



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:12 AM UTC

PDB ID : 7C9R / pdb_00007c9r
EMDB ID : EMD-30314
Title : STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF THIORHODOVIBRIO STRAIN 970
Authors : Tani, K.; Kanno, R.; Makino, Y.; Hall, M.; Takenouchi, M.; Imanishi, M.; Yu, L.-J.; Overmann, J.; Madigan, M.T.; Kimura, Y.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2020-06-07
Resolution : 2.82 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:

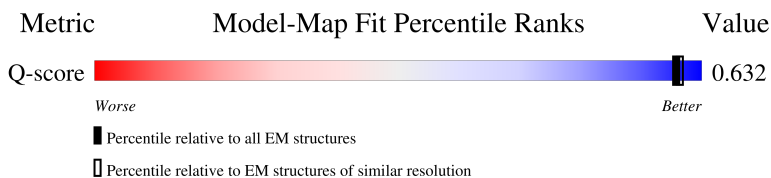
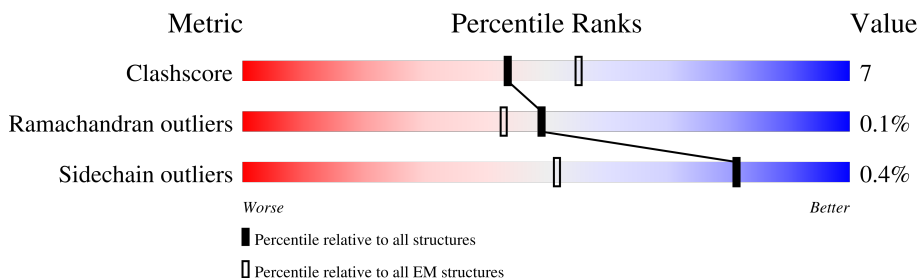
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

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 2.82 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	11795 (2.32 - 3.32)

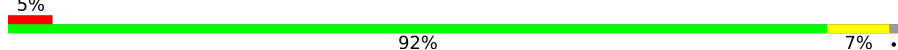
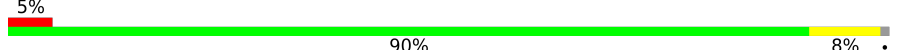
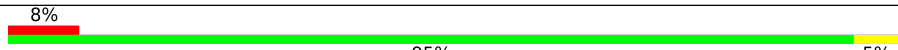
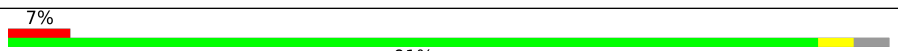
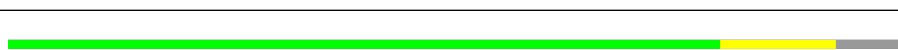
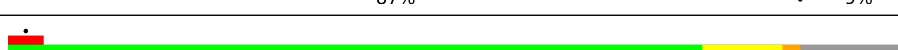
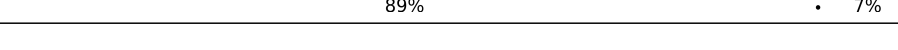
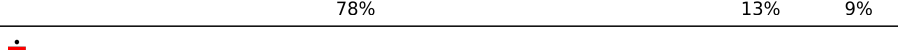
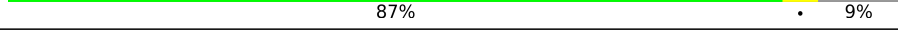
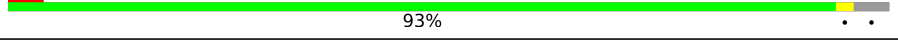
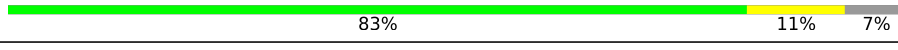
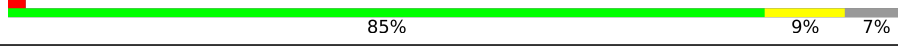
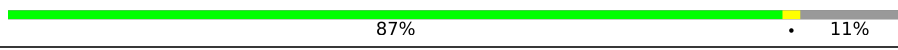
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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	396	
2	L	273	
3	M	324	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
4	H	258	
5	A	73	
5	D	73	
5	F	73	
5	I	73	
5	K	73	
5	O	73	
6	4	46	
6	B	46	
6	P	46	
7	0	46	
7	2	46	
7	6	46	
7	8	46	
7	E	46	
7	G	46	
7	J	46	
7	N	46	
7	R	46	
7	T	46	
7	V	46	
7	X	46	
7	Z	46	
8	Q	81	
9	1	77	

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Mol	Chain	Length	Quality of chain
9	3	77	6% 87% 5% • 5%
9	5	77	8% 91% 5% •
9	7	77	5% 87% 8% 5%
9	S	77	10% 81% 13% 6%
9	U	77	6% 90% • 6%
9	W	77	• 88% 5% • 5%
9	Y	77	5% 88% 6% 5%
10	9	86	5% 88% 9% •

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 29228 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	311	Total	C	N	O	S	0	0
			2433	1536	423	458	16		

- Molecule 2 is a protein called L subunit of the reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	272	Total	C	N	O	S	0	0
			2161	1459	350	344	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	318	Total	C	N	O	S	0	0
			2535	1700	408	416	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	257	Total	C	N	O	S	0	0
			2017	1298	348	366	5		

- Molecule 5 is a protein called Alpha subunit 1 of light-harvesting 1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	70	Total	C	N	O	S	0	0
			563	373	89	96	5		
5	D	72	Total	C	N	O	S	0	0
			580	382	93	100	5		
5	F	72	Total	C	N	O	S	0	0
			580	382	93	100	5		
5	I	73	Total	C	N	O	S	0	0
			588	387	94	101	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	72	Total	C	N	O	S	0	0
			580	382	93	100	5		
5	O	73	Total	C	N	O	S	0	0
			588	387	94	101	6		

- Molecule 6 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	43	Total	C	N	O	S	0	0
			352	236	55	58	3		
6	P	42	Total	C	N	O	S	0	0
			343	230	53	57	3		
6	4	44	Total	C	N	O	S	0	0
			361	241	56	61	3		

- Molecule 7 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	42	Total	C	N	O	S	0	0
			343	230	53	58	2		
7	G	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	J	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	N	42	Total	C	N	O	S	0	0
			343	230	53	58	2		
7	R	44	Total	C	N	O	S	0	0
			361	241	56	62	2		
7	T	43	Total	C	N	O	S	0	0
			352	236	55	59	2		
7	V	43	Total	C	N	O	S	0	0
			352	236	55	59	2		
7	X	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	Z	42	Total	C	N	O	S	0	0
			343	230	53	58	2		
7	2	41	Total	C	N	O	S	0	0
			337	227	52	56	2		
7	6	43	Total	C	N	O	S	0	0
			352	236	55	59	2		
7	8	42	Total	C	N	O	S	0	0
			343	230	53	58	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	0	41	Total	C	N	O	S	0	0
			337	227	52	56	2		

- Molecule 8 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	78	Total	C	N	O	S	0	0
			628	416	101	107	4		

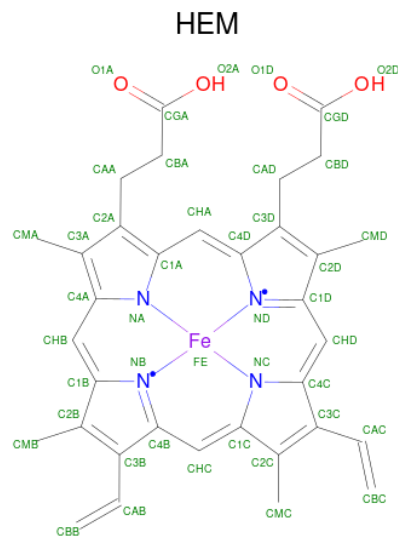
- Molecule 9 is a protein called LHC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	72	Total	C	N	O	S	0	0
			579	382	92	99	6		
9	U	72	Total	C	N	O	S	0	0
			576	382	91	98	5		
9	W	73	Total	C	N	O	S	0	0
			584	386	92	101	5		
9	Y	73	Total	C	N	O	S	0	0
			584	386	92	101	5		
9	1	72	Total	C	N	O	S	0	0
			576	382	91	98	5		
9	3	73	Total	C	N	O	S	0	0
			584	386	93	100	5		
9	5	74	Total	C	N	O	S	0	0
			589	389	94	101	5		
9	7	73	Total	C	N	O	S	0	0
			584	386	93	100	5		

- Molecule 10 is a protein called Alpha subunit 2 of light-harvesting 1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	84	Total	C	N	O	S	0	0
			668	440	113	111	4		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
12	C	1	Total Mg 1 1	0

- Molecule 13 is CALCIUM ION (CCD ID: CA) (formula: Ca).

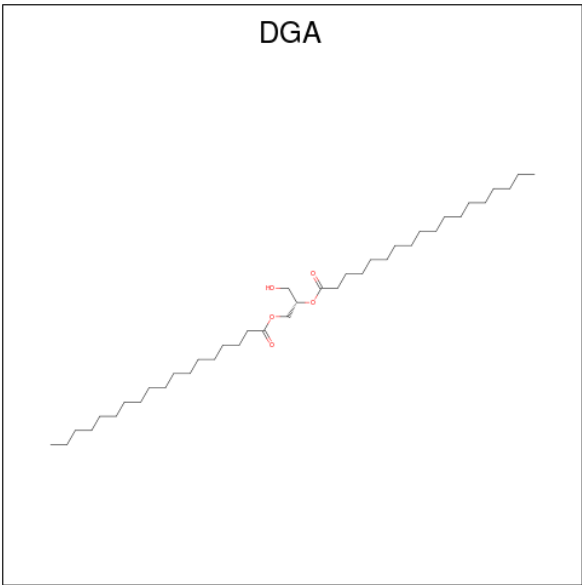
Mol	Chain	Residues	Atoms		AltConf
13	C	1	Total 1	Ca 1	0
13	A	1	Total 1	Ca 1	0
13	D	1	Total 1	Ca 1	0
13	F	1	Total 1	Ca 1	0

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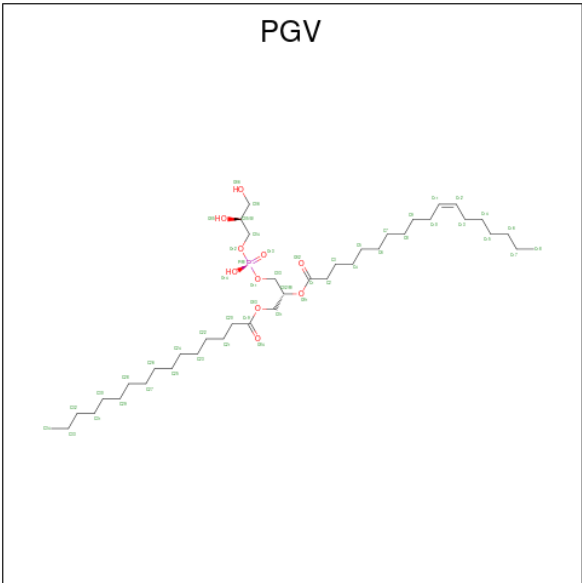
Mol	Chain	Residues	Atoms		AltConf
13	I	1	Total 1	Ca 1	0
13	K	1	Total 1	Ca 1	0
13	O	1	Total 1	Ca 1	0
13	Q	1	Total 1	Ca 1	0
13	S	1	Total 1	Ca 1	0
13	U	1	Total 1	Ca 1	0
13	W	1	Total 1	Ca 1	0
13	Y	1	Total 1	Ca 1	0
13	1	1	Total 1	Ca 1	0
13	3	1	Total 1	Ca 1	0
13	5	1	Total 1	Ca 1	0
13	7	1	Total 1	Ca 1	0
13	9	1	Total 1	Ca 1	0

- Molecule 14 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			AltConf
14	C	1	Total	C	O	0
			32	28	4	

- Molecule 15 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



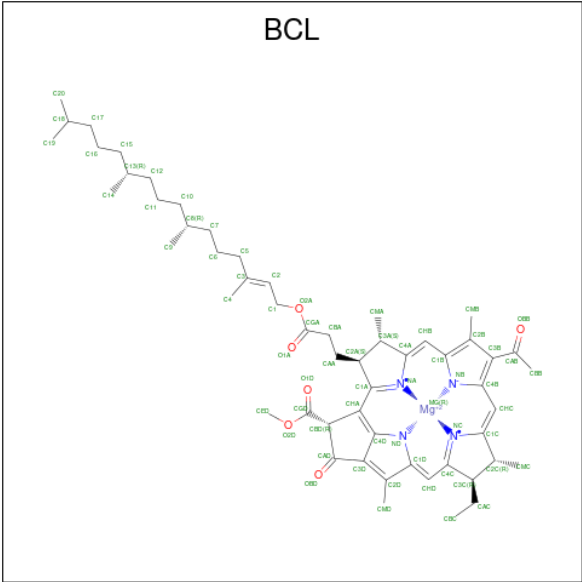
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			16	9	6	1	
15	L	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			39	28	10	1	
15	H	1	Total	C	O	P	0
			36	25	10	1	
15	A	1	Total	C	O	P	0
			23	12	10	1	
15	D	1	Total	C	O	P	0
			43	32	10	1	
15	F	1	Total	C	O	P	0
			34	25	8	1	
15	F	1	Total	C	O	P	0
			37	26	10	1	
15	I	1	Total	C	O	P	0
			41	32	8	1	
15	K	1	Total	C	O	P	0
			36	25	10	1	
15	K	1	Total	C	O	P	0
			19	10	8	1	
15	K	1	Total	C	O	P	0
			43	34	8	1	
15	O	1	Total	C	O	P	0
			44	33	10	1	
15	Q	1	Total	C	O	P	0
			38	27	10	1	
15	Y	1	Total	C	O	P	0
			27	18	8	1	
15	1	1	Total	C	O	P	0
			26	17	8	1	
15	3	1	Total	C	O	P	0
			47	36	10	1	
15	5	1	Total	C	O	P	0
			47	36	10	1	
15	9	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 16 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	K	1	Total 66	C 55	Mg 1	N 4	O 6	0

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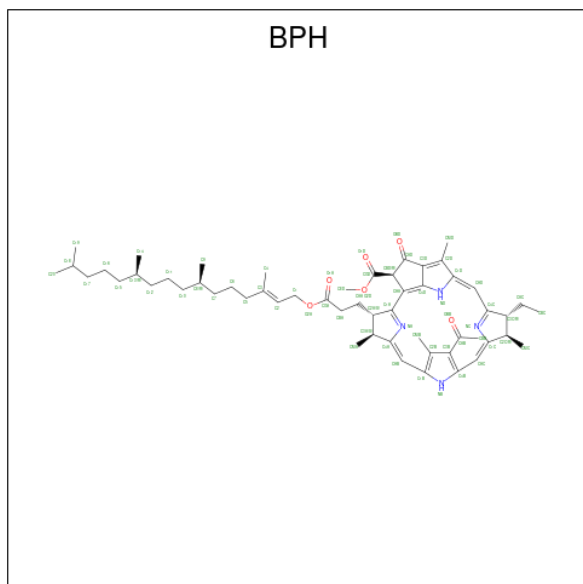
Mol	Chain	Residues	Atoms					AltConf
16	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
16	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	9	1	Total 66	C 55	Mg 1	N 4	O 6	0

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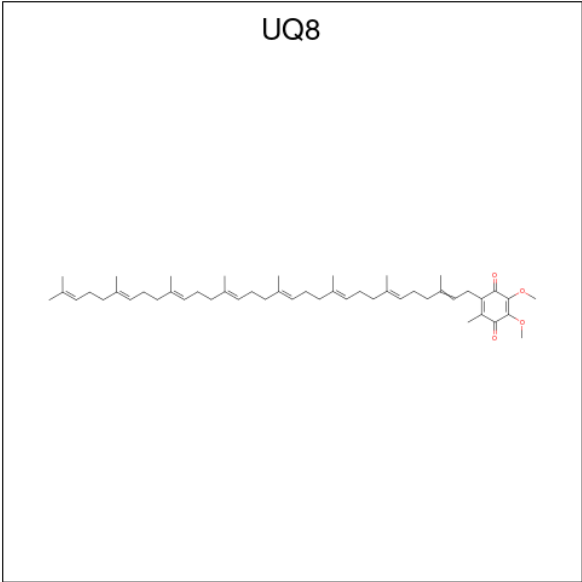
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	9	1	66	55	1	4	6	0

- Molecule 17 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



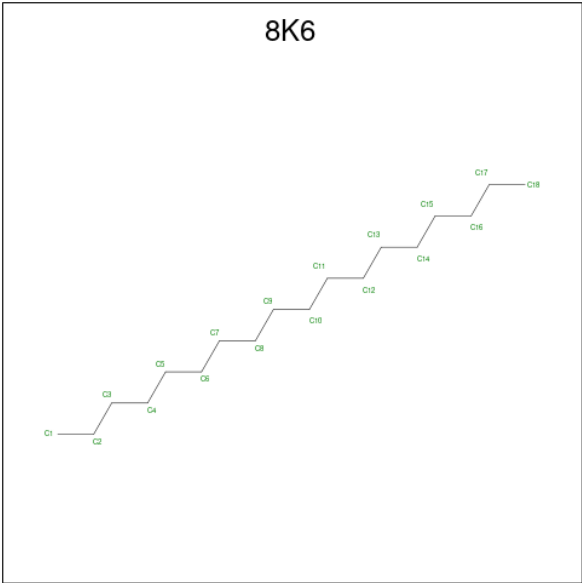
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	L	1	65	55	4	6	0
17	M	1	65	55	4	6	0

- Molecule 18 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			AltConf
18	L	1	Total	C	O	0
			33	29	4	
18	L	1	Total	C	O	0
			33	29	4	

- Molecule 19 is Octadecane (CCD ID: 8K6) (formula: C₁₈H₃₈).

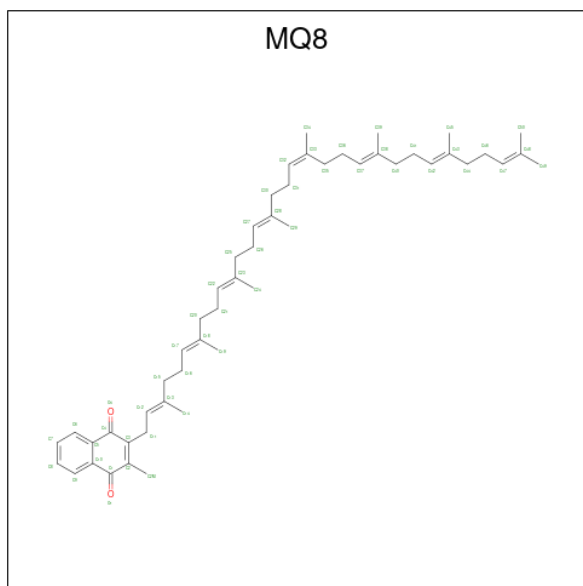


Mol	Chain	Residues	Atoms		AltConf
19	L	1	Total	C	0
			18	18	
19	5	1	Total	C	0
			15	15	

- Molecule 20 is FE (III) ION (CCD ID: FE) (formula: Fe).

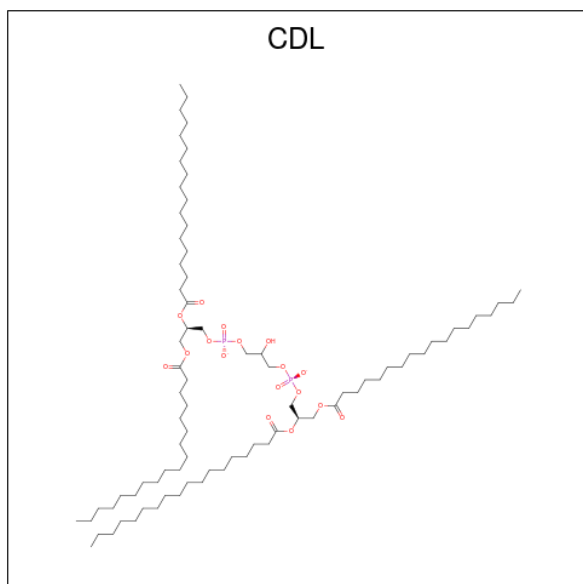
Mol	Chain	Residues	Atoms		AltConf
20	M	1	Total	Fe	0
			1	1	

- Molecule 21 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂).



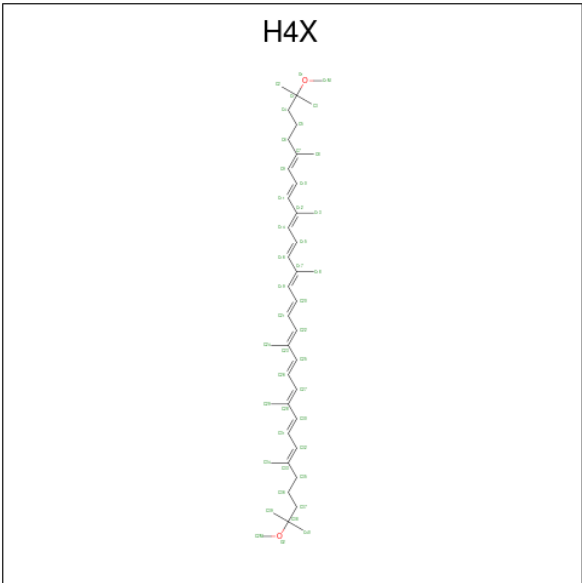
Mol	Chain	Residues	Atoms			AltConf
21	M	1	Total	C	O	0
			53	51	2	

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
22	H	1	Total	C	O	P	0
			73	54	17	2	
22	S	1	Total	C	O	P	0
			74	55	17	2	
22	Y	1	Total	C	O	P	0
			30	14	14	2	

- Molecule 23 is (6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E},26 {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-undecaene (CCD ID: H4X) (formula: C₄₂H₆₄O₂).



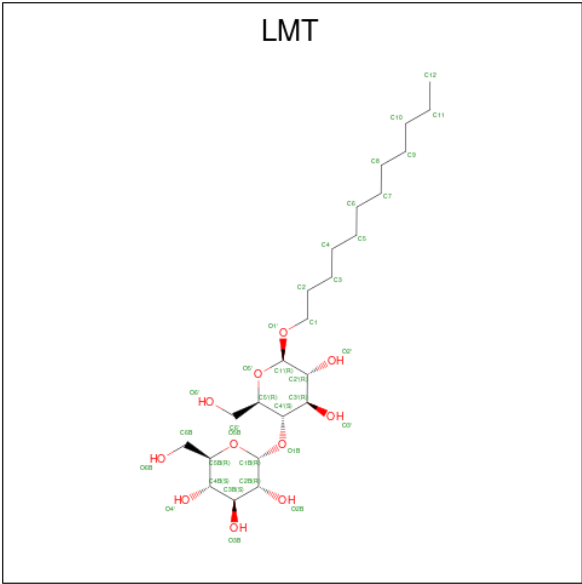
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			44	42	2	
23	E	1	Total	C	O	0
			44	42	2	
23	G	1	Total	C	O	0
			44	42	2	
23	K	1	Total	C	O	0
			44	42	2	
23	K	1	Total	C	O	0
			44	42	2	
23	O	1	Total	C	O	0
			44	42	2	
23	O	1	Total	C	O	0
			44	42	2	
23	P	1	Total	C	O	0
			44	42	2	

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Mol	Chain	Residues	Atoms			AltConf
23	Q	1	Total	C	O	0
			44	42	2	
23	U	1	Total	C	O	0
			44	42	2	
23	V	1	Total	C	O	0
			44	42	2	
23	Z	1	Total	C	O	0
			44	42	2	
23	2	1	Total	C	O	0
			44	42	2	
23	4	1	Total	C	O	0
			44	42	2	
23	5	1	Total	C	O	0
			44	42	2	
23	6	1	Total	C	O	0
			44	42	2	
23	7	1	Total	C	O	0
			44	42	2	

- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			35	24	11	
24	B	1	Total	C	O	0
			35	24	11	

Continued on next page...

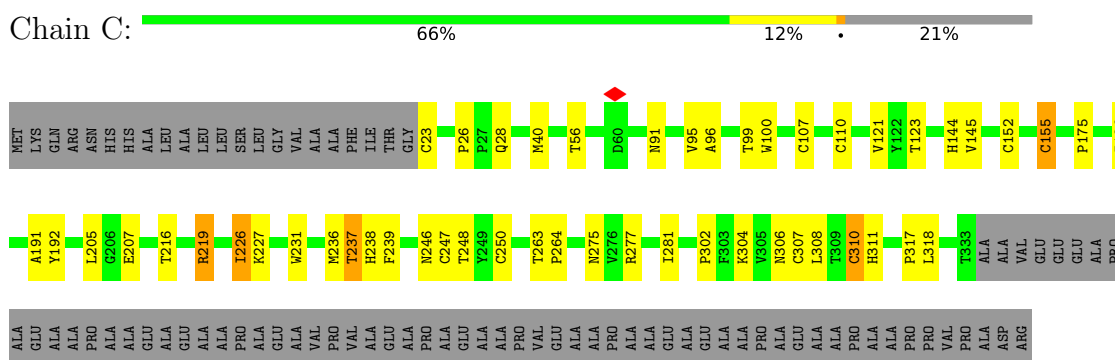
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Mol	Chain	Residues	Atoms			AltConf
24	E	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	
24	J	1	Total	C	O	0
			35	24	11	
24	N	1	Total	C	O	0
			35	24	11	
24	P	1	Total	C	O	0
			35	24	11	
24	R	1	Total	C	O	0
			35	24	11	
24	T	1	Total	C	O	0
			35	24	11	
24	V	1	Total	C	O	0
			35	24	11	
24	X	1	Total	C	O	0
			35	24	11	
24	Z	1	Total	C	O	0
			35	24	11	
24	2	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			35	24	11	
24	6	1	Total	C	O	0
			35	24	11	
24	8	1	Total	C	O	0
			35	24	11	
24	8	1	Total	C	O	0
			35	24	11	
24	0	1	Total	C	O	0
			35	24	11	

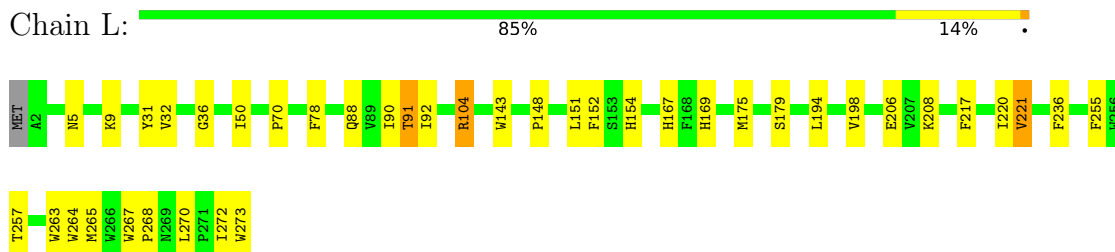
3 Residue-property plots

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.

