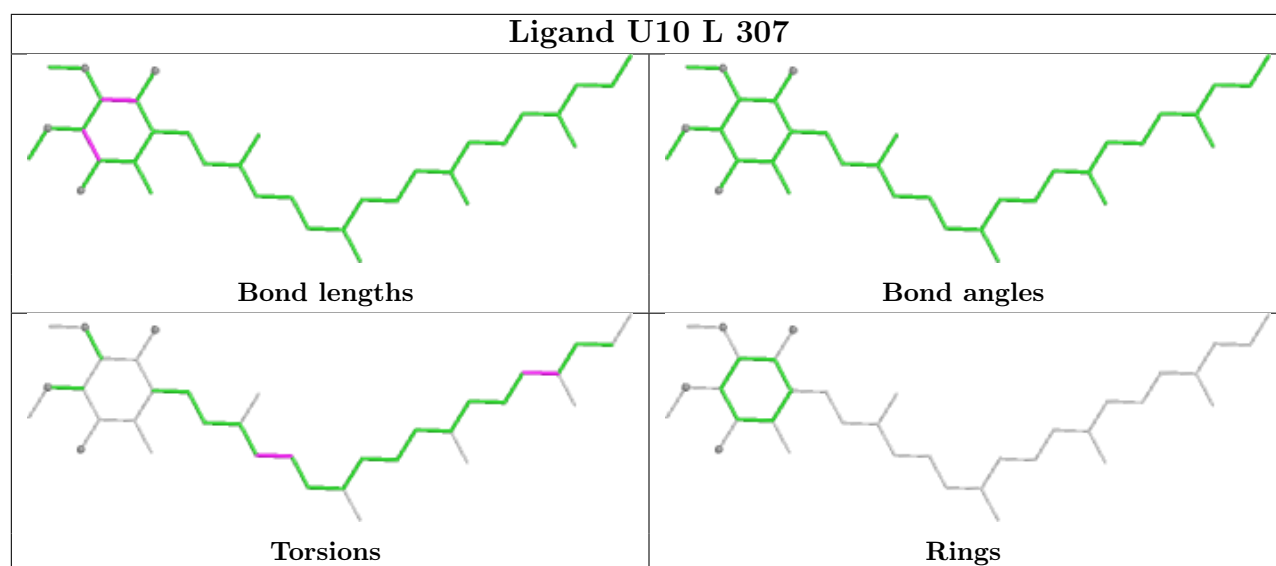
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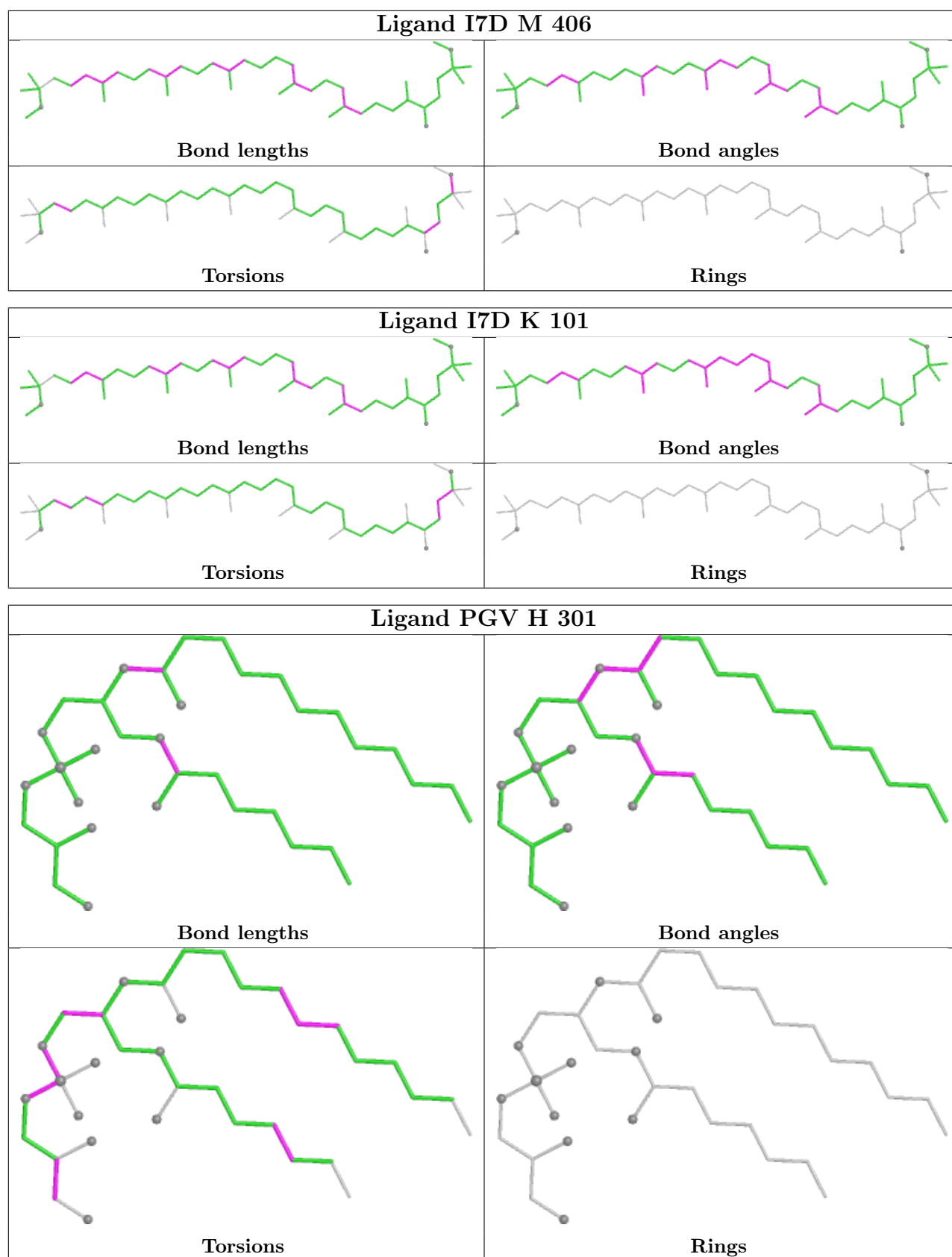
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	407	PGV	5	0
10	G	101	BCL	10	0
10	O	101	BCL	1	0
10	8	102	BCL	4	0
10	K	102	BCL	3	0
8	C	402	HEC	3	0
10	Q	102	BCL	1	0
10	Y	101	BCL	2	0
8	C	403	HEC	3	0
10	4	102	BCL	4	0
10	1	102	BCL	1	0
10	B	101	BCL	5	0
9	F	102	PGV	1	0
10	A	102	BCL	3	0
9	5	101	PGV	3	0
10	F	101	BCL	2	0
10	M	403	BCL	3	0
10	D	102	BCL	3	0
11	M	404	BPH	9	0
13	1	103	LMT	1	0
10	I	102	BCL	3	0
10	2	102	BCL	3	0
10	J	101	BCL	4	0
17	6	104	CDL	3	0
11	L	302	BPH	4	0
17	2	101	CDL	4	0
9	K	103	PGV	1	0
10	3	102	BCL	3	0
8	C	401	HEC	2	0
12	7	401	U10	9	0
17	M	407	CDL	1	0
13	3	103	LMT	8	0
10	X	102	BCL	6	0
10	T	102	BCL	3	0
12	L	306	U10	1	0
9	L	311	PGV	7	0
9	L	312	PGV	2	0
17	6	101	CDL	6	0
9	L	305	PGV	3	0
17	M	408	CDL	6	0

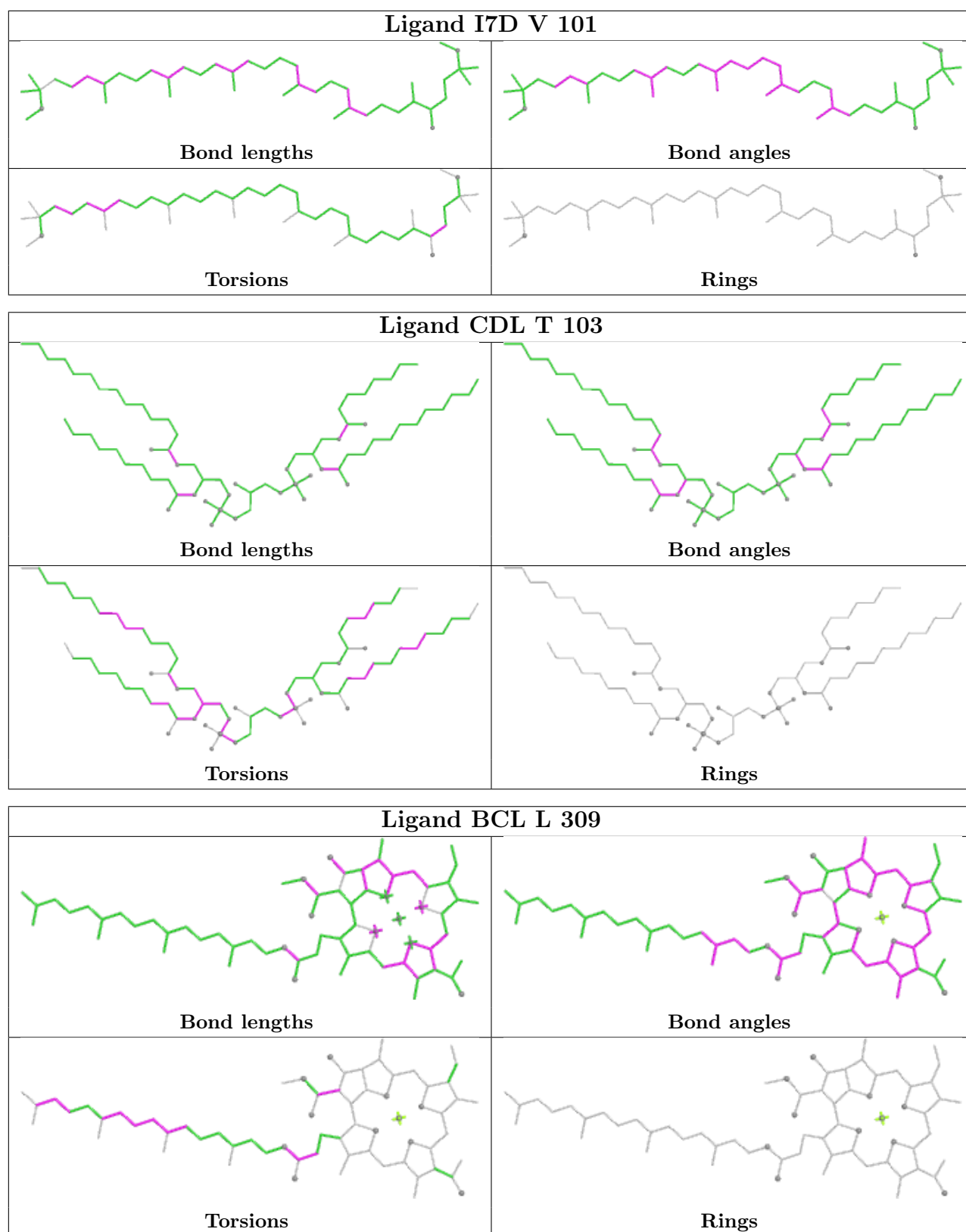
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

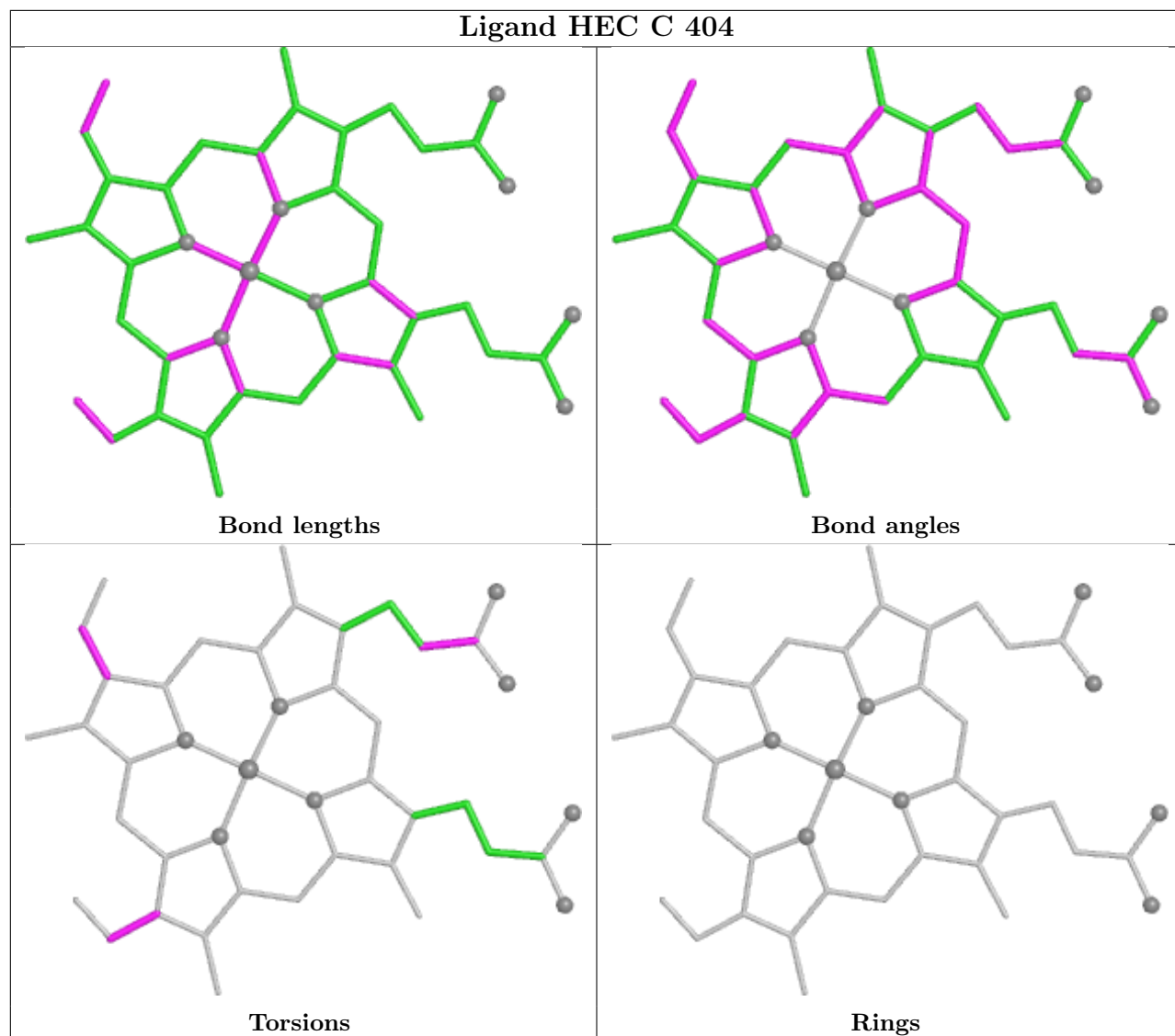
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

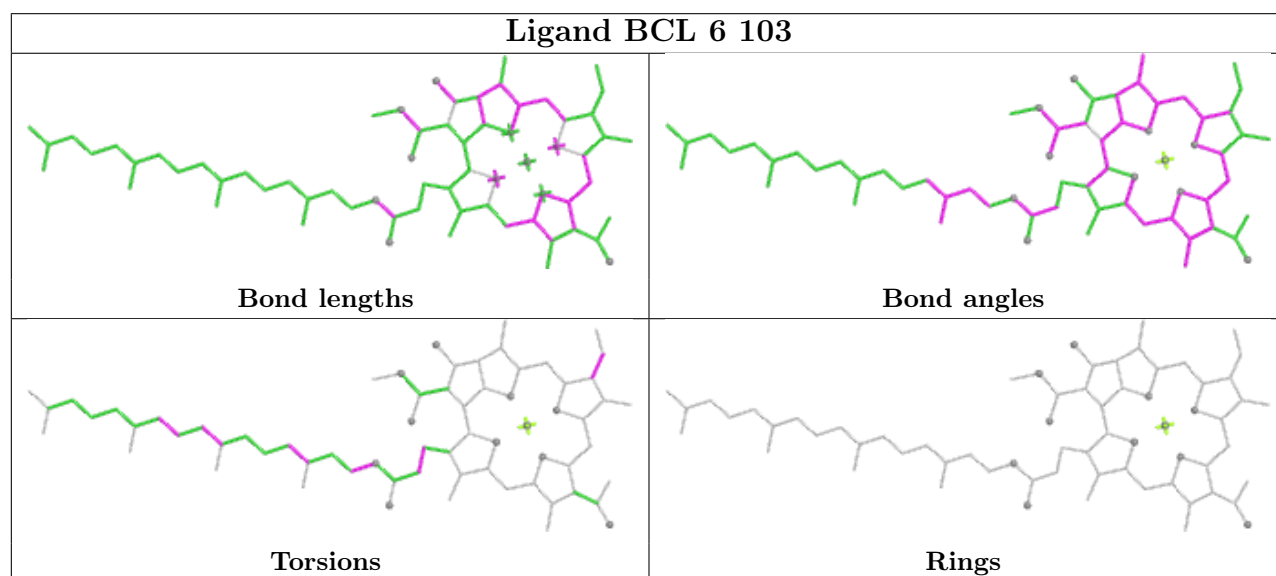
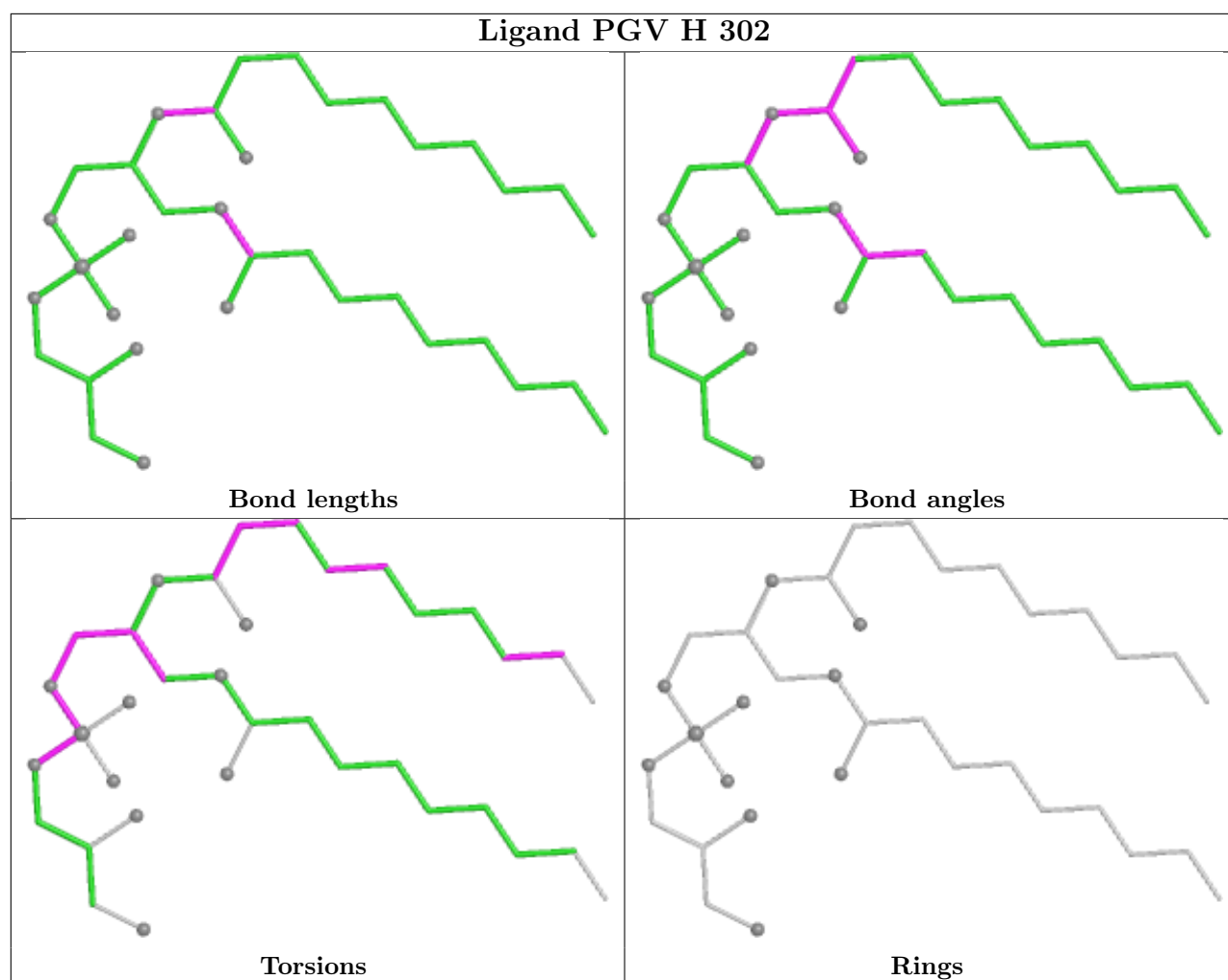


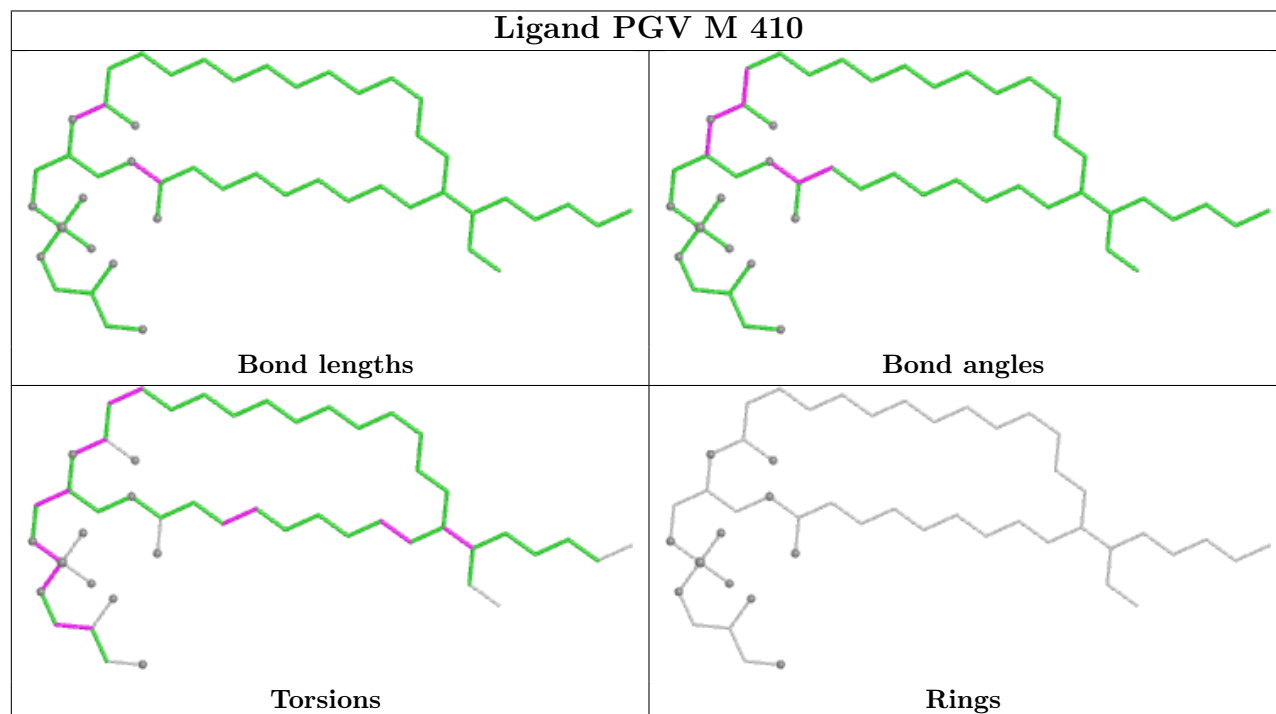
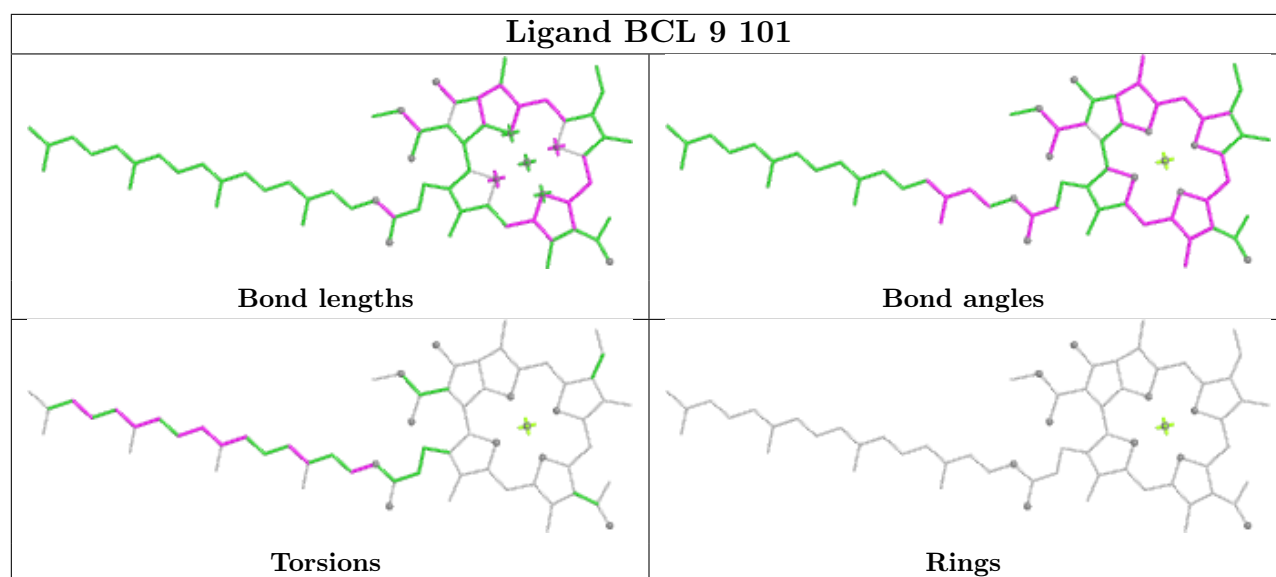


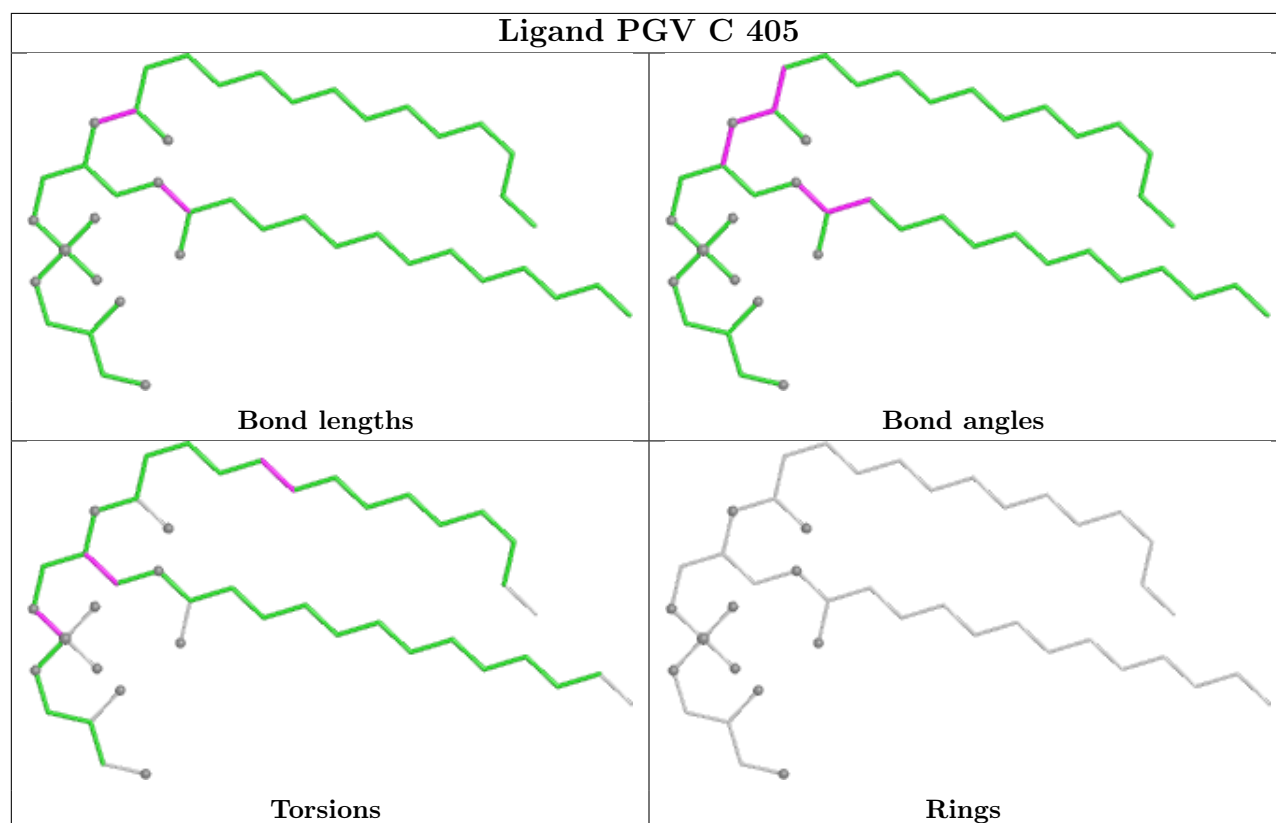
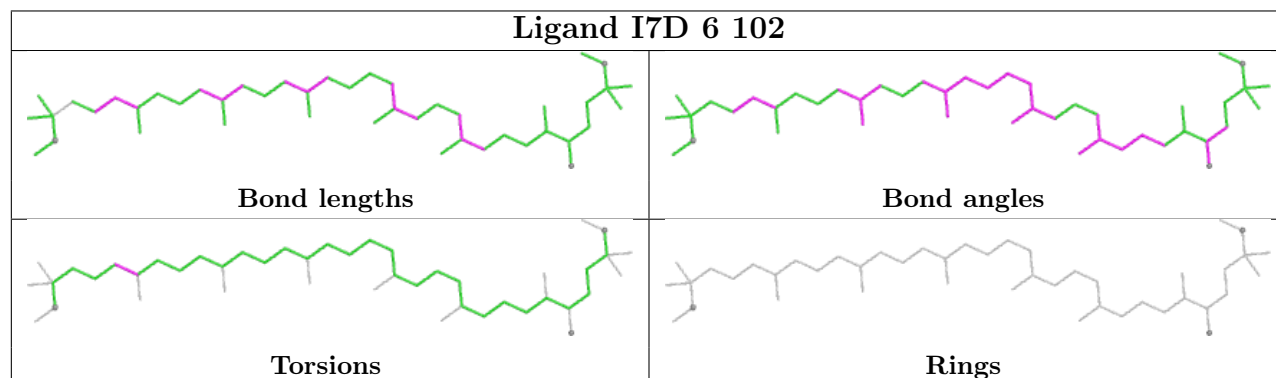
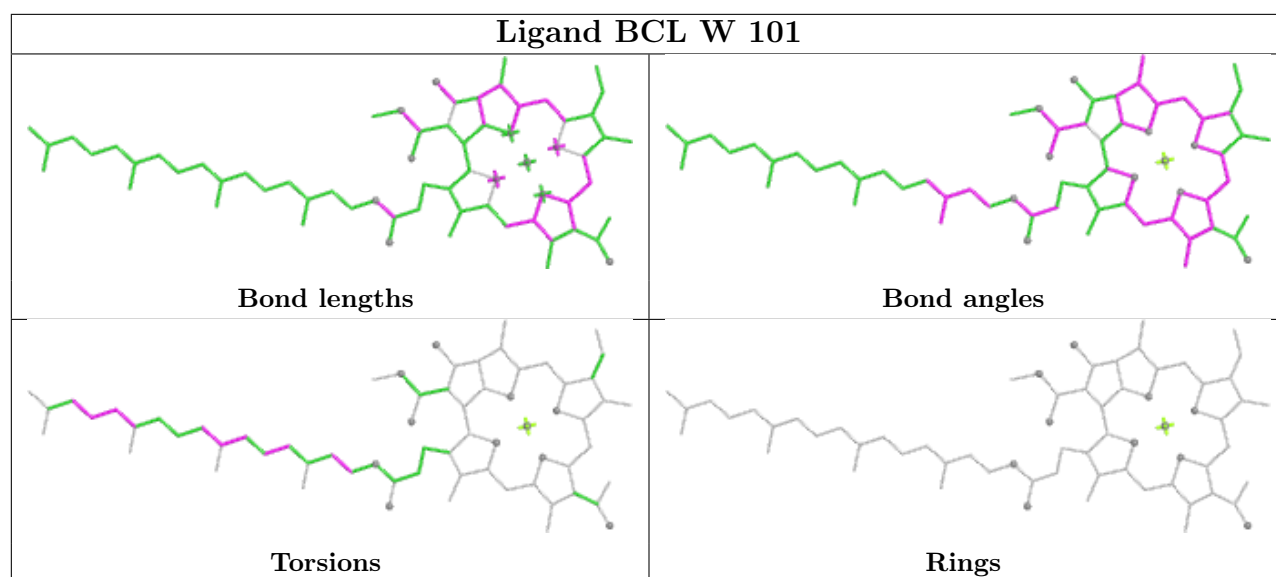