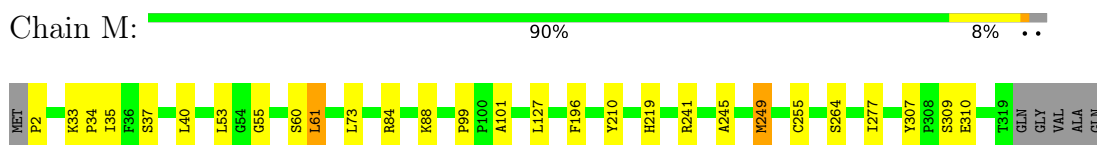
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



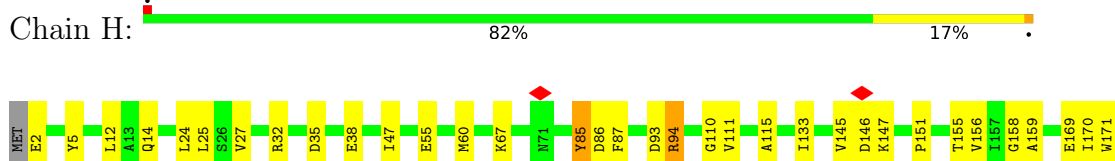
- Molecule 2: L subunit of the reaction center



- Molecule 3: Reaction center protein M chain

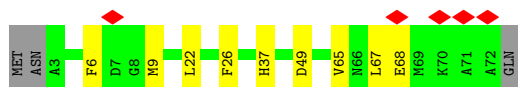
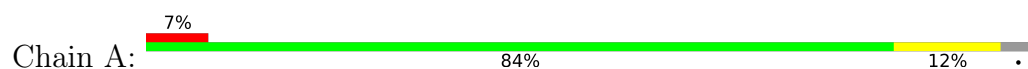


- Molecule 4: Photosynthetic reaction center, subunit H, bacterial





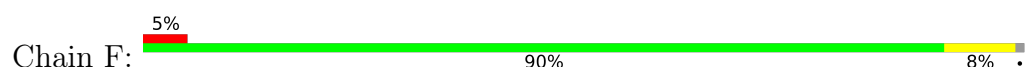
- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



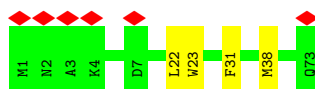
- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



- Molecule 5: Alpha subunit 1 of light-harvesting 1 complex



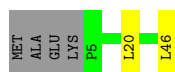
- Molecule 6: Antenna complex alpha/beta subunit

Chain B:  80% 13% 7%

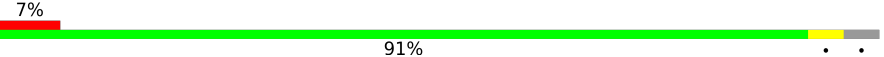


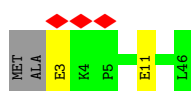
- Molecule 6: Antenna complex alpha/beta subunit

Chain P:  87% 9%



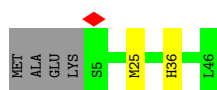
- Molecule 6: Antenna complex alpha/beta subunit

Chain 4:  7% 91%



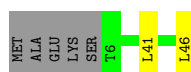
- Molecule 7: Antenna complex alpha/beta subunit

Chain E:  87% 9%



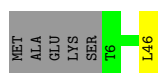
- Molecule 7: Antenna complex alpha/beta subunit

Chain G:  85% 11%



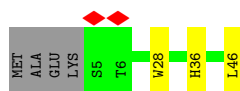
- Molecule 7: Antenna complex alpha/beta subunit

Chain J:  87% 11%



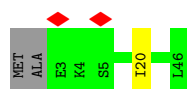
- Molecule 7: Antenna complex alpha/beta subunit

Chain N:  85% 7% 9%



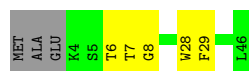
- Molecule 7: Antenna complex alpha/beta subunit

Chain R:  93%



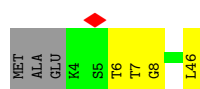
- Molecule 7: Antenna complex alpha/beta subunit

Chain T:  83% 11% 7%



- Molecule 7: Antenna complex alpha/beta subunit

Chain V:  85% 9% 7%



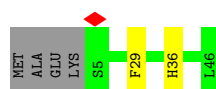
- Molecule 7: Antenna complex alpha/beta subunit

Chain X:  87% 11%



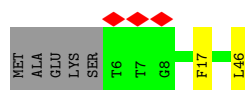
- Molecule 7: Antenna complex alpha/beta subunit

Chain Z:  87% 9%



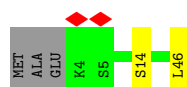
- Molecule 7: Antenna complex alpha/beta subunit

Chain 2:  85% 11% 7%



- Molecule 7: Antenna complex alpha/beta subunit

Chain 6:  89% 7%



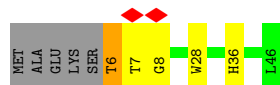
- Molecule 7: Antenna complex alpha/beta subunit

Chain 8:  78% 13% 9%



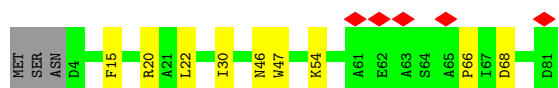
- Molecule 7: Antenna complex alpha/beta subunit

Chain 0:  78% 9% 11%



- Molecule 8: Antenna complex alpha/beta subunit

Chain Q:  6% 85% 11%

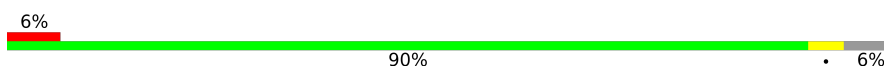


- Molecule 9: LHC domain-containing protein

Chain S:  10% 81% 13% 6%

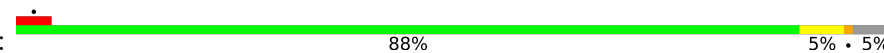


- Molecule 9: LHC domain-containing protein

Chain U:  6% 90% 6%

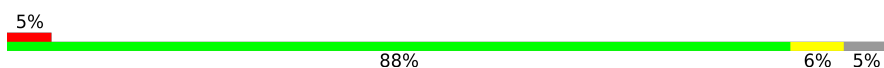


- Molecule 9: LHC domain-containing protein

Chain W:  88% 5% 5%

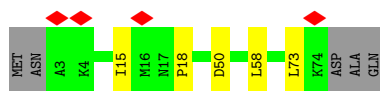
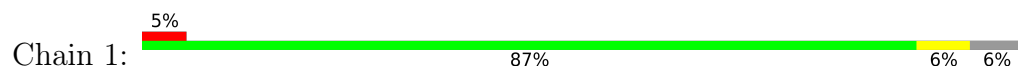


- Molecule 9: LHC domain-containing protein

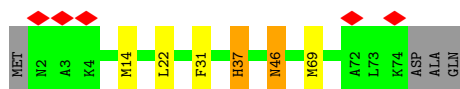
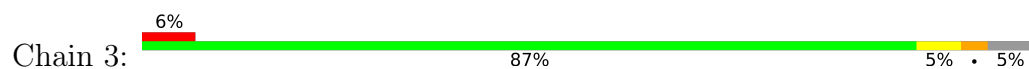
Chain Y:  5% 88% 6% 5%



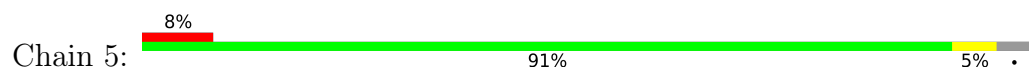
- Molecule 9: LHC domain-containing protein



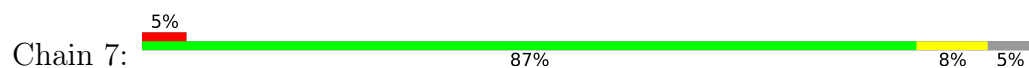
- Molecule 9: LHC domain-containing protein



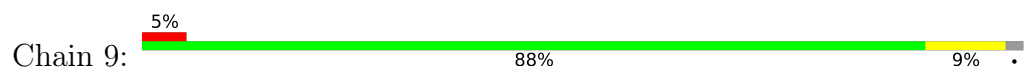
- Molecule 9: LHC domain-containing protein



- Molecule 9: LHC domain-containing protein



- Molecule 10: Alpha subunit 2 of light-harvesting 1 complex



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105234	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.263	Depositor
Minimum map value	-0.159	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.037	Depositor
Map size ($\text{\AA}$)	336.0, 336.0, 336.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, UQ8, DGA, CA, MG, MQ8, LMT, BCL, H4X, 8K6, PGV, CDL, FE, BPH

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	0.89	6/2503 (0.2%)	1.09	11/3423 (0.3%)
2	L	0.87	5/2244 (0.2%)	1.05	6/3068 (0.2%)
3	M	0.78	2/2633 (0.1%)	1.03	3/3599 (0.1%)
4	H	0.63	0/2069	1.01	2/2811 (0.1%)
5	A	0.91	1/579 (0.2%)	0.98	0/787
5	D	0.81	1/596 (0.2%)	0.97	0/810
5	F	0.80	0/596	0.92	0/810
5	I	0.75	1/604 (0.2%)	0.90	0/820
5	K	0.76	0/596	0.91	1/810 (0.1%)
5	O	0.80	0/604	0.93	0/820
6	4	0.69	0/374	0.73	0/506
6	B	1.02	3/365 (0.8%)	0.83	0/494
6	P	0.74	0/356	0.71	0/482
7	0	0.79	1/349 (0.3%)	0.91	0/474
7	2	0.64	0/349	0.69	0/474
7	6	0.76	0/364	0.78	0/493
7	8	0.78	0/355	0.79	0/482
7	E	0.81	1/355 (0.3%)	0.75	0/482
7	G	0.76	0/349	0.72	0/474
7	J	0.73	0/349	0.71	0/474
7	N	0.77	1/355 (0.3%)	0.72	0/482
7	R	0.72	0/373	0.81	0/505
7	T	0.69	0/364	0.72	0/493
7	V	0.72	0/364	0.76	0/493
7	X	0.67	0/349	0.75	1/474 (0.2%)
7	Z	0.69	1/355 (0.3%)	0.71	0/482
8	Q	0.67	0/649	0.93	0/881
9	1	0.78	0/592	0.88	0/805
9	3	0.78	1/600 (0.2%)	0.93	1/816 (0.1%)
9	5	0.79	0/605	0.85	0/823
9	7	0.88	1/600 (0.2%)	1.07	2/816 (0.2%)
9	S	0.82	0/595	1.00	1/808 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	U	0.82	0/592	0.89	0/805
9	W	0.73	0/600	0.86	0/816
9	Y	0.75	1/600 (0.2%)	0.86	0/816
10	9	0.70	0/690	1.14	0/941
All	All	0.78	26/24872 (0.1%)	0.95	28/33849 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
5	A	0	1
5	K	0	1
7	0	0	1
9	1	0	1
All	All	0	5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	ARG	CZ-NH1	18.83	1.59	1.32
1	C	219	ARG	NE-CZ	14.01	1.48	1.33
6	B	42	TYR	CZ-OH	11.38	1.61	1.38
2	L	167	HIS	CE1-NE2	8.83	1.41	1.32
2	L	154	HIS	CE1-NE2	8.28	1.40	1.32
2	L	167	HIS	CG-ND1	7.91	1.47	1.38
7	E	36	HIS	CE1-NE2	6.46	1.39	1.32
9	Y	37	HIS	CE1-NE2	6.36	1.39	1.32
1	C	219	ARG	CD-NE	6.28	1.55	1.46
9	3	37	HIS	CE1-NE2	6.28	1.38	1.32
5	A	65	VAL	C-O	-6.16	1.17	1.24
7	N	36	HIS	CE1-NE2	6.04	1.38	1.32
2	L	169	HIS	CE1-NE2	5.71	1.38	1.32
6	B	18	HIS	CE1-NE2	5.54	1.38	1.32
7	0	36	HIS	CE1-NE2	5.48	1.38	1.32
1	C	311	HIS	CE1-NE2	5.35	1.37	1.32
3	M	249	MET	CG-SD	5.35	1.94	1.80
7	Z	36	HIS	CE1-NE2	5.34	1.37	1.32
1	C	219	ARG	CZ-NH2	-5.24	1.26	1.33
9	7	48	HIS	CE1-NE2	5.19	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	179	SER	CA-CB	-5.16	1.45	1.53
5	D	37	HIS	ND1-CE1	-5.15	1.27	1.32
3	M	219	HIS	CE1-NE2	5.14	1.37	1.32
1	C	238	HIS	CG-ND1	5.10	1.43	1.38
5	I	37	HIS	CE1-NE2	5.06	1.37	1.32
6	B	36	HIS	CE1-NE2	5.03	1.37	1.32

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	ARG	NE-CZ-NH1	-7.78	113.72	121.50
1	C	219	ARG	NE-CZ-NH2	7.14	125.63	119.20
1	C	155	CYS	CB-CA-C	-6.85	98.14	109.65
5	K	46	ASN	OD1-CG-ND2	-6.70	115.91	122.60
1	C	219	ARG	CB-CA-C	6.48	119.56	109.84
9	7	3	ALA	N-CA-CB	-6.32	99.29	110.42
2	L	267	TRP	O-C-N	-6.23	115.97	120.27
2	L	148	PRO	CB-CA-C	-6.16	102.10	110.60
1	C	186	ILE	CA-C-N	-6.12	109.41	121.41
1	C	186	ILE	C-N-CA	-6.12	109.41	121.41
1	C	175	PRO	CB-CA-C	-6.02	103.69	111.39
9	S	26	PHE	CA-CB-CG	5.73	119.53	113.80
3	M	196	PHE	N-CA-C	5.69	119.73	112.34
1	C	239	PHE	CB-CA-C	-5.68	101.02	110.68
1	C	246	ASN	CB-CA-C	-5.68	99.74	111.22
3	M	61	LEU	N-CA-CB	5.58	119.92	110.49
9	7	6	PHE	CA-C-O	-5.55	113.04	119.59
1	C	310	CYS	CB-CA-C	-5.55	99.70	109.02
7	X	6	THR	CA-CB-OG1	-5.51	101.34	109.60
2	L	91	THR	OG1-CB-CG2	-5.42	98.46	109.30
9	3	46	ASN	OD1-CG-ND2	-5.39	117.21	122.60
2	L	152	PHE	N-CA-CB	5.35	119.53	110.49
4	H	85	TYR	CB-CA-C	5.33	121.03	110.42
3	M	307	TYR	N-CA-C	5.28	115.67	109.60
1	C	237	THR	OG1-CB-CG2	-5.17	98.96	109.30
2	L	104	ARG	CG-CD-NE	-5.16	100.64	112.00
2	L	5	ASN	CB-CA-C	-5.15	100.17	110.42
4	H	94	ARG	CD-NE-CZ	5.06	131.48	124.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	0	6	THR	Peptide
9	1	15	ILE	Mainchain
5	A	68	GLU	Mainchain
1	C	219	ARG	Sidechain
5	K	42	SER	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2433	0	2339	57	0
2	L	2161	0	2138	33	0
3	M	2535	0	2502	24	0
4	H	2017	0	2015	39	0
5	A	563	0	565	8	0
5	D	580	0	579	2	0
5	F	580	0	579	4	0
5	I	588	0	591	4	0
5	K	580	0	579	8	0
5	O	588	0	591	6	0
6	4	361	0	354	3	0
6	B	352	0	348	3	0
6	P	343	0	336	1	0
7	0	337	0	332	9	0
7	2	337	0	332	2	0
7	6	352	0	350	2	0
7	8	343	0	337	5	0
7	E	343	0	337	1	0
7	G	337	0	332	2	0
7	J	337	0	332	1	0
7	N	343	0	337	2	0
7	R	361	0	356	2	0
7	T	352	0	350	4	0
7	V	352	0	350	3	0
7	X	337	0	332	0	0
7	Z	343	0	337	1	0
8	Q	628	0	617	8	0
9	1	576	0	578	5	0
9	3	584	0	584	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	5	589	0	586	4	0
9	7	584	0	584	2	0
9	S	579	0	583	10	0
9	U	576	0	578	3	0
9	W	584	0	582	5	0
9	Y	584	0	582	5	0
10	9	668	0	673	7	0
11	C	172	0	120	29	0
12	C	1	0	0	0	0
13	1	1	0	0	0	0
13	3	1	0	0	0	0
13	5	1	0	0	0	0
13	7	1	0	0	0	0
13	9	1	0	0	0	0
13	A	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	F	1	0	0	0	0
13	I	1	0	0	0	0
13	K	1	0	0	0	0
13	O	1	0	0	0	0
13	Q	1	0	0	0	0
13	S	1	0	0	0	0
13	U	1	0	0	0	0
13	W	1	0	0	0	0
13	Y	1	0	0	0	0
14	C	32	0	45	6	0
15	1	26	0	25	0	0
15	3	47	0	65	4	0
15	5	47	0	65	4	0
15	9	47	0	65	2	0
15	A	23	0	18	0	0
15	C	16	0	11	0	0
15	D	43	0	59	0	0
15	F	71	0	83	2	0
15	H	36	0	42	1	0
15	I	41	0	53	0	0
15	K	98	0	117	3	0
15	L	47	0	62	3	0
15	M	39	0	48	1	0
15	O	44	0	61	5	0
15	Q	38	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Y	27	0	27	6	0
16	1	66	0	74	4	0
16	2	66	0	74	2	0
16	3	132	0	148	11	0
16	5	132	0	148	8	0
16	7	127	0	135	7	0
16	9	132	0	148	7	0
16	A	66	0	74	7	0
16	B	66	0	74	2	0
16	D	132	0	148	5	0
16	F	132	0	148	5	0
16	I	66	0	74	4	0
16	J	66	0	73	4	0
16	K	132	0	147	10	0
16	L	132	0	148	9	0
16	M	132	0	148	8	0
16	O	132	0	147	5	0
16	Q	132	0	147	8	0
16	S	66	0	74	6	0
16	T	66	0	74	3	0
16	U	132	0	147	9	0
16	W	66	0	74	3	0
16	X	66	0	74	2	0
16	Y	132	0	148	3	0
17	L	65	0	76	7	0
17	M	65	0	76	7	0
18	L	66	0	78	7	0
19	5	15	0	29	0	0
19	L	18	0	38	1	0
20	M	1	0	0	0	0
21	M	53	0	72	2	0
22	H	73	0	90	3	0
22	S	74	0	95	1	0
22	Y	30	0	17	0	0
23	2	44	0	0	0	0
23	4	44	0	0	0	0
23	5	44	0	0	0	0
23	6	44	0	0	0	0
23	7	44	0	0	0	0
23	B	44	0	0	0	0
23	E	44	0	0	1	0
23	G	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	K	88	0	0	0	0
23	O	88	0	0	1	0
23	P	44	0	0	0	0
23	Q	44	0	0	0	0
23	U	44	0	0	0	0
23	V	44	0	0	0	0
23	Z	44	0	0	0	0
24	0	35	0	46	1	0
24	2	35	0	46	2	0
24	4	35	0	46	3	0
24	6	35	0	46	2	0
24	8	70	0	92	5	0
24	B	70	0	92	5	0
24	E	35	0	46	2	0
24	G	35	0	46	1	0
24	J	35	0	46	2	0
24	N	35	0	46	3	0
24	P	35	0	46	2	0
24	R	35	0	46	2	0
24	T	35	0	46	2	0
24	V	35	0	46	1	0
24	X	35	0	46	2	0
24	Z	35	0	46	1	0
All	All	29228	0	28934	379	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 (379) 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:247:CYS:SG	11:C:403:HEM:HAB	1.52	1.47
1:C:247:CYS:SG	11:C:403:HEM:CAB	2.07	1.42
1:C:307:CYS:SG	11:C:404:HEM:HAB	1.66	1.36
1:C:155:CYS:SG	11:C:402:HEM:HAC	1.73	1.29
1:C:310:CYS:SG	11:C:404:HEM:CAC	2.28	1.21
1:C:307:CYS:SG	11:C:404:HEM:CAB	2.28	1.20
1:C:310:CYS:SG	11:C:404:HEM:HAC	1.93	1.07
1:C:250:CYS:SG	11:C:403:HEM:CAC	2.45	1.03
1:C:110:CYS:SG	11:C:401:HEM:HAC	1.99	1.01
1:C:155:CYS:SG	11:C:402:HEM:CAC	2.51	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:CYS:SG	11:C:403:HEM:CBC	2.54	0.96
17:M:404:BPH:HHC	17:M:404:BPH:HBB3	1.49	0.93
1:C:247:CYS:SG	11:C:403:HEM:CBB	2.57	0.93
1:C:152:CYS:SG	11:C:402:HEM:HAB	2.09	0.92
4:H:94:ARG:HD2	7:O:8:GLY:HA3	1.50	0.91
4:H:47:ILE:HG21	6:B:9:LEU:HD11	1.54	0.90
1:C:152:CYS:SG	11:C:402:HEM:CAB	2.60	0.90
1:C:307:CYS:CB	11:C:404:HEM:HAB	2.05	0.86
17:L:302:BPH:HHC	17:L:302:BPH:CBB	2.07	0.84
7:8:18:HIS:HE2	24:8:101:LMT:H6D	1.41	0.84
16:M:403:BCL:HMB1	16:M:403:BCL:HBB3	1.60	0.83
1:C:107:CYS:HB3	11:C:401:HEM:HAB	1.59	0.83
4:H:93:ASP:OD2	10:9:19:ARG:NH1	2.10	0.83
1:C:144:HIS:HD1	1:C:275:ASN:HD22	1.27	0.82
2:L:88:GLN:CD	18:L:306:UQ8:H4M	2.04	0.82
21:M:405:MQ8:H501	22:H:302:CDL:H631	1.63	0.80
4:H:94:ARG:HD2	7:O:8:GLY:CA	2.11	0.79
1:C:110:CYS:SG	11:C:401:HEM:CAC	2.71	0.78
3:M:73:LEU:HD11	9:S:35:LEU:HD12	1.64	0.78
2:L:272:ILE:O	9:W:38:MET:HE3	1.83	0.78
17:L:302:BPH:HHC	17:L:302:BPH:HBB3	1.63	0.77
4:H:94:ARG:CD	7:O:8:GLY:HA3	2.14	0.77
5:K:38:MET:HE3	15:K:101:PGV:H51	1.65	0.76
1:C:307:CYS:SG	11:C:404:HEM:CBB	2.74	0.75
1:C:107:CYS:CB	11:C:401:HEM:HAB	2.17	0.75
1:C:192:TYR:CD1	2:L:265:MET:HE3	2.21	0.75
2:L:31:TYR:O	2:L:104:ARG:NH1	2.21	0.73
2:L:198:VAL:HG23	2:L:208:LYS:HB2	1.69	0.73
4:H:47:ILE:HG21	6:B:9:LEU:CD1	2.18	0.73
2:L:272:ILE:HA	9:W:39:VAL:HG22	1.71	0.73
16:L:301:BCL:CBB	16:L:301:BCL:HMB3	2.20	0.72
15:F:104:PGV:H21	15:F:104:PGV:H202	1.70	0.71
16:9:103:BCL:ND	24:0:101:LMT:H101	2.06	0.71
1:C:250:CYS:SG	11:C:403:HEM:HAC	2.32	0.70
1:C:145:VAL:HG23	1:C:145:VAL:O	1.92	0.69
16:U:102:BCL:HBB3	16:U:102:BCL:HMB1	1.75	0.69
1:C:23:CYS:HA	14:C:407:DGA:HG2	1.76	0.68
2:L:92:ILE:HG21	18:L:306:UQ8:H15B	1.75	0.67
3:M:73:LEU:HD11	9:S:35:LEU:CD1	2.23	0.67
16:I:102:BCL:HBB3	16:I:102:BCL:HMB1	1.76	0.67
21:M:405:MQ8:C50	22:H:302:CDL:H631	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:PRO:HG2	10:9:70:ILE:HD13	1.75	0.66
5:K:16:MET:HE3	5:O:23:TRP:CZ2	2.30	0.66
16:D:103:BCL:ND	24:E:102:LMT:H101	2.11	0.65
9:5:10:HIS:O	7:6:14:SER:OG	2.14	0.65
2:L:220:ILE:HG22	2:L:221:VAL:HG23	1.79	0.64
17:M:404:BPH:HHC	17:M:404:BPH:CBB	2.25	0.64
23:G:101:H4X:C2M	5:I:38:MET:HE2	2.27	0.64
1:C:192:TYR:CG	2:L:265:MET:HE3	2.33	0.64
2:L:206:GLU:HG2	4:H:67:LYS:HD3	1.80	0.64
1:C:263:THR:HG22	10:9:86:ASN:HD21	1.62	0.64
14:C:407:DGA:HB41	15:Y:105:PGV:H011	1.80	0.64
16:S:103:BCL:HMB1	16:S:103:BCL:HBB3	1.80	0.64
5:A:26:PHE:HE1	16:A:102:BCL:H52	1.62	0.64
3:M:241:ARG:NH1	4:H:38:GLU:OE1	2.32	0.63
4:H:94:ARG:HB3	7:0:8:GLY:HA3	1.78	0.63
16:M:403:BCL:HMB1	16:M:403:BCL:CBB	2.29	0.62
7:J:46:LEU:HD13	24:N:101:LMT:H42	1.79	0.62
1:C:100:TRP:HB3	1:C:152:CYS:HB2	1.80	0.62
2:L:236:PHE:HB2	15:L:305:PGV:H281	1.82	0.62
16:W:102:BCL:ND	24:X:102:LMT:H101	2.15	0.62
5:A:26:PHE:CE1	16:A:102:BCL:H52	2.35	0.61
16:9:103:BCL:HMB1	16:9:103:BCL:HBB3	1.82	0.61
4:H:146:ASP:O	4:H:147:LYS:HB2	2.00	0.61
4:H:94:ARG:NH1	7:0:8:GLY:O	2.33	0.61
16:W:102:BCL:HMB1	16:W:102:BCL:HBB3	1.83	0.60
16:A:102:BCL:ND	24:B:104:LMT:H101	2.16	0.60
1:C:207:GLU:HG2	1:C:277:ARG:HD3	1.83	0.60
15:Q:101:PGV:H202	22:S:101:CDL:HA62	1.84	0.60
1:C:121:VAL:HG12	1:C:123:THR:H	1.66	0.59
16:J:101:BCL:HMB3	16:J:101:BCL:CBB	2.33	0.59
16:S:103:BCL:HMB1	16:S:103:BCL:CBB	2.33	0.59
6:P:46:LEU:HD13	24:R:101:LMT:H42	1.83	0.59
2:L:104:ARG:NH2	3:M:255:CYS:O	2.34	0.58
15:M:406:PGV:H42	5:O:38:MET:SD	2.44	0.58
16:L:301:BCL:HMB3	16:L:301:BCL:HBB3	1.85	0.57
16:D:103:BCL:HMB1	16:D:103:BCL:HBB3	1.86	0.57
9:5:38:MET:HG3	15:5:101:PGV:H231	1.85	0.57
16:S:103:BCL:ND	24:T:102:LMT:H101	2.19	0.57
7:T:6:THR:HG22	7:T:8:GLY:H	1.70	0.57
14:C:407:DGA:HG11	14:C:407:DGA:HA42	1.86	0.57
16:Q:103:BCL:ND	24:R:101:LMT:H101	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:73:LEU:CD1	9:S:35:LEU:HD12	2.33	0.57
15:3:101:PGV:O12	15:3:101:PGV:O06	2.16	0.57
16:9:103:BCL:HMB1	16:9:103:BCL:CBB	2.36	0.56
2:L:255:PHE:HZ	15:3:101:PGV:H212	1.71	0.56
15:5:101:PGV:H51	15:5:101:PGV:O01	2.05	0.56
1:C:227:LYS:O	1:C:231:TRP:HD1	1.88	0.56
16:K:108:BCL:CBB	16:K:108:BCL:HMB3	2.36	0.55
16:O:105:BCL:H42	16:Q:103:BCL:H171	1.88	0.55
1:C:307:CYS:CA	11:C:404:HEM:HAB	2.36	0.55
18:L:306:UQ8:H4MA	18:L:306:UQ8:H3MB	1.88	0.55
4:H:24:LEU:O	4:H:25:LEU:HB3	2.06	0.55
3:M:73:LEU:HD12	9:S:38:MET:HE3	1.88	0.54
15:5:101:PGV:H91	15:5:101:PGV:H202	1.89	0.54
9:5:42:SER:O	15:5:101:PGV:H061	2.07	0.54
1:C:191:ALA:HB3	1:C:237:THR:CG2	2.37	0.54
2:L:273:TRP:CD1	2:L:273:TRP:C	2.86	0.54
3:M:53:LEU:O	8:Q:20:ARG:NH1	2.41	0.54
16:U:102:BCL:HMB1	16:U:102:BCL:CBB	2.37	0.54
16:M:402:BCL:H11	17:M:404:BPH:H203	1.89	0.54
16:K:105:BCL:HBB3	16:K:105:BCL:HMB1	1.89	0.54
1:C:192:TYR:HB3	2:L:265:MET:CE	2.37	0.54
3:M:101:ALA:HB3	8:Q:66:PRO:HB3	1.89	0.54
16:O:104:BCL:ND	24:P:102:LMT:H101	2.23	0.53
16:A:102:BCL:C1D	24:B:104:LMT:H101	2.38	0.53
7:G:46:LEU:HD13	24:J:102:LMT:H42	1.91	0.53
1:C:26:PRO:HG2	15:3:101:PGV:H201	1.91	0.53
5:D:11:LYS:HG2	5:D:14:MET:HE2	1.90	0.53
3:M:55:GLY:HA3	15:O:102:PGV:H012	1.91	0.53
16:3:104:BCL:HMB3	16:3:104:BCL:CBB	2.39	0.53
9:1:58:LEU:HD23	9:3:69:MET:HE3	1.91	0.53
4:H:250:THR:HB	4:H:253:ARG:HG3	1.91	0.53
9:W:58:LEU:HD11	9:Y:70:LYS:HG3	1.91	0.53
16:1:102:BCL:ND	24:2:103:LMT:H101	2.24	0.53
16:7:102:BCL:ND	24:8:102:LMT:H101	2.23	0.52
16:F:103:BCL:ND	24:G:102:LMT:H101	2.24	0.52
5:A:49:ASP:OD1	10:9:44:ASP:N	2.43	0.52
16:1:102:BCL:CBB	16:1:102:BCL:HMB1	2.39	0.52
5:O:31:PHE:CE2	15:O:102:PGV:H281	2.45	0.52
15:Y:105:PGV:H62	15:Y:105:PGV:H201	1.90	0.52
16:M:403:BCL:CBB	16:M:403:BCL:CMB	2.87	0.52
16:D:103:BCL:HMB1	16:D:103:BCL:CBB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:6:PHE:CE1	24:B:102:LMT:H6E	2.45	0.52
16:U:102:BCL:ND	24:V:102:LMT:H101	2.24	0.52
4:H:155:THR:OG1	4:H:207:GLU:OE1	2.24	0.51
5:F:16:MET:HE3	5:I:23:TRP:CZ2	2.45	0.51
16:M:402:BCL:HBB2	16:M:402:BCL:HMB3	1.92	0.51
4:H:94:ARG:O	7:O:7:THR:O	2.28	0.51
17:L:302:BPH:H121	16:L:304:BCL:H172	1.93	0.51
5:D:57:GLN:O	5:D:61:GLU:HG2	2.10	0.51
23:O:106:H4X:C6	7:R:20:ILE:HD12	2.41	0.51
17:L:302:BPH:HHC	17:L:302:BPH:HBB2	1.90	0.51
16:S:103:BCL:H142	7:T:28:TRP:HZ3	1.75	0.51
1:C:216:THR:HB	4:H:5:TYR:CZ	2.46	0.51
7:8:18:HIS:HE2	24:8:101:LMT:C6'	2.19	0.51
16:5:103:BCL:ND	24:6:102:LMT:H101	2.27	0.50
16:L:301:BCL:CBB	16:L:301:BCL:CMB	2.89	0.50
7:V:6:THR:HG22	7:V:8:GLY:H	1.77	0.50
3:M:37:SER:HB3	3:M:40:LEU:HB2	1.94	0.50
4:H:146:ASP:O	4:H:147:LYS:CB	2.59	0.50
16:A:102:BCL:HMB1	16:A:102:BCL:HBB3	1.92	0.50
8:Q:54:LYS:HE3	9:S:69:MET:HE1	1.93	0.50
4:H:151:PRO:HD2	4:H:170:ILE:HD11	1.92	0.49
1:C:96:ALA:HA	1:C:99:THR:HG22	1.94	0.49
4:H:85:TYR:OH	4:H:110:GLY:HA3	2.12	0.49
5:K:16:MET:CE	5:O:23:TRP:CZ2	2.95	0.49
2:L:273:TRP:CD1	3:M:88:LYS:HB2	2.47	0.49
3:M:127:LEU:HB3	15:O:102:PGV:H331	1.93	0.49
4:H:145:VAL:HG12	4:H:146:ASP:O	2.13	0.49
16:K:105:BCL:C1D	24:N:101:LMT:H101	2.43	0.49
1:C:310:CYS:SG	11:C:404:HEM:CBC	2.98	0.49
4:H:85:TYR:OH	4:H:110:GLY:O	2.30	0.49
16:O:104:BCL:H62	16:O:104:BCL:H41	1.47	0.49
16:2:102:BCL:CBB	16:2:102:BCL:HMB3	2.43	0.48
17:M:404:BPH:HBC3	17:M:404:BPH:HHD	1.94	0.48
16:A:102:BCL:HMB1	16:A:102:BCL:CBB	2.43	0.48
2:L:9:LYS:HE2	4:H:115:ALA:HB1	1.95	0.48
2:L:143:TRP:NE1	18:L:306:UQ8:H4MB	2.28	0.48
17:M:404:BPH:CBB	17:M:404:BPH:CHC	2.92	0.48
16:J:101:BCL:HMB3	16:J:101:BCL:HBB2	1.95	0.48
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.95	0.48
8:Q:15:PHE:HD1	9:S:19:VAL:HG22	1.77	0.48
1:C:247:CYS:SG	11:C:403:HEM:HBB1	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:108:BCL:HMB3	16:K:108:BCL:HBB2	1.96	0.48
9:3:14:MET:HE1	6:4:11:GLU:HG3	1.95	0.48
8:Q:30:ILE:HG13	16:Q:103:BCL:H43	1.96	0.48
1:C:110:CYS:HA	1:C:123:THR:OG1	2.13	0.48
16:L:301:BCL:HMB3	16:L:301:BCL:HBB2	1.96	0.47
16:K:105:BCL:HMB1	16:K:105:BCL:CBB	2.43	0.47
5:K:38:MET:SD	15:K:101:PGV:H31	2.54	0.47
1:C:250:CYS:SG	11:C:403:HEM:HBC1	2.50	0.47
16:L:301:BCL:HBB3	16:L:301:BCL:CMB	2.44	0.47
16:A:102:BCL:H8	16:A:102:BCL:H51	1.57	0.47
9:3:46:ASN:HD21	15:3:101:PGV:H041	1.78	0.47
16:3:104:BCL:HMB3	16:3:104:BCL:HBB2	1.97	0.47
10:9:3:SER:OG	10:9:4:ASP:N	2.47	0.47
2:L:268:PRO:HA	2:L:273:TRP:HE1	1.80	0.47
2:L:273:TRP:HB2	3:M:84:ARG:HG3	1.95	0.47
4:H:252:ASN:HD21	6:4:3:GLU:HA	1.79	0.47
16:Q:103:BCL:H111	16:Q:103:BCL:H72	1.53	0.47
16:3:103:BCL:ND	24:4:102:LMT:H101	2.29	0.47
16:Q:104:BCL:CBB	16:Q:104:BCL:HMB3	2.45	0.47
17:L:302:BPH:H9C3	17:L:302:BPH:H6C1	1.71	0.47
15:L:305:PGV:O13	3:M:2:PRO:HB3	2.15	0.47
1:C:40:MET:HG2	1:C:248:THR:HB	1.96	0.47
1:C:310:CYS:SG	11:C:404:HEM:C3C	3.05	0.47
16:S:103:BCL:C1D	24:T:102:LMT:H101	2.45	0.47
15:Y:105:PGV:H241	15:Y:105:PGV:C7	2.45	0.47
7:6:46:LEU:HD13	24:8:102:LMT:H42	1.96	0.47
1:C:306:ASN:HB3	1:C:308:LEU:H	1.81	0.46
5:F:2:ASN:O	5:F:3:ALA:HB3	2.16	0.46
16:U:103:BCL:CBB	16:U:103:BCL:HMB3	2.44	0.46
7:V:46:LEU:HD13	24:X:102:LMT:H42	1.97	0.46
7:2:46:LEU:HD13	24:4:102:LMT:H42	1.96	0.46
16:K:105:BCL:H72	16:K:105:BCL:H111	1.54	0.46
16:5:103:BCL:H111	16:5:103:BCL:H71	1.59	0.46
14:C:407:DGA:HB22	14:C:407:DGA:HB51	1.54	0.46
16:Q:103:BCL:H202	16:Q:103:BCL:H161	1.84	0.46
16:Q:104:BCL:HMB3	16:Q:104:BCL:HBB2	1.97	0.46
3:M:277:ILE:HG13	17:M:404:BPH:HAC2	1.98	0.46
3:M:309:SER:O	3:M:310:GLU:HB3	2.15	0.46
15:Y:105:PGV:C7	15:Y:105:PGV:H222	2.46	0.46
1:C:191:ALA:HB3	1:C:237:THR:HG21	1.97	0.46
16:3:103:BCL:H71	16:3:103:BCL:H111	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:MET:HB3	11:C:403:HEM:C4B	2.50	0.45
2:L:143:TRP:CD1	18:L:306:UQ8:H4MB	2.51	0.45
16:U:102:BCL:H41	16:U:102:BCL:H62	1.64	0.45
16:X:101:BCL:HMB3	16:X:101:BCL:CBB	2.45	0.45
16:3:103:BCL:HMB1	16:3:103:BCL:HBB3	1.98	0.45
16:U:102:BCL:CBB	16:U:102:BCL:CMB	2.95	0.45
3:M:73:LEU:HD23	3:M:73:LEU:HA	1.80	0.45
2:L:194:LEU:HD22	2:L:217:PHE:HE2	1.81	0.45
5:A:9:MET:HE3	24:B:102:LMT:H5'	1.98	0.45
16:7:102:BCL:HMB1	16:7:102:BCL:HBB3	1.97	0.45
16:I:102:BCL:HMB1	16:I:102:BCL:CBB	2.44	0.45
16:S:103:BCL:CBB	16:S:103:BCL:CMB	2.95	0.45
16:Y:102:BCL:ND	24:Z:102:LMT:H101	2.32	0.45
1:C:110:CYS:CB	11:C:401:HEM:HAC	2.46	0.45
15:O:102:PGV:H72	8:Q:22:LEU:HD13	1.98	0.45
16:M:403:BCL:HAA2	16:M:403:BCL:HBD	1.99	0.44
3:M:264:SER:OG	4:H:35:ASP:OD1	2.26	0.44
16:I:102:BCL:C1D	24:J:102:LMT:H101	2.47	0.44
9:7:11:LYS:HE3	7:8:11:GLU:OE2	2.17	0.44
16:7:103:BCL:HMB3	16:7:103:BCL:CBB	2.47	0.44
1:C:91:ASN:O	1:C:95:VAL:HG23	2.17	0.44
4:H:169:GLU:HB3	4:H:183:GLU:HB3	1.99	0.44
16:3:104:BCL:H152	16:3:104:BCL:H112	1.77	0.44
16:5:103:BCL:C1D	24:6:102:LMT:H101	2.48	0.44
3:M:245:ALA:O	3:M:249:MET:HG2	2.18	0.44
15:Y:105:PGV:H42	15:Y:105:PGV:C19	2.47	0.44
16:Q:104:BCL:H93	16:Q:104:BCL:H111	1.81	0.44
4:H:133:ILE:HD12	4:H:180:ARG:HG3	2.00	0.44
7:N:46:LEU:HD13	24:P:102:LMT:H42	2.00	0.44
4:H:87:PHE:HB2	4:H:111:VAL:CG1	2.47	0.44
16:F:103:BCL:OBB	16:F:103:BCL:HHC	2.17	0.44
16:3:103:BCL:C1D	24:4:102:LMT:H101	2.48	0.44
16:O:105:BCL:HMB3	16:O:105:BCL:CBB	2.47	0.43
16:W:102:BCL:HMB1	16:W:102:BCL:CBB	2.46	0.43
9:3:22:LEU:HD23	9:3:22:LEU:HA	1.85	0.43
16:L:304:BCL:H11	3:M:210:TYR:HB3	1.98	0.43
16:D:104:BCL:H92	16:D:104:BCL:H62	1.76	0.43
16:5:103:BCL:HBB3	16:5:103:BCL:HMB1	1.99	0.43
16:5:104:BCL:H93	16:5:104:BCL:H111	1.77	0.43
1:C:155:CYS:HG	11:C:402:HEM:CAC	2.28	0.43
4:H:14:GLN:NE2	15:H:301:PGV:O13	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:38:MET:HG2	15:F:104:PGV:H211	1.99	0.43
16:F:103:BCL:HAA2	16:F:103:BCL:HBD	1.99	0.43
16:5:103:BCL:H62	16:5:103:BCL:H41	1.60	0.43
15:9:101:PGV:H291	15:9:101:PGV:H321	1.68	0.43
1:C:56:THR:HB	1:C:318:LEU:HD23	2.00	0.43
4:H:94:ARG:HB3	7:0:7:THR:O	2.18	0.43
5:F:31:PHE:HD1	5:F:31:PHE:HA	1.69	0.43
17:L:302:BPH:O2A	17:L:302:BPH:H4C3	2.18	0.43
5:I:16:MET:HE2	5:K:23:TRP:NE1	2.33	0.43
4:H:24:LEU:O	4:H:25:LEU:CB	2.64	0.43
16:F:105:BCL:CBB	16:F:105:BCL:HMB3	2.49	0.43
16:2:102:BCL:H92	16:2:102:BCL:H62	1.77	0.43
16:9:103:BCL:CBB	16:9:103:BCL:CMB	2.96	0.43
15:O:102:PGV:H262	15:O:102:PGV:H231	1.70	0.43
16:5:103:BCL:OB	16:5:103:BCL:HHC	2.18	0.43
16:7:102:BCL:C1D	24:8:102:LMT:H101	2.48	0.43
18:L:306:UQ8:H25	19:L:307:8K6:H181	2.01	0.43
16:I:102:BCL:H162	16:I:102:BCL:H203	1.76	0.43
16:U:103:BCL:HMB3	16:U:103:BCL:HBB2	2.00	0.43
10:9:24:PHE:HB2	15:9:101:PGV:H212	2.00	0.43
16:M:403:BCL:HHC	16:M:403:BCL:OB	2.19	0.43
24:B:102:LMT:O2B	24:B:102:LMT:O2'	2.28	0.43
16:J:101:BCL:CBB	16:J:101:BCL:CMB	2.97	0.43
2:L:78:PHE:HB3	9:7:42:SER:OG	2.18	0.42
2:L:175:MET:CE	2:L:264:TRP:CZ2	3.02	0.42
16:1:102:BCL:C1D	24:2:103:LMT:H101	2.48	0.42
7:0:6:THR:HG23	7:0:8:GLY:N	2.34	0.42
1:C:145:VAL:O	1:C:145:VAL:CG2	2.61	0.42
14:C:407:DGA:HG11	14:C:407:DGA:CA4	2.49	0.42
2:L:50:ILE:HD13	2:L:90:ILE:HD13	2.01	0.42
1:C:302:PRO:O	1:C:304:LYS:NZ	2.51	0.42
16:F:105:BCL:H152	16:F:105:BCL:H112	1.85	0.42
9:W:22:LEU:HD23	9:W:22:LEU:HA	1.87	0.42
16:L:304:BCL:HMB1	16:L:304:BCL:HBB3	2.01	0.42
16:D:103:BCL:H72	16:D:103:BCL:H111	1.73	0.42
7:G:41:LEU:HD23	7:G:41:LEU:HA	1.90	0.42
9:Y:62:THR:HG22	9:1:73:LEU:CD2	2.49	0.42
1:C:205:LEU:O	1:C:281:ILE:HD11	2.20	0.42
18:L:306:UQ8:H16A	18:L:306:UQ8:H10A	2.01	0.42
4:H:32:ARG:NH1	4:H:35:ASP:OD2	2.53	0.42
2:L:88:GLN:HA	2:L:91:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:22:LEU:HD23	9:Y:22:LEU:HA	1.87	0.42
16:3:103:BCL:HHD	16:3:103:BCL:HAC1	1.91	0.42
16:9:103:BCL:OBB	16:9:103:BCL:HHC	2.19	0.42
2:L:151:LEU:H	2:L:151:LEU:HG	1.72	0.42
9:U:22:LEU:HD23	9:U:22:LEU:HA	1.85	0.42
16:3:104:BCL:H91	16:3:104:BCL:H111	1.83	0.42
16:T:101:BCL:H92	16:T:101:BCL:H62	1.90	0.42
9:U:47:TRP:CE2	16:U:102:BCL:H2C	2.55	0.42
16:9:103:BCL:H2	7:O:28:TRP:CH2	2.55	0.42
4:H:24:LEU:HG	4:H:25:LEU:H	1.85	0.42
5:A:37:HIS:CE1	16:B:103:BCL:HMD1	2.55	0.42
16:K:105:BCL:H43	7:N:28:TRP:CZ2	2.54	0.42
8:Q:46:ASN:OD1	8:Q:47:TRP:N	2.53	0.42
16:T:101:BCL:OBB	16:T:101:BCL:HHC	2.19	0.42
1:C:28:GLN:HG2	2:L:257:THR:HG21	2.02	0.41
4:H:156:VAL:HG21	4:H:184:LEU:HD13	2.01	0.41
3:M:73:LEU:HD12	9:S:38:MET:CE	2.49	0.41
4:H:158:GLY:O	4:H:159:ALA:HB3	2.20	0.41
16:O:105:BCL:HMB3	16:O:105:BCL:HBB2	2.02	0.41
16:M:403:BCL:H192	16:M:403:BCL:H161	1.93	0.41
17:M:404:BPH:H6C1	17:M:404:BPH:H4C1	1.46	0.41
7:E:25:MET:HG3	23:E:101:H4X:C20	2.51	0.41
2:L:32:VAL:O	2:L:36:GLY:HA3	2.19	0.41
4:H:55:GLU:HG3	4:H:60:MET:HG3	2.02	0.41
5:A:22:LEU:HD23	5:A:22:LEU:HA	1.85	0.41
6:B:46:LEU:HD13	24:E:102:LMT:H42	2.03	0.41
5:K:38:MET:CE	15:K:101:PGV:H51	2.42	0.41
16:K:105:BCL:H62	16:K:105:BCL:H41	1.31	0.41
16:7:103:BCL:HMB3	16:7:103:BCL:HBB2	2.02	0.41
9:S:57:GLN:O	9:S:61:GLU:HG3	2.19	0.41
2:L:270:LEU:HD23	2:L:270:LEU:HA	1.92	0.41
16:J:101:BCL:H152	16:J:101:BCL:H112	1.94	0.41
9:S:1:MET:C	9:S:3:ALA:H	2.28	0.41
7:T:29:PHE:CE1	16:T:101:BCL:H11	2.55	0.41
16:X:101:BCL:H92	16:X:101:BCL:H62	1.96	0.41
9:5:37:HIS:CE1	16:5:104:BCL:HMD1	2.55	0.41
9:S:50:ASP:OD1	9:S:50:ASP:N	2.54	0.41
9:3:31:PHE:HD1	9:3:31:PHE:HA	1.69	0.41
1:C:107:CYS:HB2	11:C:401:HEM:HAB	1.98	0.41
2:L:70:PRO:HG3	2:L:88:GLN:HE21	1.86	0.41
15:L:305:PGV:H131	15:L:305:PGV:H102	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:93:ASP:OD1	4:H:93:ASP:O	2.39	0.41
16:K:108:BCL:H141	16:K:108:BCL:H162	1.85	0.41
5:O:22:LEU:HD23	5:O:22:LEU:HA	1.82	0.41
9:U:50:ASP:OD1	9:U:50:ASP:N	2.53	0.41
1:C:317:PRO:O	1:C:318:LEU:HB2	2.21	0.41
4:H:158:GLY:O	4:H:214:ASN:HA	2.21	0.41
16:K:105:BCL:ND	24:N:101:LMT:H101	2.35	0.41
7:T:6:THR:HG22	7:T:7:THR:N	2.36	0.41
15:Y:105:PGV:H42	15:Y:105:PGV:O03	2.20	0.41
9:1:50:ASP:N	9:1:50:ASP:OD1	2.54	0.41
3:M:33:LYS:HA	3:M:34:PRO:HD3	1.94	0.40
9:W:16:MET:HE2	9:Y:23:TRP:CE2	2.55	0.40
16:7:103:BCL:H11	7:8:29:PHE:CE1	2.56	0.40
3:M:60:SER:O	3:M:61:LEU:HB2	2.21	0.40
3:M:99:PRO:HG3	8:Q:68:ASP:OD1	2.21	0.40
16:B:103:BCL:H62	16:B:103:BCL:H92	1.88	0.40
16:Y:104:BCL:H11	7:Z:29:PHE:CE1	2.56	0.40
10:9:39:ILE:HD13	10:9:39:ILE:HG21	1.85	0.40
16:9:104:BCL:OBB	16:9:104:BCL:HHC	2.21	0.40
1:C:226:ILE:H	1:C:226:ILE:HG12	1.67	0.40
14:C:407:DGA:OG2	2:L:263:TRP:NE1	2.54	0.40
22:H:302:CDL:H141	22:H:302:CDL:H781	2.03	0.40
5:K:16:MET:HE3	5:O:23:TRP:HZ2	1.81	0.40
7:V:6:THR:HG22	7:V:7:THR:N	2.36	0.40
16:1:102:BCL:H142	16:1:102:BCL:H111	1.89	0.40
7:8:16:GLU:O	7:8:20:ILE:HD12	2.22	0.40
2:L:194:LEU:HD22	2:L:217:PHE:CE2	2.56	0.40
17:L:302:BPH:H9C1	17:L:302:BPH:H112	1.64	0.40
16:L:304:BCL:HMB1	16:L:304:BCL:CBB	2.51	0.40
4:H:2:GLU:N	4:H:2:GLU:OE1	2.54	0.40
7:R:20:ILE:HG21	7:R:20:ILE:HD13	1.81	0.40
16:U:102:BCL:H112	16:U:102:BCL:H71	1.96	0.40
9:Y:62:THR:HG22	9:1:73:LEU:HD21	2.04	0.40
9:1:18:PRO:HB3	7:2:17:PHE:CZ	2.55	0.40
9:3:37:HIS:CE1	16:3:104:BCL:HMD1	2.57	0.40
16:3:103:BCL:H203	16:3:103:BCL:H162	1.95	0.40
16:7:102:BCL:H72	16:7:102:BCL:H111	1.73	0.40
5:A:67:LEU:HD23	5:A:67:LEU:HA	1.97	0.40
5:I:16:MET:HE2	5:K:23:TRP:CE2	2.57	0.40
16:Y:104:BCL:H92	16:Y:104:BCL:H62	1.95	0.40
9:3:14:MET:CE	6:4:11:GLU:HG3	2.51	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	309/396 (78%)	287 (93%)	22 (7%)	0	100	100
2	L	270/273 (99%)	251 (93%)	19 (7%)	0	100	100
3	M	316/324 (98%)	303 (96%)	13 (4%)	0	100	100
4	H	255/258 (99%)	231 (91%)	21 (8%)	3 (1%)	10	31
5	A	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
5	D	70/73 (96%)	70 (100%)	0	0	100	100
5	F	70/73 (96%)	68 (97%)	2 (3%)	0	100	100
5	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
5	K	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
5	O	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
6	4	42/46 (91%)	40 (95%)	2 (5%)	0	100	100
6	B	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
6	P	40/46 (87%)	40 (100%)	0	0	100	100
7	0	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	2	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	6	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
7	8	40/46 (87%)	38 (95%)	1 (2%)	1 (2%)	4	15
7	E	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
7	G	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	J	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	N	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
7	R	42/46 (91%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
7	V	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
7	X	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
7	Z	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
8	Q	76/81 (94%)	73 (96%)	3 (4%)	0	100	100
9	1	70/77 (91%)	69 (99%)	1 (1%)	0	100	100
9	3	71/77 (92%)	70 (99%)	1 (1%)	0	100	100
9	5	72/77 (94%)	72 (100%)	0	0	100	100
9	7	71/77 (92%)	71 (100%)	0	0	100	100
9	S	70/77 (91%)	68 (97%)	2 (3%)	0	100	100
9	U	70/77 (91%)	68 (97%)	2 (3%)	0	100	100
9	W	71/77 (92%)	71 (100%)	0	0	100	100
9	Y	71/77 (92%)	71 (100%)	0	0	100	100
10	9	82/86 (95%)	76 (93%)	6 (7%)	0	100	100
All	All	2937/3208 (92%)	2819 (96%)	114 (4%)	4 (0%)	49	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	86	ASP
7	8	6	THR
4	H	257	VAL
4	H	256	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	266/314 (85%)	265 (100%)	1 (0%)	84	94
2	L	217/218 (100%)	216 (100%)	1 (0%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	256/260 (98%)	255 (100%)	1 (0%)	84	94
4	H	211/212 (100%)	208 (99%)	3 (1%)	59	84
5	A	62/65 (95%)	62 (100%)	0	100	100
5	D	64/65 (98%)	64 (100%)	0	100	100
5	F	64/65 (98%)	63 (98%)	1 (2%)	55	82
5	I	65/65 (100%)	65 (100%)	0	100	100
5	K	64/65 (98%)	64 (100%)	0	100	100
5	O	65/65 (100%)	65 (100%)	0	100	100
6	4	38/39 (97%)	38 (100%)	0	100	100
6	B	37/39 (95%)	36 (97%)	1 (3%)	39	72
6	P	36/39 (92%)	35 (97%)	1 (3%)	38	71
7	0	35/39 (90%)	35 (100%)	0	100	100
7	2	35/39 (90%)	35 (100%)	0	100	100
7	6	37/39 (95%)	37 (100%)	0	100	100
7	8	36/39 (92%)	36 (100%)	0	100	100
7	E	36/39 (92%)	36 (100%)	0	100	100
7	G	35/39 (90%)	35 (100%)	0	100	100
7	J	35/39 (90%)	35 (100%)	0	100	100
7	N	36/39 (92%)	36 (100%)	0	100	100
7	R	38/39 (97%)	38 (100%)	0	100	100
7	T	37/39 (95%)	37 (100%)	0	100	100
7	V	37/39 (95%)	37 (100%)	0	100	100
7	X	35/39 (90%)	35 (100%)	0	100	100
7	Z	36/39 (92%)	36 (100%)	0	100	100
8	Q	67/70 (96%)	67 (100%)	0	100	100
9	1	63/68 (93%)	63 (100%)	0	100	100
9	3	64/68 (94%)	64 (100%)	0	100	100
9	5	64/68 (94%)	64 (100%)	0	100	100
9	7	64/68 (94%)	63 (98%)	1 (2%)	55	82
9	S	64/68 (94%)	64 (100%)	0	100	100
9	U	63/68 (93%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	64/68 (94%)	63 (98%)	1 (2%)	55	82
9	Y	64/68 (94%)	64 (100%)	0	100	100
10	9	72/74 (97%)	72 (100%)	0	100	100
All	All	2562/2706 (95%)	2551 (100%)	11 (0%)	81	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	226	ILE
2	L	221	VAL
3	M	35	ILE
4	H	12	LEU
4	H	27	VAL
4	H	216	ILE
6	B	20	LEU
5	F	70	LYS
6	P	20	LEU
9	W	58	LEU
9	7	54	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	42	GLN
1	C	111	HIS
1	C	189	ASN
1	C	215	ASN
1	C	238	HIS
1	C	275	ASN
2	L	64	GLN
2	L	88	GLN
2	L	164	GLN
2	L	174	HIS
2	L	200	ASN
3	M	202	HIS
3	M	259	ASN
3	M	293	ASN
5	A	29	GLN
5	D	29	GLN
5	D	48	HIS