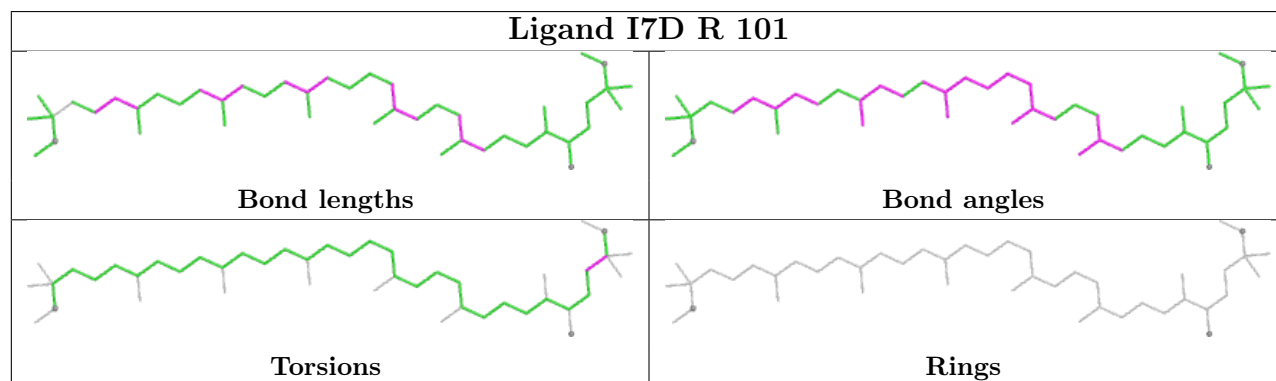
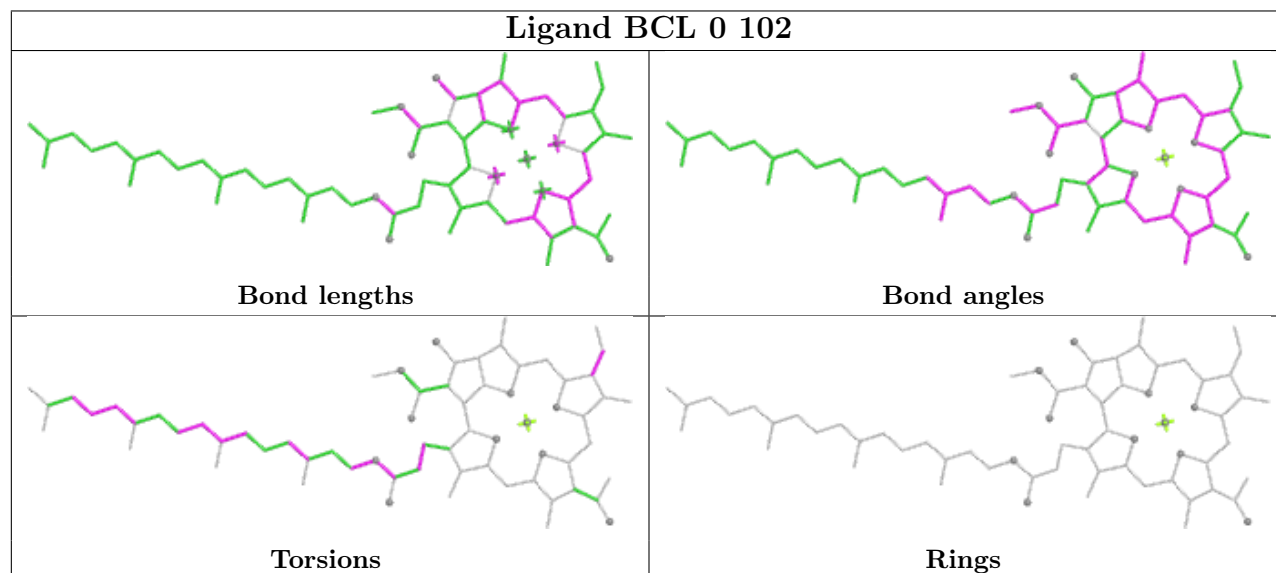
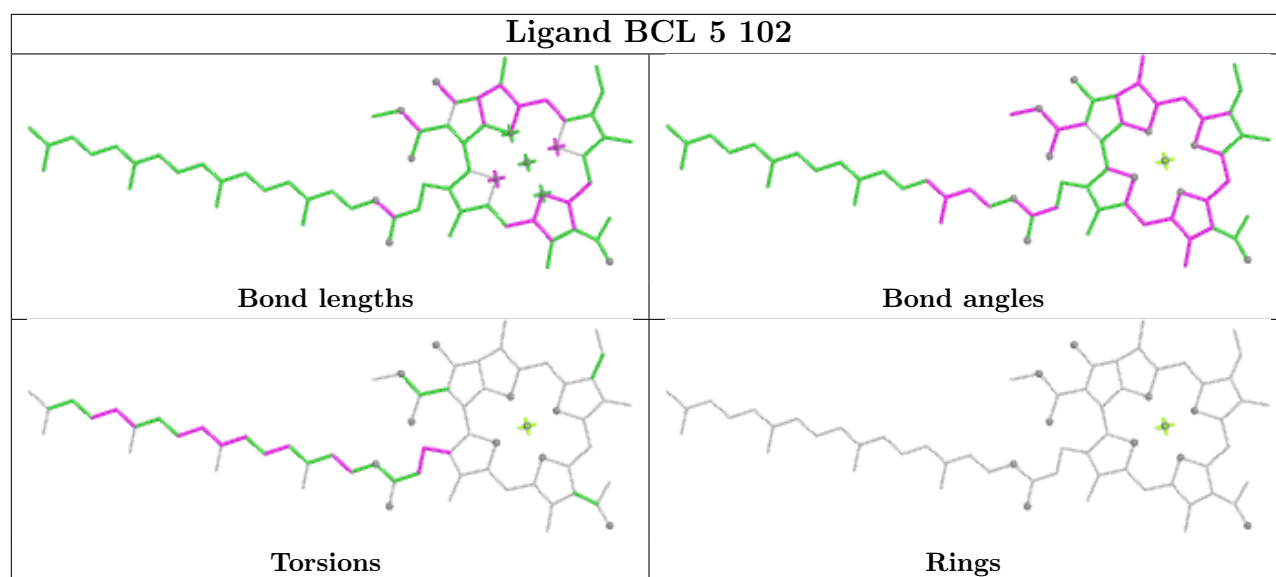


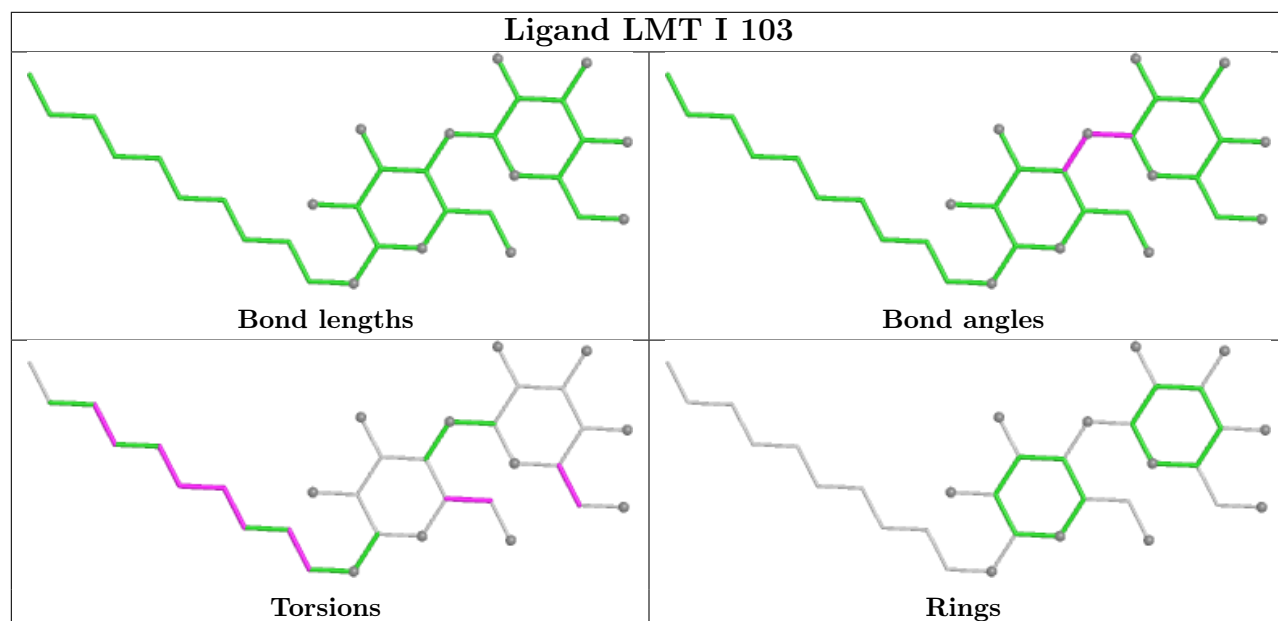
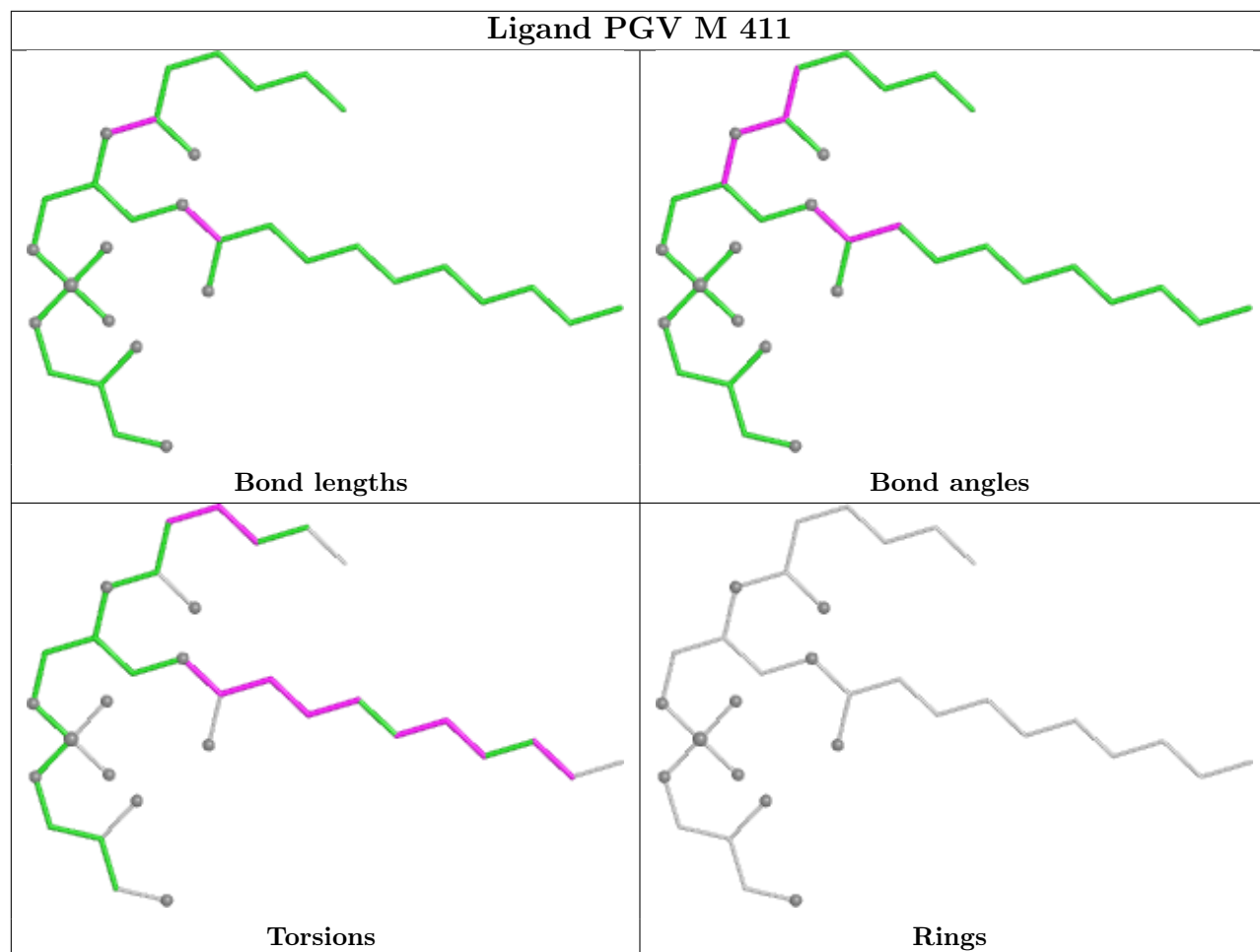


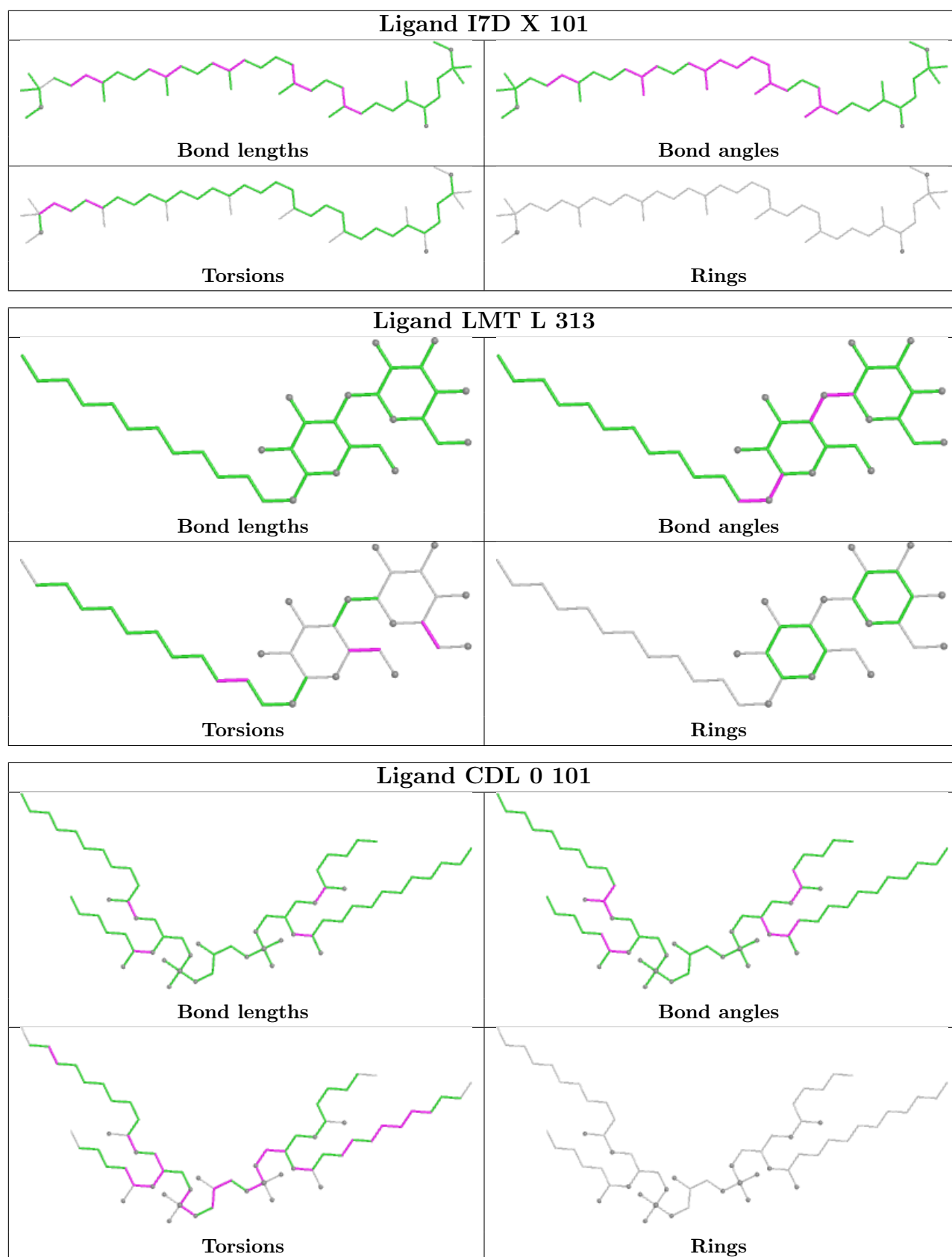


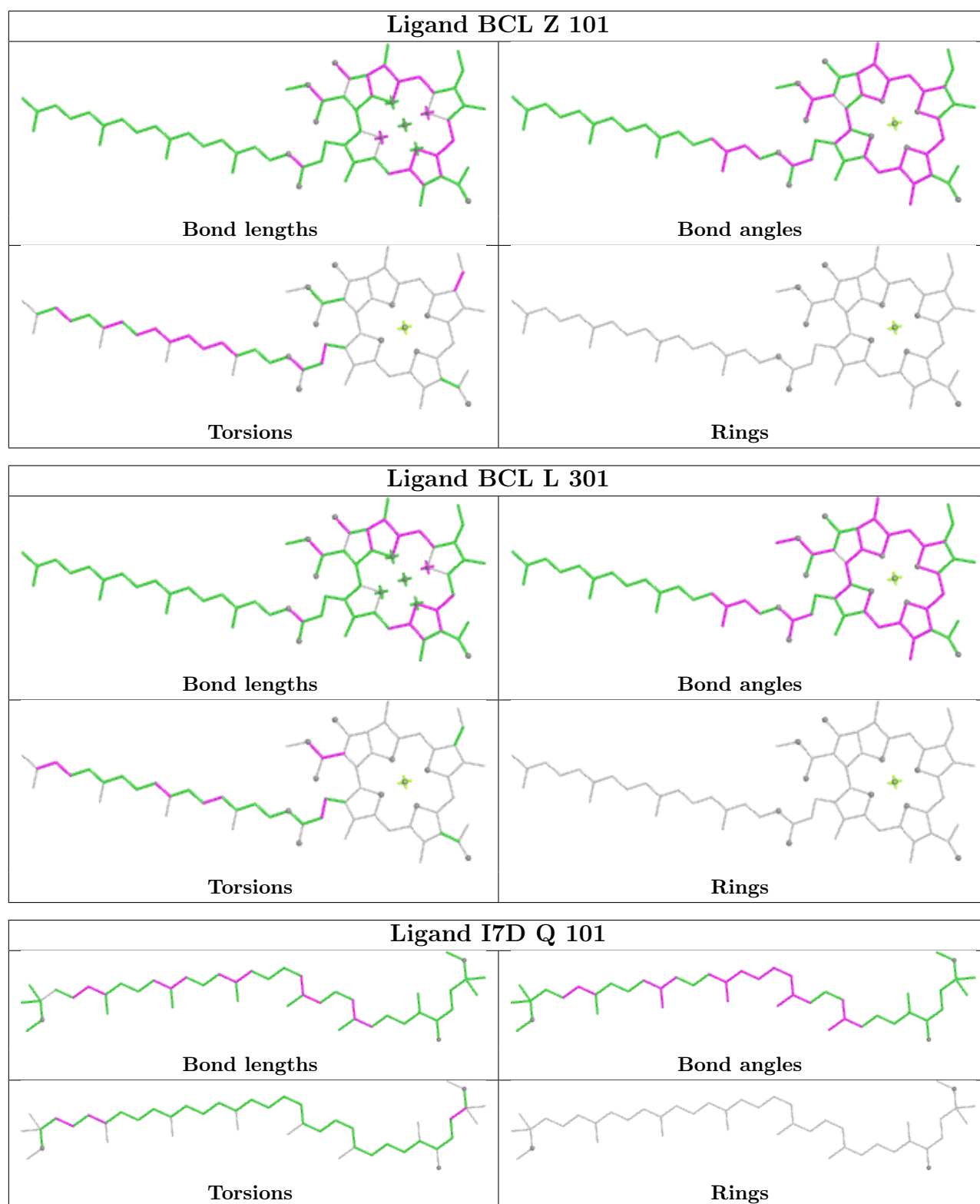


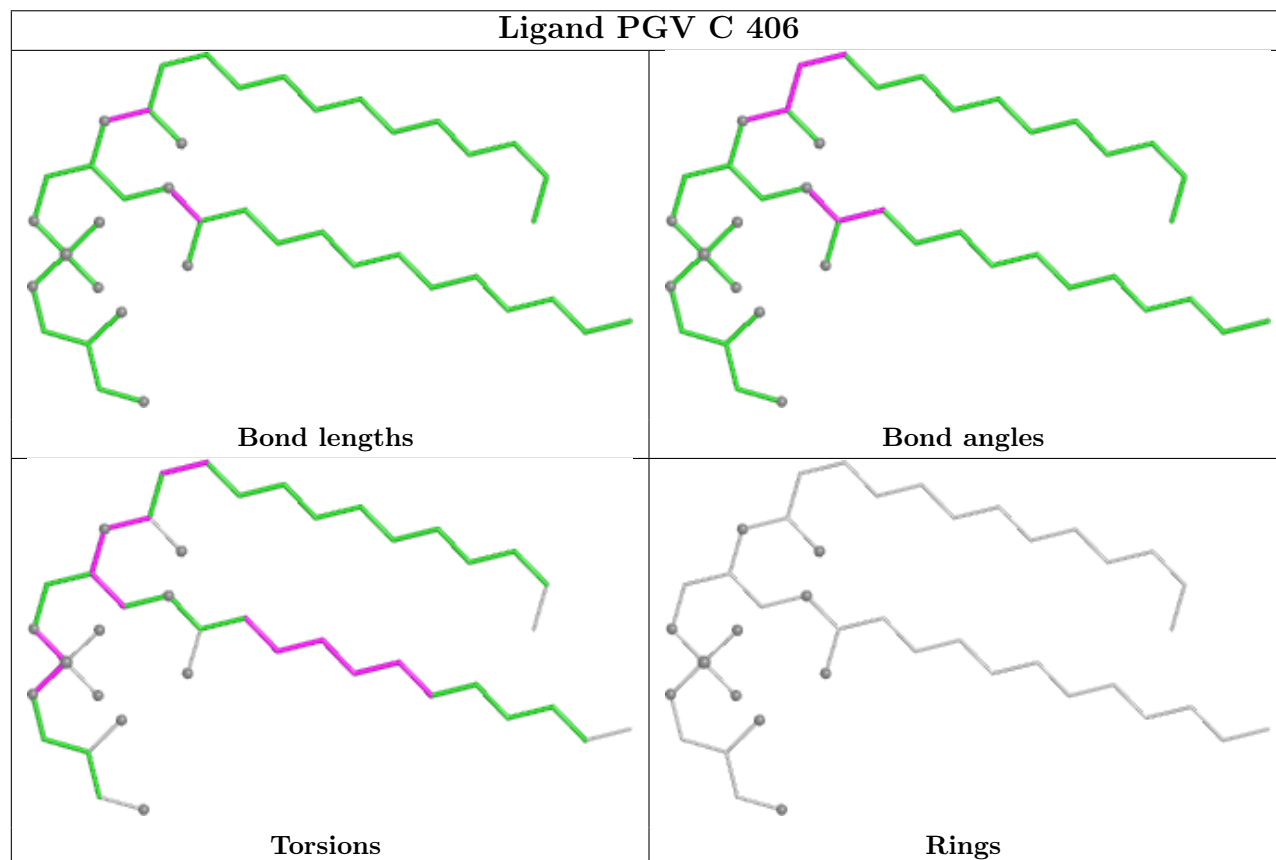
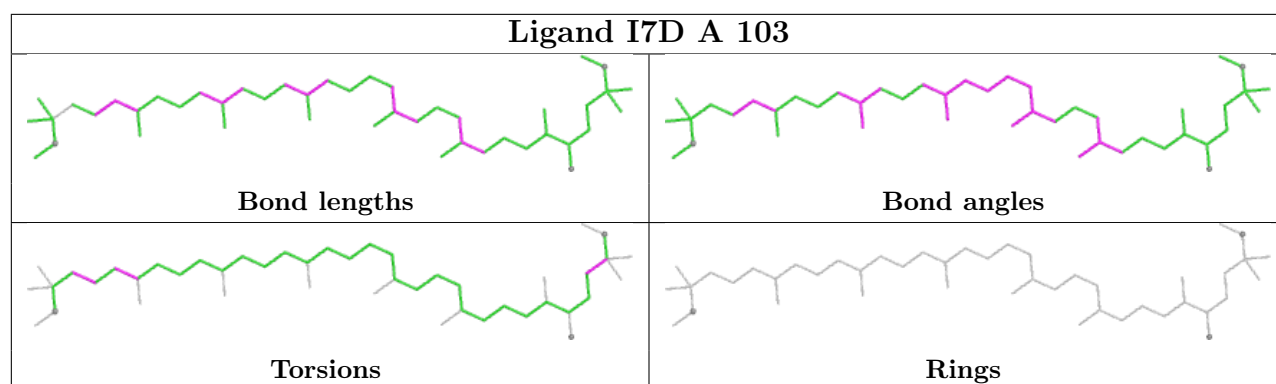