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Mol	Chain	Res	Type
5	D	59	GLN
5	F	48	HIS
5	I	48	HIS
5	O	29	GLN
5	O	48	HIS
8	Q	48	HIS
9	S	29	GLN
9	S	48	HIS
9	U	29	GLN
9	U	59	GLN
9	W	29	GLN
9	W	48	HIS
9	W	59	GLN
9	1	48	HIS
9	5	48	HIS
9	7	59	GLN
10	9	86	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 124 ligands modelled in this entry, 19 are monoatomic - leaving 105 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
16	BCL	3	104	-	69,74,74	1.96	16 (23%)	79,115,115	2.16	28 (35%)
16	BCL	T	101	-	69,74,74	1.81	17 (24%)	79,115,115	2.02	26 (32%)
16	BCL	5	104	-	69,74,74	1.88	16 (23%)	79,115,115	2.08	23 (29%)
16	BCL	9	103	-	69,74,74	1.72	15 (21%)	79,115,115	2.20	19 (24%)
24	LMT	4	102	-	36,36,36	0.99	3 (8%)	47,47,47	1.77	10 (21%)
16	BCL	D	104	-	69,74,74	1.99	18 (26%)	79,115,115	2.00	19 (24%)
17	BPH	L	302	-	59,70,70	0.93	4 (6%)	59,101,101	1.12	4 (6%)
14	DGA	C	407	-	31,31,43	0.64	0	33,33,45	0.78	1 (3%)
23	H4X	Z	101	-	43,43,43	2.28	11 (25%)	52,54,54	2.11	12 (23%)
16	BCL	Q	104	-	69,74,74	2.04	20 (28%)	79,115,115	2.32	31 (39%)
15	PGV	Y	105	-	26,26,50	1.38	2 (7%)	29,31,56	1.30	5 (17%)
23	H4X	E	101	-	43,43,43	2.50	13 (30%)	52,54,54	2.31	17 (32%)
16	BCL	S	103	-	69,74,74	1.76	15 (21%)	79,115,115	2.06	18 (22%)
17	BPH	M	404	-	59,70,70	1.09	4 (6%)	59,101,101	1.13	4 (6%)
16	BCL	F	103	-	69,74,74	1.72	14 (20%)	79,115,115	2.04	23 (29%)
16	BCL	J	101	-	69,74,74	1.87	16 (23%)	79,115,115	2.02	24 (30%)
24	LMT	N	101	-	36,36,36	0.85	2 (5%)	47,47,47	1.54	6 (12%)
16	BCL	U	103	-	69,74,74	2.12	15 (21%)	79,115,115	2.05	19 (24%)
11	HEM	C	402	1	50,50,50	1.78	11 (22%)	67,82,82	2.02	22 (32%)
15	PGV	H	301	-	35,35,50	1.28	3 (8%)	38,41,56	1.95	5 (13%)
16	BCL	D	103	-	69,74,74	1.74	15 (21%)	79,115,115	2.14	17 (21%)
24	LMT	B	102	-	36,36,36	0.54	0	47,47,47	1.16	2 (4%)
15	PGV	I	103	-	40,40,50	1.02	2 (5%)	43,45,56	1.13	6 (13%)
18	UQ8	L	303	-	33,33,53	1.73	4 (12%)	42,43,67	1.96	14 (33%)
23	H4X	5	105	-	43,43,43	2.25	12 (27%)	52,54,54	2.18	14 (26%)
24	LMT	J	102	-	36,36,36	0.91	2 (5%)	47,47,47	1.76	12 (25%)
24	LMT	8	101	-	36,36,36	0.56	1 (2%)	47,47,47	0.80	0
16	BCL	W	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.08	20 (25%)
22	CDL	S	101	-	73,73,99	0.48	0	79,85,111	0.82	3 (3%)
16	BCL	Y	102	-	69,74,74	1.83	15 (21%)	79,115,115	2.16	24 (30%)
11	HEM	C	403	1	50,50,50	1.45	7 (14%)	67,82,82	2.26	23 (34%)
15	PGV	O	102	-	43,43,50	0.94	2 (4%)	46,49,56	1.24	4 (8%)
16	BCL	K	105	-	69,74,74	1.84	14 (20%)	79,115,115	1.95	23 (29%)
23	H4X	7	104	-	43,43,43	2.31	11 (25%)	52,54,54	2.36	18 (34%)
15	PGV	9	101	-	46,46,50	0.96	3 (6%)	49,52,56	1.14	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	H4X	U	104	-	43,43,43	2.34	14 (32%)	52,54,54	2.14	15 (28%)
15	PGV	K	101	-	35,35,50	1.21	2 (5%)	38,41,56	1.16	5 (13%)
15	PGV	1	103	-	25,25,50	1.38	2 (8%)	28,30,56	1.60	4 (14%)
24	LMT	X	102	-	36,36,36	0.78	2 (5%)	47,47,47	1.36	5 (10%)
22	CDL	H	302	-	72,72,99	0.45	0	78,84,111	1.03	5 (6%)
24	LMT	8	102	-	36,36,36	0.77	1 (2%)	47,47,47	1.33	6 (12%)
23	H4X	4	101	-	43,43,43	2.10	10 (23%)	52,54,54	2.05	17 (32%)
16	BCL	Y	104	-	69,74,74	1.84	14 (20%)	79,115,115	2.07	23 (29%)
15	PGV	K	102	-	18,18,50	1.28	1 (5%)	20,22,56	1.13	2 (10%)
19	8K6	5	106	-	14,14,17	0.30	0	13,13,16	0.12	0
24	LMT	P	102	-	36,36,36	0.97	1 (2%)	47,47,47	1.37	6 (12%)
16	BCL	Q	103	-	69,74,74	1.83	14 (20%)	79,115,115	1.96	20 (25%)
21	MQ8	M	405	-	54,54,54	0.84	3 (5%)	67,69,69	0.86	2 (2%)
24	LMT	R	101	-	36,36,36	0.87	2 (5%)	47,47,47	1.37	9 (19%)
16	BCL	K	108	-	69,74,74	1.87	16 (23%)	79,115,115	2.14	25 (31%)
19	8K6	L	307	-	17,17,17	0.48	0	16,16,16	0.18	0
16	BCL	7	103	-	69,74,74	2.01	16 (23%)	79,115,115	2.02	20 (25%)
24	LMT	6	102	-	36,36,36	0.97	3 (8%)	47,47,47	1.70	9 (19%)
16	BCL	X	101	-	69,74,74	1.98	16 (23%)	79,115,115	2.10	24 (30%)
16	BCL	7	102	-	64,69,74	1.77	14 (21%)	73,109,115	2.08	23 (31%)
15	PGV	5	101	-	46,46,50	1.06	2 (4%)	49,52,56	1.04	3 (6%)
24	LMT	G	102	-	36,36,36	0.87	3 (8%)	47,47,47	1.70	8 (17%)
24	LMT	B	104	-	36,36,36	1.16	3 (8%)	47,47,47	1.39	9 (19%)
16	BCL	M	402	-	69,74,74	1.75	13 (18%)	79,115,115	2.22	23 (29%)
15	PGV	D	101	-	42,42,50	0.96	2 (4%)	45,48,56	1.53	7 (15%)
15	PGV	F	104	-	36,36,50	1.12	2 (5%)	39,42,56	1.52	6 (15%)
23	H4X	K	103	-	43,43,43	2.16	10 (23%)	52,54,54	2.05	24 (46%)
24	LMT	T	102	-	36,36,36	0.96	2 (5%)	47,47,47	1.51	10 (21%)
16	BCL	F	105	-	69,74,74	1.91	15 (21%)	79,115,115	2.04	22 (27%)
23	H4X	2	101	-	43,43,43	2.24	10 (23%)	52,54,54	1.98	18 (34%)
15	PGV	F	101	-	33,33,50	1.35	3 (9%)	36,38,56	1.63	9 (25%)
23	H4X	K	107	-	43,43,43	2.22	11 (25%)	52,54,54	2.07	16 (30%)
16	BCL	3	103	-	69,74,74	1.75	15 (21%)	79,115,115	1.94	19 (24%)
16	BCL	A	102	-	69,74,74	1.84	17 (24%)	79,115,115	2.29	19 (24%)
15	PGV	L	305	-	46,46,50	1.05	2 (4%)	49,52,56	1.47	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	H4X	O	106	-	43,43,43	2.41	15 (34%)	52,54,54	2.08	19 (36%)
15	PGV	Q	101	-	37,37,50	1.11	3 (8%)	40,43,56	1.48	6 (15%)
16	BCL	I	102	-	69,74,74	1.74	15 (21%)	79,115,115	2.12	21 (26%)
23	H4X	P	101	-	43,43,43	2.33	13 (30%)	52,54,54	1.96	17 (32%)
16	BCL	5	103	-	69,74,74	1.89	20 (28%)	79,115,115	2.07	21 (26%)
16	BCL	U	102	-	69,74,74	1.79	16 (23%)	79,115,115	2.25	23 (29%)
24	LMT	V	102	-	36,36,36	0.91	1 (2%)	47,47,47	1.72	9 (19%)
15	PGV	C	408	-	15,15,50	1.46	3 (20%)	17,19,56	2.34	5 (29%)
16	BCL	9	104	-	69,74,74	1.97	12 (17%)	79,115,115	2.01	24 (30%)
11	HEM	C	401	1	50,50,50	1.74	13 (26%)	67,82,82	1.95	21 (31%)
16	BCL	O	104	-	69,74,74	1.98	19 (27%)	79,115,115	2.05	22 (27%)
16	BCL	M	403	-	69,74,74	1.72	12 (17%)	79,115,115	2.36	26 (32%)
22	CDL	Y	103	-	29,29,99	0.59	0	33,38,111	0.81	1 (3%)
11	HEM	C	404	1	50,50,50	1.55	9 (18%)	67,82,82	2.03	17 (25%)
16	BCL	1	102	-	69,74,74	1.83	15 (21%)	79,115,115	2.06	23 (29%)
15	PGV	A	101	-	22,22,50	1.51	4 (18%)	23,27,56	1.58	6 (26%)
16	BCL	2	102	-	69,74,74	1.65	11 (15%)	79,115,115	2.20	26 (32%)
23	H4X	6	101	-	43,43,43	2.27	11 (25%)	52,54,54	2.17	22 (42%)
16	BCL	L	301	-	69,74,74	1.91	14 (20%)	79,115,115	2.32	30 (37%)
15	PGV	K	106	-	42,42,50	1.07	2 (4%)	45,47,56	1.05	3 (6%)
23	H4X	Q	105	-	43,43,43	2.24	12 (27%)	52,54,54	2.40	24 (46%)
24	LMT	2	103	-	36,36,36	0.95	3 (8%)	47,47,47	1.94	14 (29%)
24	LMT	E	102	-	36,36,36	0.95	2 (5%)	47,47,47	1.54	9 (19%)
23	H4X	V	101	-	43,43,43	2.31	13 (30%)	52,54,54	2.78	20 (38%)
15	PGV	3	101	-	46,46,50	1.06	2 (4%)	49,52,56	1.41	8 (16%)
23	H4X	G	101	-	43,43,43	2.29	13 (30%)	52,54,54	2.35	17 (32%)
16	BCL	L	304	-	69,74,74	1.83	16 (23%)	79,115,115	3.13	26 (32%)
23	H4X	B	101	-	43,43,43	2.22	12 (27%)	52,54,54	2.19	21 (40%)
15	PGV	M	406	-	38,38,50	1.15	2 (5%)	41,44,56	1.21	3 (7%)
24	LMT	Z	102	-	36,36,36	0.86	1 (2%)	47,47,47	1.63	12 (25%)
23	H4X	O	101	-	43,43,43	2.24	14 (32%)	52,54,54	2.51	20 (38%)
24	LMT	0	101	-	36,36,36	0.87	2 (5%)	47,47,47	1.39	8 (17%)
16	BCL	O	105	-	69,74,74	1.94	15 (21%)	79,115,115	2.19	27 (34%)
16	BCL	B	103	-	69,74,74	2.05	15 (21%)	79,115,115	2.13	29 (36%)
18	UQ8	L	306	-	33,33,53	1.71	2 (6%)	42,43,67	1.79	11 (26%)

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
16	BCL	3	104	-	-	16/41/137/137	-
16	BCL	T	101	-	-	15/41/137/137	-
16	BCL	5	104	-	-	18/41/137/137	-
16	BCL	9	103	-	-	21/41/137/137	-
24	LMT	4	102	-	-	10/21/61/61	0/2/2/2
16	BCL	D	104	-	-	16/41/137/137	-
17	BPH	L	302	-	-	17/37/105/105	0/5/6/6
14	DGA	C	407	-	-	20/32/32/45	-
23	H4X	Z	101	-	-	9/51/51/51	-
16	BCL	Q	104	-	-	14/41/137/137	-
15	PGV	Y	105	-	-	9/28/28/55	-
23	H4X	E	101	-	-	5/51/51/51	-
16	BCL	S	103	-	-	3/41/137/137	-
17	BPH	M	404	-	-	18/37/105/105	0/5/6/6
16	BCL	F	103	-	-	13/41/137/137	-
16	BCL	J	101	-	-	14/41/137/137	-
24	LMT	N	101	-	-	11/21/61/61	0/2/2/2
16	BCL	U	103	-	-	15/41/137/137	-
11	HEM	C	402	1	-	7/14/54/54	-
15	PGV	H	301	-	-	16/40/40/55	-
16	BCL	D	103	-	-	6/41/137/137	-
24	LMT	B	102	-	-	12/21/61/61	0/2/2/2
15	PGV	I	103	-	-	19/42/42/55	-
18	UQ8	L	303	-	-	6/27/51/75	0/1/1/1
23	H4X	5	105	-	-	10/51/51/51	-
24	LMT	J	102	-	-	10/21/61/61	0/2/2/2
24	LMT	8	101	-	-	8/21/61/61	0/2/2/2
16	BCL	W	102	-	-	6/41/137/137	-
22	CDL	S	101	-	-	32/84/84/110	-
16	BCL	Y	102	-	-	10/41/137/137	-
11	HEM	C	403	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PGV	O	102	-	-	23/48/48/55	-
16	BCL	K	105	-	-	19/41/137/137	-
23	H4X	7	104	-	-	7/51/51/51	-
15	PGV	9	101	-	-	23/51/51/55	-
23	H4X	U	104	-	-	5/51/51/51	-
15	PGV	K	101	-	-	16/40/40/55	-
15	PGV	1	103	-	-	11/27/27/55	-
24	LMT	X	102	-	-	10/21/61/61	0/2/2/2
22	CDL	H	302	-	-	28/83/83/110	-
24	LMT	8	102	-	-	11/21/61/61	0/2/2/2
23	H4X	4	101	-	-	10/51/51/51	-
16	BCL	Y	104	-	-	19/41/137/137	-
15	PGV	K	102	-	-	4/20/20/55	-
19	8K6	5	106	-	-	4/12/12/15	-
24	LMT	P	102	-	-	11/21/61/61	0/2/2/2
16	BCL	Q	103	-	-	17/41/137/137	-
21	MQ8	M	405	-	-	10/47/67/67	0/2/2/2
24	LMT	R	101	-	-	9/21/61/61	0/2/2/2
16	BCL	K	108	-	-	19/41/137/137	-
19	8K6	L	307	-	-	11/15/15/15	-
16	BCL	7	103	-	-	13/41/137/137	-
24	LMT	6	102	-	-	10/21/61/61	0/2/2/2
16	BCL	X	101	-	-	16/41/137/137	-
16	BCL	7	102	-	-	8/35/131/137	-
15	PGV	5	101	-	-	20/51/51/55	-
24	LMT	G	102	-	-	12/21/61/61	0/2/2/2
24	LMT	B	104	-	-	13/21/61/61	0/2/2/2
16	BCL	M	402	-	-	14/41/137/137	-
15	PGV	D	101	-	-	13/47/47/55	-
15	PGV	F	104	-	-	22/41/41/55	-
23	H4X	K	103	-	-	10/51/51/51	-
24	LMT	T	102	-	-	11/21/61/61	0/2/2/2
16	BCL	F	105	-	-	13/41/137/137	-
23	H4X	2	101	-	-	10/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PGV	F	101	-	-	13/35/35/55	-
23	H4X	K	107	-	-	9/51/51/51	-
16	BCL	3	103	-	-	17/41/137/137	-
16	BCL	A	102	-	-	14/41/137/137	-
15	PGV	L	305	-	-	13/51/51/55	-
23	H4X	O	106	-	-	7/51/51/51	-
15	PGV	Q	101	-	-	21/42/42/55	-
16	BCL	I	102	-	-	13/41/137/137	-
23	H4X	P	101	-	-	6/51/51/51	-
16	BCL	5	103	-	-	14/41/137/137	-
16	BCL	U	102	-	-	13/41/137/137	-
24	LMT	V	102	-	-	10/21/61/61	0/2/2/2
15	PGV	C	408	-	-	9/15/15/55	-
16	BCL	9	104	-	-	13/41/137/137	-
11	HEM	C	401	1	-	9/14/54/54	-
16	BCL	O	104	-	-	13/41/137/137	-
16	BCL	M	403	-	-	12/41/137/137	-
22	CDL	Y	103	-	-	10/35/35/110	-
11	HEM	C	404	1	-	7/14/54/54	-
16	BCL	1	102	-	-	7/41/137/137	-
15	PGV	A	101	-	-	8/26/26/55	-
16	BCL	2	102	-	-	15/41/137/137	-
23	H4X	6	101	-	-	5/51/51/51	-
16	BCL	L	301	-	-	7/41/137/137	-
15	PGV	K	106	-	-	17/44/44/55	-
23	H4X	Q	105	-	-	10/51/51/51	-
24	LMT	2	103	-	-	11/21/61/61	0/2/2/2
24	LMT	E	102	-	-	12/21/61/61	0/2/2/2
23	H4X	V	101	-	-	11/51/51/51	-
15	PGV	3	101	-	-	23/51/51/55	-
23	H4X	G	101	-	-	7/51/51/51	-
16	BCL	L	304	-	-	7/41/137/137	-
23	H4X	B	101	-	-	3/51/51/51	-
15	PGV	M	406	-	-	22/43/43/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMT	Z	102	-	-	11/21/61/61	0/2/2/2
23	H4X	O	101	-	-	14/51/51/51	-
24	LMT	0	101	-	-	10/21/61/61	0/2/2/2
16	BCL	O	105	-	-	15/41/137/137	-
16	BCL	B	103	-	-	13/41/137/137	-
18	UQ8	L	306	-	-	7/27/51/75	0/1/1/1

All (892) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	306	UQ8	C6-C1	8.22	1.49	1.35
18	L	303	UQ8	C6-C1	7.36	1.48	1.35
16	U	103	BCL	C3D-C4D	-6.75	1.29	1.44
16	L	301	BCL	O2D-CGD	6.48	1.49	1.33
16	B	103	BCL	C3D-C4D	-6.31	1.30	1.44
16	3	104	BCL	C3D-C4D	-6.27	1.30	1.44
16	U	103	BCL	OBD-CAD	6.08	1.33	1.22
16	M	402	BCL	C3D-C4D	-5.98	1.30	1.44
16	D	104	BCL	C3D-C4D	-5.96	1.30	1.44
16	5	104	BCL	C3D-C4D	-5.95	1.30	1.44
16	7	103	BCL	C3D-C4D	-5.83	1.31	1.44
16	Q	104	BCL	OBD-CAD	5.80	1.32	1.22
16	J	101	BCL	OBD-CAD	5.79	1.32	1.22
16	U	103	BCL	C1D-ND	-5.77	1.30	1.37
23	O	106	H4X	C25-C23	5.76	1.58	1.46
16	B	103	BCL	CHD-C1D	5.75	1.49	1.38
16	X	101	BCL	C3D-C4D	-5.74	1.31	1.44
23	6	101	H4X	C25-C23	5.69	1.58	1.46
16	F	105	BCL	C3D-C4D	-5.68	1.31	1.44
16	K	108	BCL	C3D-C4D	-5.68	1.31	1.44
16	K	105	BCL	C3D-C4D	-5.67	1.31	1.44
16	L	301	BCL	C3D-C4D	-5.63	1.31	1.44
16	M	403	BCL	O2A-CGA	5.62	1.49	1.33
16	9	103	BCL	C3D-C4D	-5.60	1.31	1.44
16	7	103	BCL	O2A-CGA	5.60	1.49	1.33
23	7	104	H4X	C25-C23	5.59	1.57	1.46
16	B	103	BCL	OBD-CAD	5.56	1.32	1.22
16	7	103	BCL	OBD-CAD	5.54	1.32	1.22
16	Y	102	BCL	C3D-C4D	-5.51	1.31	1.44
16	J	101	BCL	C3D-C4D	-5.50	1.31	1.44
16	K	108	BCL	O2D-CGD	5.43	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	104	BCL	C3D-C4D	-5.42	1.32	1.44
16	Q	103	BCL	C3D-C4D	-5.40	1.32	1.44
16	9	104	BCL	CHD-C1D	5.39	1.48	1.38
16	U	103	BCL	O2A-CGA	5.39	1.49	1.33
23	O	101	H4X	C16-C17	5.32	1.57	1.46
16	Q	104	BCL	C3D-C4D	-5.31	1.32	1.44
16	9	104	BCL	O2A-CGA	5.31	1.48	1.33
16	3	104	BCL	OBD-CAD	5.30	1.31	1.22
16	7	102	BCL	C3D-C4D	-5.27	1.32	1.44
16	B	103	BCL	C3C-C4C	-5.26	1.45	1.51
23	U	104	H4X	C11-C12	5.23	1.57	1.46
16	Q	104	BCL	CHD-C1D	5.22	1.48	1.38
23	V	101	H4X	C25-C23	5.21	1.57	1.46
16	5	104	BCL	O2A-CGA	5.18	1.48	1.33
23	K	107	H4X	C16-C17	5.17	1.57	1.46
16	A	102	BCL	C3D-C4D	-5.17	1.32	1.44
16	O	105	BCL	C3D-C4D	-5.17	1.32	1.44
16	2	102	BCL	O2A-CGA	5.17	1.48	1.33
16	9	104	BCL	C3D-C4D	-5.13	1.32	1.44
16	5	103	BCL	O2A-CGA	5.13	1.48	1.33
23	2	101	H4X	C11-C12	5.12	1.56	1.46
16	D	103	BCL	C3D-C4D	-5.11	1.32	1.44
16	O	104	BCL	O2A-CGA	5.11	1.48	1.33
16	Y	102	BCL	O2D-CGD	5.10	1.45	1.33
23	E	101	H4X	C25-C23	5.10	1.56	1.46
16	L	304	BCL	O2A-CGA	5.08	1.48	1.33
16	1	102	BCL	C3D-C4D	-5.08	1.32	1.44
16	3	104	BCL	O2A-CGA	5.07	1.48	1.33
16	U	102	BCL	C3C-C4C	-5.07	1.45	1.51
11	C	401	HEM	FE-NB	5.06	2.10	1.94
16	B	103	BCL	O2A-CGA	5.06	1.48	1.33
23	O	101	H4X	C25-C23	5.06	1.56	1.46
16	D	104	BCL	O2A-CGA	5.06	1.48	1.33
23	G	101	H4X	C21-C22	5.05	1.58	1.43
16	T	101	BCL	O2A-CGA	5.05	1.48	1.33
23	2	101	H4X	C25-C23	5.05	1.56	1.46
16	F	105	BCL	C1D-ND	-5.05	1.31	1.37
16	U	102	BCL	CHD-C1D	5.04	1.48	1.38
16	3	103	BCL	C3D-C4D	-5.04	1.32	1.44
16	7	103	BCL	C1D-ND	-5.03	1.31	1.37
23	P	101	H4X	C16-C17	5.03	1.56	1.46
23	Z	101	H4X	C26-C27	5.03	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	101	BCL	O2A-CGA	5.02	1.48	1.33
23	Z	101	H4X	C25-C23	5.01	1.56	1.46
23	E	101	H4X	C16-C17	5.00	1.56	1.46
23	V	101	H4X	C21-C22	4.99	1.58	1.43
15	K	102	PGV	O01-C1	4.99	1.47	1.33
23	Q	105	H4X	C26-C27	4.98	1.58	1.43
16	S	103	BCL	O2A-CGA	4.98	1.47	1.33
23	B	101	H4X	C20-C19	4.98	1.58	1.43
16	F	103	BCL	C3D-C4D	-4.96	1.33	1.44
23	E	101	H4X	C21-C22	4.96	1.58	1.43
23	5	105	H4X	C21-C22	4.96	1.58	1.43
23	Q	105	H4X	C16-C17	4.95	1.56	1.46
16	K	108	BCL	O2A-CGA	4.92	1.47	1.33
23	K	103	H4X	C16-C17	4.92	1.56	1.46
16	3	104	BCL	CHD-C1D	4.92	1.48	1.38
16	O	105	BCL	CHD-C1D	4.91	1.48	1.38
15	5	101	PGV	O01-C1	4.90	1.48	1.34
23	P	101	H4X	C26-C27	4.90	1.58	1.43
23	6	101	H4X	C21-C22	4.89	1.58	1.43
16	Q	104	BCL	O2A-CGA	4.88	1.47	1.33
23	P	101	H4X	C21-C22	4.86	1.58	1.43
16	K	108	BCL	OBD-CAD	4.86	1.30	1.22
23	Z	101	H4X	C21-C22	4.86	1.58	1.43
16	T	101	BCL	OBD-CAD	4.86	1.30	1.22
16	O	105	BCL	O2D-CGD	4.85	1.45	1.33
16	X	101	BCL	C3C-C4C	-4.84	1.45	1.51
16	Y	104	BCL	O2A-CGA	4.84	1.47	1.33
23	K	103	H4X	C25-C23	4.84	1.56	1.46
16	9	103	BCL	O2A-CGA	4.83	1.47	1.33
15	F	101	PGV	O03-C19	4.82	1.47	1.33
16	O	105	BCL	O2A-CGA	4.82	1.47	1.33
23	K	107	H4X	C26-C27	4.81	1.58	1.43
23	4	101	H4X	C21-C22	4.80	1.58	1.43
16	Q	103	BCL	CHD-C1D	4.80	1.47	1.38
16	9	104	BCL	C1D-ND	-4.79	1.31	1.37
16	T	101	BCL	C3D-C4D	-4.79	1.33	1.44
23	O	106	H4X	C16-C17	4.78	1.56	1.46
23	K	103	H4X	C26-C27	4.78	1.58	1.43
16	F	105	BCL	O2A-CGA	4.78	1.47	1.33
23	E	101	H4X	C11-C12	4.77	1.56	1.46
16	X	101	BCL	CHD-C1D	4.77	1.47	1.38
23	B	101	H4X	C26-C27	4.77	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	101	BCL	OBD-CAD	4.75	1.30	1.22
15	K	101	PGV	O03-C19	4.75	1.47	1.33
23	7	104	H4X	C26-C27	4.75	1.57	1.43
15	3	101	PGV	O03-C19	4.75	1.47	1.33
23	O	101	H4X	C11-C12	4.75	1.56	1.46
15	H	301	PGV	O03-C19	4.74	1.47	1.33
16	K	105	BCL	CHD-C1D	4.74	1.47	1.38
23	5	105	H4X	C15-C14	4.74	1.57	1.43
23	P	101	H4X	C25-C23	4.73	1.56	1.46
16	M	403	BCL	O2D-CGD	4.72	1.44	1.33
23	E	101	H4X	C26-C27	4.72	1.57	1.43
16	D	104	BCL	O2D-CGD	4.71	1.44	1.33
16	O	104	BCL	O2D-CGD	4.70	1.44	1.33
15	K	106	PGV	O03-C19	4.70	1.47	1.33
16	A	102	BCL	O2A-CGA	4.69	1.47	1.33
23	2	101	H4X	C21-C22	4.69	1.57	1.43
23	O	106	H4X	C26-C27	4.68	1.57	1.43
23	V	101	H4X	C26-C27	4.68	1.57	1.43
16	1	102	BCL	O2A-CGA	4.67	1.47	1.33
16	U	103	BCL	O2D-CGD	4.66	1.44	1.33
15	L	305	PGV	O01-C1	4.66	1.47	1.34
16	7	102	BCL	O2D-CGD	4.65	1.44	1.33
23	E	101	H4X	C31-C32	4.65	1.57	1.43
15	M	406	PGV	O01-C1	4.64	1.47	1.34
23	K	107	H4X	C31-C32	4.64	1.57	1.43
16	1	102	BCL	CHD-C1D	4.63	1.47	1.38
23	7	104	H4X	C11-C12	4.63	1.55	1.46
15	1	103	PGV	O01-C1	4.63	1.47	1.34
16	L	301	BCL	CHB-C1B	4.63	1.49	1.39
23	K	107	H4X	C25-C23	4.62	1.55	1.46
23	U	104	H4X	C21-C22	4.62	1.57	1.43
23	6	101	H4X	C20-C19	4.62	1.57	1.43
16	9	104	BCL	OBD-CAD	4.60	1.30	1.22
23	7	104	H4X	C21-C22	4.60	1.57	1.43
23	7	104	H4X	C20-C19	4.60	1.57	1.43
23	G	101	H4X	C11-C12	4.59	1.55	1.46
16	2	102	BCL	C3D-C4D	-4.59	1.33	1.44
11	C	402	HEM	C1C-C2C	-4.58	1.36	1.45
15	Y	105	PGV	O03-C19	4.57	1.46	1.33
23	Q	105	H4X	C20-C19	4.57	1.57	1.43
23	P	101	H4X	C11-C12	4.57	1.55	1.46
16	F	105	BCL	O2D-CGD	4.57	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	E	101	H4X	C15-C14	4.56	1.57	1.43
23	K	103	H4X	C21-C22	4.56	1.57	1.43
16	5	104	BCL	O2D-CGD	4.56	1.44	1.33
23	O	106	H4X	C20-C19	4.56	1.57	1.43
16	5	104	BCL	C3B-C4B	4.56	1.50	1.41
16	W	102	BCL	C3D-C4D	-4.56	1.33	1.44
16	F	105	BCL	OBD-CAD	4.56	1.30	1.22
23	Q	105	H4X	C10-C9	4.56	1.57	1.43
16	L	304	BCL	C3D-C4D	-4.55	1.34	1.44
23	6	101	H4X	C16-C17	4.54	1.55	1.46
23	E	101	H4X	C20-C19	4.54	1.57	1.43
16	X	101	BCL	O2A-CGA	4.54	1.46	1.33
11	C	402	HEM	FE-NB	4.53	2.08	1.94
23	B	101	H4X	C21-C22	4.53	1.57	1.43
16	D	104	BCL	C3C-C4C	-4.52	1.45	1.51
23	U	104	H4X	C26-C27	4.52	1.57	1.43
23	U	104	H4X	C16-C17	4.51	1.55	1.46
23	V	101	H4X	C20-C19	4.50	1.57	1.43
16	Y	104	BCL	OBD-CAD	4.50	1.30	1.22
16	T	101	BCL	CHD-C1D	4.50	1.47	1.38
11	C	404	HEM	FE-NB	4.49	2.08	1.94
23	Z	101	H4X	C11-C12	4.49	1.55	1.46
16	3	104	BCL	O2D-CGD	4.48	1.44	1.33
16	T	101	BCL	C3C-C4C	-4.48	1.46	1.51
16	D	104	BCL	CHD-C1D	4.47	1.47	1.38
23	5	105	H4X	C26-C27	4.47	1.57	1.43
23	Z	101	H4X	C20-C19	4.47	1.57	1.43
16	K	105	BCL	O2A-CGA	4.46	1.46	1.33
23	2	101	H4X	C20-C19	4.45	1.57	1.43
16	3	103	BCL	CHD-C1D	4.45	1.47	1.38
23	Z	101	H4X	C31-C32	4.45	1.57	1.43
23	U	104	H4X	C20-C19	4.45	1.57	1.43
23	2	101	H4X	C26-C27	4.45	1.57	1.43
15	F	101	PGV	O01-C1	4.44	1.46	1.34
16	D	103	BCL	O2A-CGA	4.44	1.46	1.33
16	W	102	BCL	CHD-C1D	4.44	1.47	1.38
15	L	305	PGV	O03-C19	4.44	1.46	1.33
16	L	301	BCL	OBD-CAD	4.43	1.30	1.22
23	4	101	H4X	C26-C27	4.43	1.56	1.43
23	K	107	H4X	C20-C19	4.42	1.56	1.43
23	P	101	H4X	C20-C19	4.42	1.56	1.43
16	Q	104	BCL	C3C-C4C	-4.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	102	BCL	O2A-CGA	4.41	1.46	1.33
23	G	101	H4X	C16-C17	4.40	1.55	1.46
23	5	105	H4X	C25-C23	4.40	1.55	1.46
23	5	105	H4X	C16-C17	4.40	1.55	1.46
16	5	103	BCL	CHD-C1D	4.39	1.47	1.38
16	5	104	BCL	C1D-ND	-4.39	1.32	1.37
23	U	104	H4X	C25-C23	4.39	1.55	1.46
16	F	103	BCL	O2A-CGA	4.38	1.46	1.33
23	G	101	H4X	C30-C28	4.38	1.55	1.46
23	Z	101	H4X	C16-C17	4.38	1.55	1.46
23	O	101	H4X	C26-C27	4.37	1.56	1.43
16	O	104	BCL	CHC-C4B	4.37	1.49	1.39
16	3	103	BCL	O2A-CGA	4.37	1.46	1.33
16	1	102	BCL	O2D-CGD	4.36	1.44	1.33
16	J	101	BCL	O2D-CGD	4.36	1.43	1.33
16	5	103	BCL	C3C-C4C	-4.34	1.46	1.51
23	G	101	H4X	C25-C23	4.34	1.55	1.46
16	U	102	BCL	C3D-C4D	-4.34	1.34	1.44
23	5	105	H4X	C30-C28	4.34	1.55	1.46
23	O	106	H4X	C15-C14	4.33	1.56	1.43
16	I	102	BCL	O2D-CGD	4.33	1.43	1.33
16	M	403	BCL	C3D-C4D	-4.33	1.34	1.44
23	Q	105	H4X	C21-C22	4.31	1.56	1.43
16	F	103	BCL	O2D-CGD	4.31	1.43	1.33
16	M	402	BCL	CHD-C1D	4.31	1.46	1.38
15	3	101	PGV	O01-C1	4.31	1.46	1.34
23	K	107	H4X	C21-C22	4.29	1.56	1.43
23	6	101	H4X	C15-C14	4.29	1.56	1.43
23	E	101	H4X	C10-C9	4.28	1.56	1.43
23	4	101	H4X	C20-C19	4.28	1.56	1.43
16	L	304	BCL	CHD-C1D	4.28	1.46	1.38
23	4	101	H4X	C25-C23	4.28	1.55	1.46
23	Q	105	H4X	C25-C23	4.28	1.55	1.46
16	X	101	BCL	O2D-CGD	4.28	1.43	1.33
23	O	106	H4X	C21-C22	4.27	1.56	1.43
23	2	101	H4X	C16-C17	4.27	1.55	1.46
16	S	103	BCL	C3D-C4D	-4.26	1.34	1.44
23	O	106	H4X	C31-C32	4.26	1.56	1.43
15	Q	101	PGV	O03-C19	4.26	1.45	1.33
16	A	102	BCL	C1D-ND	-4.26	1.32	1.37
16	I	102	BCL	C3D-C4D	-4.26	1.34	1.44
23	K	107	H4X	C10-C9	4.26	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	6	101	H4X	C30-C28	4.25	1.55	1.46
23	V	101	H4X	C16-C17	4.25	1.55	1.46
16	3	103	BCL	O2D-CGD	4.25	1.43	1.33
23	O	106	H4X	C11-C12	4.25	1.55	1.46
16	O	104	BCL	C3D-C4D	-4.24	1.34	1.44
16	K	105	BCL	O2D-CGD	4.24	1.43	1.33
23	4	101	H4X	C15-C14	4.24	1.56	1.43
23	G	101	H4X	C26-C27	4.23	1.56	1.43
16	M	402	BCL	CHB-C1B	4.23	1.48	1.39
16	D	104	BCL	OBD-CAD	4.23	1.29	1.22
23	4	101	H4X	C11-C12	4.22	1.55	1.46
15	F	104	PGV	O03-C19	4.22	1.45	1.33
16	Q	104	BCL	C3B-C4B	4.22	1.49	1.41
16	D	103	BCL	CHD-C1D	4.22	1.46	1.38
23	P	101	H4X	C15-C14	4.21	1.56	1.43
16	5	103	BCL	O2D-CGD	4.20	1.43	1.33
23	5	105	H4X	C20-C19	4.19	1.56	1.43
16	9	103	BCL	O2D-CGD	4.19	1.43	1.33
16	I	102	BCL	CHC-C4B	4.19	1.48	1.39
23	7	104	H4X	C31-C32	4.19	1.56	1.43
15	D	101	PGV	O01-C1	4.19	1.46	1.34
23	Q	105	H4X	C31-C32	4.18	1.56	1.43
16	O	105	BCL	CHB-C1B	4.18	1.48	1.39
23	K	103	H4X	C20-C19	4.17	1.56	1.43
15	9	101	PGV	O03-C19	4.16	1.45	1.33
16	Q	103	BCL	O2A-CGA	4.16	1.45	1.33
23	V	101	H4X	C11-C12	4.15	1.54	1.46
23	B	101	H4X	C25-C23	4.14	1.54	1.46
15	1	103	PGV	O03-C19	4.14	1.45	1.33
15	K	101	PGV	O01-C1	4.14	1.46	1.34
23	5	105	H4X	C31-C32	4.13	1.56	1.43
23	6	101	H4X	C31-C32	4.13	1.56	1.43
11	C	403	HEM	FE-NB	4.13	2.07	1.94
23	B	101	H4X	C11-C12	4.12	1.54	1.46
16	Y	102	BCL	CHD-C1D	4.11	1.46	1.38
16	X	101	BCL	C3B-C4B	4.11	1.49	1.41
23	5	105	H4X	C11-C12	4.11	1.54	1.46
16	D	103	BCL	CHC-C4B	4.11	1.48	1.39
15	A	101	PGV	O03-C19	4.11	1.49	1.33
16	M	402	BCL	O2A-CGA	4.10	1.45	1.33
16	I	102	BCL	O2A-CGA	4.10	1.45	1.33
16	I	102	BCL	CHB-C1B	4.10	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	105	BCL	CHB-C1B	4.09	1.48	1.39
16	F	103	BCL	CHD-C1D	4.09	1.46	1.38
23	5	105	H4X	C10-C9	4.09	1.55	1.43
23	2	101	H4X	C31-C32	4.08	1.55	1.43
23	6	101	H4X	C10-C9	4.07	1.55	1.43
15	Y	105	PGV	O01-C1	4.07	1.45	1.34
15	M	406	PGV	O03-C19	4.06	1.45	1.33
16	O	104	BCL	C1D-ND	-4.06	1.32	1.37
23	B	101	H4X	C10-C9	4.05	1.55	1.43
16	U	103	BCL	CHD-C1D	4.05	1.46	1.38
23	E	101	H4X	C30-C28	4.05	1.54	1.46
16	2	102	BCL	C3B-C4B	4.04	1.49	1.41
16	J	101	BCL	CHD-C1D	4.03	1.46	1.38
16	O	105	BCL	C1D-ND	-4.03	1.32	1.37
23	Z	101	H4X	C15-C14	4.02	1.55	1.43
15	I	103	PGV	O03-C19	4.01	1.45	1.33
23	K	103	H4X	C31-C32	4.01	1.55	1.43
11	C	402	HEM	FE-NC	4.01	2.08	1.95
16	O	104	BCL	CHD-C1D	4.01	1.46	1.38
16	B	103	BCL	C3B-C4B	4.01	1.49	1.41
16	Q	104	BCL	O2D-CGD	4.00	1.43	1.33
16	7	102	BCL	CHD-C1D	4.00	1.46	1.38
16	O	104	BCL	C3B-C4B	3.99	1.49	1.41
16	9	103	BCL	CHD-C1D	3.99	1.46	1.38
23	K	107	H4X	C15-C14	3.99	1.55	1.43
16	9	104	BCL	O2D-CGD	3.99	1.43	1.33
16	M	402	BCL	OBD-CAD	3.98	1.29	1.22
16	Q	103	BCL	CHC-C4B	3.98	1.48	1.39
23	Z	101	H4X	C10-C9	3.97	1.55	1.43
16	O	104	BCL	CHB-C1B	3.97	1.48	1.39
15	C	408	PGV	O01-C1	3.97	1.45	1.34
16	S	103	BCL	CMA-C3A	-3.96	1.44	1.53
16	7	103	BCL	C3C-C4C	-3.96	1.46	1.51
23	B	101	H4X	C31-C32	3.96	1.55	1.43
16	W	102	BCL	O2D-CGD	3.95	1.42	1.33
16	Y	102	BCL	CHB-C1B	3.95	1.48	1.39
23	B	101	H4X	C15-C14	3.95	1.55	1.43
23	G	101	H4X	C20-C19	3.94	1.55	1.43
16	O	105	BCL	CHC-C4B	3.94	1.48	1.39
16	7	102	BCL	O2A-CGA	3.93	1.44	1.33
23	P	101	H4X	C31-C32	3.93	1.55	1.43
16	3	104	BCL	C3C-C4C	-3.93	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	402	BCL	O2D-CGD	3.93	1.42	1.33
16	T	101	BCL	O2D-CGD	3.92	1.42	1.33
16	K	105	BCL	OBD-CAD	3.92	1.29	1.22
23	U	104	H4X	C30-C28	3.91	1.54	1.46
16	U	102	BCL	O2A-CGA	3.91	1.44	1.33
16	5	103	BCL	C3D-C4D	-3.90	1.35	1.44
16	Y	104	BCL	C3B-C4B	3.90	1.48	1.41
16	1	102	BCL	CHC-C4B	3.90	1.48	1.39
23	V	101	H4X	C30-C28	3.90	1.54	1.46
16	Q	104	BCL	MG-ND	-3.90	1.98	2.05
23	4	101	H4X	C10-C9	3.89	1.55	1.43
16	M	403	BCL	C3B-C4B	3.89	1.48	1.41
16	9	104	BCL	C3B-C4B	3.88	1.48	1.41
16	A	102	BCL	CHD-C1D	3.88	1.46	1.38
23	2	101	H4X	C15-C14	3.88	1.55	1.43
23	Q	105	H4X	C11-C12	3.87	1.54	1.46
23	6	101	H4X	C26-C27	3.87	1.55	1.43
23	O	101	H4X	C21-C22	3.86	1.55	1.43
16	3	103	BCL	CHC-C4B	3.86	1.48	1.39
17	M	404	BPH	C4D-CHA	3.86	1.45	1.39
16	D	104	BCL	CHB-C1B	3.85	1.48	1.39
23	7	104	H4X	C16-C17	3.84	1.54	1.46
23	K	103	H4X	C10-C9	3.84	1.55	1.43
23	B	101	H4X	C30-C28	3.83	1.54	1.46
23	P	101	H4X	C30-C28	3.83	1.54	1.46
23	V	101	H4X	C10-C9	3.83	1.55	1.43
16	B	103	BCL	C1D-ND	-3.83	1.32	1.37
23	2	101	H4X	C10-C9	3.83	1.55	1.43
23	P	101	H4X	C10-C9	3.82	1.55	1.43
16	O	105	BCL	C3B-C4B	3.82	1.48	1.41
16	U	103	BCL	C3B-C4B	3.82	1.48	1.41
23	Q	105	H4X	C15-C14	3.81	1.55	1.43
23	E	101	H4X	C18-C17	3.81	1.58	1.50
23	O	106	H4X	C30-C28	3.81	1.54	1.46
23	V	101	H4X	C15-C14	3.81	1.55	1.43
16	7	102	BCL	CAA-C2A	-3.80	1.47	1.54
16	U	102	BCL	O2D-CGD	3.80	1.42	1.33
16	L	304	BCL	C3B-C4B	3.79	1.48	1.41
16	W	102	BCL	C3B-C4B	3.79	1.48	1.41
16	A	102	BCL	CHB-C1B	3.79	1.47	1.39
16	1	102	BCL	C3C-C4C	-3.79	1.46	1.51
16	L	301	BCL	C3D-C2D	3.79	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	102	BCL	O2D-CGD	3.77	1.42	1.33
16	L	304	BCL	CHB-C1B	3.77	1.47	1.39
23	B	101	H4X	C16-C17	3.77	1.54	1.46
16	Q	103	BCL	CHB-C1B	3.77	1.47	1.39
23	K	103	H4X	C11-C12	3.75	1.54	1.46
23	Q	105	H4X	C30-C28	3.75	1.54	1.46
16	B	103	BCL	O2D-CGD	3.73	1.42	1.33
16	Y	104	BCL	O2D-CGD	3.72	1.42	1.33
23	G	101	H4X	C10-C9	3.72	1.54	1.43
23	U	104	H4X	C31-C32	3.72	1.54	1.43
16	K	105	BCL	C3C-C4C	-3.72	1.46	1.51
16	F	103	BCL	CHC-C4B	3.72	1.47	1.39
16	Y	102	BCL	CHC-C4B	3.72	1.47	1.39
23	V	101	H4X	C24-C23	3.72	1.58	1.50
16	K	105	BCL	CHB-C1B	3.72	1.47	1.39
16	D	103	BCL	C3C-C4C	-3.71	1.46	1.51
23	2	101	H4X	C30-C28	3.71	1.53	1.46
23	V	101	H4X	C31-C32	3.70	1.54	1.43
16	Q	103	BCL	O2D-CGD	3.70	1.42	1.33
16	F	103	BCL	C3B-C4B	3.70	1.48	1.41
23	U	104	H4X	C18-C17	3.69	1.58	1.50
15	I	103	PGV	O01-C1	3.69	1.44	1.34
15	O	102	PGV	O03-C19	3.69	1.44	1.33
23	O	101	H4X	C10-C9	3.68	1.54	1.43
23	U	104	H4X	C10-C9	3.67	1.54	1.43
16	1	102	BCL	OBD-CAD	3.67	1.28	1.22
23	K	103	H4X	C15-C14	3.67	1.54	1.43
23	6	101	H4X	C11-C12	3.66	1.53	1.46
23	G	101	H4X	C31-C32	3.66	1.54	1.43
16	F	105	BCL	CHD-C1D	3.66	1.45	1.38
23	K	107	H4X	C11-C12	3.65	1.53	1.46
16	Q	104	BCL	C1D-ND	-3.65	1.33	1.37
16	D	103	BCL	CHB-C1B	3.64	1.47	1.39
23	7	104	H4X	C30-C28	3.64	1.53	1.46
23	4	101	H4X	C31-C32	3.63	1.54	1.43
16	F	105	BCL	CHC-C4B	3.63	1.47	1.39
23	4	101	H4X	C16-C17	3.63	1.53	1.46
15	O	102	PGV	O01-C1	3.62	1.44	1.34
23	U	104	H4X	C15-C14	3.62	1.54	1.43
16	Q	103	BCL	CAC-C3C	-3.61	1.47	1.54
16	L	304	BCL	CAA-C2A	-3.61	1.47	1.54
16	7	103	BCL	CHD-C1D	3.61	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	5	101	PGV	O03-C19	3.61	1.43	1.33
11	C	402	HEM	C1B-NB	-3.60	1.34	1.40
16	K	108	BCL	CHD-C1D	3.60	1.45	1.38
16	B	103	BCL	CHB-C1B	3.59	1.47	1.39
16	2	102	BCL	O2D-CGD	3.59	1.42	1.33
15	H	301	PGV	O01-C1	3.58	1.44	1.34
16	Y	104	BCL	C3D-C2D	3.57	1.48	1.39
16	Y	104	BCL	CHD-C1D	3.57	1.45	1.38
16	9	104	BCL	C3C-C4C	-3.57	1.47	1.51
11	C	402	HEM	C4D-ND	-3.57	1.34	1.40
16	L	304	BCL	O2D-CED	3.56	1.53	1.45
16	L	301	BCL	CHC-C4B	3.55	1.47	1.39
17	M	404	BPH	CBD-CGD	-3.55	1.48	1.52
16	7	103	BCL	O2D-CGD	3.55	1.41	1.33
23	G	101	H4X	C15-C14	3.54	1.54	1.43
16	W	102	BCL	CHC-C4B	3.54	1.47	1.39
16	I	102	BCL	CHD-C1D	3.54	1.45	1.38
15	K	106	PGV	O01-C1	3.54	1.44	1.34
23	O	101	H4X	C15-C14	3.53	1.54	1.43
16	2	102	BCL	C3D-C2D	3.53	1.48	1.39
16	X	101	BCL	C1D-ND	-3.52	1.33	1.37
11	C	401	HEM	C1B-NB	-3.52	1.34	1.40
16	O	105	BCL	OBD-CAD	3.51	1.28	1.22
16	7	103	BCL	C3D-C2D	3.51	1.48	1.39
16	A	102	BCL	C4B-NB	-3.50	1.33	1.37
23	4	101	H4X	C30-C28	3.49	1.53	1.46
23	7	104	H4X	C15-C14	3.49	1.54	1.43
16	7	103	BCL	C3B-C4B	3.49	1.48	1.41
16	5	103	BCL	C3B-C4B	3.49	1.48	1.41
16	7	102	BCL	CHB-C1B	3.49	1.47	1.39
16	3	103	BCL	C3B-C4B	3.47	1.48	1.41
16	Y	102	BCL	O2A-CGA	3.46	1.43	1.33
23	O	106	H4X	C10-C9	3.46	1.53	1.43
16	S	103	BCL	CHC-C4B	3.46	1.47	1.39
23	7	104	H4X	C10-C9	3.45	1.53	1.43
16	Y	104	BCL	CAC-C3C	-3.44	1.47	1.54
23	O	101	H4X	C31-C32	3.44	1.53	1.43