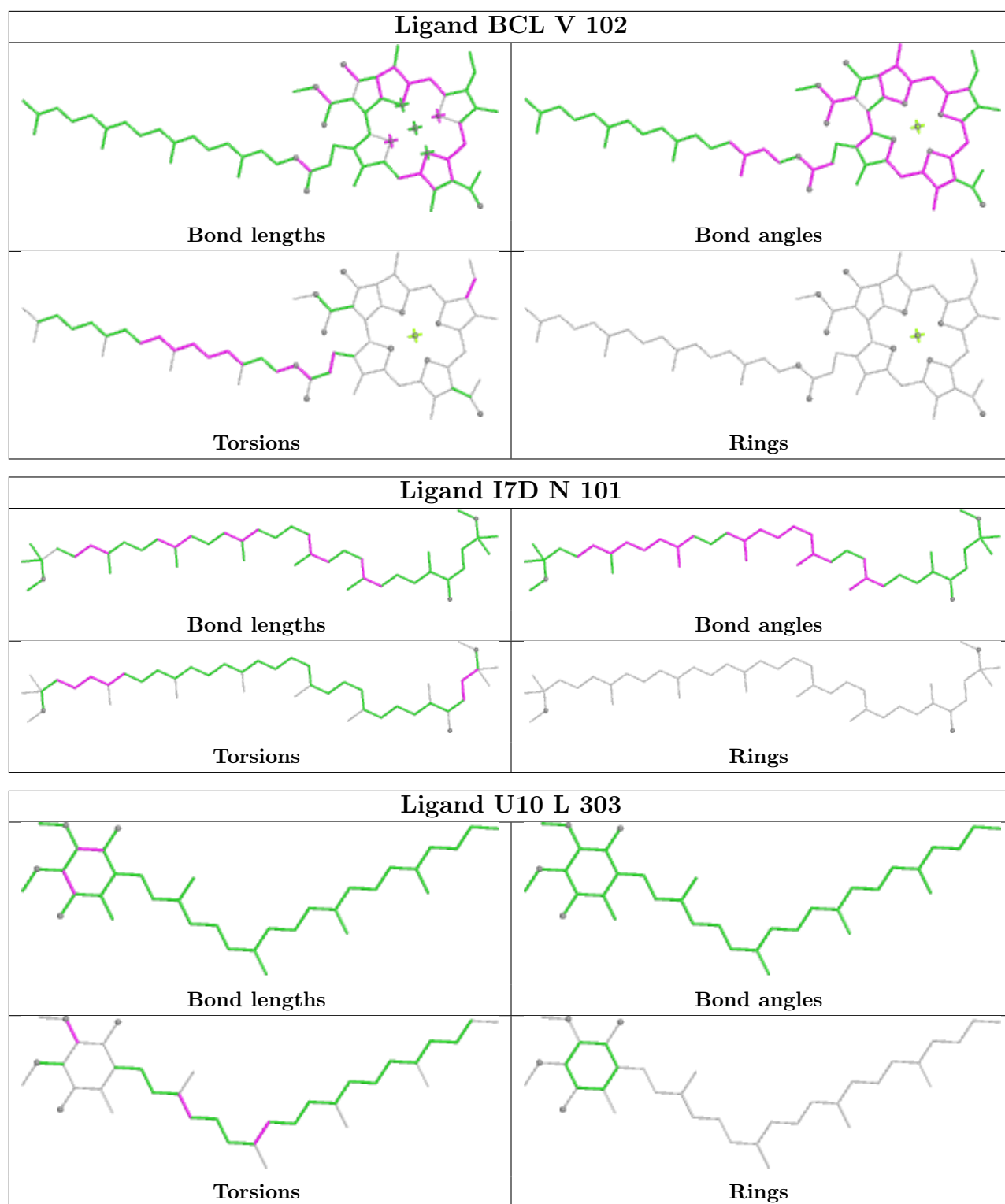


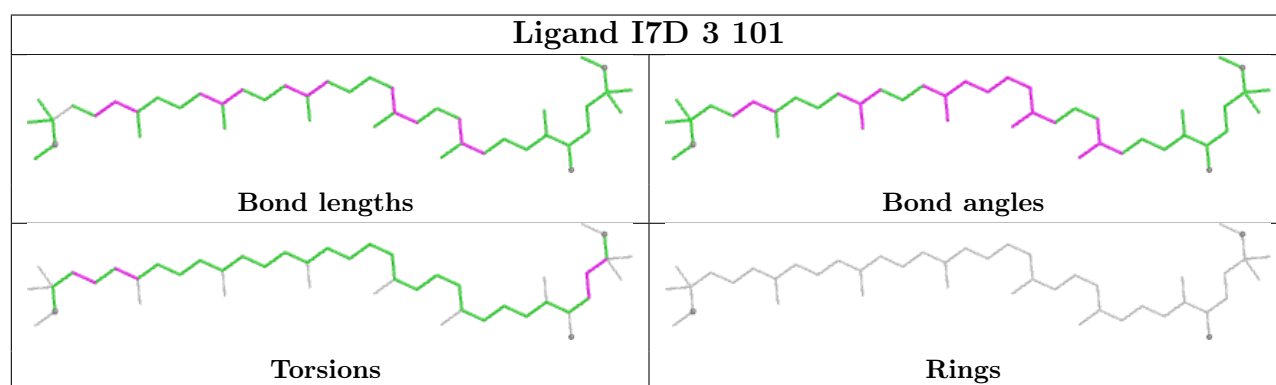
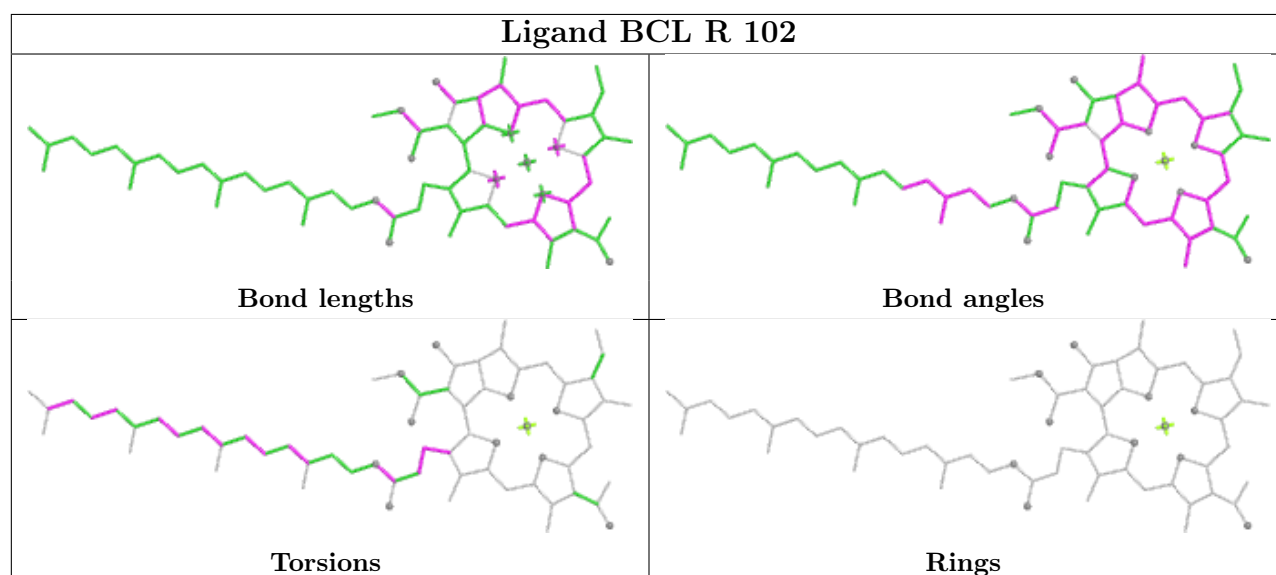
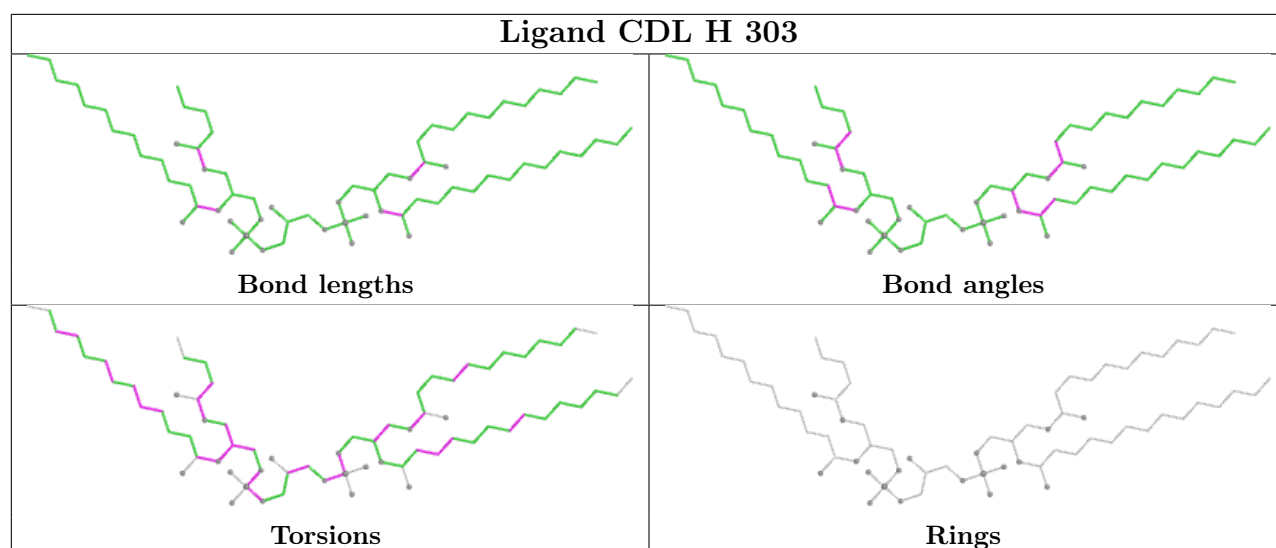


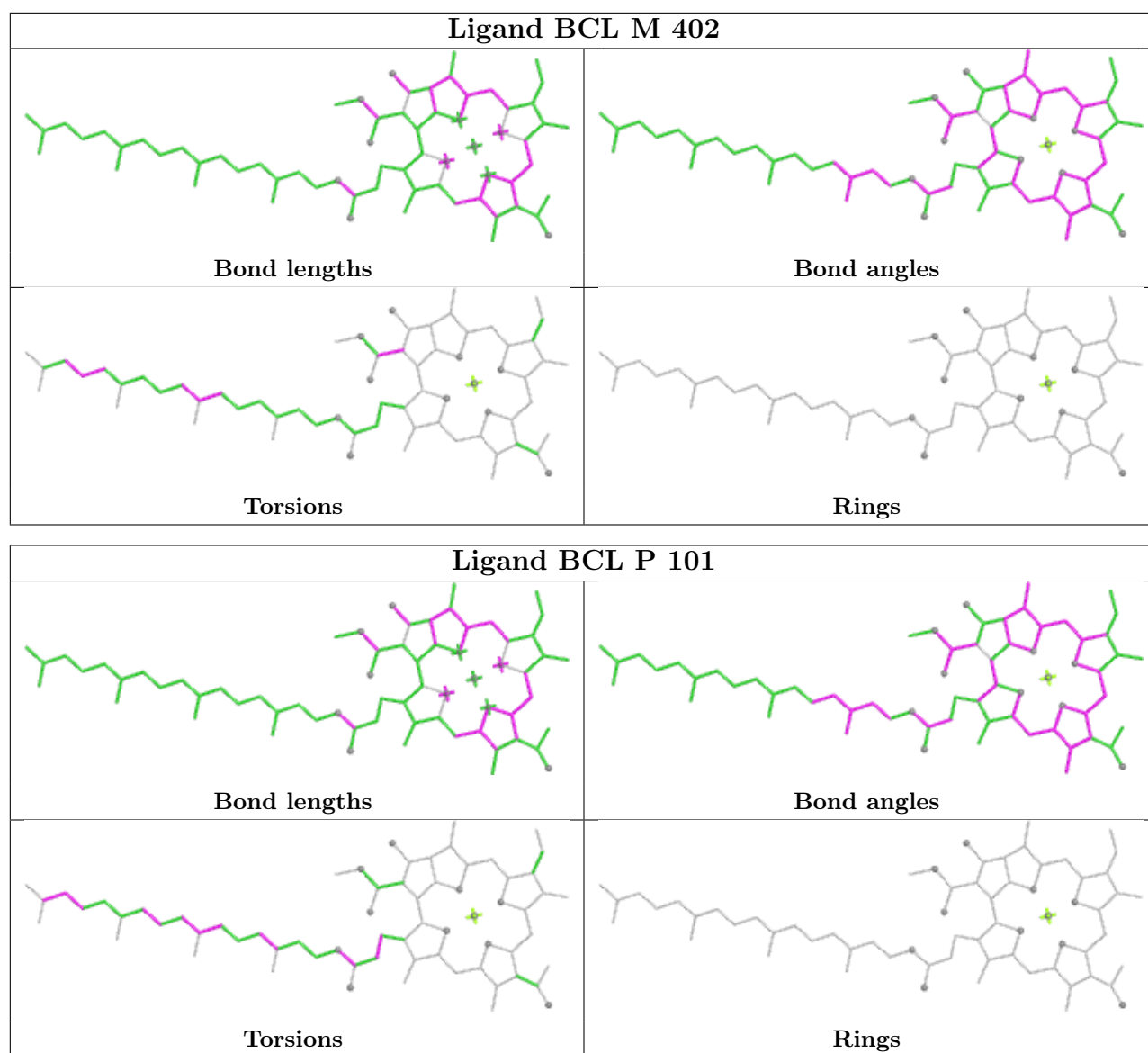


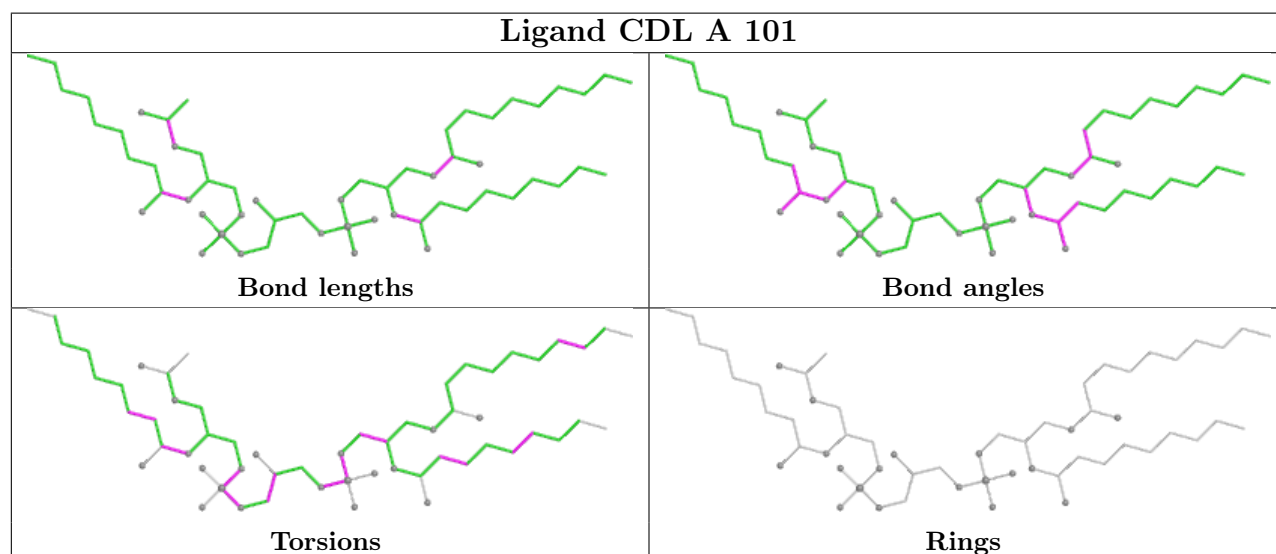
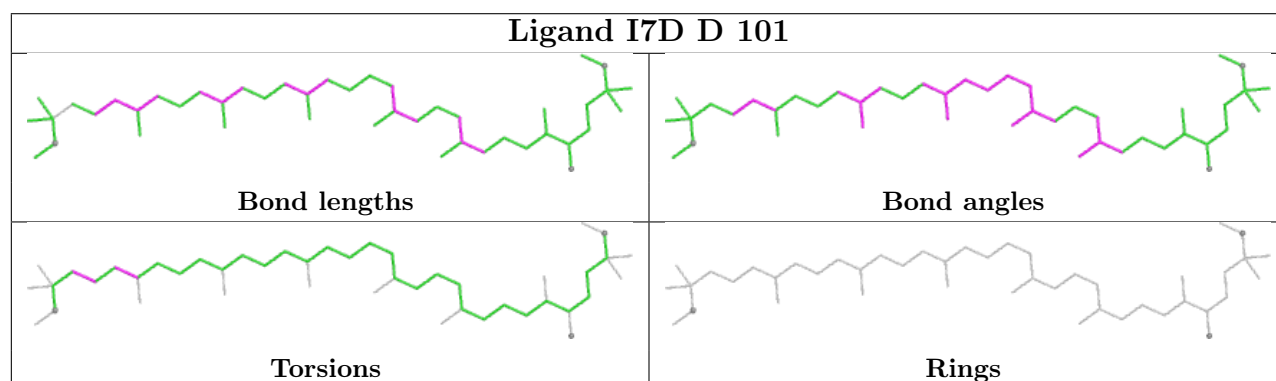
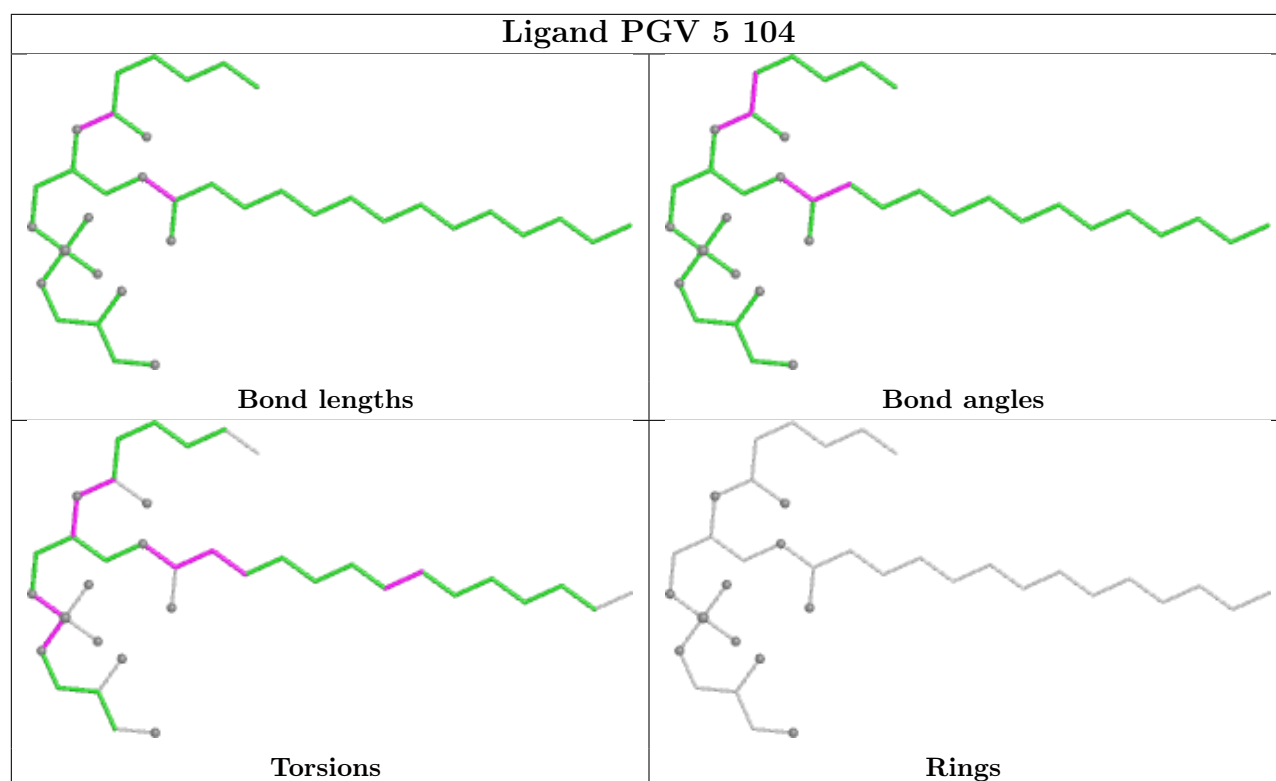


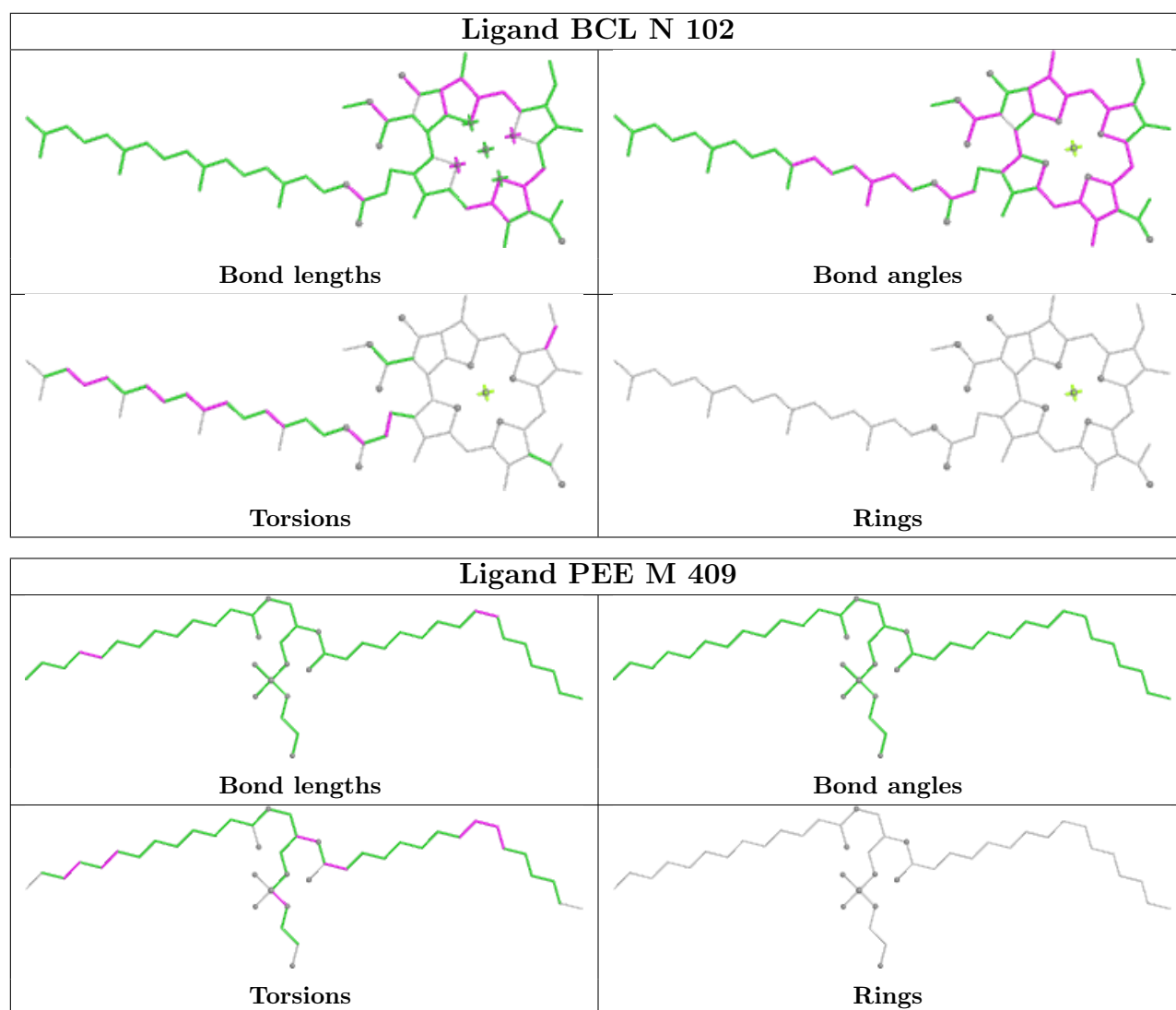


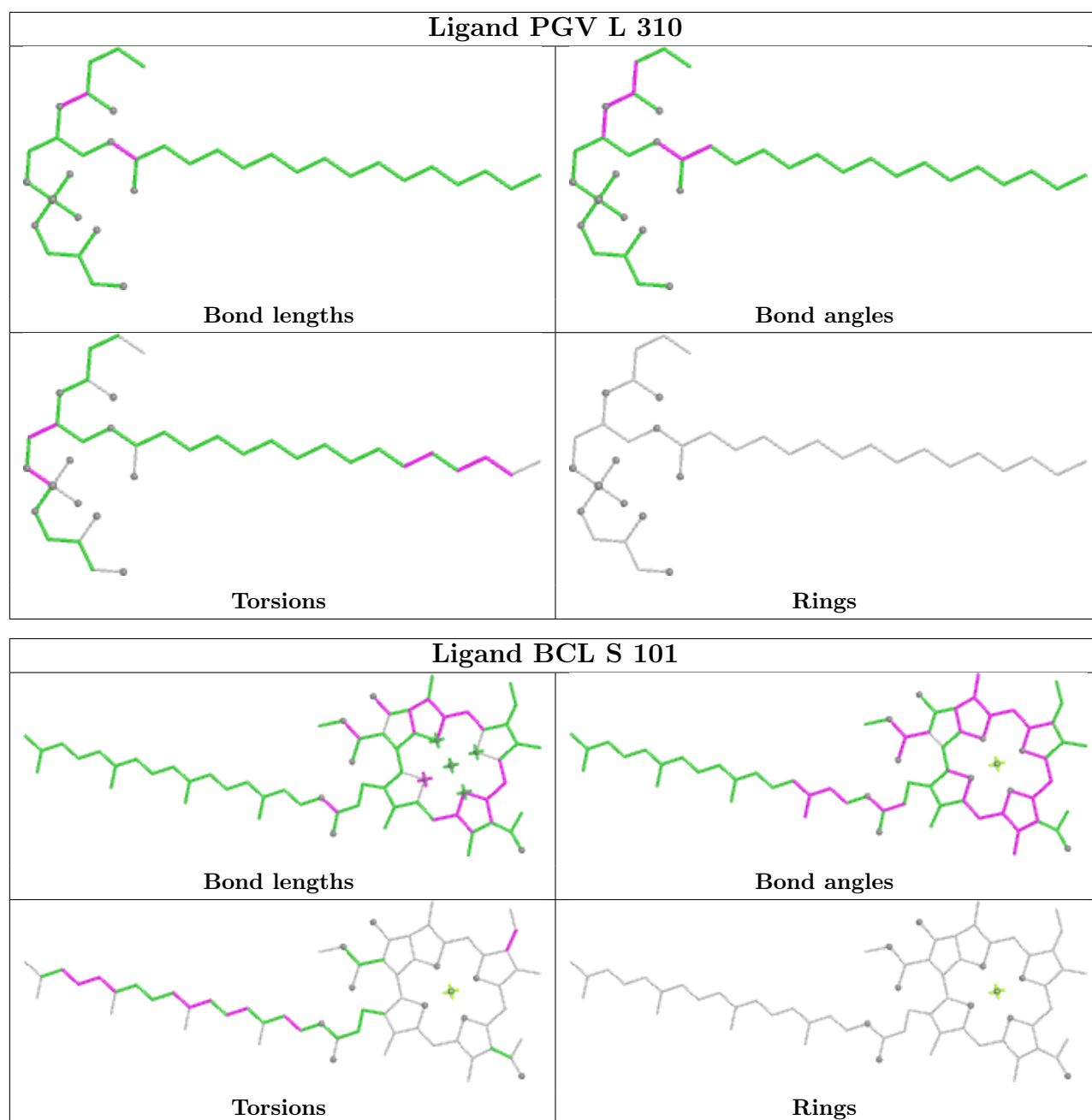


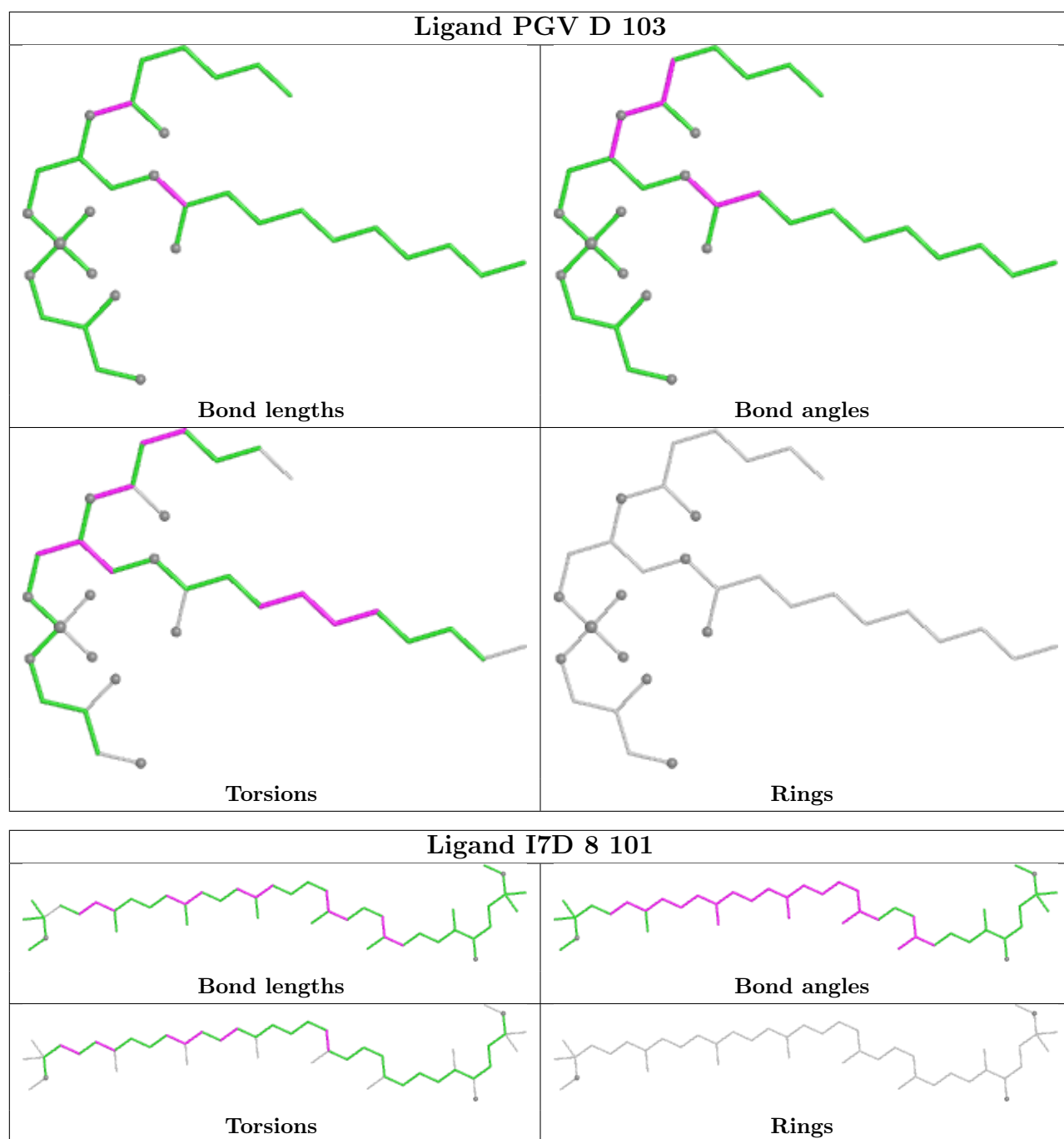


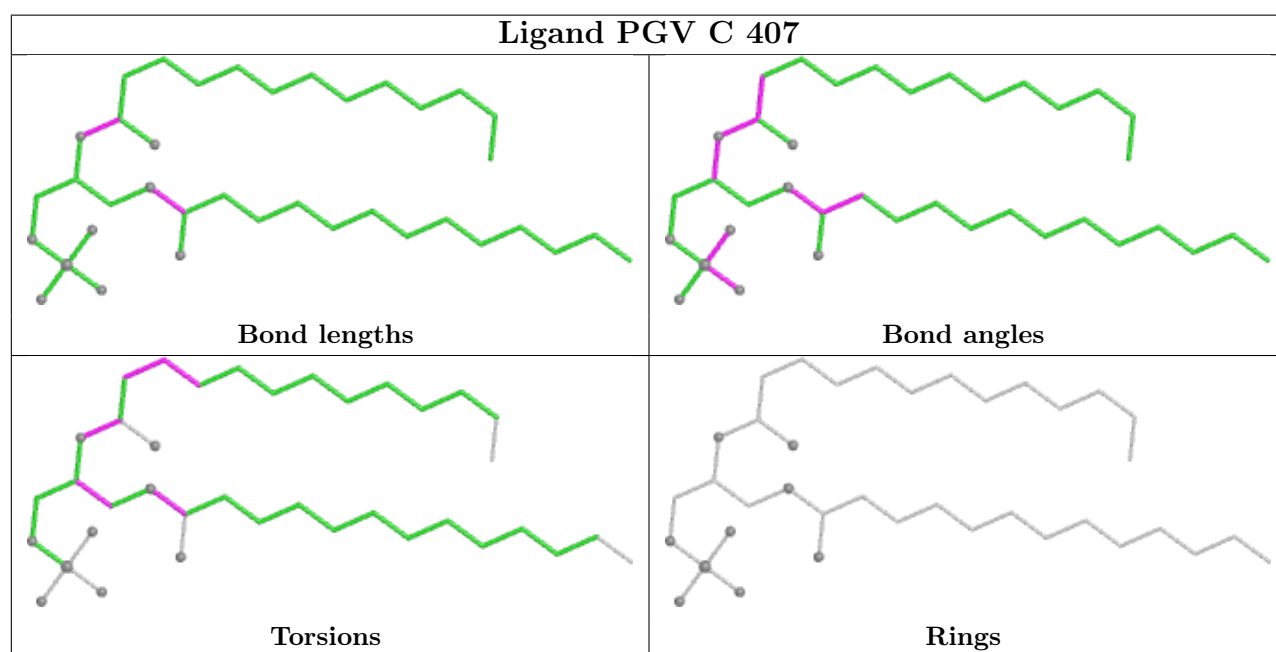
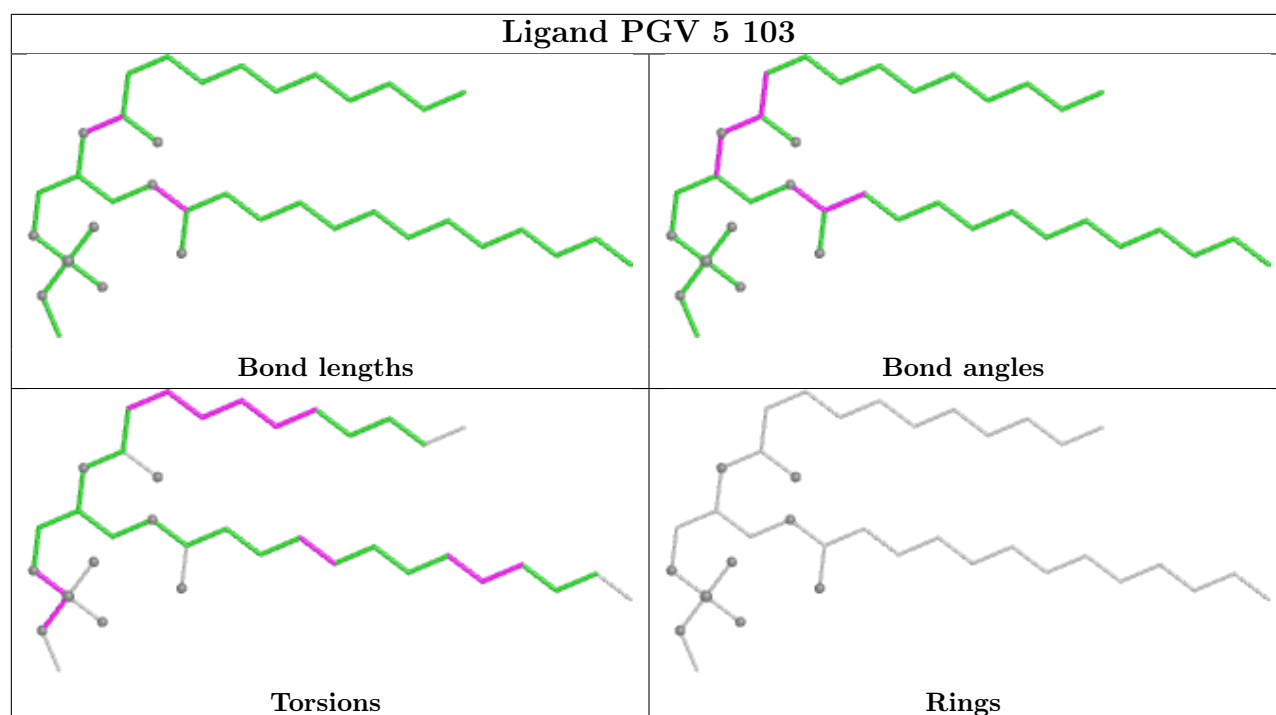