16	5	103	BCL	C3D-C2D	3.43	1.48	1.39
16	D	104	BCL	C3D-C2D	3.43	1.48	1.39
16	M	403	BCL	C3D-C2D	3.43	1.48	1.39
17	L	302	BPH	C4D-CHA	3.42	1.44	1.39
16	D	104	BCL	CHC-C4B	3.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	5	104	BCL	CHD-C1D	3.41	1.45	1.38
23	O	101	H4X	C30-C28	3.40	1.53	1.46
16	U	103	BCL	CAA-C2A	-3.40	1.47	1.54
16	Q	103	BCL	C3B-C4B	3.39	1.47	1.41
16	Q	103	BCL	C3C-C4C	-3.38	1.47	1.51
16	L	301	BCL	O2A-CGA	3.38	1.43	1.33
16	L	304	BCL	C3D-C2D	3.37	1.48	1.39
11	C	404	HEM	C1C-C2C	-3.37	1.38	1.45
16	5	103	BCL	MG-ND	-3.36	1.99	2.05
15	F	104	PGV	O01-C1	3.36	1.43	1.34
21	M	405	MQ8	C3-C2	3.36	1.41	1.35
16	Y	102	BCL	C3B-C4B	3.36	1.47	1.41
24	P	102	LMT	C12-C11	3.35	1.74	1.50
16	O	104	BCL	MG-ND	-3.34	1.99	2.05
16	O	105	BCL	C3C-C4C	-3.33	1.47	1.51
16	S	103	BCL	CHB-C1B	3.33	1.46	1.39
16	O	105	BCL	C4B-NB	-3.33	1.33	1.37
16	Y	104	BCL	C1B-C2B	3.32	1.50	1.43
16	J	101	BCL	C1D-ND	-3.31	1.33	1.37
16	9	104	BCL	MG-ND	-3.31	1.99	2.05
16	S	103	BCL	C4B-NB	-3.31	1.33	1.37
16	A	102	BCL	OBD-CAD	3.30	1.28	1.22
16	B	103	BCL	CHC-C4B	3.29	1.46	1.39
16	U	102	BCL	CHB-C1B	3.29	1.46	1.39
16	X	101	BCL	CHC-C4B	3.29	1.46	1.39
16	L	301	BCL	CHD-C1D	3.29	1.44	1.38
16	D	104	BCL	C3B-C4B	3.27	1.47	1.41
16	5	104	BCL	CAA-C2A	-3.27	1.48	1.54
24	T	102	LMT	C12-C11	3.26	1.73	1.50
16	Y	102	BCL	C1D-ND	-3.26	1.33	1.37
15	Q	101	PGV	O01-C1	3.26	1.43	1.34
23	7	104	H4X	C24-C23	3.26	1.57	1.50
16	J	101	BCL	MG-ND	-3.25	1.99	2.05
16	2	102	BCL	CMC-C2C	-3.24	1.46	1.53
16	Q	103	BCL	C1D-ND	-3.24	1.33	1.37
16	T	101	BCL	CHB-C1B	3.24	1.46	1.39
16	S	103	BCL	CHD-C1D	3.24	1.44	1.38
16	X	101	BCL	CAA-C2A	-3.22	1.48	1.54
16	J	101	BCL	C3B-C4B	3.22	1.47	1.41
16	O	104	BCL	C1B-NB	-3.21	1.33	1.37
15	9	101	PGV	O01-C1	3.21	1.43	1.34
16	9	104	BCL	CHB-C1B	3.19	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	7	102	BCL	OBD-CAD	3.18	1.28	1.22
16	S	103	BCL	C3B-C4B	3.17	1.47	1.41
16	F	103	BCL	CHB-C1B	3.17	1.46	1.39
16	O	104	BCL	C3D-C2D	3.17	1.47	1.39
16	O	104	BCL	CAC-C3C	-3.17	1.48	1.54
16	U	103	BCL	C3C-C4C	-3.16	1.47	1.51
16	3	104	BCL	C1D-ND	-3.16	1.33	1.37
16	F	105	BCL	C3B-C4B	3.15	1.47	1.41
23	K	103	H4X	C30-C28	3.14	1.52	1.46
16	3	104	BCL	C3B-C4B	3.14	1.47	1.41
16	J	101	BCL	CHB-C1B	3.14	1.46	1.39
16	K	108	BCL	CHB-C1B	3.13	1.46	1.39
16	2	102	BCL	CHC-C4B	3.13	1.46	1.39
11	C	401	HEM	FE-NC	3.12	2.05	1.95
16	A	102	BCL	C3B-C4B	3.12	1.47	1.41
16	J	101	BCL	C3C-C4C	-3.12	1.47	1.51
18	L	303	UQ8	C4-C3	3.12	1.47	1.36
16	3	103	BCL	OBD-CAD	3.11	1.27	1.22
16	L	301	BCL	C3B-C4B	3.11	1.47	1.41
16	M	402	BCL	CHC-C4B	3.09	1.46	1.39
17	M	404	BPH	C1D-C2D	3.09	1.43	1.39
11	C	403	HEM	FE-NC	3.09	2.05	1.95
16	7	103	BCL	CAA-C2A	-3.09	1.48	1.54
16	O	104	BCL	C4D-CHA	3.09	1.49	1.38
16	I	102	BCL	C3C-C4C	-3.08	1.47	1.51
16	U	102	BCL	C3B-C4B	3.08	1.47	1.41
16	O	104	BCL	C4B-NB	-3.08	1.33	1.37
23	Z	101	H4X	C30-C28	3.07	1.52	1.46
16	M	403	BCL	MG-ND	-3.07	1.99	2.05
16	U	103	BCL	CHB-C1B	3.07	1.46	1.39
16	7	103	BCL	CHB-C1B	3.06	1.46	1.39
16	1	102	BCL	C3B-C4B	3.06	1.47	1.41
16	U	102	BCL	CAA-C2A	-3.06	1.48	1.54
16	5	103	BCL	CHB-C1B	3.06	1.46	1.39
16	K	105	BCL	C3B-C4B	3.04	1.47	1.41
16	9	103	BCL	CHC-C4B	3.04	1.46	1.39
16	X	101	BCL	CHB-C1B	3.04	1.46	1.39
16	M	402	BCL	C4B-NB	-3.03	1.33	1.37
16	Y	102	BCL	OBD-CAD	3.02	1.27	1.22
16	Y	102	BCL	C4D-CHA	3.01	1.48	1.38
16	I	102	BCL	C4B-NB	-3.01	1.33	1.37
16	9	103	BCL	C1B-C2B	3.01	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	101	PGV	O01-C02	-3.01	1.39	1.46
16	S	103	BCL	C3D-C2D	3.00	1.47	1.39
16	Y	104	BCL	CHC-C4B	3.00	1.46	1.39
16	5	103	BCL	CHC-C4B	2.99	1.46	1.39
23	K	107	H4X	C30-C28	2.99	1.52	1.46
23	O	106	H4X	C39-C38	2.99	1.59	1.52
16	W	102	BCL	CAA-C2A	-2.99	1.48	1.54
16	S	103	BCL	O2D-CGD	2.98	1.40	1.33
16	9	104	BCL	CHC-C4B	2.98	1.46	1.39
16	7	102	BCL	C3D-C2D	2.96	1.47	1.39
16	L	301	BCL	C4D-CHA	2.96	1.48	1.38
16	J	101	BCL	CHC-C4B	2.96	1.46	1.39
16	M	403	BCL	CHD-C1D	2.95	1.44	1.38
23	E	101	H4X	C39-C38	2.94	1.59	1.52
16	L	301	BCL	C1B-C2B	2.94	1.50	1.43
11	C	401	HEM	C1A-C2A	-2.94	1.38	1.44
16	9	103	BCL	CMC-C2C	-2.94	1.47	1.53
16	I	102	BCL	C3D-C2D	2.94	1.47	1.39
16	A	102	BCL	C3C-C4C	-2.93	1.47	1.51
23	O	106	H4X	C18-C17	2.92	1.56	1.50
16	K	108	BCL	CHC-C4B	2.91	1.45	1.39
16	K	105	BCL	CHC-C4B	2.90	1.45	1.39
16	B	103	BCL	C4D-CHA	2.90	1.48	1.38
16	U	103	BCL	C3D-C2D	2.90	1.46	1.39
16	3	104	BCL	C3D-C2D	2.89	1.46	1.39
16	S	103	BCL	C3C-C4C	-2.88	1.48	1.51
16	1	102	BCL	CHB-C1B	2.88	1.45	1.39
16	5	104	BCL	OBD-CAD	2.88	1.27	1.22
16	K	105	BCL	C4D-CHA	2.87	1.48	1.38
16	M	403	BCL	CMD-C2D	-2.87	1.44	1.50
16	Q	103	BCL	C4D-CHA	2.87	1.48	1.38
16	9	103	BCL	C4D-CHA	2.87	1.48	1.38
16	A	102	BCL	C4D-CHA	2.86	1.48	1.38
21	M	405	MQ8	C8-C7	2.85	1.44	1.38
15	D	101	PGV	O03-C19	2.84	1.41	1.33
23	P	101	H4X	C18-C17	2.84	1.56	1.50
16	D	103	BCL	O2D-CGD	2.83	1.40	1.33
16	3	103	BCL	MG-ND	-2.83	2.00	2.05
16	D	104	BCL	C4B-NB	-2.83	1.34	1.37
15	A	101	PGV	O01-C1	2.82	1.42	1.34
16	5	104	BCL	C3D-C2D	2.82	1.46	1.39
16	9	104	BCL	C4D-CHA	2.82	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	M	404	BPH	C1B-C2B	2.82	1.42	1.39
16	W	102	BCL	CHB-C1B	2.82	1.45	1.39
16	U	102	BCL	CHC-C4B	2.82	1.45	1.39
16	3	103	BCL	CHB-C1B	2.82	1.45	1.39
16	X	101	BCL	C3D-C2D	2.81	1.46	1.39
16	K	105	BCL	C4B-NB	-2.81	1.34	1.37
16	L	304	BCL	CBD-CGD	-2.79	1.44	1.52
16	O	104	BCL	C3C-C4C	-2.77	1.48	1.51
16	L	304	BCL	C1B-C2B	2.76	1.49	1.43
11	C	401	HEM	FE-ND	-2.76	1.86	1.94
16	D	103	BCL	C3B-C4B	2.76	1.46	1.41
16	A	102	BCL	CAA-C2A	-2.75	1.49	1.54
16	X	101	BCL	CHD-C4C	2.75	1.46	1.39
18	L	306	UQ8	C4-C3	2.74	1.46	1.36
11	C	402	HEM	C1B-C2B	-2.74	1.38	1.44
24	4	102	LMT	C12-C11	2.74	1.69	1.50
16	D	103	BCL	C1D-ND	-2.73	1.34	1.37
23	P	101	H4X	C13-C12	2.73	1.56	1.50
16	Q	104	BCL	CAC-C3C	-2.73	1.48	1.54
16	W	102	BCL	C4D-CHA	2.71	1.47	1.38
16	5	103	BCL	CMC-C2C	-2.71	1.47	1.53
24	T	102	LMT	O1'-C1'	2.70	1.44	1.40
16	M	402	BCL	CHD-C4C	2.70	1.46	1.39
24	R	101	LMT	O1'-C1'	2.70	1.44	1.40
24	E	102	LMT	C12-C11	2.69	1.69	1.50
16	3	103	BCL	C3D-C2D	2.69	1.46	1.39
16	F	103	BCL	CMA-C3A	-2.68	1.47	1.53
16	2	102	BCL	CHD-C4C	2.68	1.46	1.39
16	L	304	BCL	OBD-CAD	2.68	1.27	1.22
16	1	102	BCL	CAC-C3C	-2.67	1.48	1.54
16	D	104	BCL	C1D-ND	-2.67	1.34	1.37
15	C	408	PGV	O01-C02	-2.67	1.42	1.47
16	M	402	BCL	C3D-C2D	2.66	1.46	1.39
16	L	304	BCL	CAC-C3C	-2.66	1.48	1.54
18	L	303	UQ8	O3-C3M	-2.66	1.39	1.45
16	5	103	BCL	C1B-NB	-2.65	1.34	1.37
16	L	301	BCL	CHD-C4C	2.65	1.46	1.39
16	U	103	BCL	C4B-NB	-2.65	1.34	1.37
16	W	102	BCL	C3D-C2D	2.65	1.46	1.39
16	3	103	BCL	CAA-C2A	-2.65	1.49	1.54
16	7	102	BCL	C3B-C4B	2.64	1.46	1.41
16	9	103	BCL	C3B-C4B	2.64	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	302	BPH	C1B-C2B	2.64	1.42	1.39
16	K	105	BCL	CAA-C2A	-2.63	1.49	1.54
16	9	103	BCL	C3D-C2D	2.63	1.46	1.39
23	E	101	H4X	C29-C28	2.63	1.56	1.50
16	Y	104	BCL	CHB-C4A	-2.63	1.31	1.37
16	3	104	BCL	CAA-C2A	-2.62	1.49	1.54
24	6	102	LMT	O1'-C1'	2.62	1.44	1.40
16	J	101	BCL	C3D-C2D	2.62	1.46	1.39
16	U	102	BCL	C4D-CHA	2.61	1.47	1.38
16	5	104	BCL	CHC-C4B	2.61	1.45	1.39
23	U	104	H4X	C35-C33	2.59	1.56	1.51
24	0	101	LMT	C12-C11	2.59	1.68	1.50
16	I	102	BCL	C3B-C4B	2.59	1.46	1.41
24	6	102	LMT	C12-C11	2.59	1.68	1.50
16	O	105	BCL	C4D-CHA	2.59	1.47	1.38
16	W	102	BCL	CMB-C2B	-2.59	1.45	1.50
11	C	404	HEM	CAB-C3B	2.59	1.54	1.47
16	K	108	BCL	C3B-C4B	2.59	1.46	1.41
16	5	103	BCL	C1D-ND	-2.59	1.34	1.37
16	D	104	BCL	C1B-C2B	2.58	1.49	1.43
11	C	404	HEM	CMC-C2C	-2.58	1.45	1.50
16	5	103	BCL	CHB-C4A	-2.58	1.31	1.37
16	7	102	BCL	CHD-C4C	2.58	1.46	1.39
16	D	103	BCL	C3D-C2D	2.57	1.46	1.39
24	2	103	LMT	C12-C11	2.57	1.68	1.50
24	4	102	LMT	O1'-C1'	2.57	1.44	1.40
16	5	104	BCL	CHB-C1B	2.57	1.45	1.39
16	M	402	BCL	C4D-CHA	2.57	1.47	1.38
16	Q	104	BCL	C4D-CHA	2.57	1.47	1.38
16	9	103	BCL	OBD-CAD	2.57	1.26	1.22
16	D	103	BCL	OBD-CAD	2.56	1.26	1.22
16	O	105	BCL	C3D-C2D	2.56	1.46	1.39
16	7	103	BCL	CHC-C1C	-2.56	1.31	1.37
16	L	304	BCL	MG-ND	-2.56	2.00	2.05
23	O	101	H4X	C31-C30	-2.56	1.28	1.34
23	K	107	H4X	C18-C17	2.56	1.56	1.50
11	C	403	HEM	C1C-C2C	-2.55	1.40	1.45
16	U	102	BCL	C3D-C2D	2.55	1.46	1.39
16	F	103	BCL	C2C-C3C	-2.54	1.47	1.54
24	E	102	LMT	O1'-C1'	2.54	1.44	1.40
16	F	103	BCL	CHD-C4C	2.54	1.46	1.39
16	D	103	BCL	C4D-CHA	2.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	102	BCL	CAA-C2A	-2.53	1.49	1.54
16	K	108	BCL	C1D-ND	-2.52	1.34	1.37
16	Y	104	BCL	CHB-C1B	2.52	1.45	1.39
16	K	108	BCL	C3D-C2D	2.52	1.45	1.39
16	U	102	BCL	C1B-C2B	2.52	1.49	1.43
16	7	103	BCL	CHC-C4B	2.51	1.45	1.39
16	L	301	BCL	C2A-C1A	-2.51	1.46	1.52
24	B	104	LMT	O5B-C1B	2.51	1.48	1.41
23	O	101	H4X	C6-C7	2.50	1.56	1.51
16	7	102	BCL	C4D-CHA	2.50	1.47	1.38
16	Q	103	BCL	CAA-C2A	-2.50	1.49	1.54
16	W	102	BCL	OBD-CAD	2.50	1.26	1.22
16	Y	102	BCL	O2A-C1	-2.50	1.39	1.46
24	R	101	LMT	C12-C11	2.50	1.68	1.50
23	Q	105	H4X	C18-C17	2.50	1.55	1.50
16	Y	102	BCL	CAA-C2A	-2.49	1.49	1.54
16	F	105	BCL	CAA-C2A	-2.49	1.49	1.54
23	6	101	H4X	C18-C17	2.48	1.55	1.50
16	3	104	BCL	C4D-CHA	2.48	1.46	1.38
16	K	108	BCL	CMA-C3A	-2.48	1.47	1.53
16	O	105	BCL	CHD-C4C	2.48	1.46	1.39
16	1	102	BCL	CMA-C3A	-2.48	1.48	1.53
16	Q	104	BCL	C3D-C2D	2.48	1.45	1.39
16	5	103	BCL	C4D-CHA	2.47	1.46	1.38
16	F	103	BCL	OBD-CAD	2.47	1.26	1.22
11	C	404	HEM	C3C-C2C	2.47	1.42	1.37
16	W	102	BCL	CHD-C4C	2.47	1.46	1.39
16	T	101	BCL	CMD-C2D	-2.47	1.45	1.50
16	3	104	BCL	CMC-C2C	-2.47	1.48	1.53
16	D	104	BCL	CHD-C4C	2.46	1.46	1.39
16	K	108	BCL	C3C-C4C	-2.46	1.48	1.51
11	C	403	HEM	C1B-C2B	-2.46	1.39	1.44
16	3	103	BCL	C3C-C4C	-2.46	1.48	1.51
16	A	102	BCL	CHC-C4B	2.46	1.44	1.39
11	C	402	HEM	CBC-CAC	2.45	1.42	1.30
16	M	403	BCL	C1B-C2B	2.45	1.48	1.43
16	7	102	BCL	O2A-C1	-2.44	1.39	1.46
24	J	102	LMT	C1'-C2'	2.44	1.59	1.52
24	2	103	LMT	C1'-C2'	2.44	1.59	1.52
16	5	103	BCL	C1B-C2B	2.44	1.48	1.43
16	S	103	BCL	C1B-C2B	2.43	1.48	1.43
16	U	103	BCL	O1D-CGD	2.42	1.27	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	U	103	BCL	CHC-C4B	2.42	1.44	1.39
16	9	103	BCL	CHB-C1B	2.42	1.44	1.39
24	J	102	LMT	O1'-C1'	2.42	1.44	1.40
15	H	301	PGV	O03-C01	-2.42	1.39	1.45
16	F	105	BCL	C4D-CHA	2.42	1.46	1.38
16	Q	104	BCL	CHD-C4C	2.41	1.46	1.39
16	2	102	BCL	C4B-NB	-2.41	1.34	1.37
15	C	408	PGV	P-O12	2.41	1.63	1.54
16	L	304	BCL	C1D-C2D	2.40	1.50	1.45
11	C	401	HEM	C3C-C4C	-2.40	1.41	1.46
23	5	105	H4X	C18-C17	2.40	1.55	1.50
24	4	102	LMT	C1'-C2'	2.40	1.59	1.52
16	D	104	BCL	CHB-C4A	-2.40	1.31	1.37
23	B	101	H4X	C24-C23	2.40	1.55	1.50
16	L	301	BCL	C2-C3	2.40	1.38	1.33
16	5	104	BCL	C4D-CHA	2.39	1.46	1.38
16	Y	102	BCL	OBB-CAB	-2.39	1.17	1.23
16	D	104	BCL	MG-ND	-2.39	2.01	2.05
24	N	101	LMT	O1'-C1'	2.39	1.44	1.40
16	Q	104	BCL	CHB-C1B	2.38	1.44	1.39
16	1	102	BCL	CBD-CGD	-2.38	1.45	1.52
16	J	101	BCL	CMA-C3A	-2.38	1.48	1.53
11	C	401	HEM	C1D-ND	-2.38	1.34	1.38
11	C	401	HEM	C4B-NB	-2.37	1.34	1.38
16	T	101	BCL	C1D-ND	-2.37	1.34	1.37
16	1	102	BCL	C4D-CHA	2.37	1.46	1.38
24	Z	102	LMT	C12-C11	2.37	1.67	1.50
24	B	104	LMT	C12-C11	2.37	1.67	1.50
16	3	103	BCL	C1D-ND	-2.36	1.34	1.37
24	G	102	LMT	C1'-C2'	2.36	1.59	1.52
16	S	103	BCL	MG-ND	-2.36	2.01	2.05
16	3	103	BCL	C4D-CHA	2.35	1.46	1.38
24	0	101	LMT	O1'-C1'	2.35	1.44	1.40
16	U	102	BCL	CAC-C3C	-2.35	1.49	1.54
11	C	402	HEM	C3C-C2C	2.35	1.41	1.37
16	S	103	BCL	OBD-CAD	2.35	1.26	1.22
24	B	104	LMT	O1'-C1'	2.35	1.44	1.40
16	O	104	BCL	CAA-C2A	-2.35	1.49	1.54
11	C	402	HEM	C4B-NB	-2.34	1.34	1.38
16	Q	104	BCL	CAA-C2A	-2.34	1.49	1.54
16	Q	104	BCL	CMB-C2B	-2.34	1.46	1.50
16	3	104	BCL	CMA-C3A	-2.34	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	105	BCL	O1D-CGD	2.33	1.27	1.21
16	I	102	BCL	CHD-C4C	2.33	1.45	1.39
16	T	101	BCL	MG-ND	-2.32	2.01	2.05
11	C	401	HEM	CBD-CGD	2.32	1.55	1.50
16	1	102	BCL	C4B-NB	-2.32	1.34	1.37
16	Q	103	BCL	C3D-C2D	2.32	1.45	1.39
16	L	304	BCL	C4B-NB	-2.32	1.34	1.37
16	9	103	BCL	C3C-C4C	-2.32	1.48	1.51
23	O	101	H4X	C24-C23	2.31	1.55	1.50
23	B	101	H4X	C2-C1	2.31	1.57	1.52
16	T	101	BCL	C3D-C2D	2.31	1.45	1.39
11	C	401	HEM	FE-NA	2.30	2.02	1.95
11	C	404	HEM	FE-NA	2.30	2.02	1.95
16	Y	104	BCL	C1D-ND	-2.30	1.34	1.37
16	A	102	BCL	CHB-C4A	-2.30	1.31	1.37
23	P	101	H4X	C39-C38	2.30	1.57	1.52
16	U	102	BCL	C1D-ND	-2.30	1.34	1.37
23	U	104	H4X	C37-C38	2.30	1.56	1.53
11	C	403	HEM	C1A-C2A	-2.30	1.40	1.44
16	T	101	BCL	CAA-C2A	-2.29	1.49	1.54
16	7	103	BCL	CHB-C4A	-2.29	1.32	1.37
16	5	104	BCL	MG-NC	-2.29	2.00	2.06
16	O	105	BCL	CHB-C4A	-2.29	1.32	1.37
23	G	101	H4X	C24-C23	2.28	1.55	1.50
16	M	403	BCL	C4D-CHA	2.28	1.46	1.38
11	C	404	HEM	C1B-C2B	-2.27	1.39	1.44
16	A	102	BCL	C1B-C2B	2.27	1.48	1.43
16	9	103	BCL	CAA-C2A	-2.27	1.50	1.54
16	D	103	BCL	CMA-C3A	-2.27	1.48	1.53
16	X	101	BCL	C3A-C2A	-2.27	1.48	1.54
16	7	102	BCL	CHC-C4B	2.26	1.44	1.39
16	3	104	BCL	CHD-C4C	2.26	1.45	1.39
16	T	101	BCL	CHC-C4B	2.26	1.44	1.39
16	W	102	BCL	C3C-C4C	-2.26	1.48	1.51
16	O	104	BCL	CBD-CAD	-2.26	1.46	1.56
16	5	103	BCL	C4B-NB	-2.26	1.34	1.37
16	Q	104	BCL	CBD-CGD	-2.25	1.45	1.52
24	2	103	LMT	O1'-C1'	2.24	1.43	1.40
16	Y	104	BCL	MG-ND	-2.24	2.01	2.05
16	3	103	BCL	CHD-C4C	2.24	1.45	1.39
16	F	105	BCL	O2D-CED	-2.24	1.40	1.45
21	M	405	MQ8	C15-C16	-2.24	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	101	PGV	O05-C05	-2.24	1.36	1.43
16	1	102	BCL	O2A-C1	-2.23	1.40	1.46
16	7	103	BCL	MG-ND	-2.23	2.01	2.05
16	U	103	BCL	C4D-CHA	2.23	1.46	1.38
16	I	102	BCL	OBD-CAD	2.23	1.26	1.22
16	K	108	BCL	CHD-C4C	2.23	1.45	1.39
24	X	102	LMT	C12-C11	2.23	1.66	1.50
16	Q	103	BCL	C1B-NB	-2.23	1.34	1.37
16	K	108	BCL	CMC-C2C	-2.22	1.48	1.53
16	2	102	BCL	CHD-C1D	2.22	1.42	1.38
11	C	404	HEM	CMD-C2D	-2.21	1.46	1.50
16	A	102	BCL	O2A-C1	-2.21	1.40	1.46
16	W	102	BCL	O2A-C1	-2.21	1.40	1.46
11	C	402	HEM	CAB-C3B	2.20	1.53	1.47
16	F	103	BCL	C3D-C2D	2.20	1.45	1.39
16	Q	104	BCL	C3A-C2A	-2.20	1.48	1.54
23	5	105	H4X	C8-C7	2.20	1.56	1.50
16	F	105	BCL	C3C-C4C	-2.20	1.48	1.51
16	B	103	BCL	CAA-C2A	-2.19	1.50	1.54
16	9	103	BCL	C1D-ND	-2.19	1.35	1.37
16	5	104	BCL	CHD-C4C	2.19	1.45	1.39
16	A	102	BCL	C3D-C2D	2.19	1.45	1.39
16	D	103	BCL	CMD-C2D	-2.19	1.46	1.50
23	Z	101	H4X	C18-C17	2.19	1.55	1.50
16	B	103	BCL	CMB-C2B	-2.19	1.46	1.50
16	M	402	BCL	C3C-C4C	-2.18	1.48	1.51
16	J	101	BCL	C1D-C2D	2.18	1.49	1.45
16	M	403	BCL	CHC-C4B	2.18	1.44	1.39
16	T	101	BCL	C3B-C4B	2.18	1.45	1.41
16	M	402	BCL	C3B-C4B	2.17	1.45	1.41
16	M	403	BCL	CAC-C3C	-2.17	1.49	1.54
16	D	104	BCL	CAA-C2A	-2.17	1.50	1.54
23	V	101	H4X	C18-C17	2.16	1.55	1.50
17	L	302	BPH	C3B-C2B	2.16	1.43	1.39
15	A	101	PGV	P-O12	2.16	1.67	1.59
16	K	108	BCL	CHB-C4A	-2.16	1.32	1.37
16	F	103	BCL	C1B-C2B	2.16	1.48	1.43
16	7	103	BCL	O2D-CED	-2.15	1.40	1.45
24	X	102	LMT	O1'-C1'	2.15	1.43	1.40
16	I	102	BCL	C4D-CHA	2.15	1.45	1.38
16	F	105	BCL	C3D-C2D	2.15	1.44	1.39
16	K	105	BCL	C3D-C2D	2.15	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	102	BCL	C1B-C2B	2.15	1.48	1.43
16	X	101	BCL	C4B-NB	-2.15	1.35	1.37
16	K	105	BCL	CMA-C3A	-2.15	1.48	1.53
16	T	101	BCL	C4D-CHA	2.15	1.45	1.38
16	Y	102	BCL	C1B-NB	-2.14	1.35	1.37
16	X	101	BCL	C4D-CHA	2.14	1.45	1.38
23	V	101	H4X	C2-C1	2.14	1.57	1.52
16	3	104	BCL	CHC-C4B	2.14	1.44	1.39
16	B	103	BCL	CBD-CGD	-2.14	1.46	1.52
16	U	102	BCL	MG-NB	-2.13	2.01	2.05
18	L	303	UQ8	C7-C8	-2.13	1.47	1.50
16	2	102	BCL	MG-ND	-2.13	2.01	2.05
16	7	102	BCL	C1B-C2B	2.13	1.48	1.43
23	O	106	H4X	C6-C7	2.13	1.55	1.51
16	5	103	BCL	CAA-C2A	-2.13	1.50	1.54
17	L	302	BPH	CBD-CGD	-2.12	1.49	1.52
16	O	104	BCL	CMC-C2C	-2.11	1.48	1.53
16	B	103	BCL	C4B-NB	-2.11	1.35	1.37
11	C	401	HEM	C4D-ND	-2.11	1.36	1.40
16	Q	104	BCL	CHC-C4B	2.11	1.44	1.39
16	U	102	BCL	C1B-NB	-2.11	1.35	1.37
23	O	101	H4X	C37-C38	2.11	1.56	1.53
23	O	106	H4X	C4-C1	2.11	1.56	1.53
16	5	103	BCL	CBD-CAD	-2.10	1.47	1.56
16	K	108	BCL	MG-ND	-2.09	2.01	2.05
24	6	102	LMT	C1'-C2'	2.09	1.58	1.52
24	G	102	LMT	O1'-C1'	2.09	1.43	1.40
23	G	101	H4X	C18-C17	2.09	1.55	1.50
16	T	101	BCL	MG-NB	2.08	2.09	2.05
23	O	106	H4X	C29-C28	2.08	1.55	1.50
16	5	104	BCL	C4B-NB	-2.08	1.35	1.37
16	5	104	BCL	CBD-CAD	-2.08	1.47	1.56
11	C	401	HEM	C3B-C2B	-2.08	1.32	1.37
16	J	101	BCL	CHB-C4A	-2.07	1.32	1.37
23	O	101	H4X	C4-C1	2.07	1.56	1.53
24	G	102	LMT	C12-C11	2.06	1.65	1.50
11	C	403	HEM	C1B-NB	-2.06	1.36	1.40
16	D	104	BCL	CAC-C3C	-2.06	1.50	1.54
16	O	104	BCL	O2A-C1	-2.05	1.40	1.46
23	G	101	H4X	C6-C7	2.05	1.55	1.51
24	N	101	LMT	C12-C11	2.05	1.64	1.50
11	C	403	HEM	C3B-C2B	2.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	102	BCL	CMD-C2D	-2.04	1.46	1.50
16	T	101	BCL	CAC-C3C	-2.04	1.50	1.54
16	Q	104	BCL	C3B-C2B	2.03	1.49	1.42
11	C	402	HEM	CBD-CGD	-2.03	1.45	1.50
16	S	103	BCL	CHD-C4C	2.03	1.44	1.39
16	3	104	BCL	O2D-CED	-2.03	1.40	1.45
15	9	101	PGV	O01-C02	-2.03	1.41	1.46
16	Y	102	BCL	C3D-C2D	2.03	1.44	1.39
24	V	102	LMT	C12-C11	2.03	1.64	1.50
16	L	304	BCL	C2-C3	2.03	1.37	1.33
16	5	103	BCL	CHD-C4C	2.03	1.44	1.39
16	D	103	BCL	C4B-NB	-2.02	1.35	1.37
23	Q	105	H4X	C24-C23	2.02	1.54	1.50
11	C	404	HEM	CBB-CAB	2.02	1.40	1.30
11	C	401	HEM	C3D-C2D	-2.02	1.32	1.36
15	F	101	PGV	P-O12	2.01	1.62	1.54
24	8	102	LMT	O1'-C1'	2.01	1.43	1.40
24	8	101	LMT	O1'-C1'	2.01	1.43	1.40
16	F	103	BCL	C4D-CHA	2.01	1.45	1.38
23	U	104	H4X	C24-C23	2.01	1.54	1.50
16	J	101	BCL	C4D-CHA	2.00	1.45	1.38