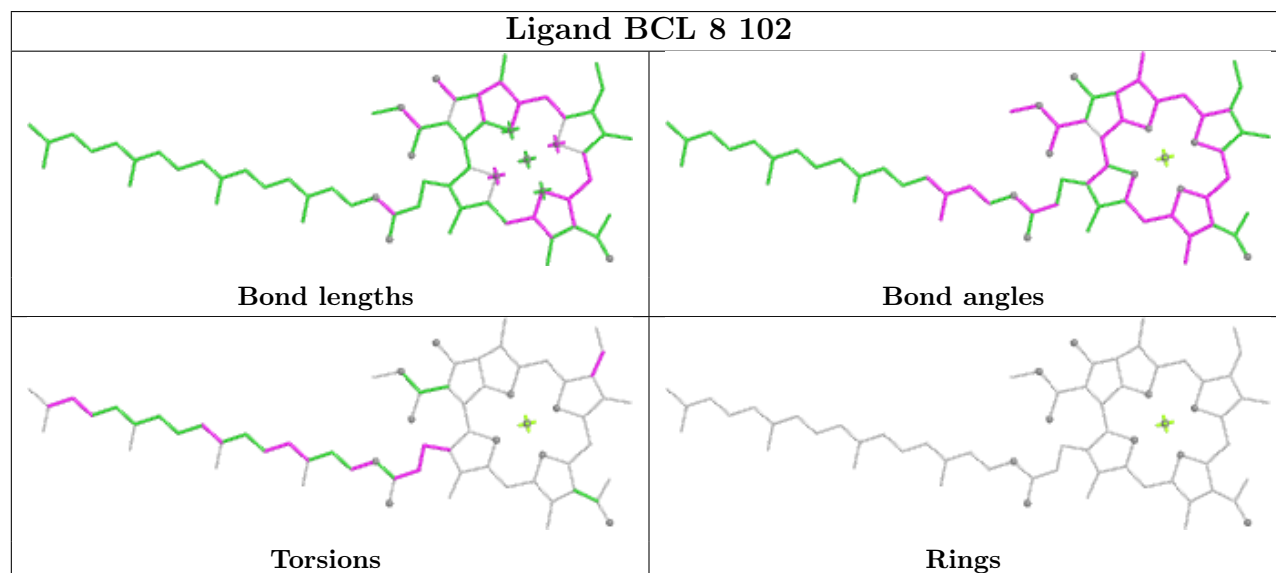
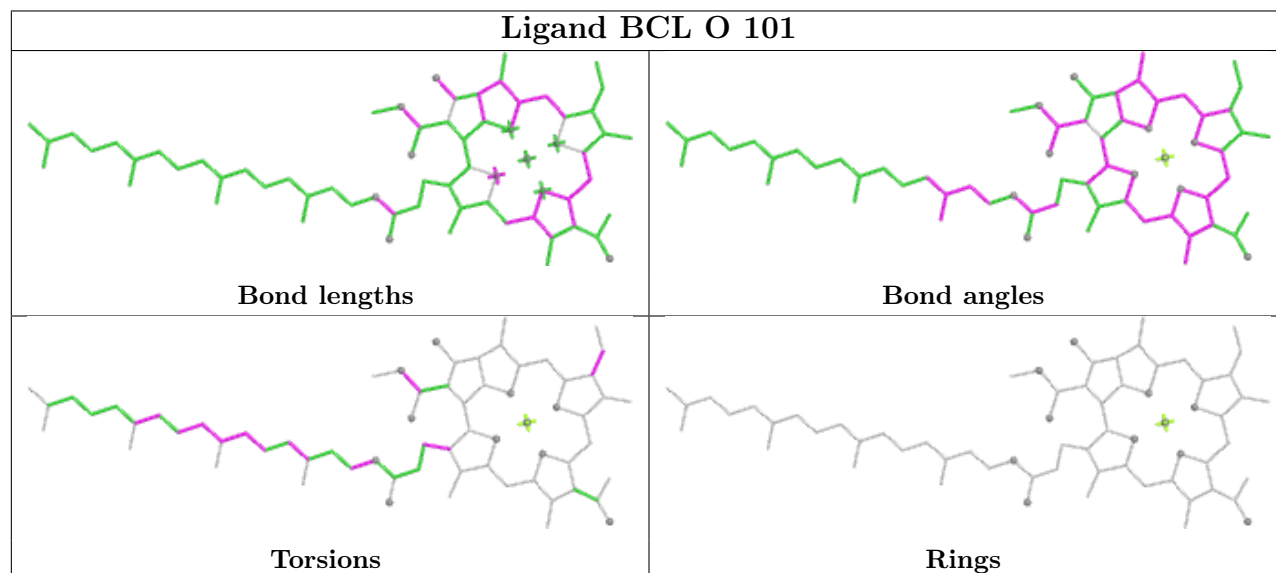
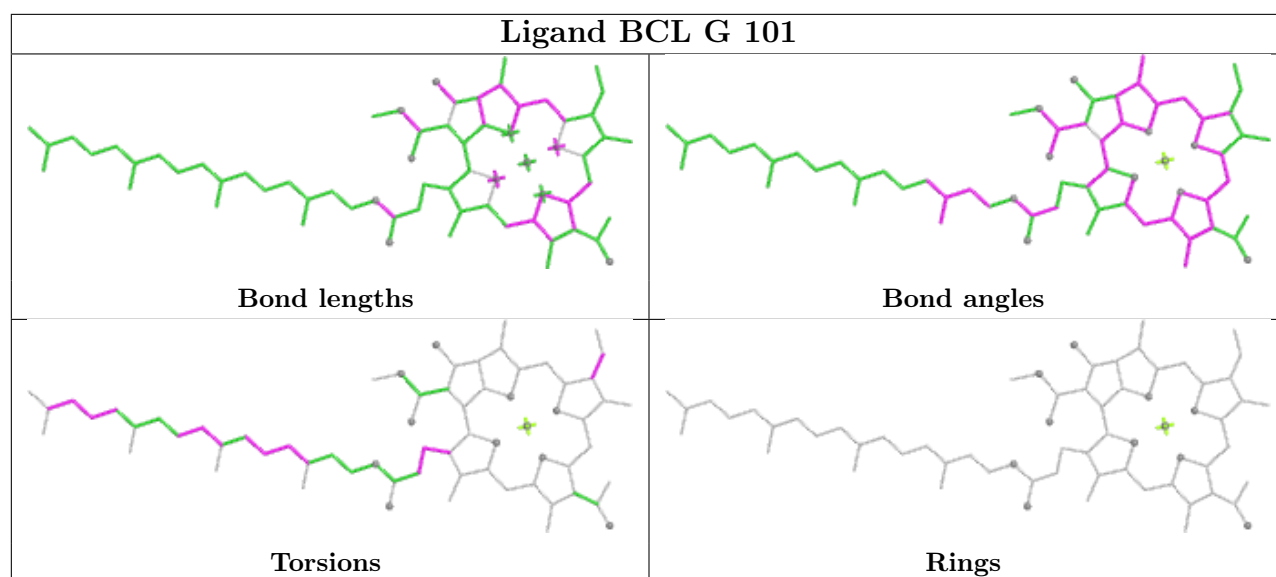


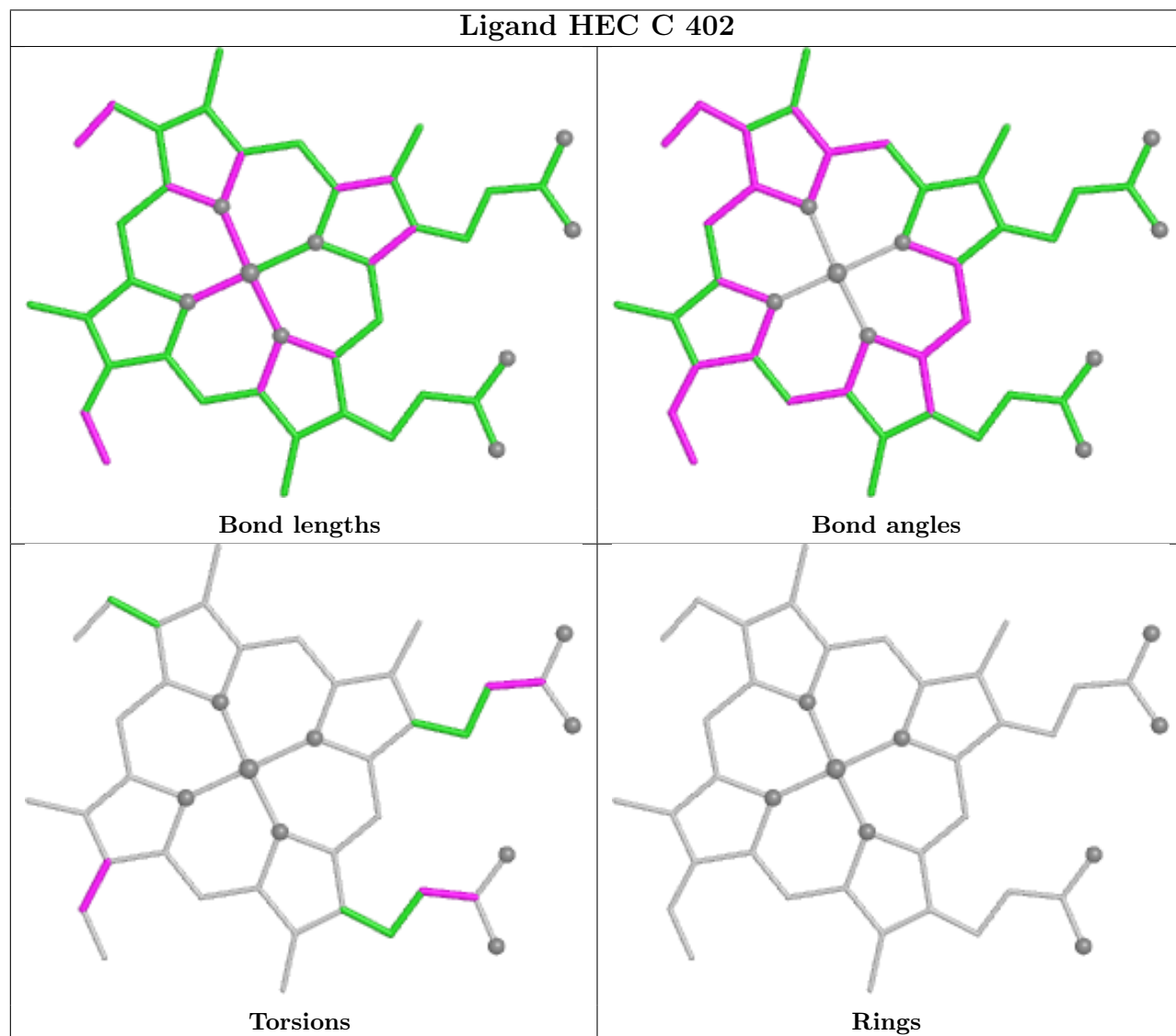
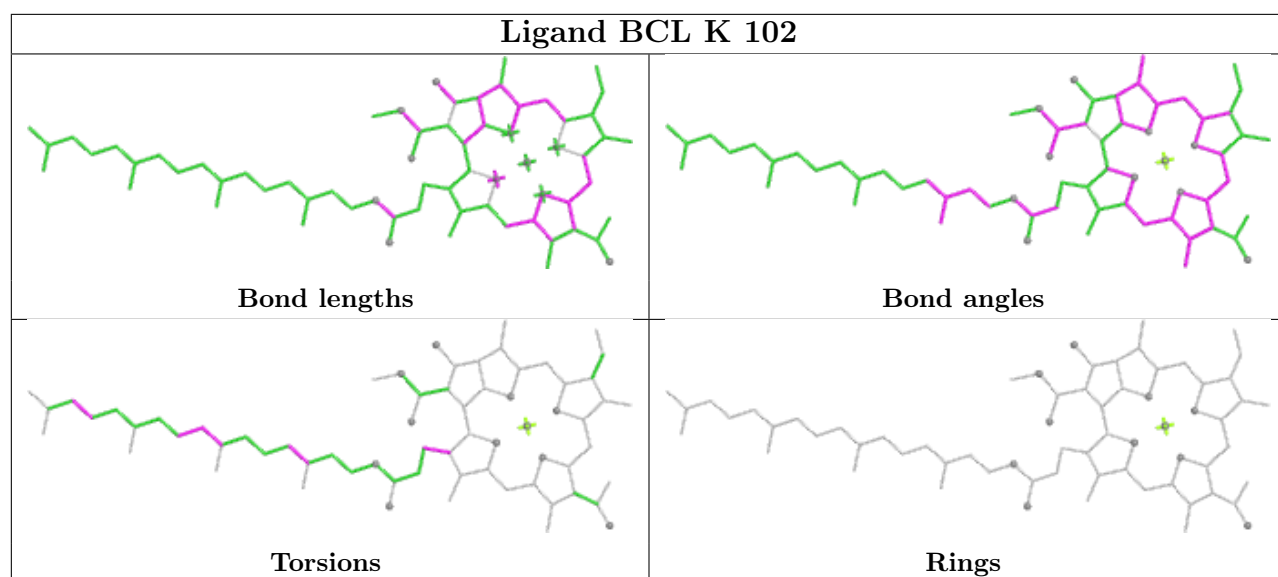


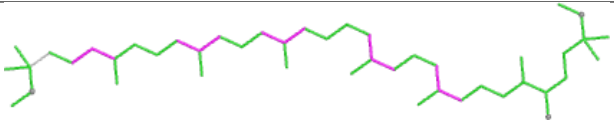
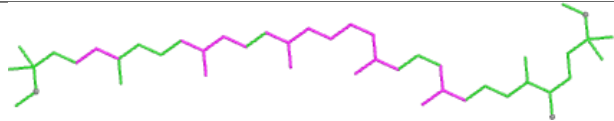
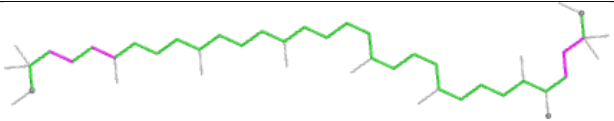
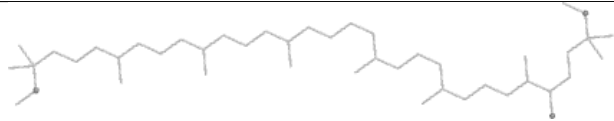


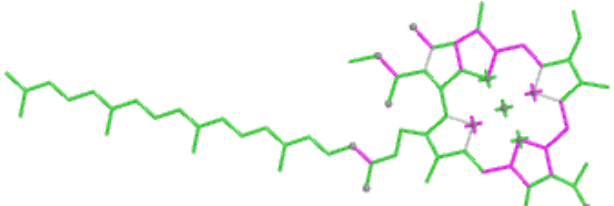
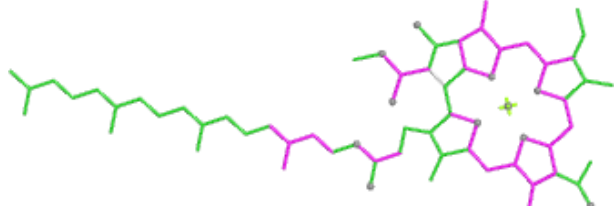
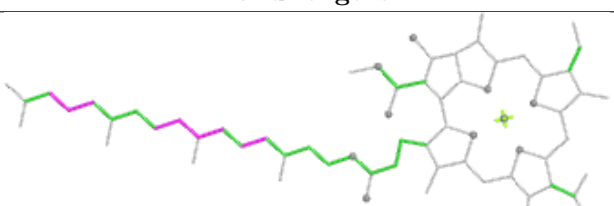
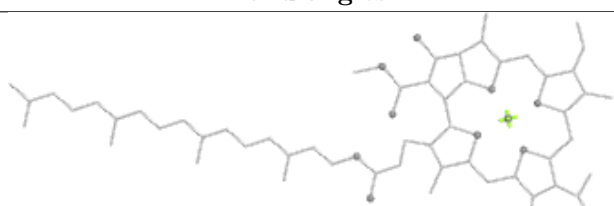


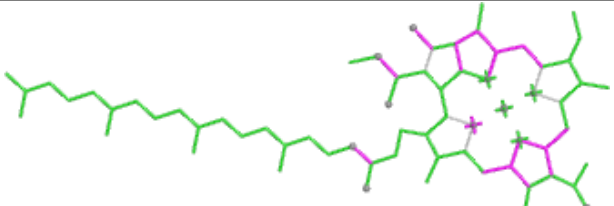
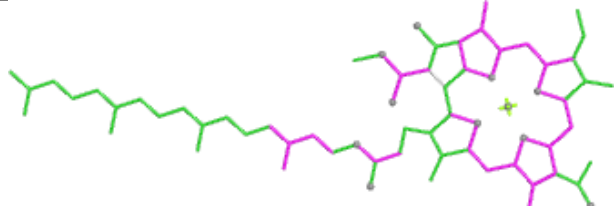
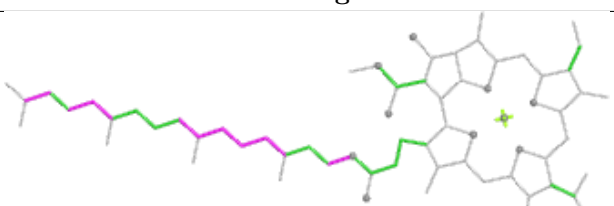
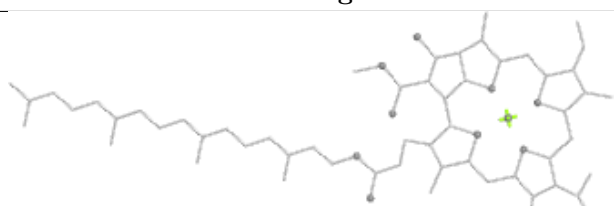


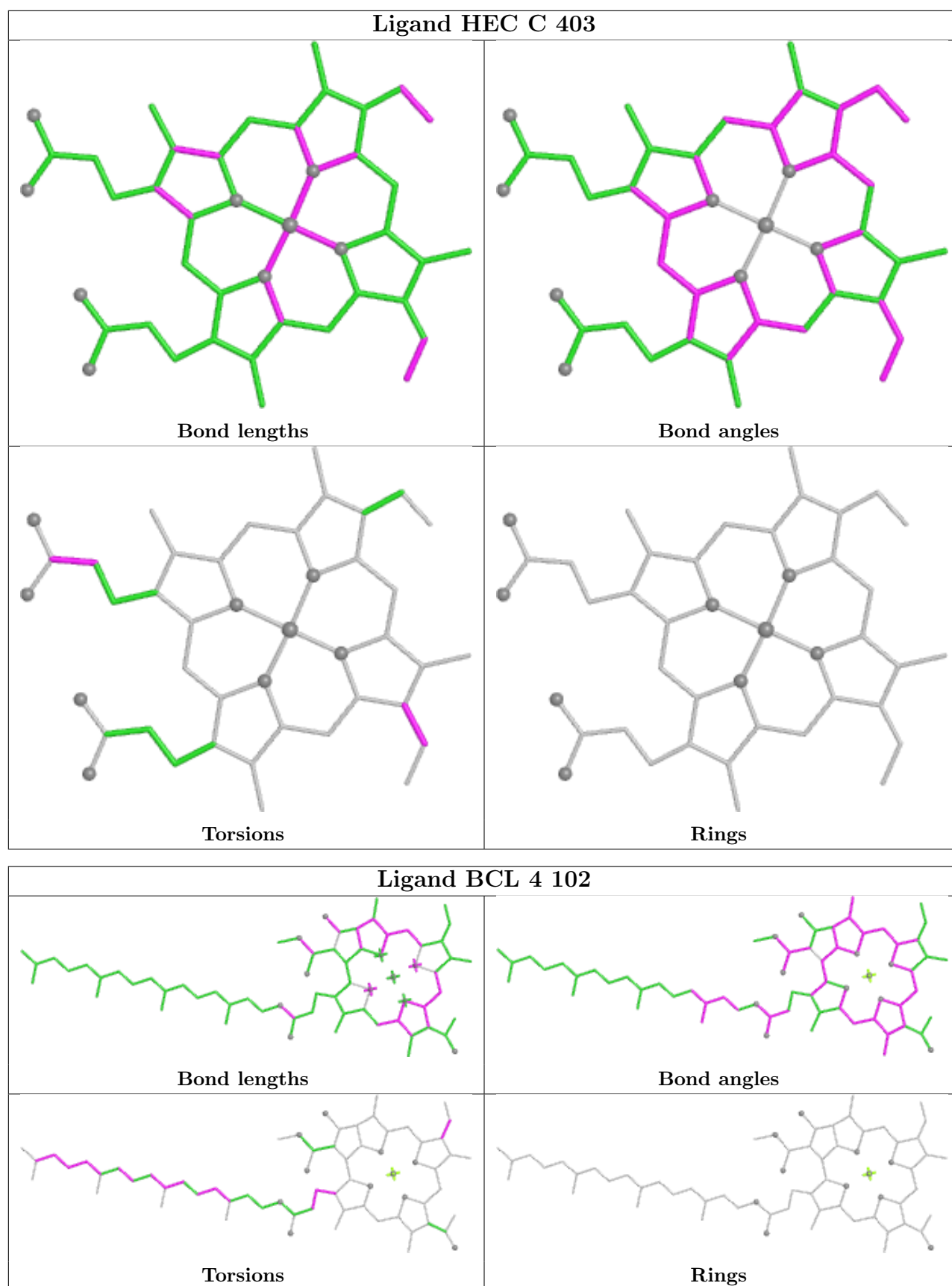


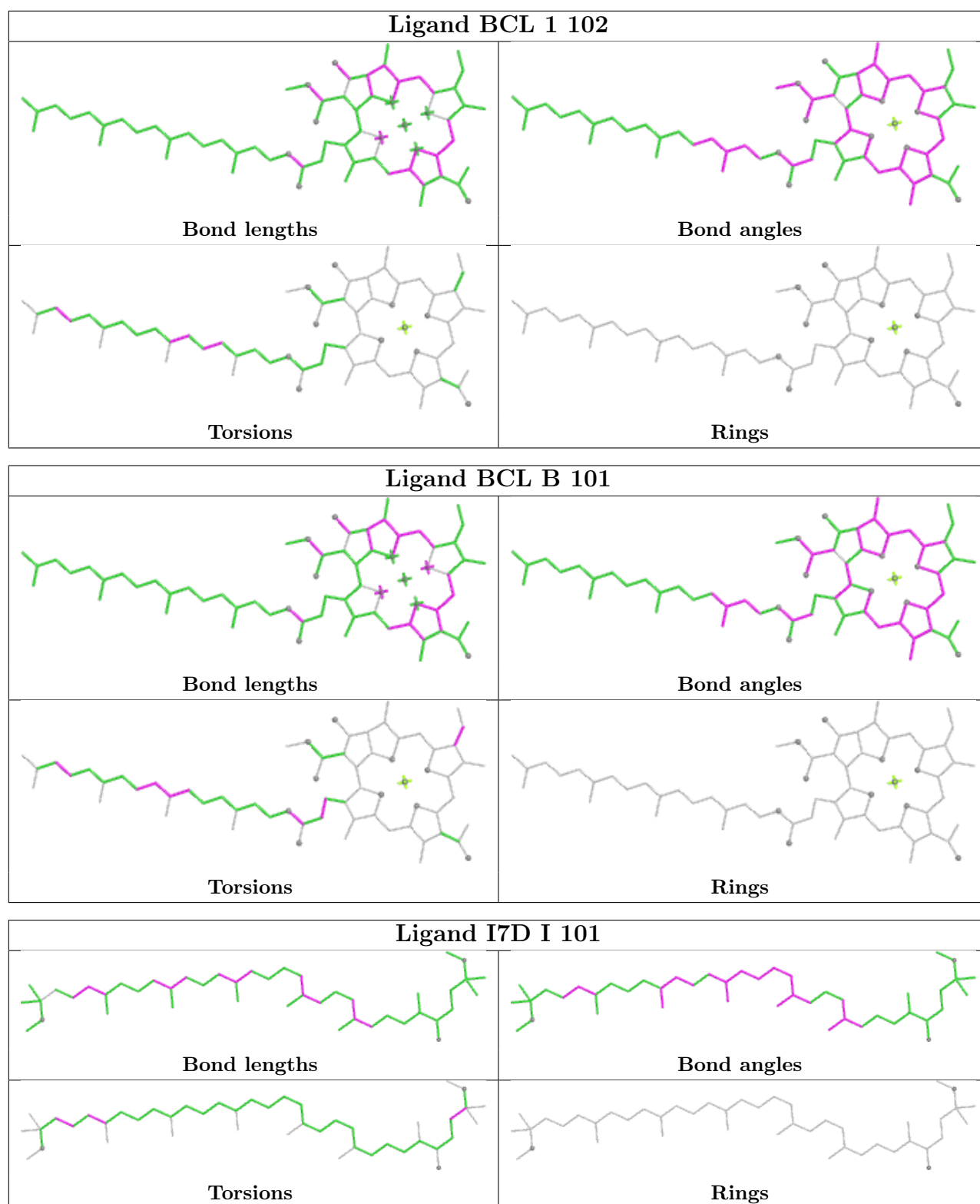


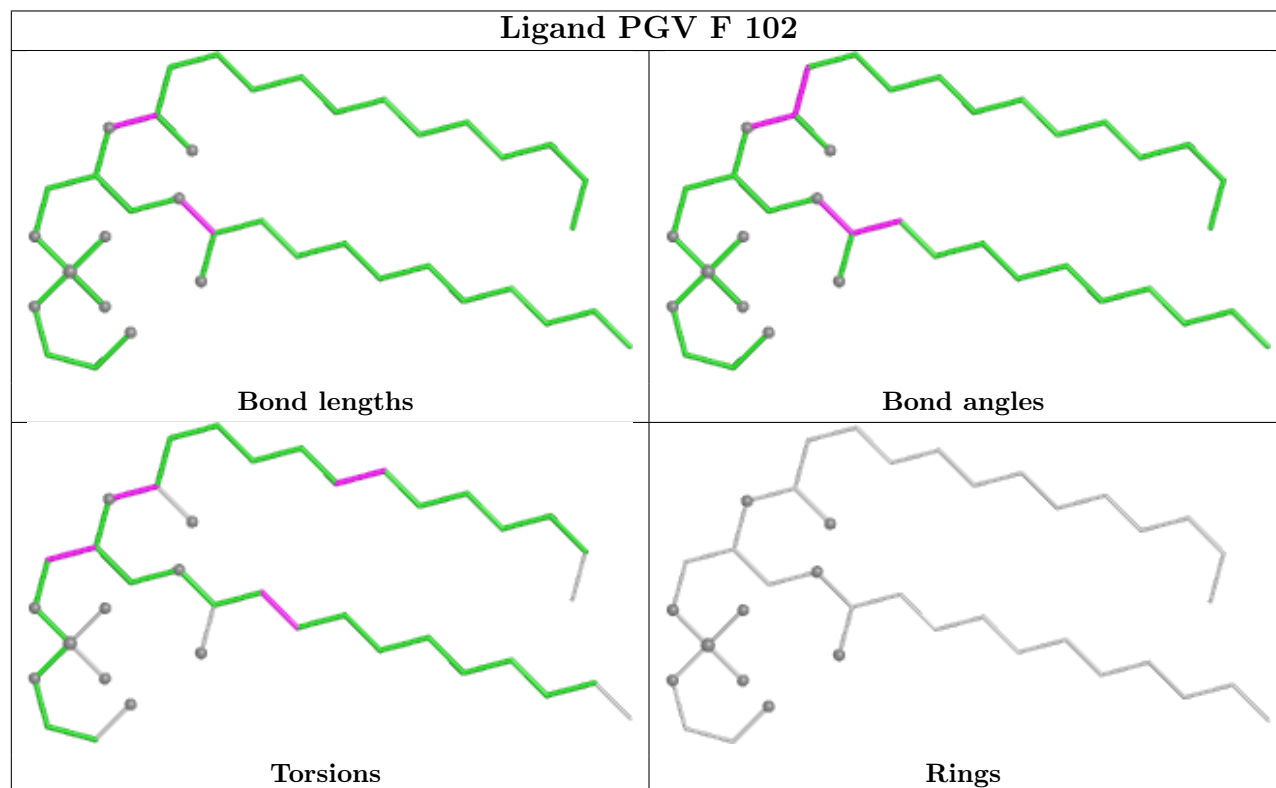
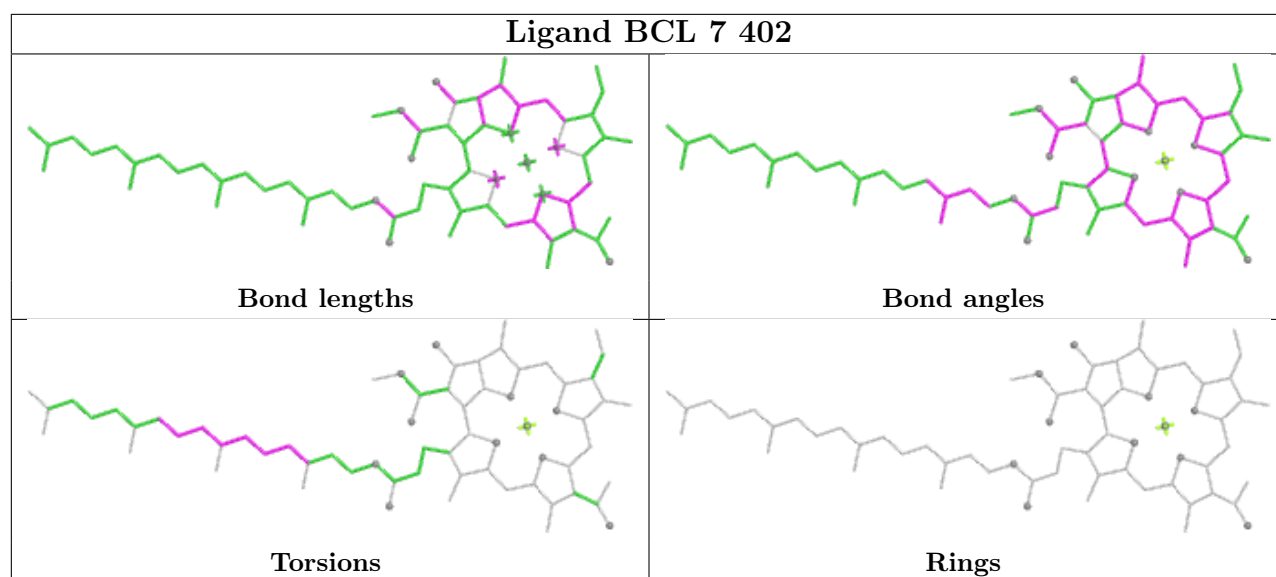
Ligand I7D 4 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

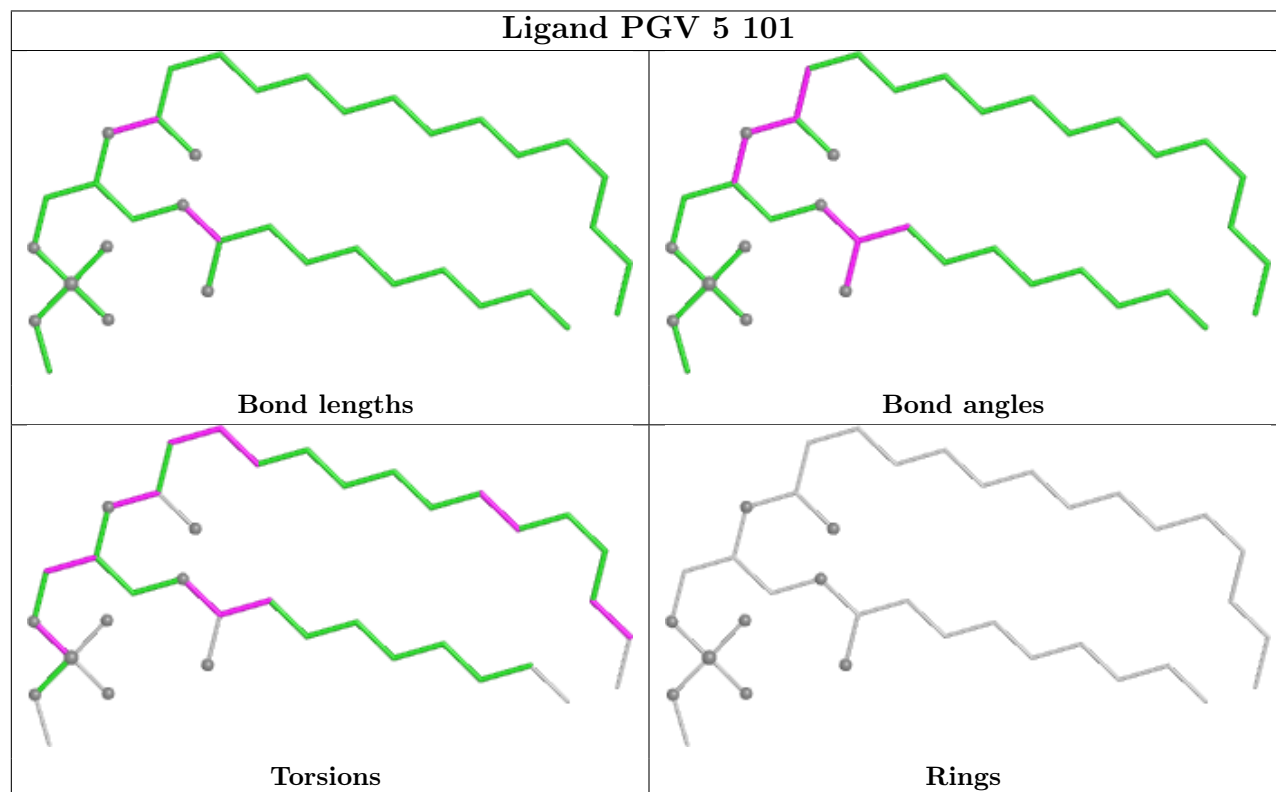
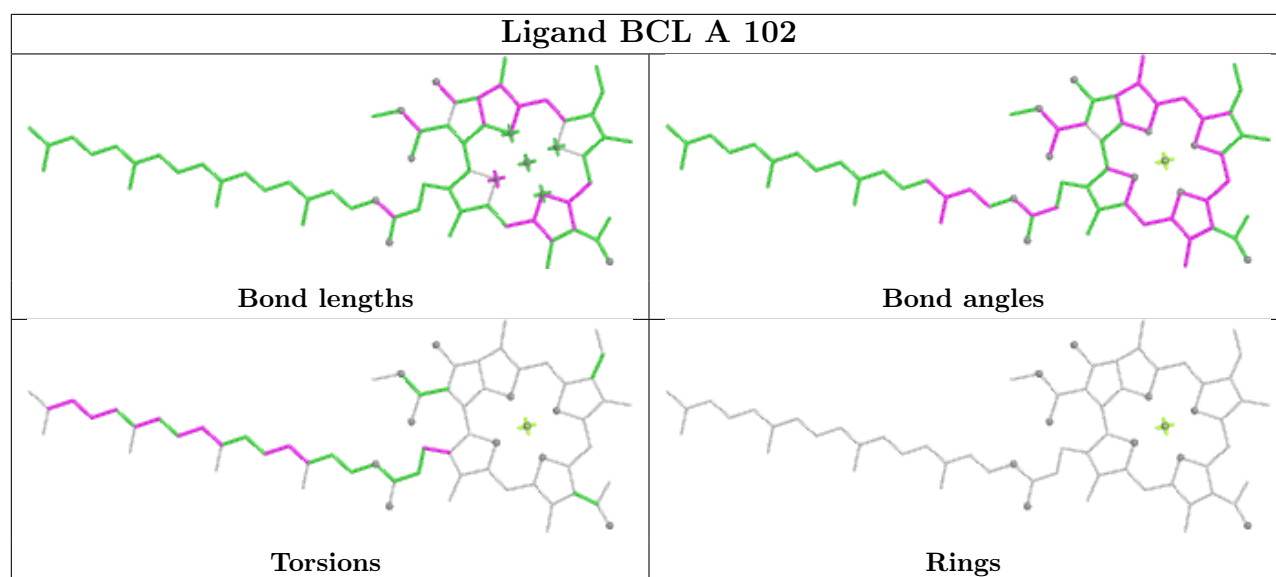
Ligand BCL Q 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

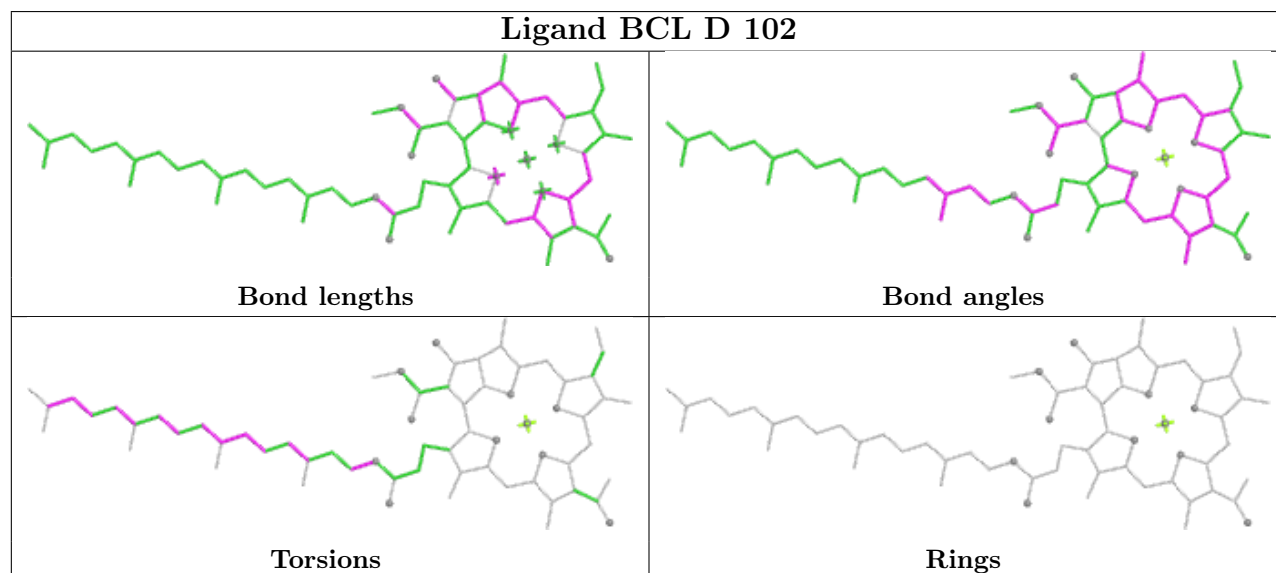
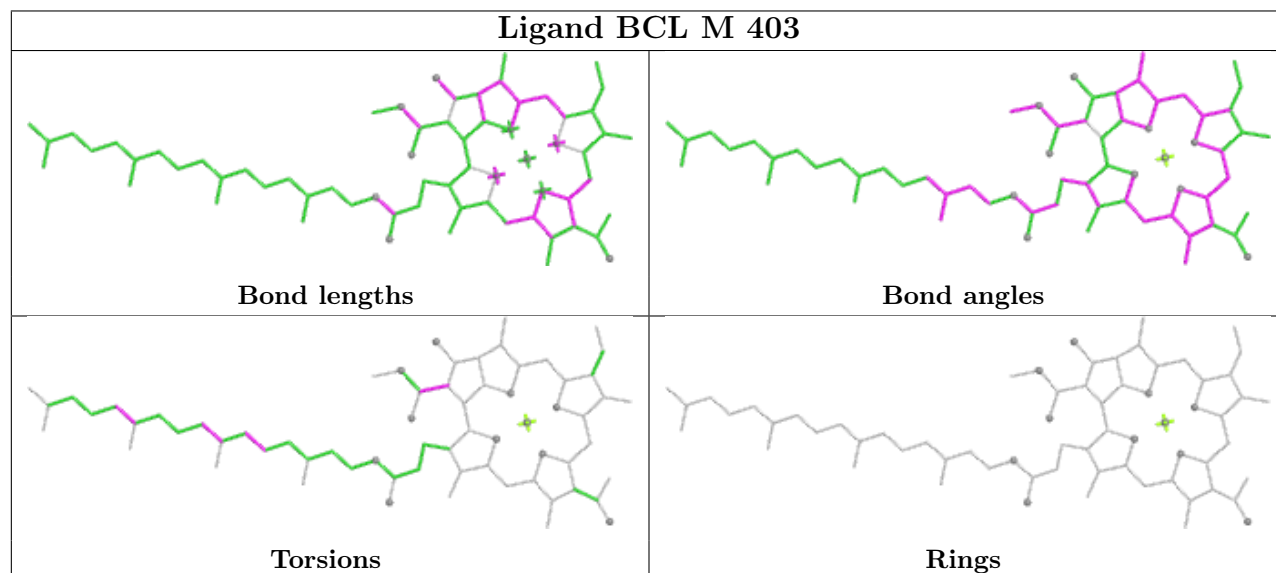
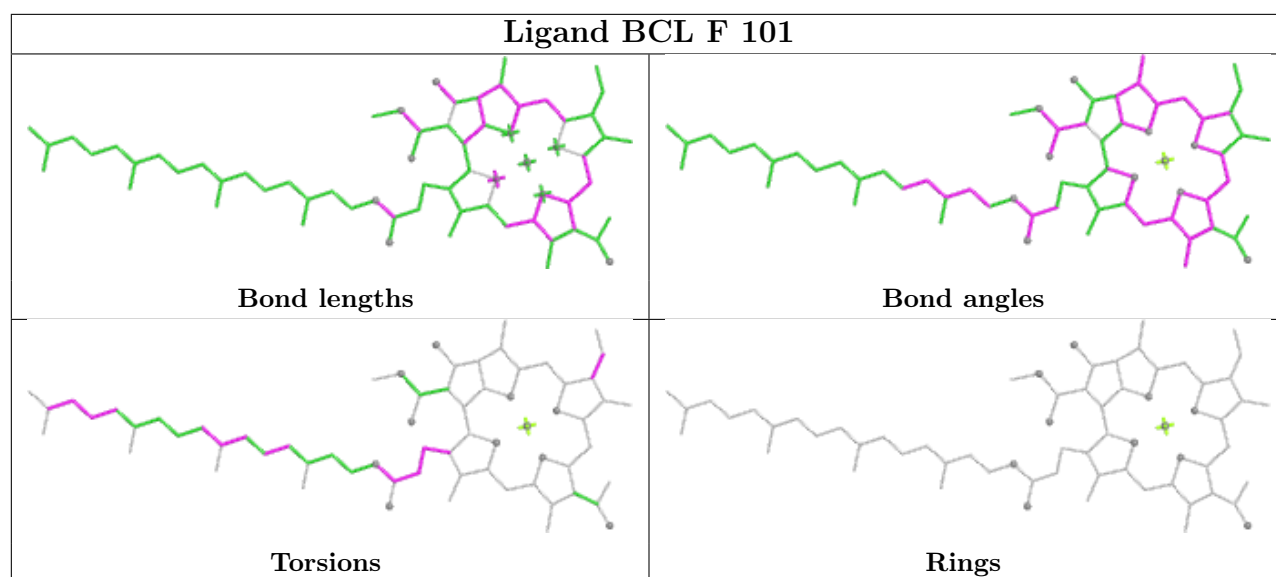
Ligand BCL Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

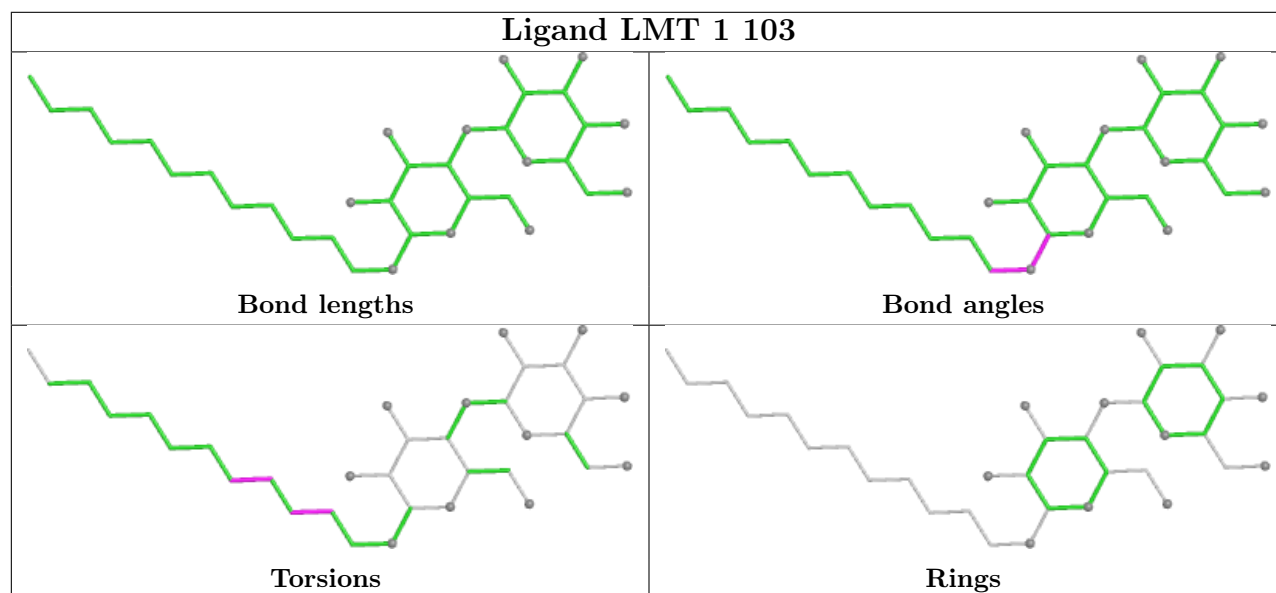
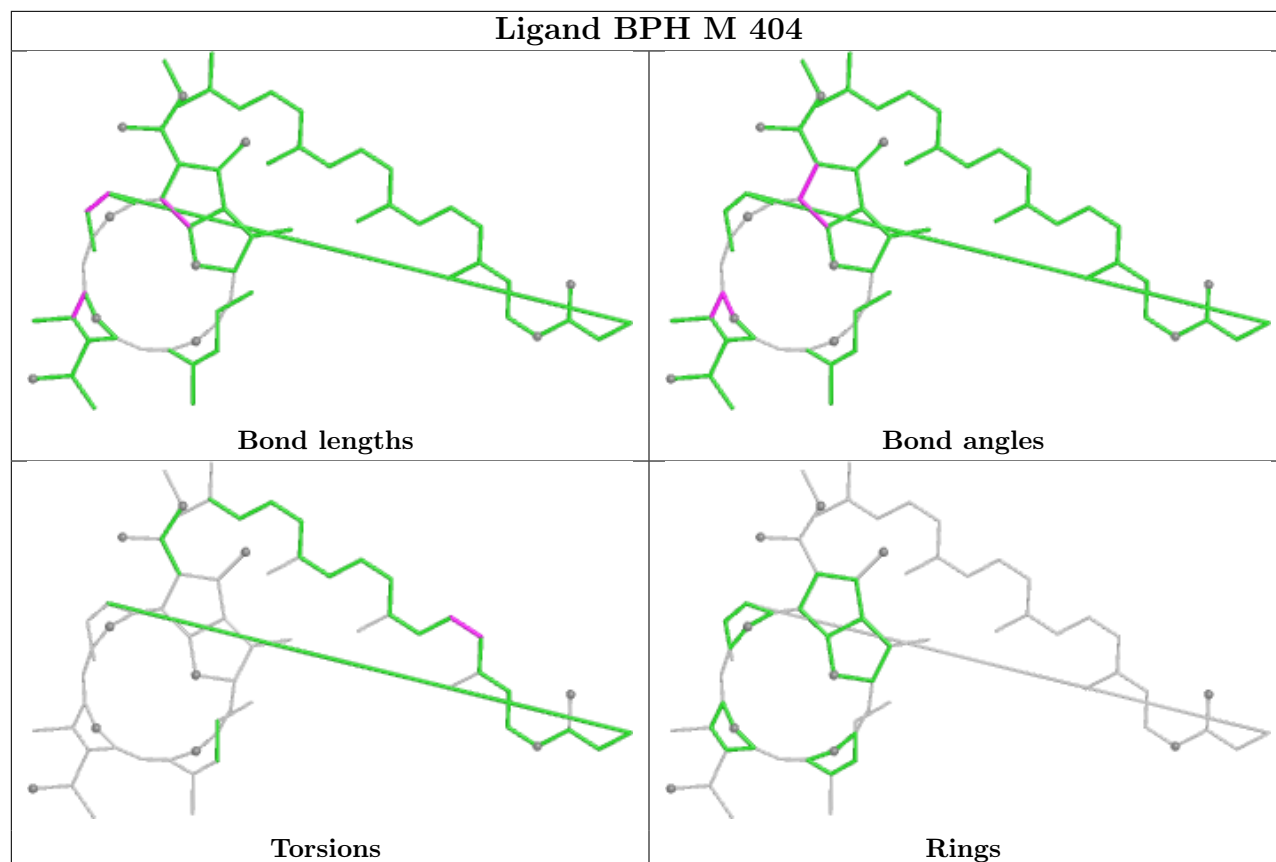


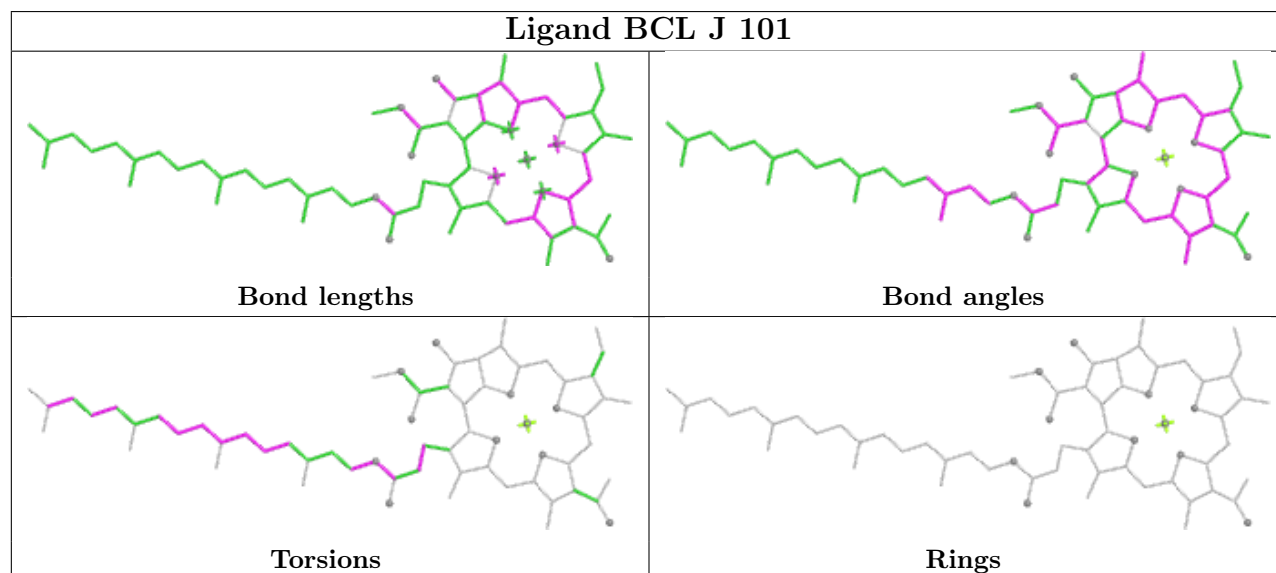
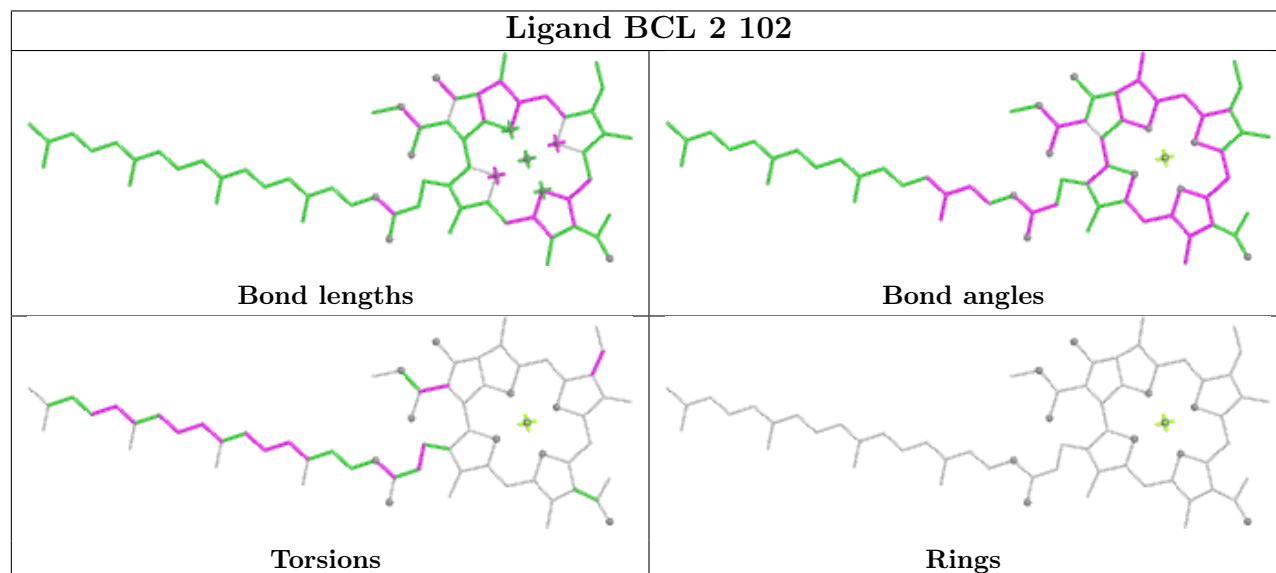
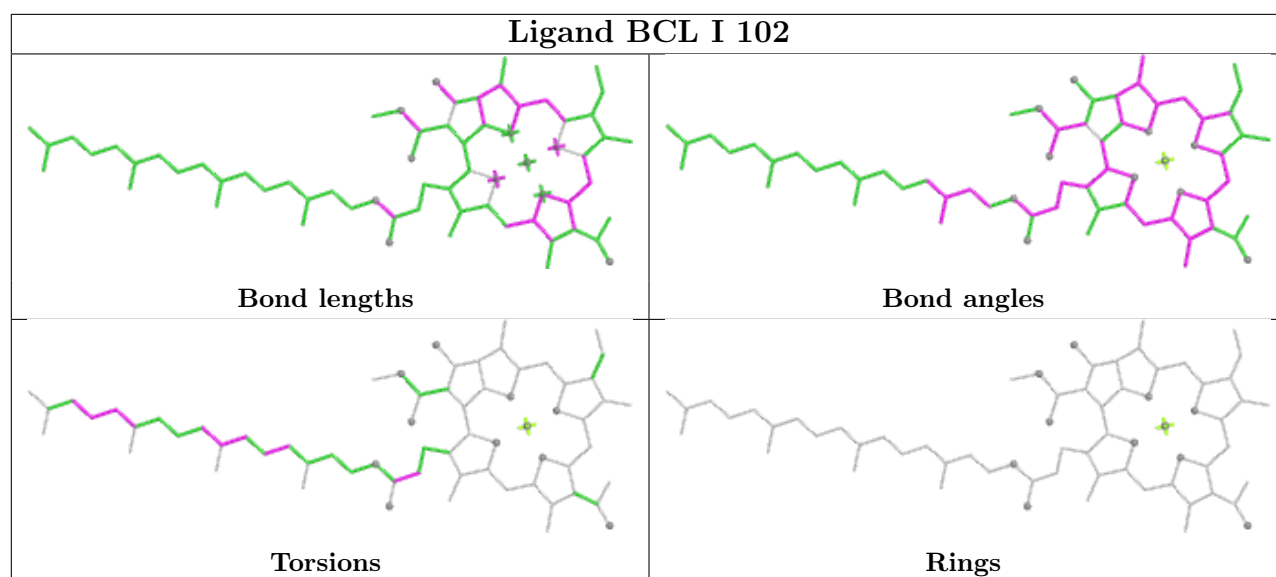