All (1510) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	304	BCL	O2D-CGD-CBD	15.98	139.16	111.23
16	L	304	BCL	O2D-CGD-O1D	-13.30	97.96	123.85
23	V	101	H4X	C21-C22-C23	-9.39	114.11	127.28
16	D	103	BCL	O2D-CGD-CBD	8.65	126.36	111.23
16	A	102	BCL	O2D-CGD-CBD	8.41	125.94	111.23
16	S	103	BCL	O2D-CGD-CBD	8.07	125.34	111.23
16	I	102	BCL	O2D-CGD-CBD	7.93	125.10	111.23
15	H	301	PGV	O01-C1-C2	7.86	128.49	111.48
16	U	102	BCL	O2D-CGD-CBD	7.85	124.95	111.23
16	M	403	BCL	C1C-NC-C4C	-7.68	103.17	106.68
23	5	105	H4X	C21-C22-C23	-7.61	116.60	127.28
16	9	103	BCL	O2D-CGD-CBD	7.58	124.49	111.23
16	3	103	BCL	O2D-CGD-CBD	7.58	124.47	111.23
16	M	402	BCL	O2D-CGD-CBD	7.34	124.05	111.23
16	K	108	BCL	C6-C5-C3	-7.26	95.79	113.47
23	V	101	H4X	C20-C19-C17	-7.23	117.13	127.28
11	C	403	HEM	CHC-C4B-NB	7.11	132.07	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	301	BCL	C1C-NC-C4C	-7.09	103.44	106.68
16	Q	103	BCL	O2D-CGD-CBD	7.08	123.60	111.23
18	L	303	UQ8	C15-C14-C16	7.04	127.45	115.23
16	A	102	BCL	O2D-CGD-O1D	-6.96	110.31	123.85
16	M	403	BCL	O2D-CGD-CBD	6.94	123.37	111.23
23	G	101	H4X	C31-C32-C33	-6.91	117.97	127.69
23	7	104	H4X	C21-C22-C23	-6.84	117.68	127.28
16	M	402	BCL	O2D-CGD-O1D	-6.74	110.73	123.85
23	Z	101	H4X	C21-C22-C23	-6.74	117.83	127.28
16	1	102	BCL	O2D-CGD-CBD	6.71	122.96	111.23
23	E	101	H4X	C36-C35-C33	6.69	129.77	113.47
16	9	103	BCL	CMB-C2B-C1B	6.65	135.54	125.42
16	2	102	BCL	C2B-C1B-NB	6.56	117.13	110.33
11	C	404	HEM	C3B-C4B-NB	-6.45	104.83	109.47
16	F	103	BCL	O2D-CGD-CBD	6.44	122.48	111.23
15	D	101	PGV	O01-C1-C2	6.40	125.32	111.48
16	7	102	BCL	O2D-CGD-CBD	6.40	122.41	111.23
16	Q	104	BCL	C2B-C1B-NB	6.38	116.94	110.33
16	F	103	BCL	CMD-C2D-C1D	6.34	135.90	124.73
16	Y	102	BCL	O2D-CGD-CBD	6.33	122.30	111.23
16	B	103	BCL	C2B-C1B-NB	6.29	116.85	110.33
16	2	102	BCL	C4-C3-C5	6.29	126.14	115.23
23	Z	101	H4X	C10-C9-C7	-6.27	118.88	127.69
16	X	101	BCL	C2B-C1B-NB	6.22	116.78	110.33
16	U	103	BCL	CMD-C2D-C1D	6.19	135.63	124.73
16	L	301	BCL	CMB-C2B-C1B	6.16	134.80	125.42
23	V	101	H4X	C39-C38-C37	-6.14	100.20	111.12
16	M	402	BCL	CHD-C1D-ND	-6.12	116.19	124.80
23	Q	105	H4X	C21-C22-C23	-6.10	118.72	127.28
18	L	306	UQ8	C15-C14-C16	6.05	125.73	115.23
23	G	101	H4X	C8-C7-C6	6.01	125.67	115.23
11	C	404	HEM	CHC-C4B-NB	6.01	130.89	124.42
16	F	105	BCL	CMD-C2D-C1D	5.96	135.22	124.73
16	S	103	BCL	O2D-CGD-O1D	-5.95	112.26	123.85
23	B	101	H4X	C10-C9-C7	-5.95	119.33	127.69
16	F	103	BCL	CHD-C1D-ND	-5.94	116.44	124.80
16	5	104	BCL	C2B-C1B-NB	5.91	116.45	110.33
16	1	102	BCL	CMD-C2D-C1D	5.91	135.13	124.73
16	L	304	BCL	C1-O2A-CGA	5.90	130.94	116.65
16	K	105	BCL	O2D-CGD-CBD	5.90	121.54	111.23
16	T	101	BCL	C2B-C1B-NB	5.86	116.41	110.33
23	O	101	H4X	C20-C21-C22	5.86	135.52	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	104	BCL	C2B-C1B-NB	5.86	116.41	110.33
16	W	102	BCL	O2D-CGD-CBD	5.86	121.47	111.23
16	5	103	BCL	CMD-C2D-C1D	5.86	135.04	124.73
16	O	104	BCL	O2D-CGD-CBD	5.86	121.47	111.23
15	C	408	PGV	O01-C1-C2	5.84	124.11	111.48
16	9	104	BCL	C2B-C1B-NB	5.83	116.37	110.33
16	5	103	BCL	O2D-CGD-CBD	5.82	121.41	111.23
23	G	101	H4X	C21-C22-C23	-5.82	119.12	127.28
11	C	403	HEM	C3B-C4B-NB	-5.78	105.32	109.47
16	O	105	BCL	C2B-C1B-NB	5.77	116.31	110.33
16	F	105	BCL	C2B-C1B-NB	5.76	116.30	110.33
16	U	103	BCL	C2B-C1B-NB	5.76	116.30	110.33
23	U	104	H4X	C34-C33-C35	5.75	125.20	115.23
23	E	101	H4X	C21-C22-C23	-5.74	119.22	127.28
16	Y	104	BCL	C2B-C1B-NB	5.73	116.27	110.33
23	7	104	H4X	C10-C9-C7	-5.71	119.66	127.69
16	I	102	BCL	O2D-CGD-O1D	-5.68	112.79	123.85
23	6	101	H4X	C20-C19-C17	-5.65	119.35	127.28
16	A	102	BCL	CMD-C2D-C1D	5.65	134.68	124.73
16	7	103	BCL	CMD-C2D-C1D	5.64	134.67	124.73
16	O	105	BCL	C6-C5-C3	-5.61	99.79	113.47
16	D	104	BCL	C2B-C1B-NB	5.58	116.11	110.33
24	V	102	LMT	O5B-C5B-C6B	5.57	120.23	106.44
16	D	103	BCL	O2D-CGD-O1D	-5.56	113.03	123.85
16	U	102	BCL	O2D-CGD-O1D	-5.55	113.04	123.85
16	5	103	BCL	C2B-C1B-NB	5.55	116.08	110.33
23	U	104	H4X	C31-C32-C33	-5.55	119.89	127.69
16	5	104	BCL	CMD-C2D-C1D	5.53	134.47	124.73
16	7	103	BCL	C1-C2-C3	-5.51	117.17	126.20
16	9	104	BCL	C6-C5-C3	-5.50	100.08	113.47
16	M	403	BCL	CMB-C2B-C1B	5.46	133.73	125.42
16	S	103	BCL	CMD-C2D-C1D	5.45	134.32	124.73
16	Q	104	BCL	C6-C5-C3	-5.45	100.20	113.47
16	3	104	BCL	C2B-C1B-NB	5.42	115.94	110.33
23	V	101	H4X	C31-C32-C33	-5.40	120.09	127.69
16	I	102	BCL	CHD-C1D-ND	-5.40	117.21	124.80
24	2	103	LMT	O5B-C5B-C6B	5.36	119.72	106.44
23	4	101	H4X	C31-C32-C33	-5.33	120.20	127.69
23	O	101	H4X	C13-C12-C11	5.30	126.19	118.09
24	Z	102	LMT	O5B-C5B-C6B	5.29	119.54	106.44
16	1	102	BCL	CHD-C1D-ND	-5.28	117.37	124.80
16	U	103	BCL	C1-C2-C3	-5.27	117.56	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	101	H4X	C4-C5-C6	5.27	125.00	112.33
15	H	301	PGV	O01-C1-O02	-5.25	111.43	123.70
16	3	103	BCL	O2D-CGD-O1D	-5.25	113.64	123.85
16	D	104	BCL	CED-O2D-CGD	5.24	127.81	115.92
16	U	102	BCL	CMD-C2D-C1D	5.24	133.96	124.73
16	L	304	BCL	CMD-C2D-C1D	5.24	133.95	124.73
16	A	102	BCL	C4-C3-C5	5.23	124.31	115.23
23	7	104	H4X	C26-C27-C28	-5.23	119.95	127.28
11	C	401	HEM	CHC-C4B-NB	5.21	130.03	124.42
23	6	101	H4X	C21-C22-C23	-5.21	119.97	127.28
16	K	105	BCL	CMD-C2D-C1D	5.20	133.88	124.73
16	L	304	BCL	C3D-C2D-C1D	-5.18	98.76	105.83
16	O	104	BCL	CMD-C2D-C1D	5.18	133.84	124.73
22	H	302	CDL	OA6-CA5-C11	5.17	122.66	111.48
15	L	305	PGV	O01-C1-C2	5.15	122.63	111.48
16	9	103	BCL	CMD-C2D-C1D	5.12	133.75	124.73
16	O	105	BCL	C3C-C4C-CHD	-5.12	112.59	123.39
16	7	102	BCL	C3C-C4C-CHD	-5.11	112.61	123.39
16	J	101	BCL	C2B-C1B-NB	5.11	115.62	110.33
11	C	403	HEM	O2D-CGD-O1D	-5.09	110.23	123.33
23	U	104	H4X	C21-C22-C23	-5.09	120.14	127.28
16	Q	103	BCL	O2D-CGD-O1D	-5.08	113.95	123.85
24	6	102	LMT	C1'-C2'-C3'	5.08	120.70	110.01
23	O	101	H4X	C8-C7-C6	5.08	124.04	115.23
16	L	304	BCL	CED-O2D-CGD	-5.07	104.42	115.92
16	3	104	BCL	CMD-C2D-C1D	5.07	133.66	124.73
24	4	102	LMT	O5B-C5B-C6B	5.06	118.99	106.44
23	4	101	H4X	C21-C22-C23	-5.06	120.18	127.28
16	J	101	BCL	CMD-C2D-C1D	5.05	133.61	124.73
16	U	103	BCL	C6-C5-C3	-5.04	101.19	113.47
16	Y	102	BCL	CMD-C2D-C1D	5.02	133.56	124.73
16	L	301	BCL	O2D-CGD-CBD	5.01	119.98	111.23
24	G	102	LMT	O5B-C5B-C6B	5.01	118.85	106.44
23	2	101	H4X	C21-C22-C23	-5.00	120.27	127.28
23	E	101	H4X	C20-C19-C17	-4.98	120.29	127.28
16	L	301	BCL	C3D-C2D-C1D	-4.97	99.04	105.83
16	Q	104	BCL	C1C-NC-C4C	-4.97	104.41	106.68
23	B	101	H4X	C39-C38-C37	-4.97	102.29	111.12
16	5	104	BCL	C3C-C4C-CHD	-4.93	113.00	123.39
16	T	101	BCL	C3C-C4C-CHD	-4.93	113.00	123.39
23	O	101	H4X	C21-C22-C23	-4.92	120.38	127.28
16	M	402	BCL	CMD-C2D-C1D	4.92	133.39	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	108	BCL	C3C-C4C-CHD	-4.91	113.04	123.39
16	I	102	BCL	CMD-C2D-C1D	4.90	133.35	124.73
16	Y	102	BCL	CHD-C1D-ND	-4.88	117.93	124.80
16	Y	102	BCL	C2B-C1B-NB	4.87	115.38	110.33
23	U	104	H4X	C20-C19-C17	-4.87	120.44	127.28
16	9	103	BCL	O2D-CGD-O1D	-4.87	114.37	123.85
16	D	103	BCL	C4A-NA-C1A	-4.86	104.46	106.68
16	W	102	BCL	C2B-C1B-NB	4.86	115.36	110.33
16	M	402	BCL	C3C-C4C-CHD	-4.85	113.17	123.39
23	7	104	H4X	C20-C19-C17	-4.84	120.50	127.28
23	V	101	H4X	C8-C7-C6	4.83	123.61	115.23
24	2	103	LMT	C1'-C2'-C3'	4.83	120.17	110.01
16	Y	104	BCL	O2D-CGD-CBD	4.82	119.66	111.23
16	W	102	BCL	CMD-C2D-C1D	4.82	133.22	124.73
16	X	101	BCL	C1-C2-C3	-4.82	118.30	126.20
15	L	305	PGV	O03-C19-C20	4.82	126.53	111.83
15	3	101	PGV	O03-C19-C20	4.81	126.50	111.83
17	M	404	BPH	C4D-CHA-CBD	-4.81	106.15	108.45
16	W	102	BCL	CMB-C2B-C1B	4.80	132.73	125.42
23	Q	105	H4X	C10-C9-C7	-4.80	120.94	127.69
11	C	404	HEM	CHD-C4C-NC	4.80	129.68	124.45
16	M	403	BCL	CMD-C2D-C1D	4.80	133.18	124.73
24	4	102	LMT	C1'-C2'-C3'	4.79	120.09	110.01
16	O	105	BCL	CMD-C2D-C1D	4.79	133.16	124.73
16	9	104	BCL	C1-C2-C3	-4.79	118.36	126.20
16	1	102	BCL	C3C-C4C-CHD	-4.78	113.31	123.39
16	U	102	BCL	CHD-C1D-ND	-4.78	118.08	124.80
23	V	101	H4X	C2-C1-C3	-4.77	101.71	110.43
24	J	102	LMT	C1'-C2'-C3'	4.76	120.02	110.01
16	L	304	BCL	C3C-C4C-CHD	-4.76	113.36	123.39
23	K	107	H4X	C31-C32-C33	-4.75	121.01	127.69
16	K	108	BCL	CMD-C2D-C1D	4.75	133.09	124.73
16	D	103	BCL	CHD-C1D-ND	-4.71	118.17	124.80
16	7	103	BCL	C6-C5-C3	-4.71	102.00	113.47
16	X	101	BCL	O2D-CGD-CBD	4.70	119.45	111.23
16	2	102	BCL	C3C-C4C-CHD	-4.70	113.49	123.39
23	Z	101	H4X	C2-C1-C3	-4.68	101.86	110.43
16	L	304	BCL	C2B-C1B-NB	4.68	115.18	110.33
16	1	102	BCL	C2B-C1B-NB	4.68	115.18	110.33
16	L	301	BCL	C3C-C4C-CHD	-4.68	113.52	123.39
16	Q	104	BCL	C4A-NA-C1A	-4.68	104.54	106.68
23	5	105	H4X	C20-C19-C17	-4.68	120.72	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	103	BCL	CED-O2D-CGD	4.68	126.52	115.92
11	C	403	HEM	C1B-NB-C4B	4.67	110.74	105.21
16	U	103	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
16	B	103	BCL	CMD-C2D-C1D	4.66	132.94	124.73
16	M	403	BCL	C3C-C4C-CHD	-4.65	113.59	123.39
11	C	403	HEM	CHB-C1B-NB	4.63	130.09	124.37
16	2	102	BCL	CMD-C2D-C1D	4.62	132.87	124.73
16	9	104	BCL	CMD-C2D-C1D	4.62	132.86	124.73
16	X	101	BCL	C3C-C4C-CHD	-4.61	113.66	123.39
16	2	102	BCL	O2D-CGD-CBD	4.61	119.29	111.23
23	2	101	H4X	C26-C27-C28	-4.60	120.83	127.28
16	K	105	BCL	C2B-C1B-NB	4.59	115.09	110.33
16	B	103	BCL	C3C-C4C-CHD	-4.59	113.71	123.39
16	Q	103	BCL	CMD-C2D-C1D	4.59	132.81	124.73
16	W	102	BCL	CHD-C1D-ND	-4.59	118.34	124.80
16	F	105	BCL	C1-C2-C3	-4.59	118.68	126.20
16	D	104	BCL	CMD-C2D-C1D	4.59	132.80	124.73
16	Q	104	BCL	C3C-C4C-CHD	-4.58	113.72	123.39
11	C	402	HEM	CHC-C4B-NB	4.58	129.35	124.42
23	5	105	H4X	C31-C32-C33	-4.58	121.25	127.69
23	O	106	H4X	C4-C5-C6	4.58	123.33	112.33
16	3	103	BCL	C2B-C1B-NB	4.58	115.07	110.33
16	7	102	BCL	CHD-C1D-ND	-4.57	118.37	124.80
16	7	103	BCL	C1-O2A-CGA	4.57	127.72	116.65
16	B	103	BCL	C3D-C2D-C1D	-4.57	99.60	105.83
23	E	101	H4X	C10-C9-C7	-4.56	121.28	127.69
24	V	102	LMT	C1'-C2'-C3'	4.56	119.60	110.01
16	W	102	BCL	O2D-CGD-O1D	-4.55	115.00	123.85
24	E	102	LMT	O5B-C5B-C6B	4.54	117.70	106.44
16	Y	102	BCL	C4-C3-C5	4.54	123.11	115.23
16	M	403	BCL	C2B-C1B-NB	4.54	115.03	110.33
16	O	104	BCL	O2D-CGD-O1D	-4.54	115.02	123.85
16	Q	104	BCL	C1-C2-C3	-4.54	118.77	126.20
11	C	403	HEM	CHD-C4C-NC	4.53	129.39	124.45
11	C	402	HEM	CHB-C1B-NB	4.53	129.97	124.37
15	F	104	PGV	O01-C1-C2	4.52	121.25	111.48
16	Y	104	BCL	C3C-C4C-CHD	-4.51	113.88	123.39
24	J	102	LMT	O5B-C5B-C6B	4.50	117.59	106.44
15	O	102	PGV	O01-C1-C2	4.50	121.21	111.48
23	E	101	H4X	C26-C27-C28	-4.49	120.98	127.28
16	X	101	BCL	CMD-C2D-C1D	4.49	132.64	124.73
16	U	102	BCL	C3C-C4C-CHD	-4.49	113.92	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	103	BCL	CMB-C2B-C1B	4.48	132.25	125.42
23	P	101	H4X	C21-C22-C23	-4.48	120.99	127.28
23	O	101	H4X	C39-C38-C37	-4.47	103.18	111.12
16	5	104	BCL	C1-C2-C3	-4.47	118.88	126.20
16	D	103	BCL	C3C-C4C-CHD	-4.46	113.98	123.39
23	6	101	H4X	C24-C23-C22	-4.46	115.59	122.82
24	J	102	LMT	O5'-C5'-C6'	-4.45	95.40	106.44
16	A	102	BCL	CHD-C1D-ND	-4.45	118.54	124.80
16	L	301	BCL	CMD-C2D-C1D	4.44	132.55	124.73
24	2	103	LMT	O5'-C5'-C6'	-4.44	95.44	106.44
24	N	101	LMT	O5B-C5B-C6B	4.43	117.41	106.44
16	O	104	BCL	CHD-C1D-ND	-4.41	118.59	124.80
16	U	102	BCL	C2B-C1B-NB	4.41	114.90	110.33
16	I	102	BCL	CMB-C2B-C1B	4.41	132.13	125.42
16	F	103	BCL	C2B-C1B-NB	4.40	114.89	110.33
24	G	102	LMT	C1'-C2'-C3'	4.40	119.26	110.01
16	3	104	BCL	C3C-C4C-CHD	-4.40	114.12	123.39
16	3	104	BCL	C4A-NA-C1A	-4.39	104.67	106.68
15	1	103	PGV	O01-C1-C2	4.39	120.98	111.48
23	O	101	H4X	C5-C6-C7	4.39	124.15	113.47
23	K	107	H4X	C21-C22-C23	-4.37	121.14	127.28
23	E	101	H4X	C5-C6-C7	4.37	124.12	113.47
16	7	103	BCL	CED-O2D-CGD	4.37	125.83	115.92
16	Y	102	BCL	OBb-CAB-CBB	-4.35	110.03	119.77
16	L	304	BCL	CHD-C1D-ND	-4.35	118.68	124.80
16	Y	104	BCL	CMD-C2D-C1D	4.35	132.39	124.73
16	7	103	BCL	C2B-C1B-NB	4.35	114.83	110.33
15	F	104	PGV	O01-C1-O02	-4.34	113.56	123.70
16	L	301	BCL	C2B-C1B-NB	4.34	114.82	110.33
11	C	402	HEM	C1B-NB-C4B	4.33	110.34	105.21
16	J	101	BCL	C3C-C4C-CHD	-4.33	114.27	123.39
15	K	101	PGV	O01-C1-C2	4.32	120.83	111.48
16	J	101	BCL	O2D-CGD-CBD	4.32	118.78	111.23
16	K	105	BCL	CHD-C1D-ND	-4.32	118.73	124.80
24	6	102	LMT	O5B-C5B-C6B	4.31	117.13	106.44
15	C	408	PGV	O01-C1-O02	-4.31	113.63	123.70
16	K	108	BCL	C3D-C2D-C1D	-4.31	99.95	105.83
16	Y	102	BCL	C3C-C4C-CHD	-4.30	114.32	123.39
16	K	108	BCL	C2B-C1B-NB	4.30	114.79	110.33
16	M	403	BCL	O2D-CGD-O1D	-4.29	115.50	123.85
16	U	102	BCL	CAA-C2A-C3A	-4.29	101.42	113.00
23	4	101	H4X	C20-C19-C17	-4.28	121.28	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	301	PGV	O03-C19-C20	4.28	124.88	111.83
16	B	103	BCL	C6-C5-C3	-4.27	103.06	113.47
16	D	104	BCL	C1-C2-C3	-4.27	119.20	126.20
16	J	101	BCL	C1-C2-C3	-4.27	119.20	126.20
15	Q	101	PGV	O03-C19-C20	4.27	124.84	111.83
16	2	102	BCL	C4-C3-C2	-4.25	112.72	123.63
16	B	103	BCL	C1-C2-C3	-4.24	119.25	126.20
16	O	105	BCL	CED-O2D-CGD	4.24	125.53	115.92