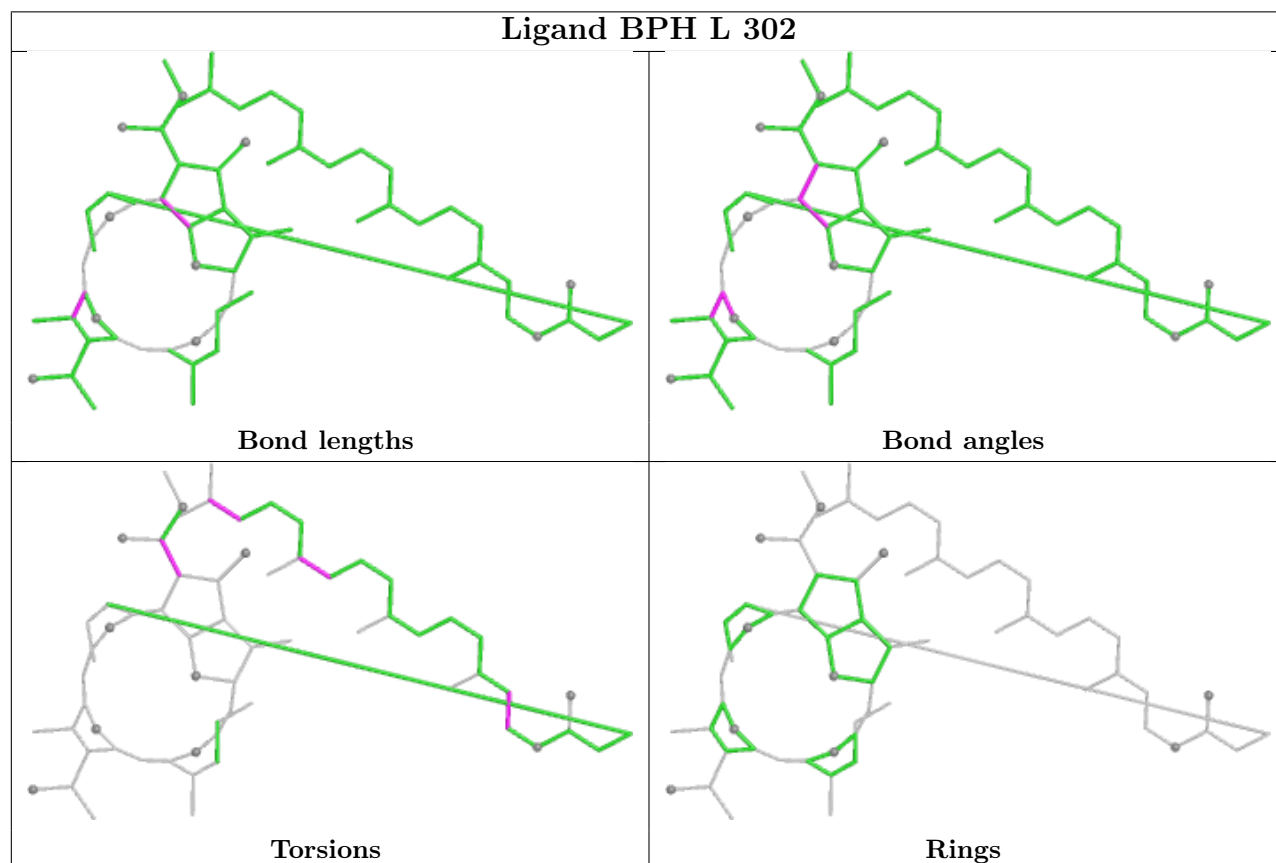
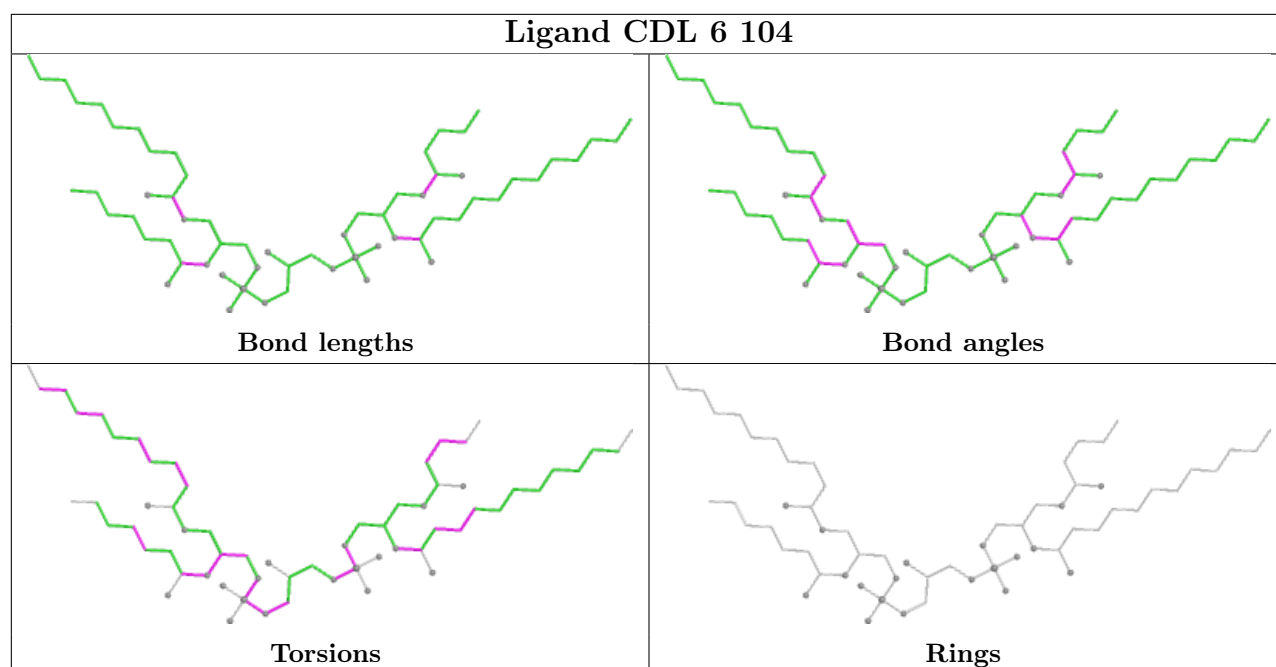


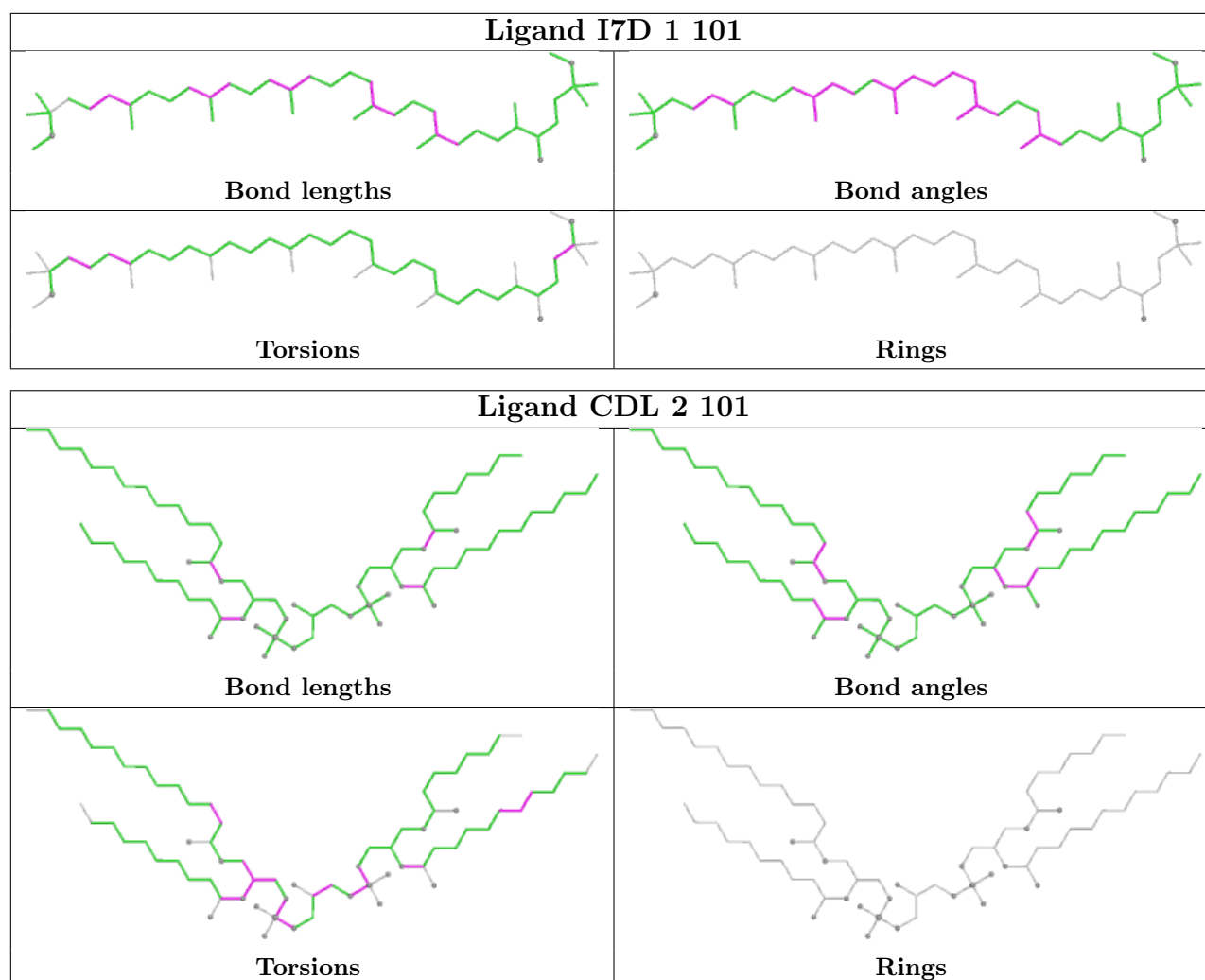


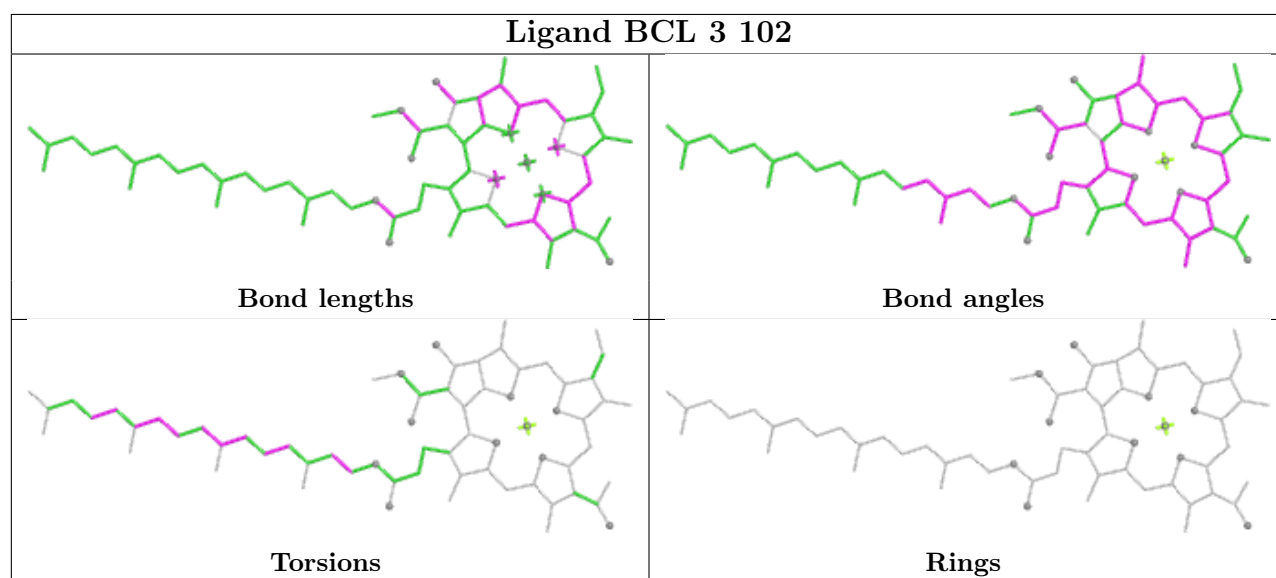
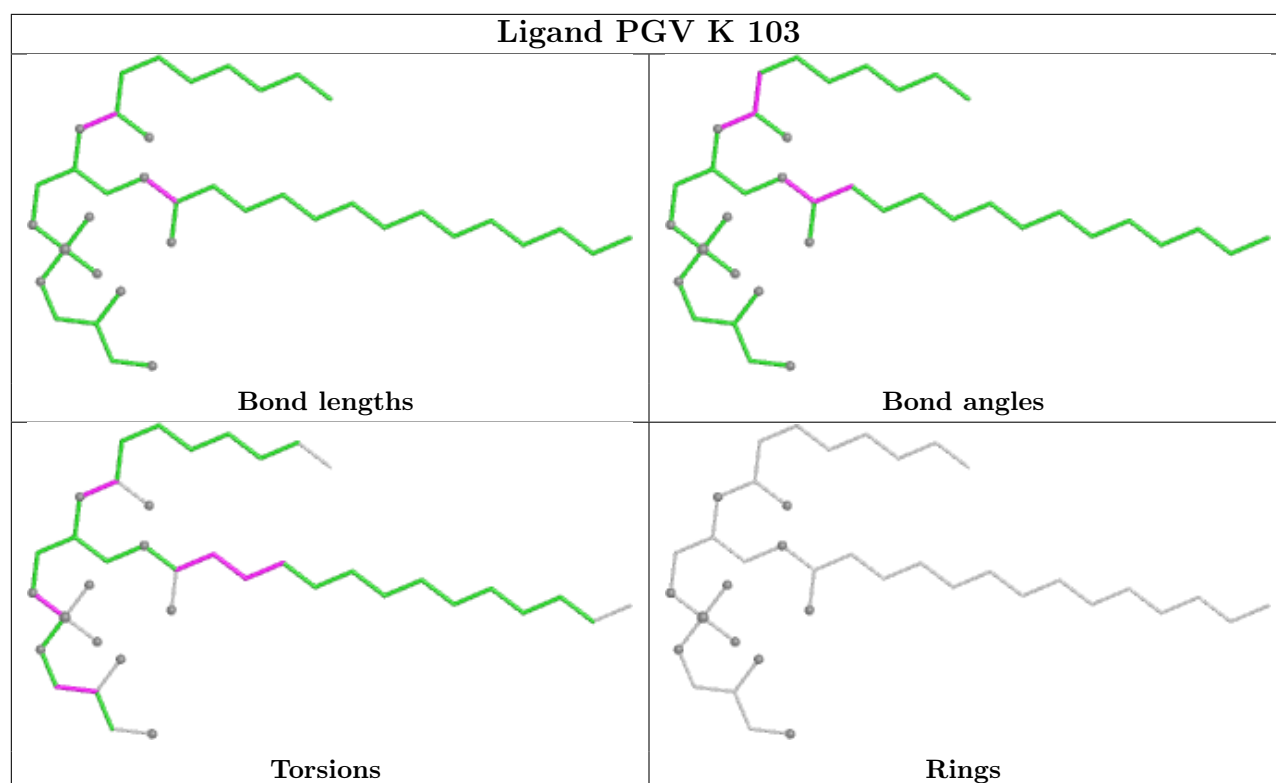




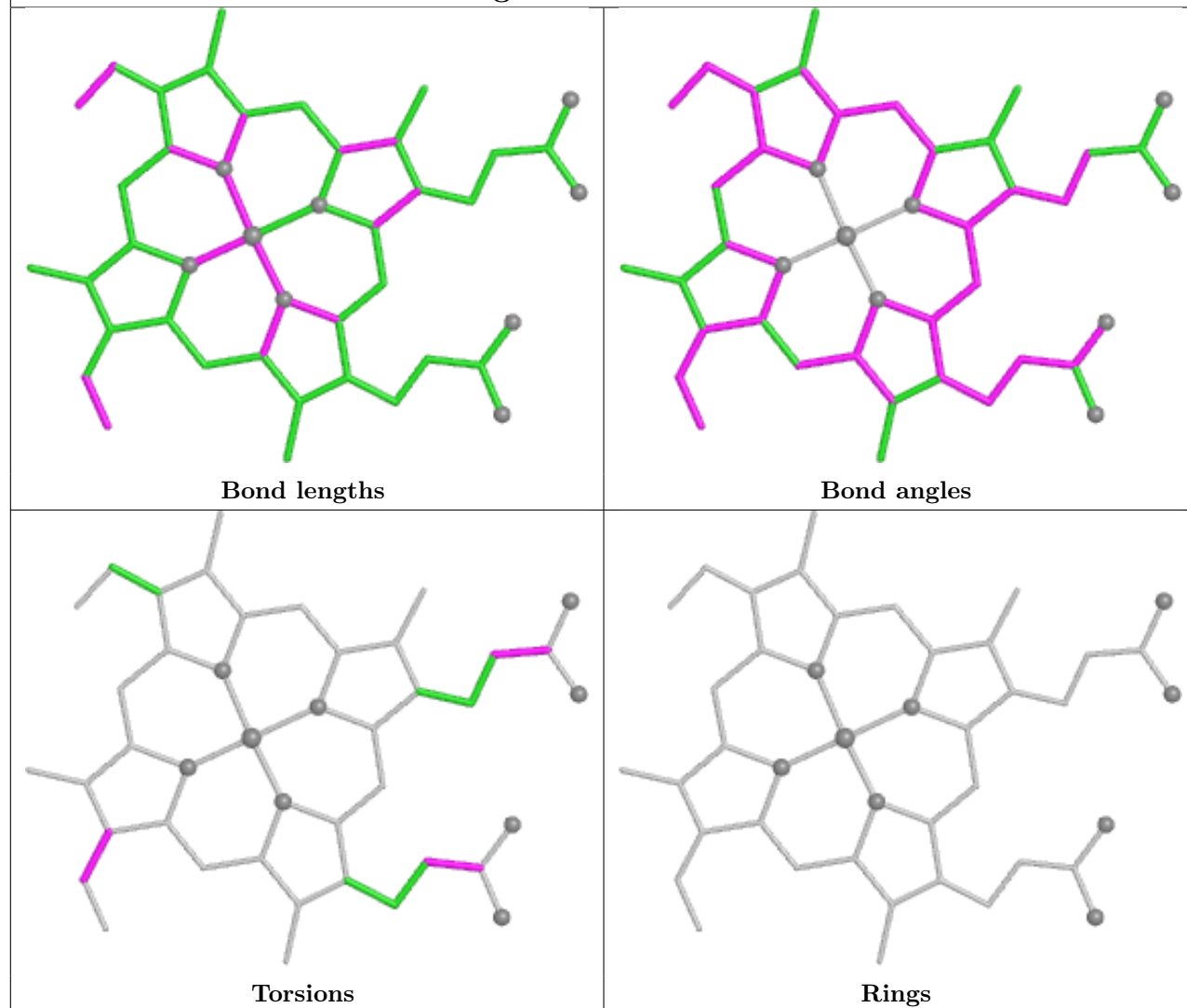




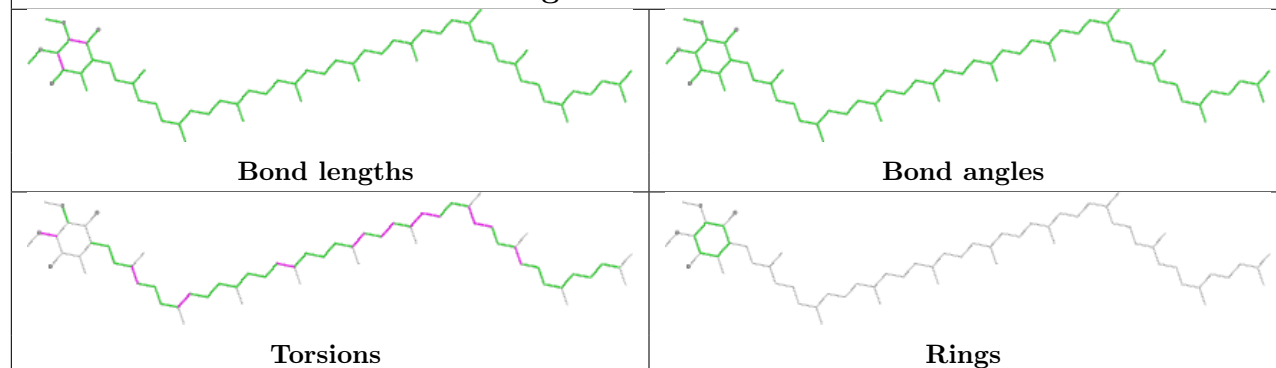


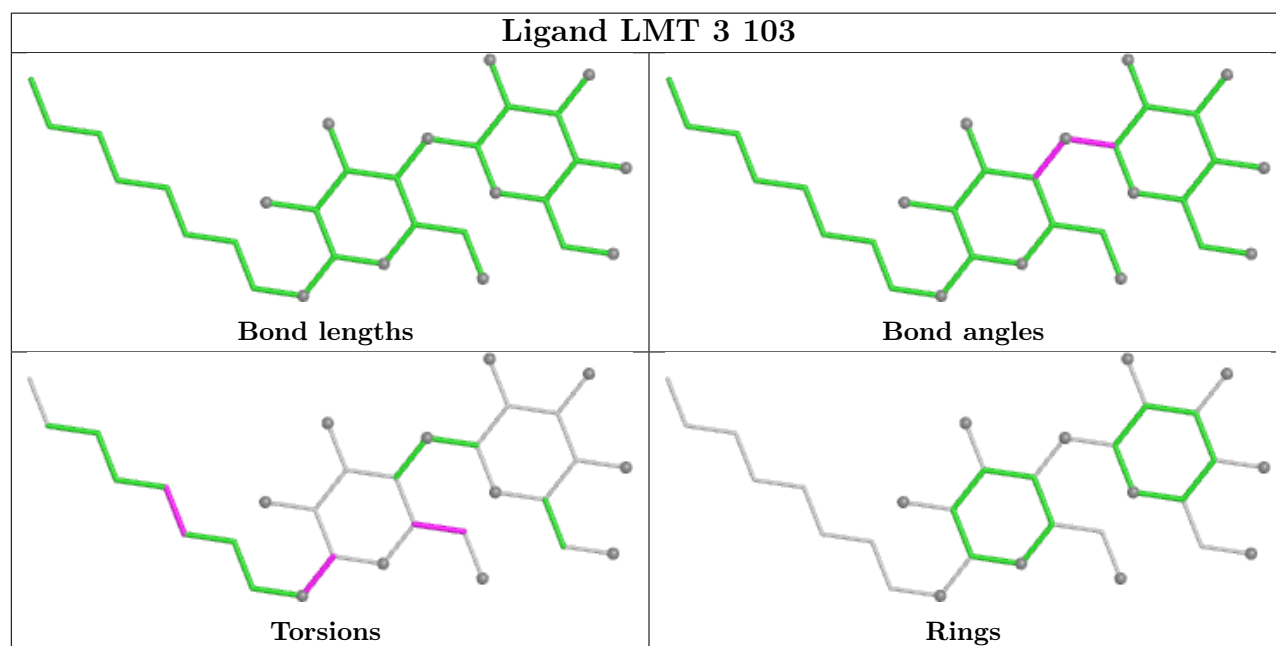
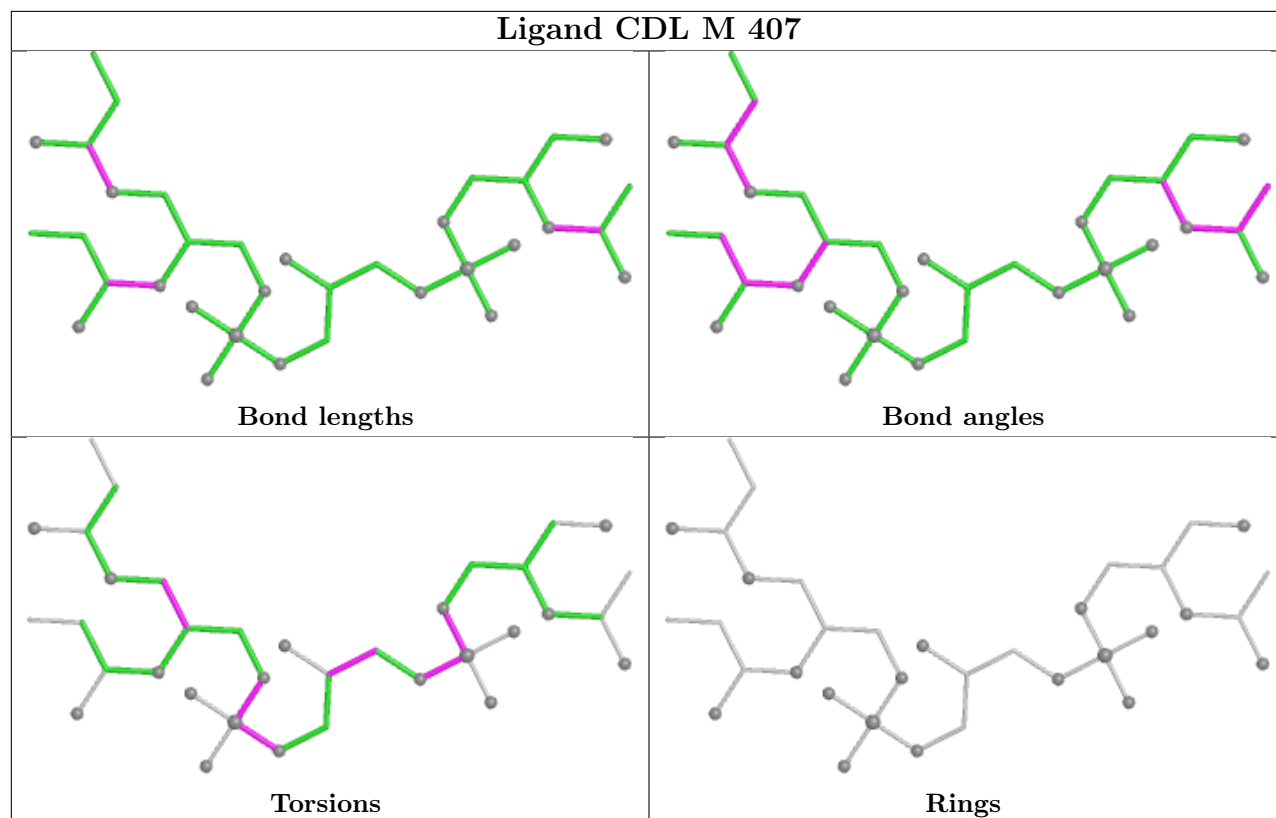


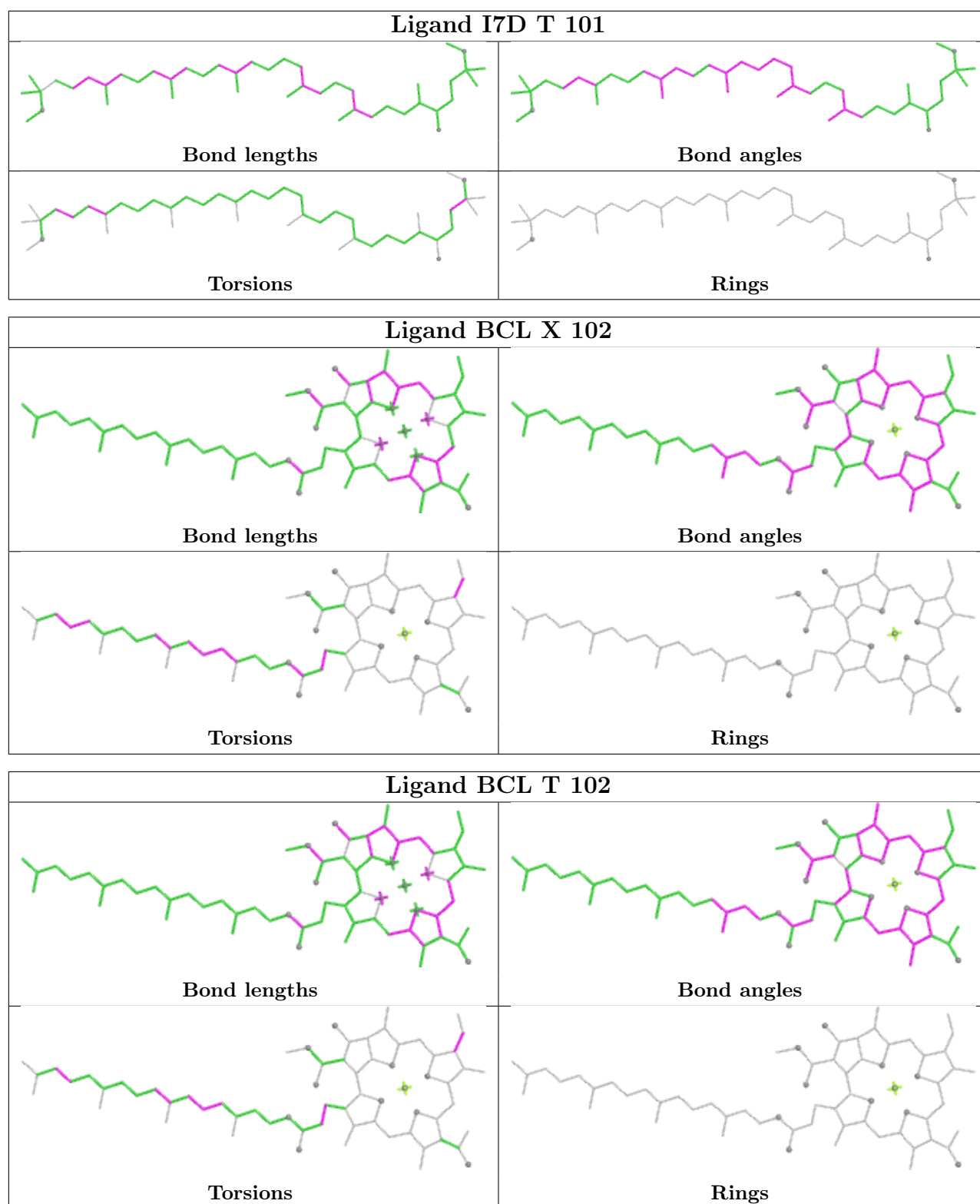
Ligand HEC C 401



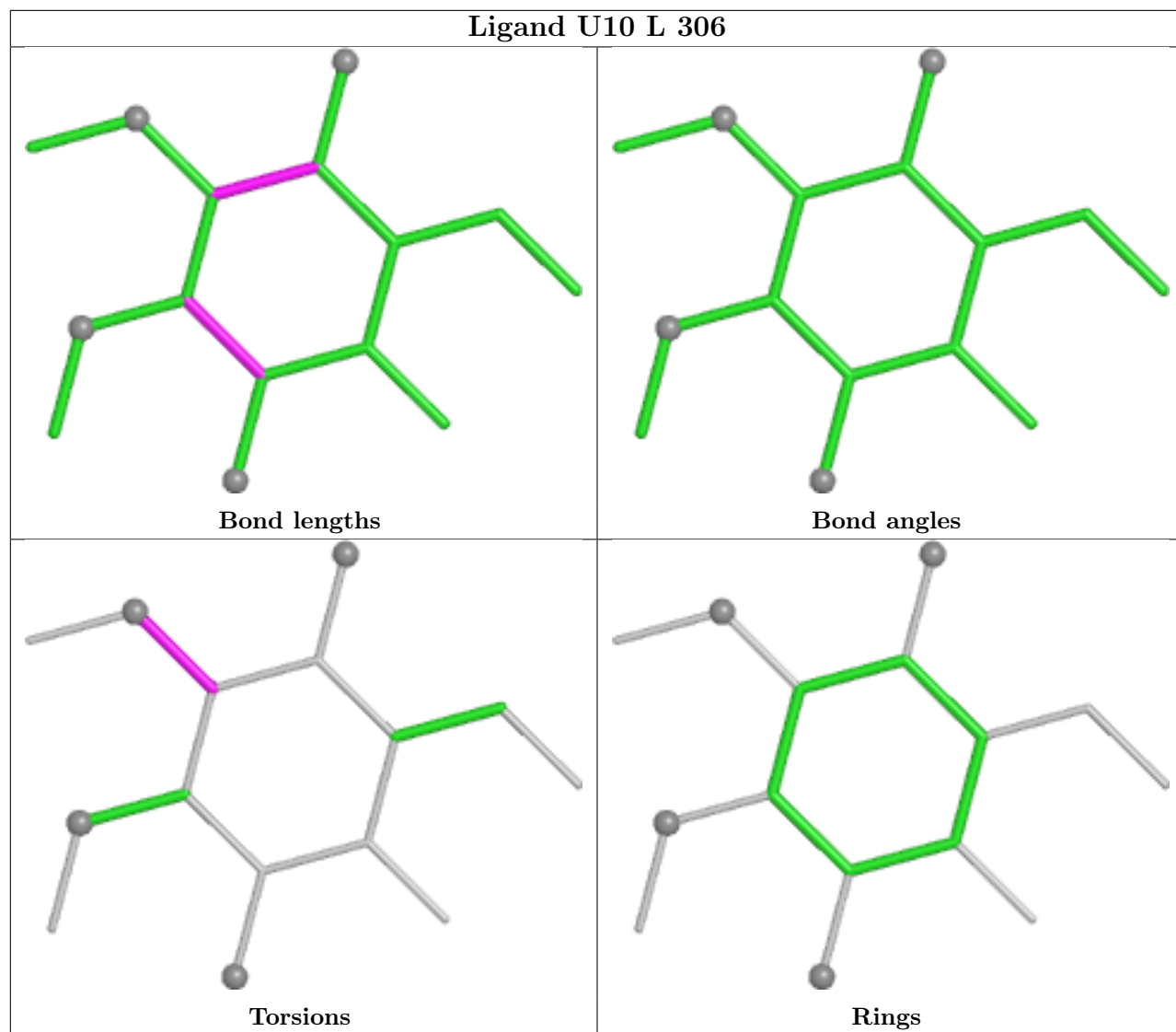
Ligand U10 7 401

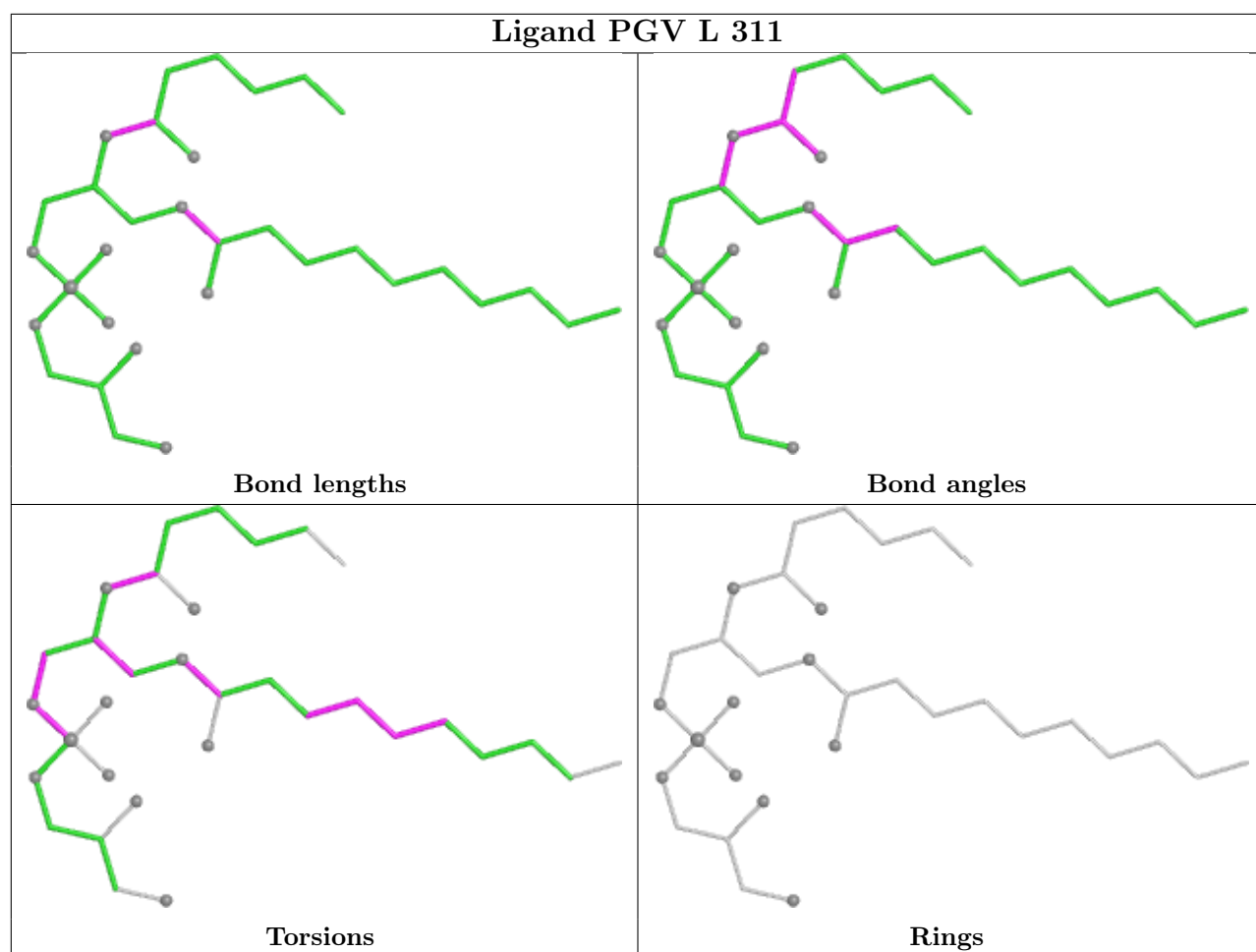


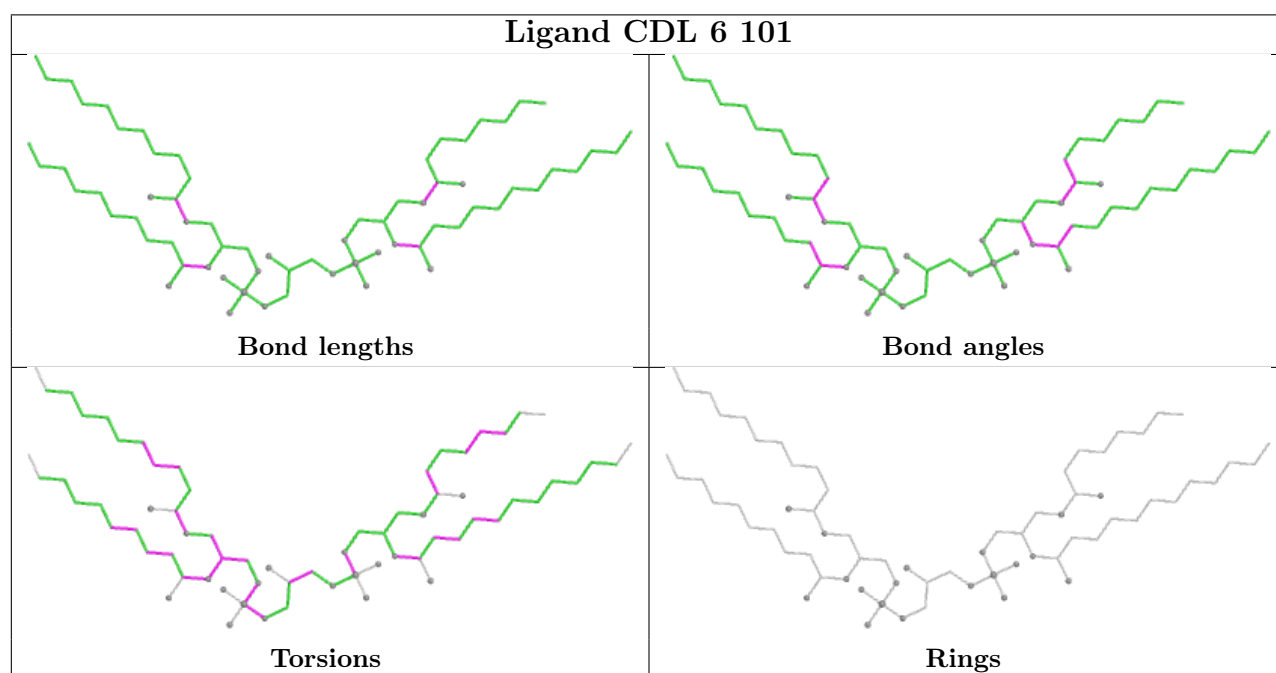
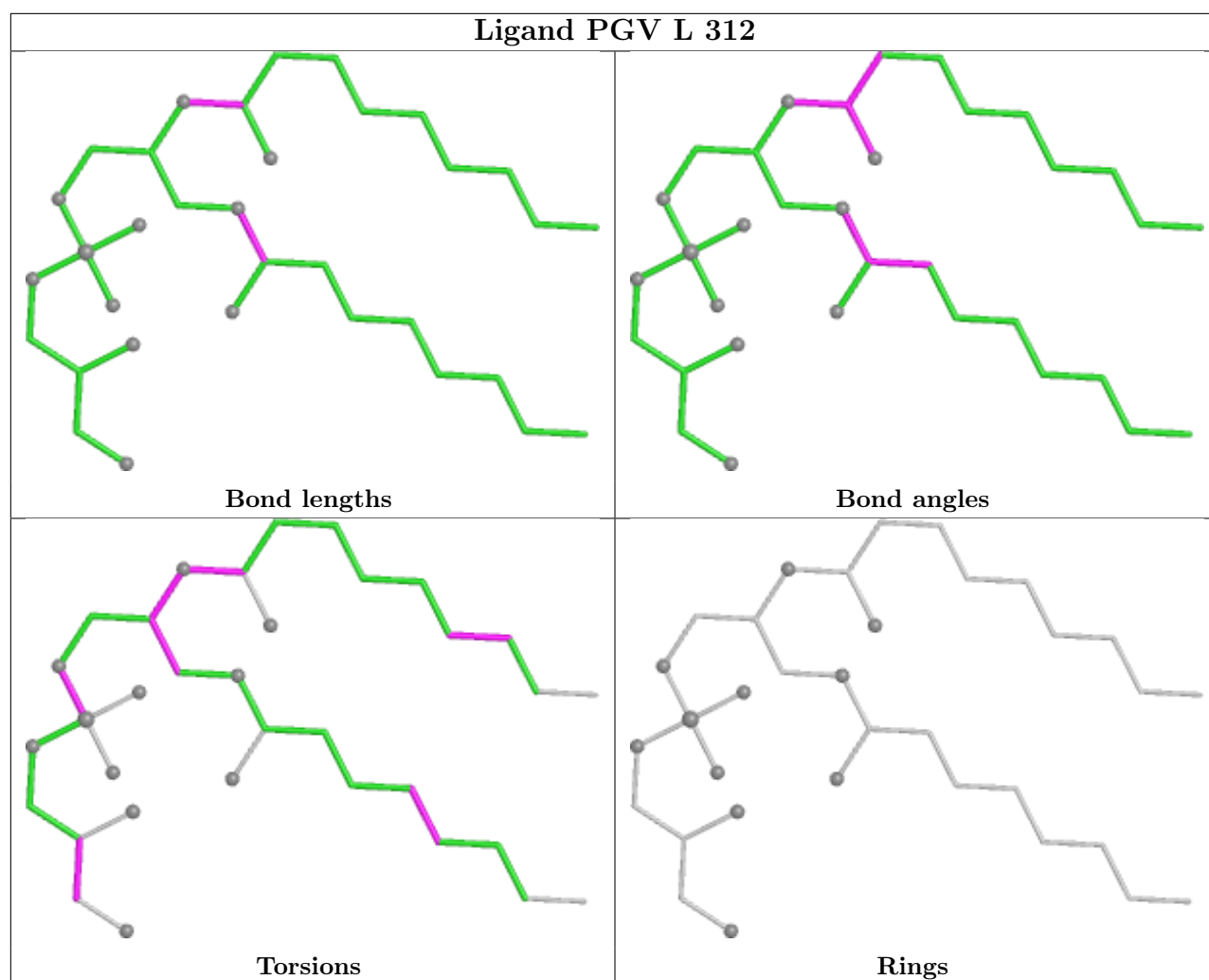


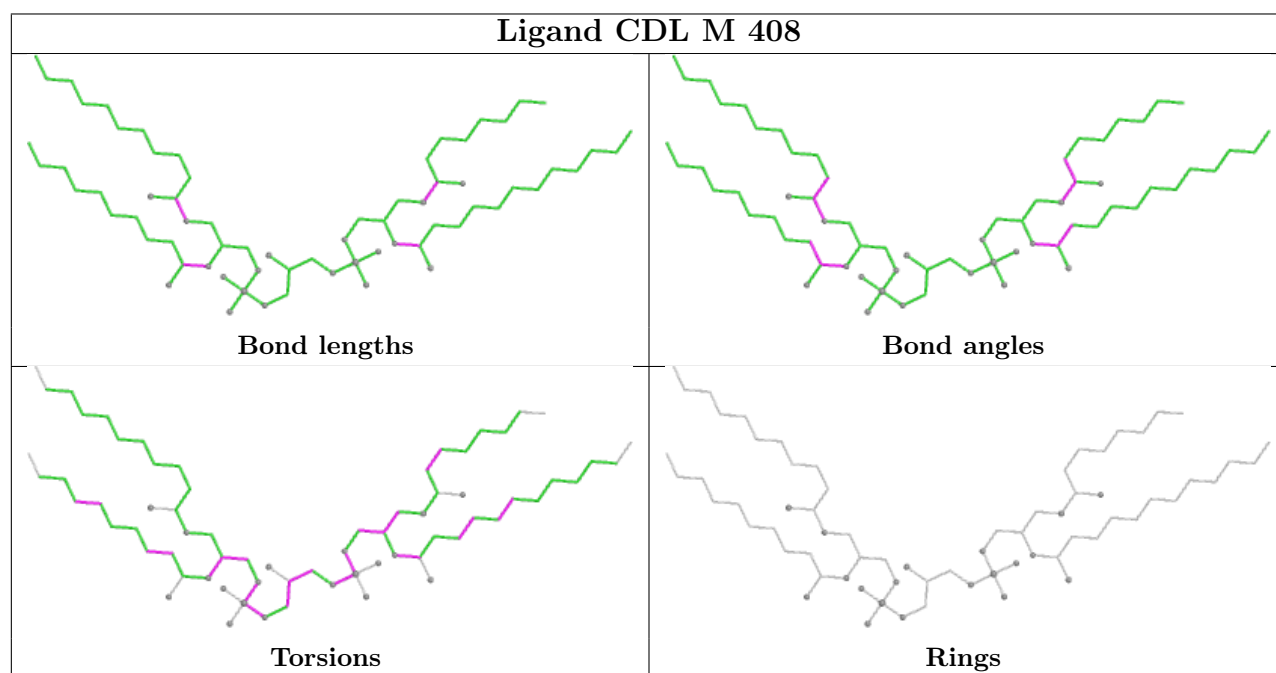
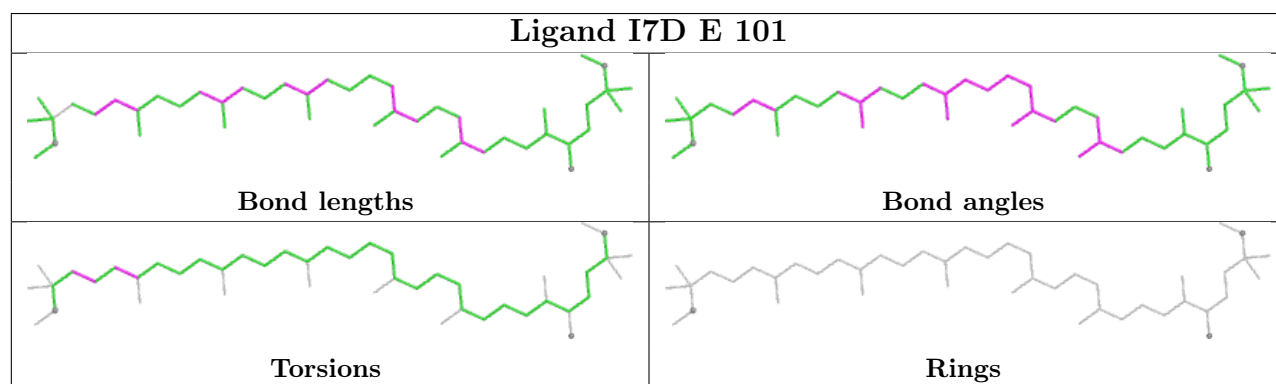
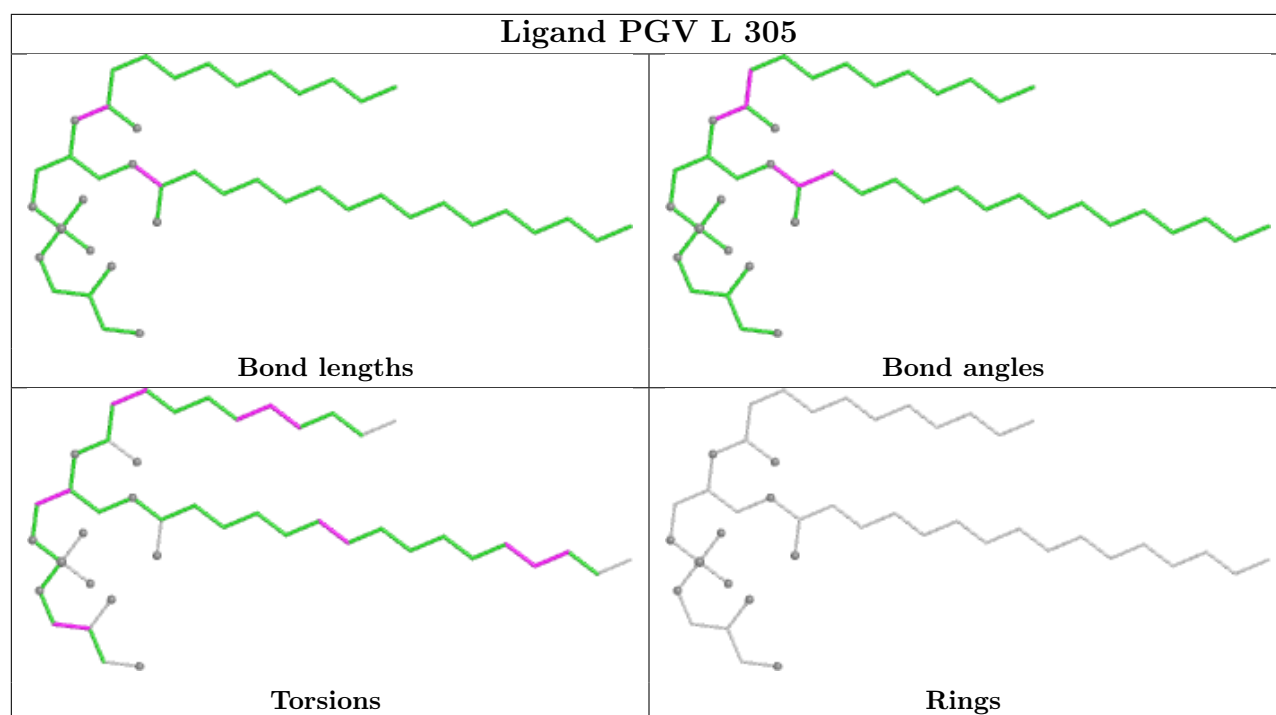


Ligand U10 L 306









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.

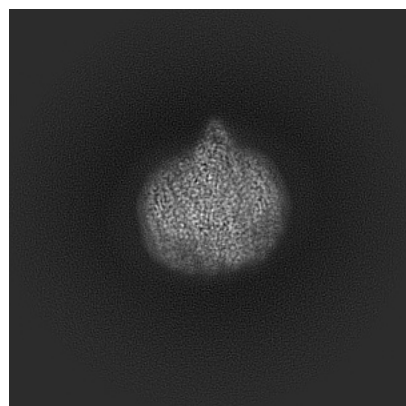
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33501. These allow visual inspection of the internal detail of the map and identification of artifacts.

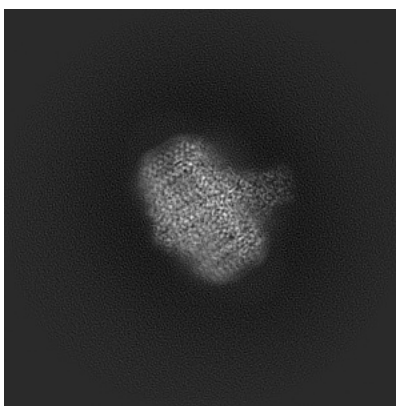
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

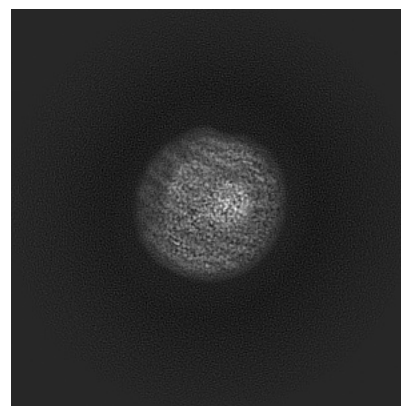
6.1.1 Primary map



X

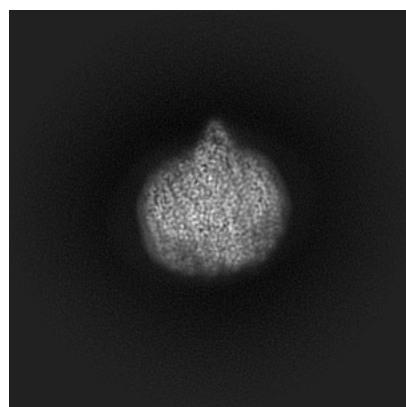


Y

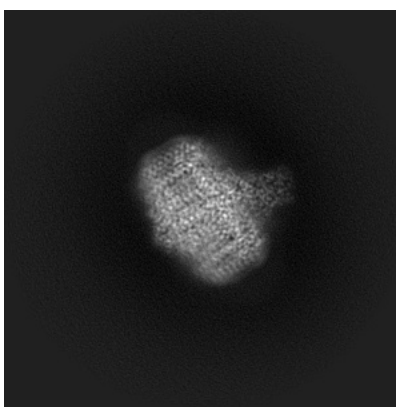


Z

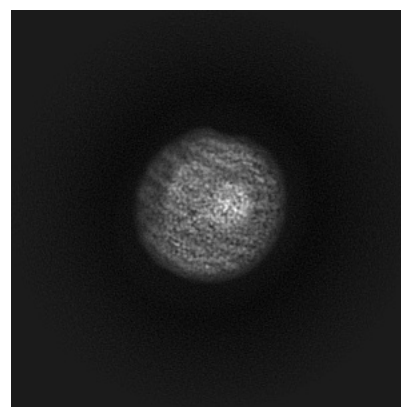
6.1.2 Raw map



X



Y

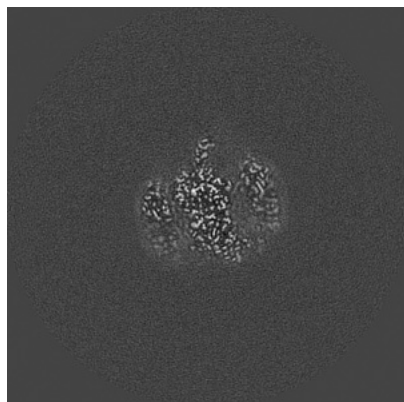


Z

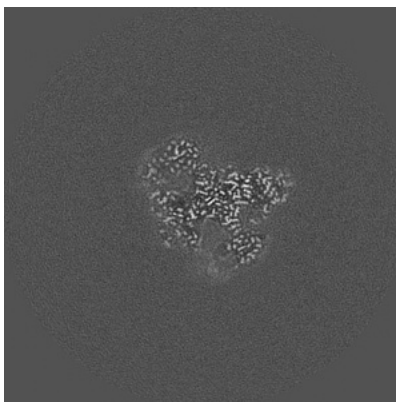
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

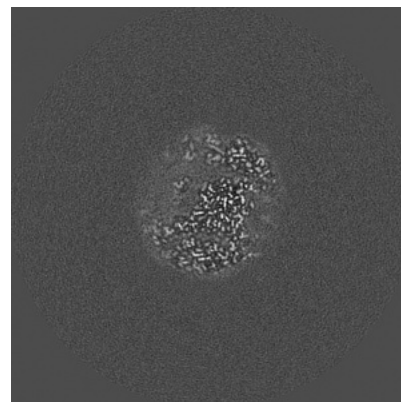
6.2.1 Primary map



X Index: 200

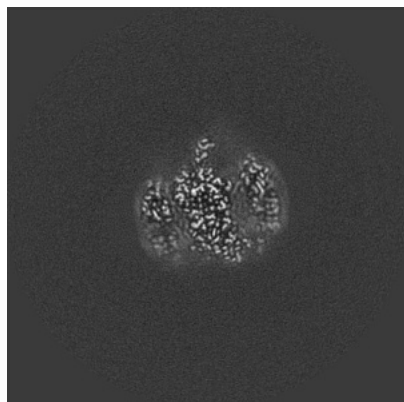


Y Index: 200

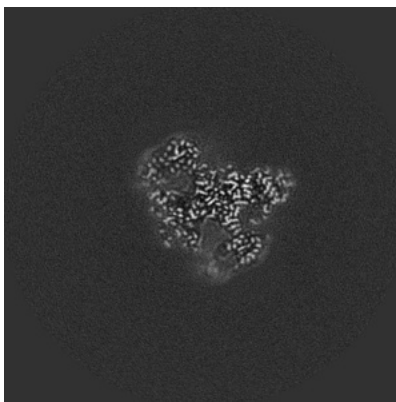


Z Index: 200

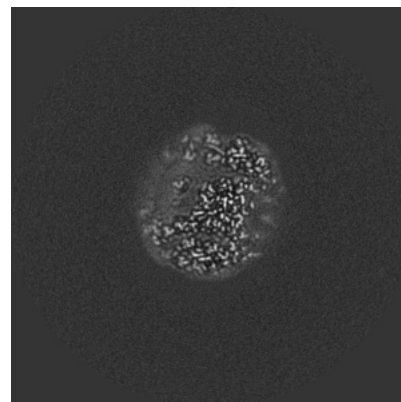
6.2.2 Raw map



X Index: 200



Y Index: 200

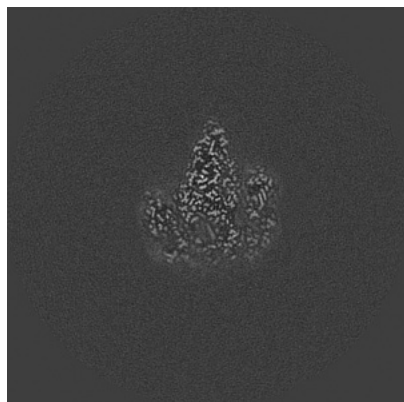


Z Index: 200

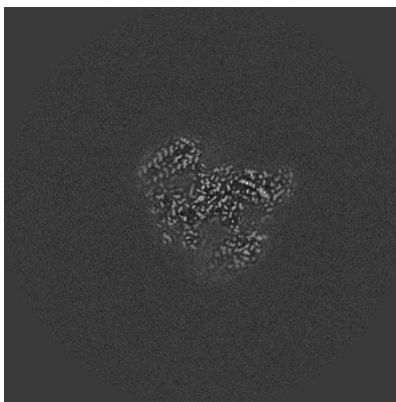
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

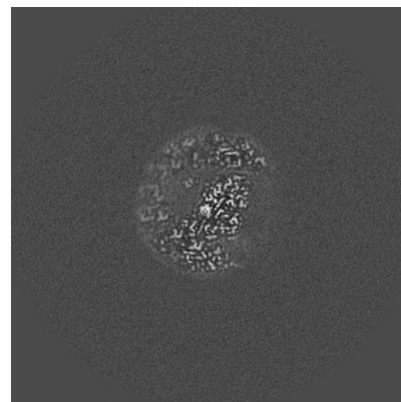
6.3.1 Primary map



X Index: 217

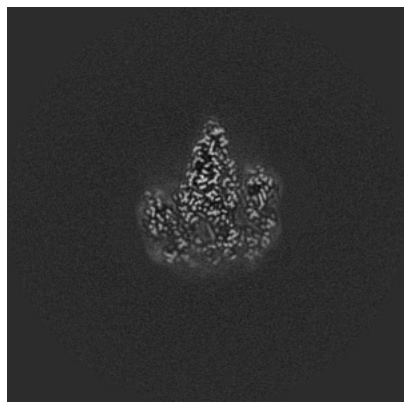


Y Index: 203

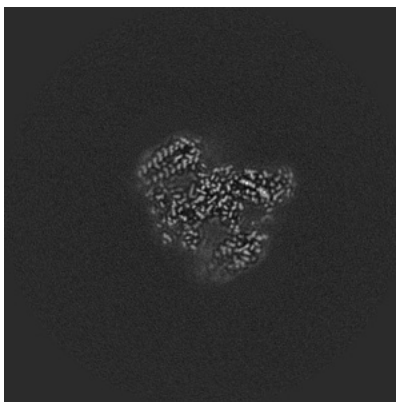


Z Index: 209

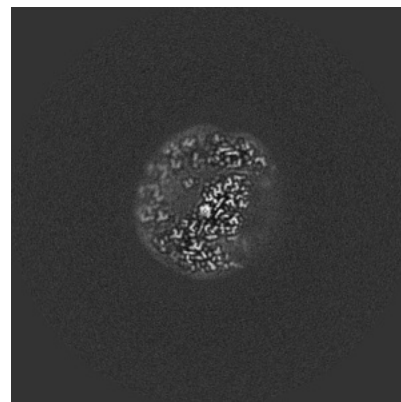
6.3.2 Raw map



X Index: 217



Y Index: 203

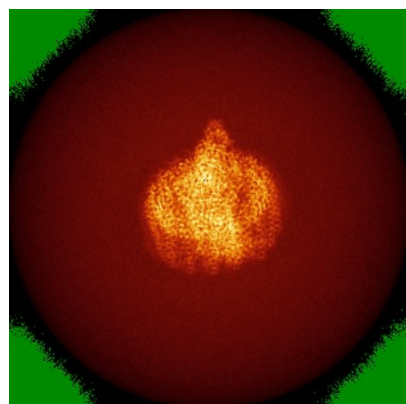


Z Index: 209

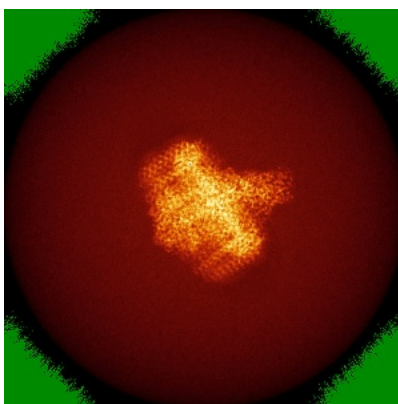
The images above show the largest variance slices of the map in three orthogonal directions.

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

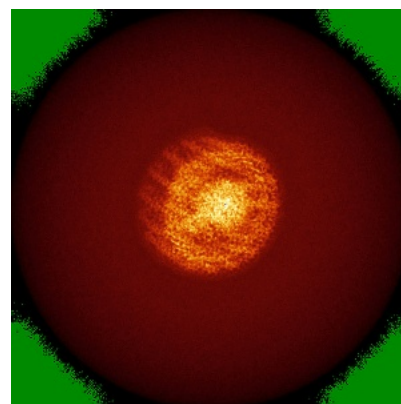
6.4.1 Primary map



X

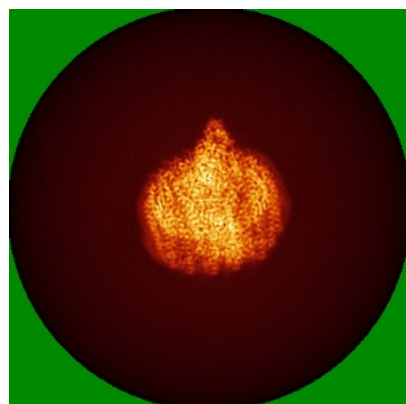


Y

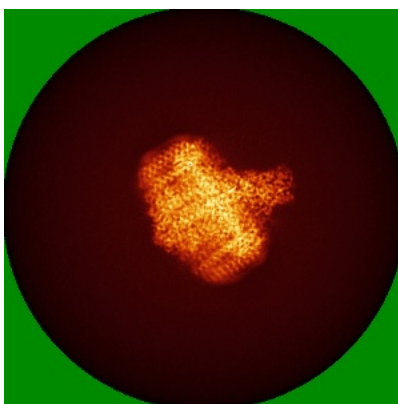


Z

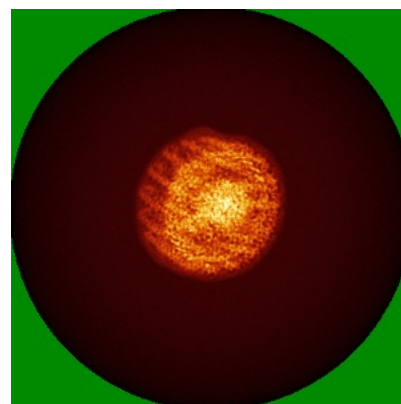
6.4.2 Raw map



X



Y

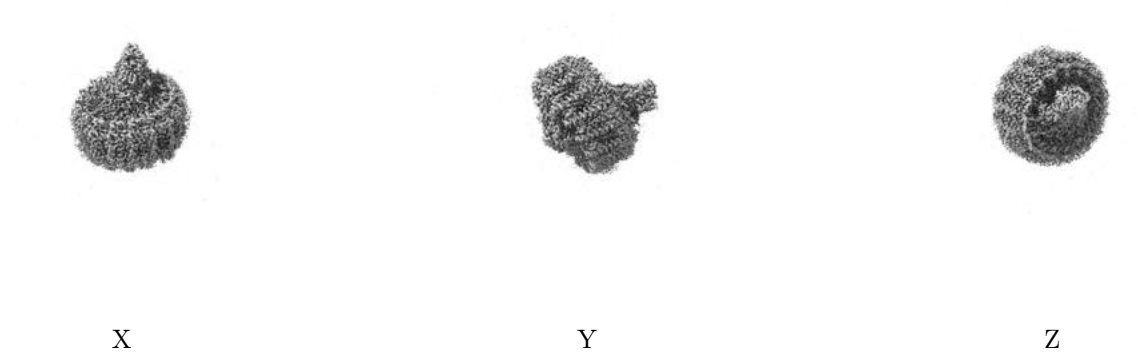


Z

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

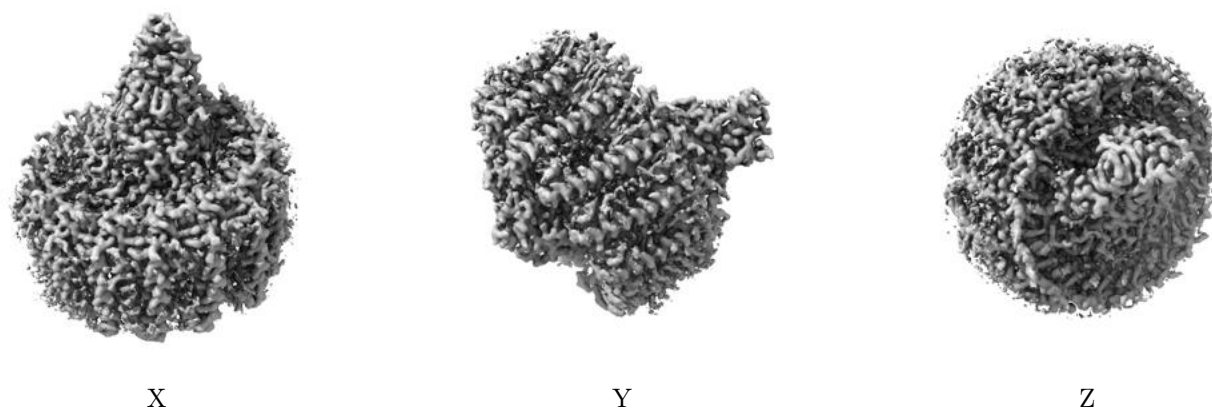
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

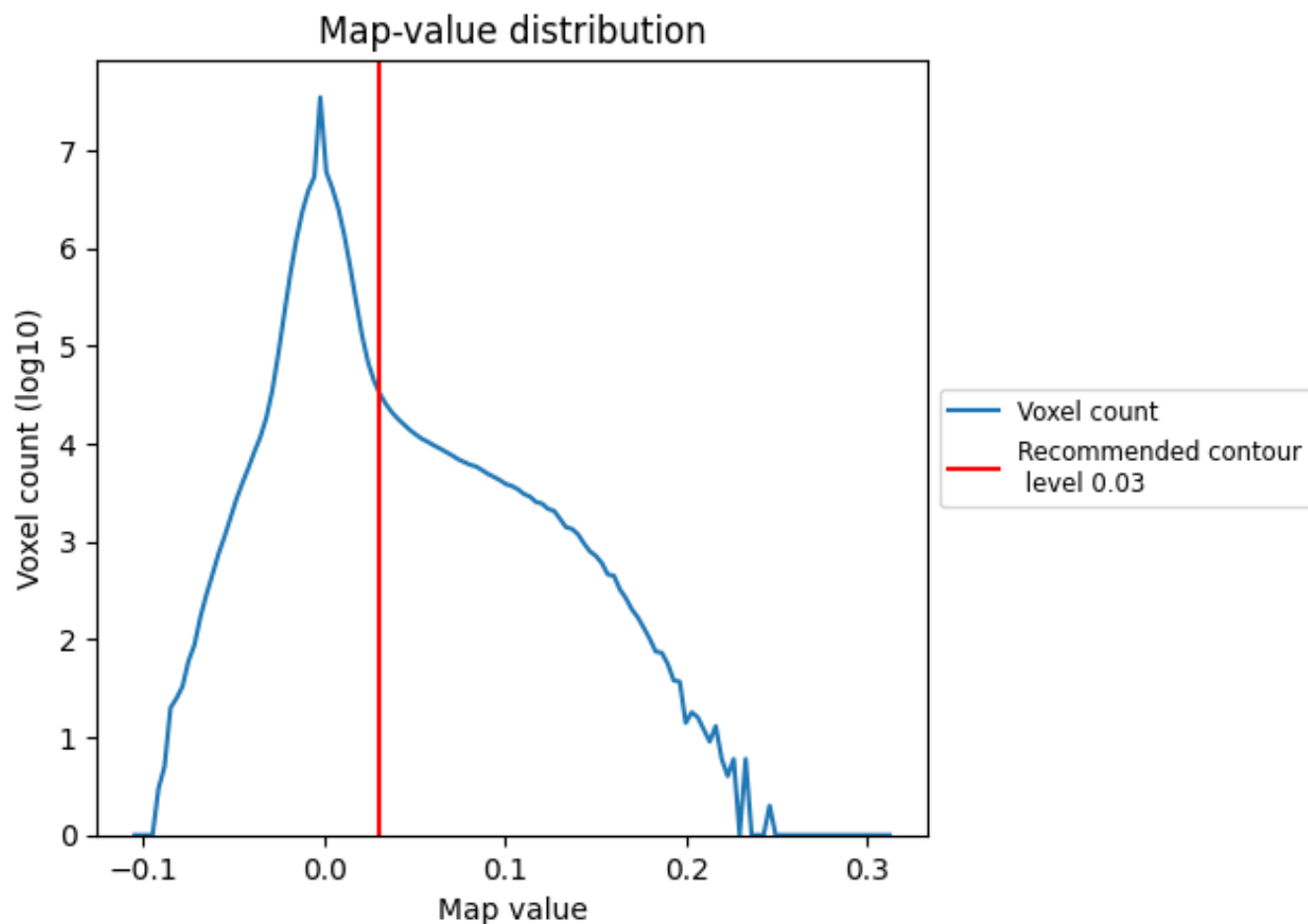
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

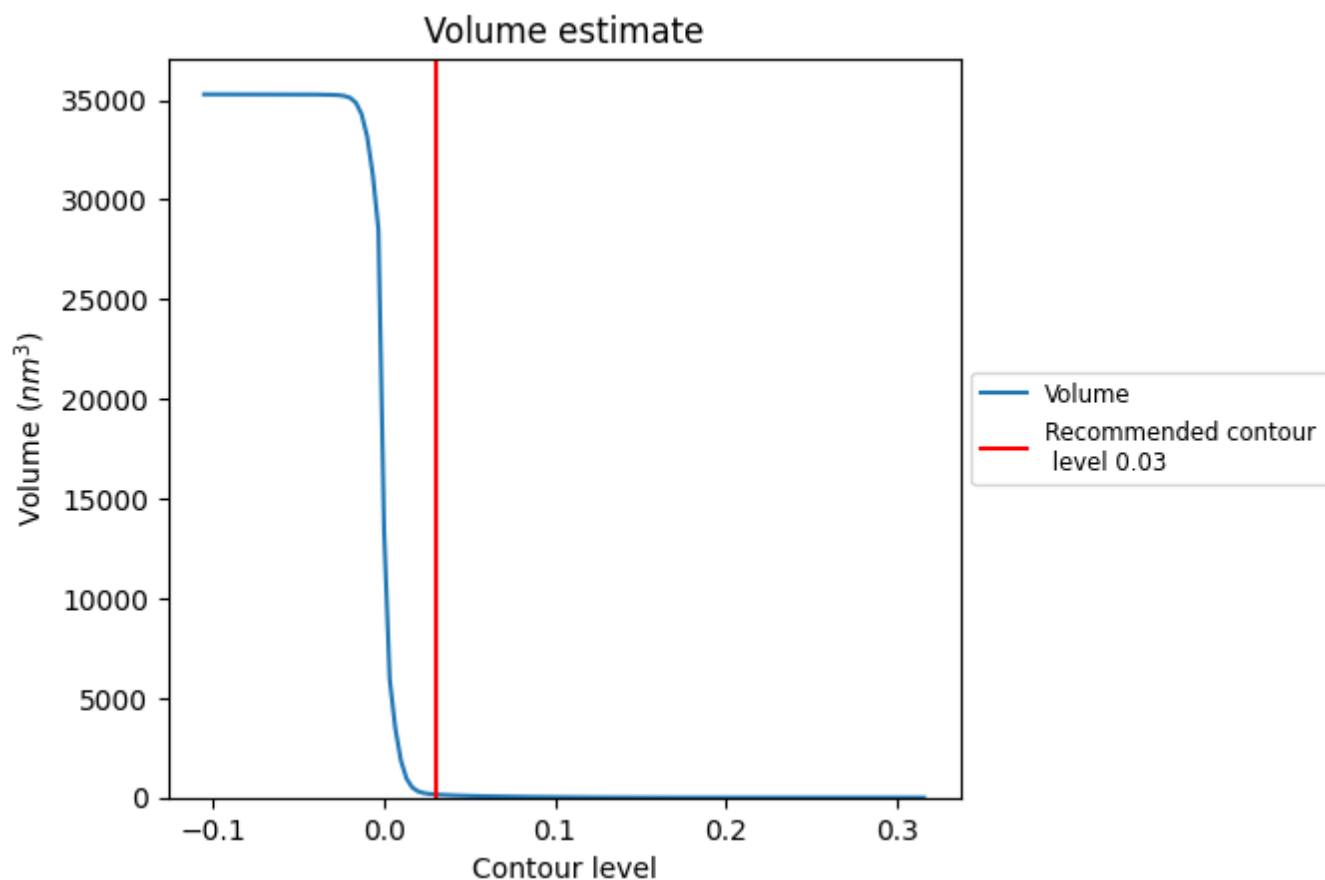
This section contains the results of statistical analysis of the map.

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.

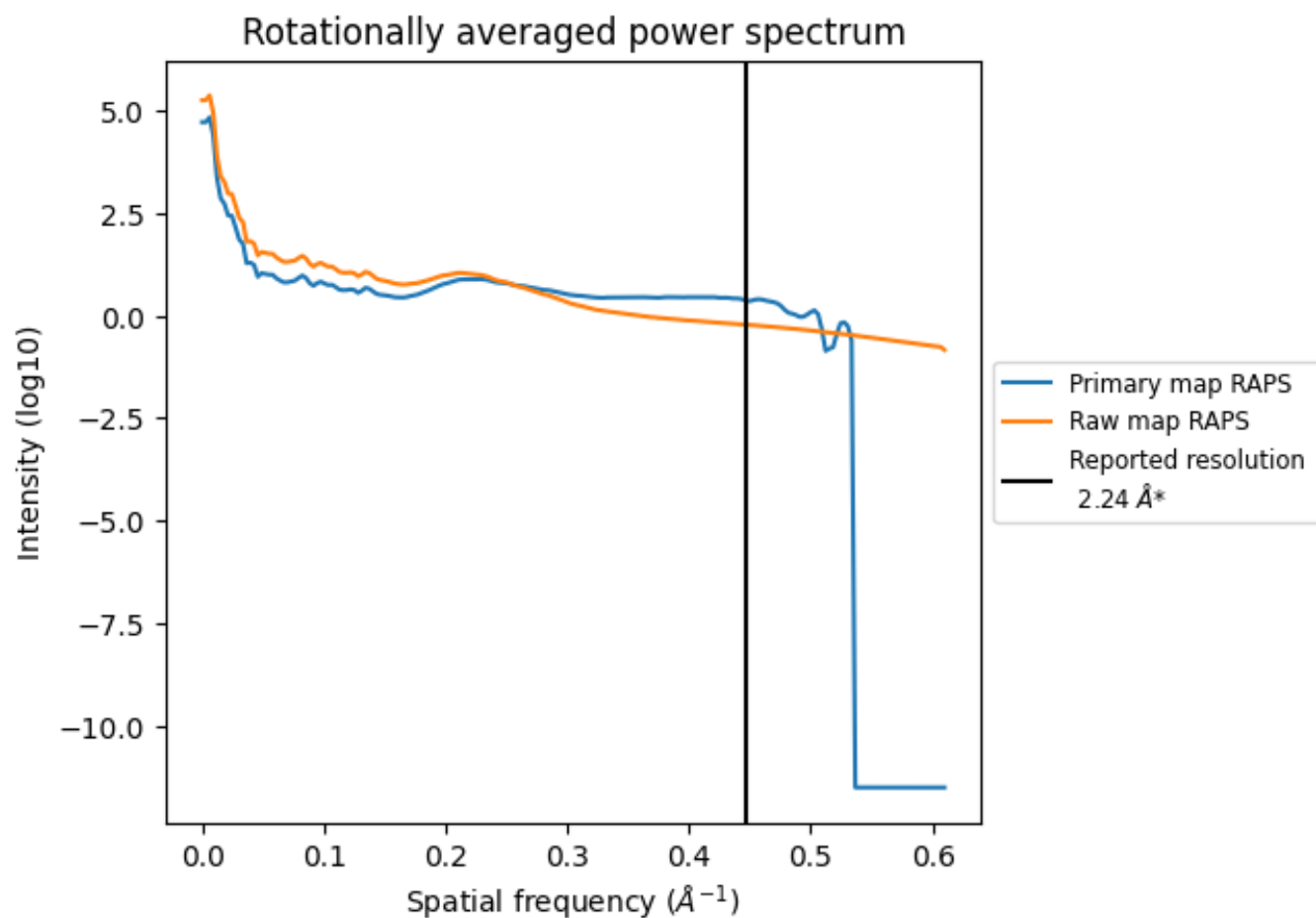
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm³; this corresponds to an approximate mass of 142 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 ⓘ

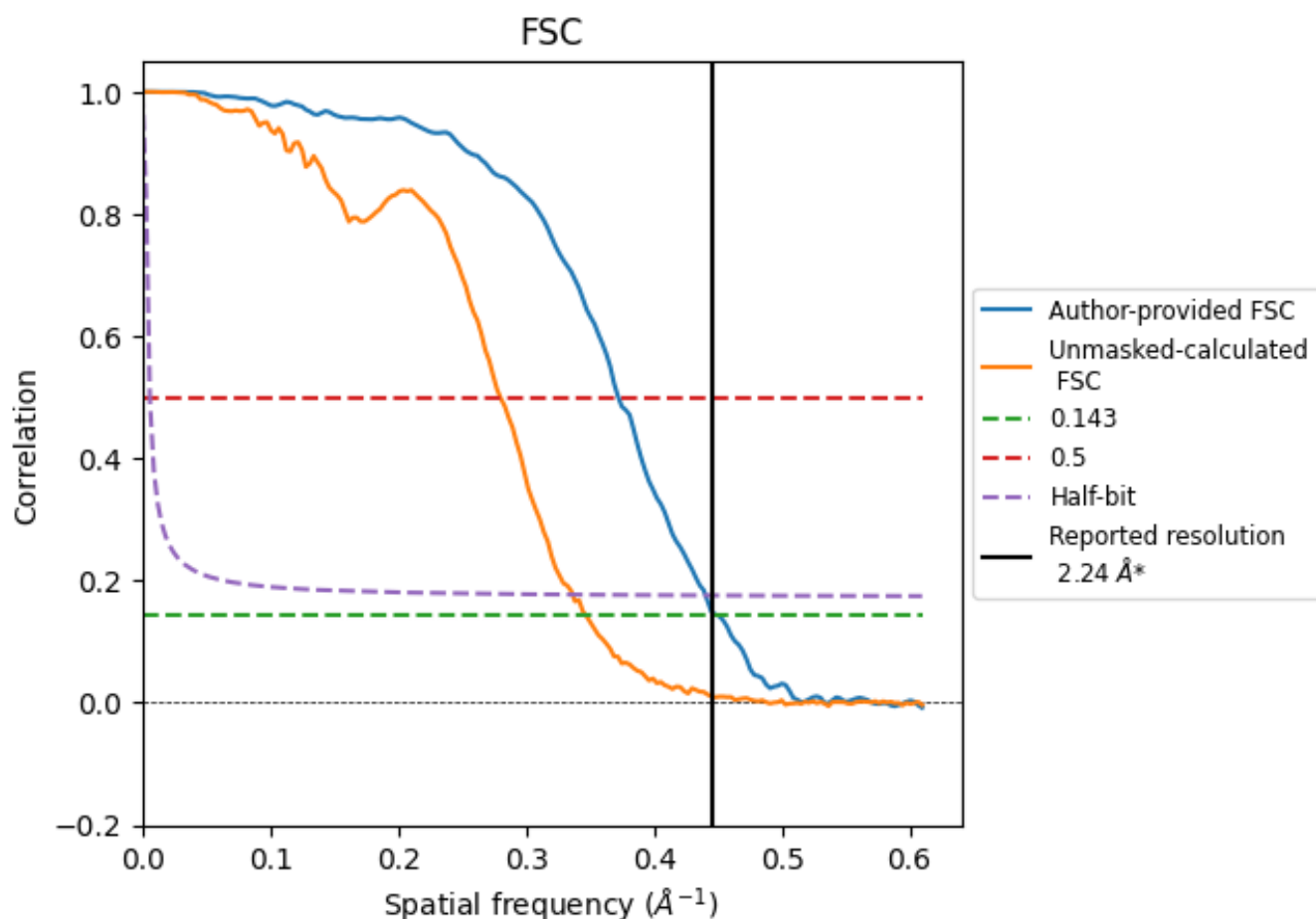


*Reported resolution corresponds to spatial frequency of 0.446 Å⁻¹

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 0.446 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

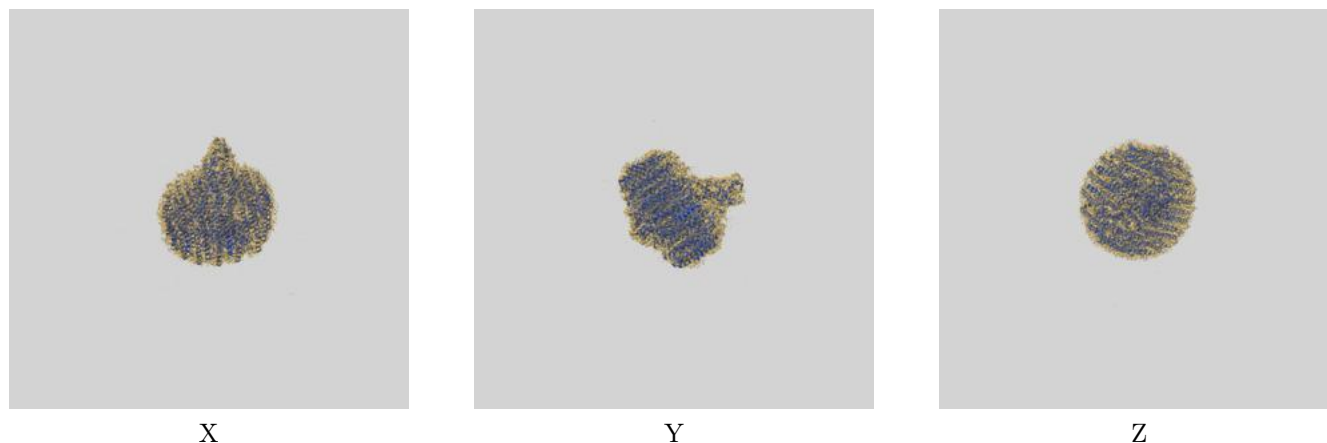
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.22	2.69	2.27
Unmasked-calculated*	2.88	3.57	2.97

*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 2.88 differs from the reported value 2.24 by more than 10 %

9 Map-model fit [i](#)

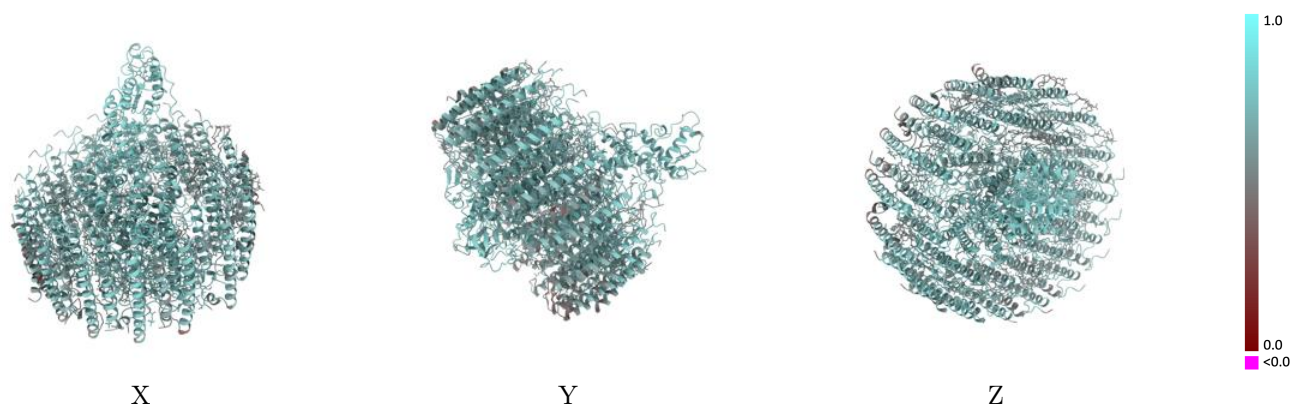
This section contains information regarding the fit between EMDB map EMD-33501 and PDB model 7XXF. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



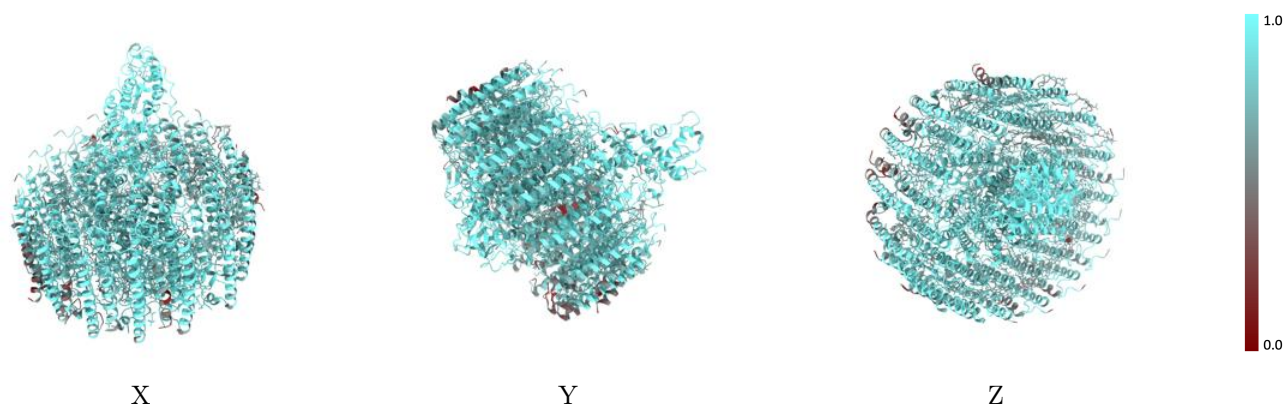
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



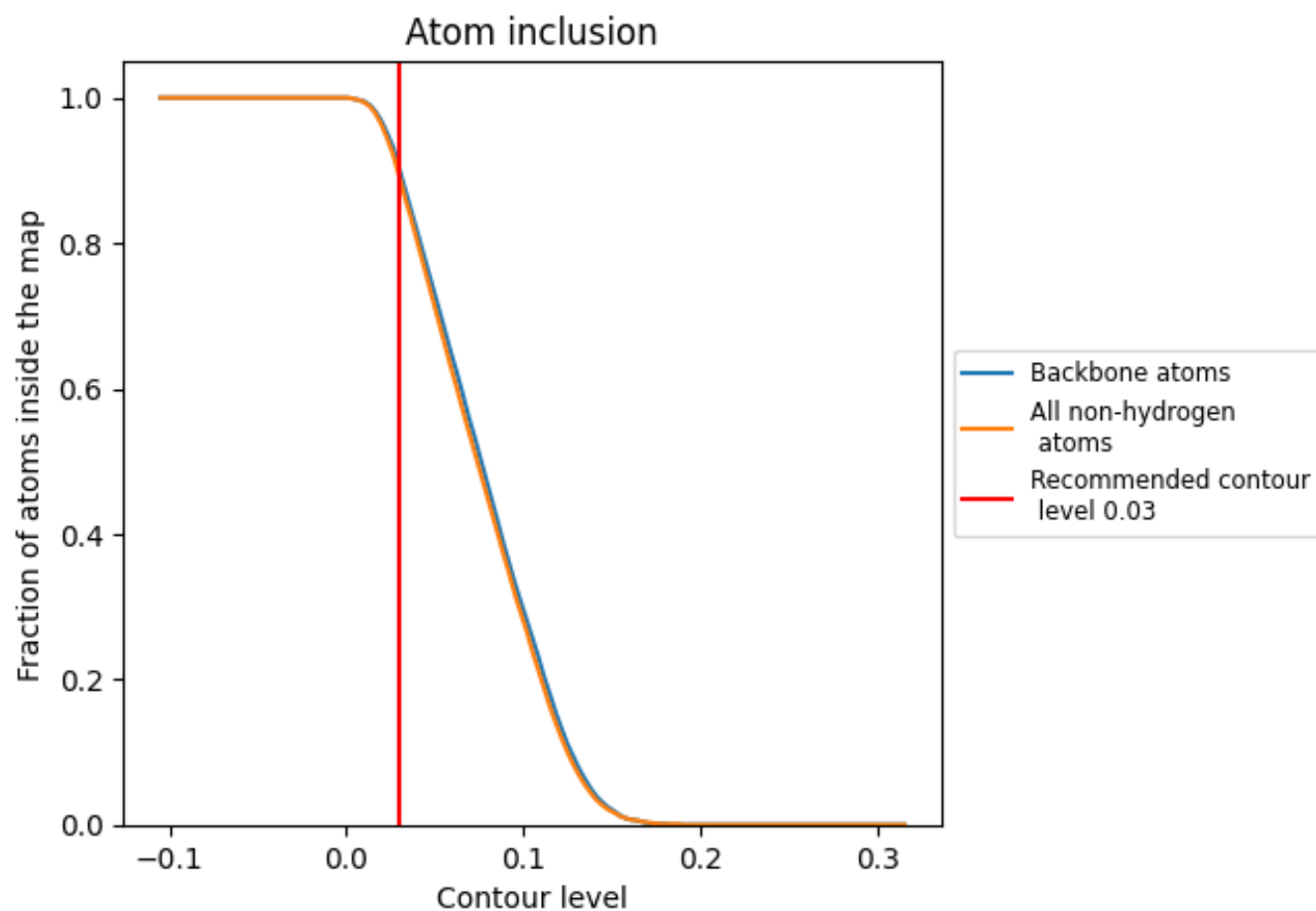
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.6760
0	 0.8830	 0.6580
1	 0.8970	 0.6610
2	 0.8000	 0.6200
3	 0.8760	 0.6530
4	 0.8550	 0.6490
5	 0.9020	 0.6750
6	 0.8410	 0.6380
7	 0.9080	 0.6750
8	 0.8690	 0.6580
9	 0.9380	 0.7020
A	 0.8920	 0.6700
B	 0.9050	 0.6820
C	 0.9680	 0.7240
D	 0.9040	 0.6730
E	 0.8750	 0.6610
F	 0.9390	 0.6820
G	 0.8720	 0.6590
H	 0.9370	 0.6960
I	 0.8910	 0.6690
J	 0.8450	 0.6430
K	 0.8860	 0.6530
L	 0.9620	 0.7280
M	 0.9680	 0.7290
N	 0.8610	 0.6580
O	 0.9430	 0.6890
P	 0.9110	 0.6720
Q	 0.9300	 0.6860
R	 0.8950	 0.6780
S	 0.9080	 0.6710
T	 0.7890	 0.6170
U	 0.8660	 0.6510
V	 0.8130	 0.6360
W	 0.8630	 0.6590
X	 0.8190	 0.6330



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.8870	 0.6590
Z	 0.8560	 0.6430
a	 0.5780	 0.5470
b	 0.8150	 0.6400
c	 0.6010	 0.5570
d	 0.4510	 0.5070
e	 0.4970	 0.5040
f	 0.8210	 0.6180
g	 0.6880	 0.5940
h	 0.8270	 0.6330
i	 0.5670	 0.5550
j	 0.6470	 0.5740
k	 0.5140	 0.4980