16	5	103	BCL	CHD-C1D-ND	-4.22	118.86	124.80
16	T	101	BCL	CMD-C2D-C1D	4.22	132.16	124.73
23	K	103	H4X	C21-C22-C23	-4.22	121.36	127.28
24	P	102	LMT	C1B-O5B-C5B	4.22	121.96	113.72
16	D	103	BCL	CMD-C2D-C1D	4.21	132.14	124.73
16	Q	103	BCL	C2B-C1B-NB	4.19	114.67	110.33
16	Y	104	BCL	C6-C5-C3	-4.19	103.27	113.47
16	7	103	BCL	C3D-C2D-C1D	-4.18	100.12	105.83
16	7	102	BCL	CMD-C2D-C1D	4.18	132.10	124.73
16	7	102	BCL	O2D-CGD-O1D	-4.18	115.71	123.85
16	T	101	BCL	C3D-C2D-C1D	-4.18	100.13	105.83
16	I	102	BCL	C2B-C1B-NB	4.17	114.65	110.33
23	Z	101	H4X	C5-C6-C7	4.17	123.63	113.47
16	3	103	BCL	C3C-C4C-CHD	-4.17	114.60	123.39
16	J	101	BCL	C3D-C2D-C1D	-4.17	100.14	105.83
23	Q	105	H4X	C36-C35-C33	4.16	123.61	113.47
16	D	103	BCL	C3D-C2D-C1D	-4.16	100.15	105.83
16	A	102	BCL	C1C-NC-C4C	-4.16	104.78	106.68
17	L	302	BPH	C4D-CHA-CBD	-4.14	106.47	108.45
15	C	408	PGV	C02-O01-C1	-4.14	111.81	117.78
23	Z	101	H4X	C20-C19-C17	-4.14	121.47	127.28
16	Q	104	BCL	C1-O2A-CGA	4.14	126.67	116.65
16	A	102	BCL	C2B-C1B-NB	4.14	114.61	110.33
23	Q	105	H4X	C5-C6-C7	4.14	123.54	113.47
16	F	103	BCL	O2D-CGD-O1D	-4.13	115.80	123.85
16	O	105	BCL	C1-C2-C3	-4.13	119.43	126.20
24	T	102	LMT	C1'-C2'-C3'	4.10	118.64	110.01
23	B	101	H4X	C34-C33-C35	4.09	122.33	115.23
16	B	103	BCL	O2D-CGD-CBD	4.09	118.39	111.23
16	Y	102	BCL	C1C-NC-C4C	-4.09	104.81	106.68
23	7	104	H4X	C2-C1-C3	-4.09	102.96	110.43
23	2	101	H4X	C20-C19-C17	-4.08	121.56	127.28
23	O	101	H4X	C31-C32-C33	-4.06	121.98	127.69
15	F	101	PGV	O01-C1-C2	4.04	120.23	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	102	BCL	CMB-C2B-C1B	4.04	131.57	125.42
24	T	102	LMT	O5B-C5B-C6B	4.04	116.44	106.44
16	Q	103	BCL	C3C-C4C-CHD	-4.03	114.90	123.39
16	I	102	BCL	C4-C3-C5	4.02	122.21	115.23
23	Q	105	H4X	C39-C38-C37	-4.01	103.99	111.12
16	O	105	BCL	C4-C3-C5	4.01	122.18	115.23
16	W	102	BCL	C1C-NC-C4C	-4.00	104.85	106.68
16	A	102	BCL	C3D-C2D-C1D	-4.00	100.37	105.83
23	5	105	H4X	C4-C5-C6	4.00	121.95	112.33
16	D	103	BCL	CMB-C2B-C1B	4.00	131.51	125.42
22	H	302	CDL	OB6-CB5-C51	4.00	120.13	111.48
23	Q	105	H4X	C34-C33-C35	3.99	122.16	115.23
16	S	103	BCL	C3C-C4C-CHD	-3.99	114.97	123.39
16	S	103	BCL	CHD-C1D-ND	-3.99	119.18	124.80
16	7	102	BCL	C3D-C2D-C1D	-3.99	100.38	105.83
23	O	106	H4X	C20-C19-C17	-3.98	121.70	127.28
23	O	101	H4X	C36-C35-C33	3.97	123.14	113.47
23	O	101	H4X	C2-C1-C3	-3.97	103.17	110.43
16	O	105	BCL	O2D-CGD-CBD	3.97	118.17	111.23
16	7	103	BCL	C3C-C4C-CHD	-3.96	115.03	123.39
23	P	101	H4X	C26-C27-C28	-3.96	121.72	127.28
16	5	103	BCL	O2D-CGD-O1D	-3.96	116.14	123.85
11	C	404	HEM	C1B-NB-C4B	3.96	109.89	105.21
16	Y	104	BCL	C3D-C2D-C1D	-3.96	100.43	105.83
16	Q	104	BCL	O2D-CGD-CBD	3.95	118.14	111.23
23	4	101	H4X	C15-C14-C12	-3.95	121.73	127.28
16	M	402	BCL	C4-C3-C5	3.95	122.08	115.23
16	D	104	BCL	C3C-C4C-CHD	-3.94	115.09	123.39
16	U	102	BCL	C3D-C2D-C1D	-3.93	100.46	105.83
16	D	104	BCL	C3D-C2D-C1D	-3.93	100.46	105.83
16	9	103	BCL	C3C-C4C-CHD	-3.93	115.10	123.39
16	W	102	BCL	C4A-NA-C1A	-3.93	104.89	106.68
23	P	101	H4X	C5-C6-C7	3.93	123.03	113.47
11	C	401	HEM	CHA-C4D-ND	3.92	129.22	124.37
24	0	101	LMT	C1B-O5B-C5B	3.92	121.37	113.72
23	V	101	H4X	C3-C1-C4	-3.92	104.16	111.12
16	M	402	BCL	CMB-C2B-C1B	3.91	131.37	125.42
16	F	105	BCL	C1-O2A-CGA	3.90	126.10	116.65
16	Y	104	BCL	C1-C2-C3	-3.89	119.82	126.20
24	R	101	LMT	C1'-C2'-C3'	3.89	118.19	110.01
16	Q	104	BCL	CMD-C2D-C1D	3.89	131.57	124.73
24	N	101	LMT	C1'-C2'-C3'	3.88	118.18	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	102	BCL	C3D-C2D-C1D	-3.88	100.54	105.83
16	K	108	BCL	CED-O2D-CGD	3.88	124.71	115.92
16	F	103	BCL	C3C-C4C-CHD	-3.88	115.22	123.39
23	5	105	H4X	C39-C38-C37	-3.87	104.24	111.12
23	K	107	H4X	C36-C35-C33	3.87	122.89	113.47
16	K	105	BCL	O2D-CGD-O1D	-3.86	116.33	123.85
23	2	101	H4X	C10-C9-C7	-3.86	122.26	127.69
16	O	104	BCL	C3D-C2D-C1D	-3.86	100.57	105.83
16	3	104	BCL	C1C-NC-C4C	-3.85	104.92	106.68
16	Q	104	BCL	C3D-C2D-C1D	-3.85	100.57	105.83
16	Q	104	BCL	C4-C3-C5	3.85	121.91	115.23
16	Q	103	BCL	C3D-C2D-C1D	-3.85	100.58	105.83
11	C	402	HEM	CHD-C1D-ND	3.84	128.56	124.42
16	Y	104	BCL	O2D-CGD-O1D	-3.84	116.37	123.85
18	L	306	UQ8	C10-C9-C11	3.84	121.89	115.23
16	U	103	BCL	C3C-C4C-CHD	-3.82	115.33	123.39
16	3	104	BCL	C4-C3-C5	3.82	121.86	115.23
23	7	104	H4X	C31-C32-C33	-3.82	122.32	127.69
16	X	101	BCL	C3D-C2D-C1D	-3.82	100.62	105.83
16	9	103	BCL	CAA-C2A-C3A	-3.82	102.69	113.00
16	3	104	BCL	CED-O2D-CGD	3.82	124.57	115.92
16	W	102	BCL	C3C-C4C-CHD	-3.81	115.36	123.39
16	U	103	BCL	O2D-CGD-CBD	3.80	117.88	111.23
23	K	107	H4X	C26-C27-C28	-3.80	121.95	127.28
16	1	102	BCL	O2D-CGD-O1D	-3.79	116.46	123.85
16	5	104	BCL	O2D-CGD-CBD	3.79	117.85	111.23
15	F	101	PGV	O01-C02-C01	3.78	121.92	108.34
23	G	101	H4X	C14-C15-C16	-3.78	112.24	123.20
23	G	101	H4X	C20-C19-C17	-3.78	121.98	127.28
16	3	104	BCL	C1-O2A-CGA	3.78	125.80	116.65
16	M	403	BCL	C3D-C2D-C1D	-3.78	100.68	105.83
23	K	107	H4X	C20-C19-C17	-3.77	121.98	127.28
16	U	102	BCL	CMB-C2B-C1B	3.77	131.15	125.42
16	F	105	BCL	C4-C3-C5	3.76	121.75	115.23
16	L	301	BCL	C4-C3-C5	3.76	121.75	115.23
24	4	102	LMT	O5'-C5'-C6'	-3.76	97.12	106.44
16	Q	104	BCL	O2D-CGD-O1D	-3.76	116.53	123.85
16	S	103	BCL	C2B-C1B-NB	3.75	114.22	110.33
23	K	103	H4X	C31-C32-C33	-3.75	122.42	127.69
16	3	103	BCL	CHD-C1D-ND	-3.74	119.53	124.80
23	6	101	H4X	C9-C10-C11	-3.74	112.35	123.20
11	C	404	HEM	CHB-C1B-NB	3.74	129.00	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	101	H4X	C40-C38-C39	3.74	117.27	110.43
16	Q	103	BCL	CHD-C1D-ND	-3.74	119.54	124.80
16	F	105	BCL	C3C-C4C-CHD	-3.73	115.52	123.39
16	5	103	BCL	CMB-C2B-C1B	3.73	131.10	125.42
16	W	102	BCL	CAA-C2A-C3A	-3.73	102.92	113.00
16	O	104	BCL	C3C-C4C-CHD	-3.72	115.54	123.39
24	G	102	LMT	O5'-C5'-C6'	-3.71	97.24	106.44
23	G	101	H4X	C4-C5-C6	3.71	121.24	112.33
15	3	101	PGV	O01-C1-C2	3.71	119.50	111.48
16	D	103	BCL	C2B-C1B-NB	3.70	114.17	110.33
23	K	103	H4X	C32-C31-C30	-3.70	112.48	123.20
16	X	101	BCL	O2D-CGD-O1D	-3.70	116.65	123.85
23	U	104	H4X	C36-C35-C33	3.70	122.47	113.47
23	7	104	H4X	C34-C33-C35	3.69	121.64	115.23
16	L	301	BCL	CMC-C2C-C3C	-3.69	99.72	113.98
16	9	104	BCL	O2D-CGD-CBD	3.69	117.68	111.23
16	5	103	BCL	C3D-C2D-C1D	-3.69	100.80	105.83
16	9	103	BCL	O2A-CGA-CBA	3.69	123.08	111.83
23	6	101	H4X	C34-C33-C35	3.67	121.60	115.23
23	Q	105	H4X	C9-C10-C11	-3.66	112.58	123.20
16	K	105	BCL	C3C-C4C-CHD	-3.66	115.68	123.39
16	2	102	BCL	C7-C6-C5	3.65	123.00	113.26
16	T	101	BCL	O2D-CGD-CBD	3.65	117.61	111.23
16	7	103	BCL	CMB-C2B-C1B	3.65	130.97	125.42
11	C	401	HEM	CHD-C4C-NC	3.65	128.42	124.45
11	C	402	HEM	C2A-C1A-NA	-3.64	106.11	110.15
23	O	106	H4X	C24-C23-C25	3.64	123.65	118.09
16	M	402	BCL	C2B-C1B-NB	3.64	114.10	110.33
23	6	101	H4X	C24-C23-C25	3.64	123.64	118.09
16	L	304	BCL	C4A-NA-C1A	-3.64	105.02	106.68
16	3	104	BCL	C3D-C2D-C1D	-3.63	100.88	105.83
24	B	102	LMT	C1B-O5B-C5B	3.63	120.80	113.72
16	3	104	BCL	O2D-CGD-CBD	3.62	117.56	111.23
23	O	106	H4X	C32-C31-C30	-3.62	112.71	123.20
15	M	406	PGV	O01-C1-C2	3.62	119.31	111.48
16	3	103	BCL	CMD-C2D-C1D	3.62	131.10	124.73
16	7	102	BCL	C2B-C1B-NB	3.62	114.08	110.33
16	U	103	BCL	C1-O2A-CGA	3.62	125.40	116.65
16	K	105	BCL	CMB-C2B-C1B	3.61	130.92	125.42
24	X	102	LMT	O5B-C5B-C6B	3.61	115.39	106.44
23	O	106	H4X	C21-C22-C23	-3.60	122.22	127.28
16	3	104	BCL	CAA-C2A-C3A	-3.60	103.26	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	104	BCL	C3D-C2D-C1D	-3.60	100.92	105.83
16	I	102	BCL	C3C-C4C-CHD	-3.60	115.80	123.39
23	K	103	H4X	C39-C38-C37	-3.59	104.73	111.12
16	O	104	BCL	C2D-C1D-ND	3.59	113.68	110.13
16	2	102	BCL	O2D-CGD-O1D	-3.59	116.86	123.85
23	Z	101	H4X	C26-C27-C28	-3.59	122.25	127.28
24	V	102	LMT	O5'-C5'-C6'	-3.59	97.55	106.44
11	C	401	HEM	O2D-CGD-O1D	-3.58	114.12	123.33
23	2	101	H4X	C40-C38-C37	-3.58	104.76	111.12
16	X	101	BCL	C6-C5-C3	-3.57	104.77	113.47
16	Y	104	BCL	CHC-C4B-NB	-3.57	118.69	124.05
23	K	107	H4X	C4-C5-C6	3.57	120.91	112.33
23	Q	105	H4X	C20-C19-C17	-3.56	122.28	127.28
23	5	105	H4X	C9-C10-C11	-3.56	112.88	123.20
24	E	102	LMT	O5'-C5'-C6'	-3.56	97.62	106.44
16	O	105	BCL	C3D-C2D-C1D	-3.56	100.98	105.83
23	E	101	H4X	C2-C1-C3	-3.54	103.95	110.43
16	T	101	BCL	C1-C2-C3	-3.54	120.40	126.20
11	C	401	HEM	CHD-C1D-ND	3.53	128.23	124.42
16	Q	103	BCL	CAA-C2A-C3A	-3.53	103.45	113.00
15	9	101	PGV	O01-C1-C2	3.53	119.13	111.48
23	Q	105	H4X	C26-C27-C28	-3.53	122.33	127.28
16	S	103	BCL	C3D-C2D-C1D	-3.53	101.01	105.83
15	5	101	PGV	O03-C19-O04	-3.53	114.80	123.63
23	O	106	H4X	C26-C27-C28	-3.53	122.33	127.28
23	K	103	H4X	C5-C6-C7	3.53	122.06	113.47
16	5	103	BCL	C1-C2-C3	-3.52	120.42	126.20
16	X	101	BCL	C1-O2A-CGA	3.52	125.18	116.65
16	O	104	BCL	CHB-C1B-C2B	-3.52	117.20	127.43
16	9	103	BCL	C3D-C2D-C1D	-3.52	101.03	105.83
23	O	101	H4X	C13-C12-C14	-3.52	117.12	122.82
16	M	403	BCL	CAA-C2A-C3A	-3.51	103.52	113.00
16	D	104	BCL	C3B-C4B-NB	3.49	114.37	109.76
16	9	103	BCL	C2B-C1B-NB	3.49	113.95	110.33
24	E	102	LMT	C1'-C2'-C3'	3.49	117.36	110.01
16	9	103	BCL	CHD-C1D-ND	-3.49	119.89	124.80
16	K	108	BCL	CAA-C2A-C3A	-3.49	103.57	113.00
23	P	101	H4X	C36-C35-C33	3.49	121.97	113.47
11	C	402	HEM	C3B-C4B-NB	-3.48	106.97	109.47
23	O	106	H4X	C34-C33-C35	3.48	121.27	115.23
16	Y	104	BCL	C3B-C4B-NB	3.48	114.35	109.76
16	5	104	BCL	CHD-C1D-ND	-3.47	119.91	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	9	104	BCL	C3D-C2D-C1D	-3.47	101.10	105.83
16	D	103	BCL	C2D-C1D-ND	3.46	113.55	110.13
16	M	403	BCL	OB B-CAB-CBB	3.46	127.53	119.77
16	Y	104	BCL	C1-O2A-CGA	3.46	125.02	116.65
16	M	402	BCL	C1D-ND-C4D	-3.45	103.89	106.31
11	C	401	HEM	C1B-NB-C4B	3.44	109.28	105.21
16	5	104	BCL	CAA-C2A-C3A	-3.43	103.72	113.00
23	U	104	H4X	C26-C27-C28	-3.43	122.47	127.28
23	P	101	H4X	C32-C31-C30	-3.43	113.27	123.20
15	F	101	PGV	O03-C19-C20	3.43	122.28	111.83
16	W	102	BCL	O2A-CGA-CBA	3.42	122.27	111.83
15	Q	101	PGV	O01-C1-C2	3.42	118.89	111.48
16	5	103	BCL	CED-O2D-CGD	3.42	123.68	115.92
16	K	105	BCL	C3D-C2D-C1D	-3.42	101.16	105.83
16	K	108	BCL	CMB-C2B-C1B	3.42	130.62	125.42
16	M	402	BCL	C3D-C2D-C1D	-3.42	101.17	105.83
16	3	103	BCL	C3D-C2D-C1D	-3.42	101.17	105.83
23	G	101	H4X	C36-C35-C33	3.42	121.79	113.47
16	7	102	BCL	CMB-C2B-C1B	3.41	130.62	125.42
23	V	101	H4X	C2-C1-C4	3.41	117.19	111.12
16	S	103	BCL	CAC-C3C-C4C	-3.41	105.02	112.58
23	Z	101	H4X	C31-C32-C33	-3.41	122.90	127.69
23	V	101	H4X	C14-C15-C16	-3.40	113.33	123.20
23	O	101	H4X	C14-C15-C16	-3.40	113.34	123.20
11	C	403	HEM	CBA-CAA-C2A	-3.40	103.14	112.53
16	D	104	BCL	C1-O2A-CGA	3.39	124.86	116.65
16	Y	102	BCL	C1D-ND-C4D	-3.39	103.94	106.31
16	T	101	BCL	C4-C3-C2	-3.38	114.94	123.63
15	A	101	PGV	O01-C1-O02	-3.38	115.80	123.70
23	7	104	H4X	C36-C35-C33	3.38	121.70	113.47
16	2	102	BCL	CAA-C2A-C3A	-3.36	103.91	113.00
15	A	101	PGV	O01-C1-C2	3.36	118.75	111.48
11	C	401	HEM	CMD-C2D-C1D	3.36	130.29	125.03
16	B	103	BCL	O2D-CGD-O1D	-3.36	117.31	123.85
11	C	403	HEM	CMC-C2C-C1C	3.35	130.63	124.73
24	X	102	LMT	C1'-C2'-C3'	3.35	117.06	110.01
11	C	404	HEM	CBA-CAA-C2A	-3.35	103.27	112.53
11	C	402	HEM	CHA-C4D-ND	3.35	128.51	124.37
16	X	101	BCL	OB B-CAB-CBB	3.34	127.26	119.77
24	B	104	LMT	C1'-C2'-C3'	3.34	117.04	110.01
23	O	106	H4X	C21-C20-C19	-3.34	116.69	123.52
16	T	101	BCL	CHC-C4B-NB	-3.34	119.04	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	102	BCL	C3D-C2D-C1D	-3.34	101.28	105.83
16	Y	104	BCL	C1D-CHD-C4C	-3.33	118.58	126.62
16	D	104	BCL	O2D-CGD-CBD	3.33	117.05	111.23
23	4	101	H4X	C4-C5-C6	3.33	120.33	112.33
16	5	103	BCL	C3C-C4C-CHD	-3.33	116.38	123.39
16	7	103	BCL	O2D-CGD-CBD	3.32	117.04	111.23
16	U	102	BCL	C1D-ND-C4D	-3.32	103.98	106.31
23	K	107	H4X	C24-C23-C22	-3.32	117.44	122.82
16	B	103	BCL	C1D-CHD-C4C	-3.31	118.63	126.62
24	Z	102	LMT	C1'-C2'-C3'	3.31	116.97	110.01
16	F	105	BCL	O2D-CGD-CBD	3.31	117.01	111.23
23	2	101	H4X	C32-C31-C30	-3.30	113.63	123.20
22	S	101	CDL	OB6-CB5-C51	3.30	118.62	111.48
23	K	103	H4X	C9-C10-C11	-3.29	113.65	123.20
23	E	101	H4X	C20-C21-C22	-3.29	116.78	123.52
11	C	404	HEM	CHD-C1D-ND	3.29	127.97	124.42
16	3	104	BCL	C4-C3-C2	-3.29	115.17	123.63
16	L	301	BCL	O2A-CGA-CBA	3.29	121.87	111.83
16	7	102	BCL	C1C-NC-C4C	-3.29	105.18	106.68
23	E	101	H4X	C9-C10-C11	-3.28	113.69	123.20
23	B	101	H4X	C9-C10-C11	-3.28	113.70	123.20
23	K	107	H4X	C10-C9-C7	-3.28	123.08	127.69
16	F	103	BCL	C3D-C2D-C1D	-3.28	101.36	105.83
16	U	102	BCL	C1-C2-C3	-3.28	120.83	126.20
16	F	103	BCL	CMB-C2B-C1B	3.27	130.40	125.42
16	9	103	BCL	C1-C2-C3	-3.27	120.84	126.20
16	2	102	BCL	C3D-C2D-C1D	-3.27	101.38	105.83
15	F	104	PGV	O03-C19-O04	-3.26	115.47	123.63
16	F	105	BCL	C4-C3-C2	-3.25	115.27	123.63
16	5	104	BCL	C4-C3-C5	3.25	120.87	115.23
16	F	105	BCL	C3D-C2D-C1D	-3.25	101.40	105.83
16	9	103	BCL	C4-C3-C5	3.25	120.86	115.23
16	T	101	BCL	CHD-C1D-ND	-3.24	120.24	124.80
23	K	107	H4X	C18-C17-C16	3.24	123.04	118.09
16	M	403	BCL	C4A-NA-C1A	3.24	108.16	106.68
23	K	103	H4X	C24-C23-C22	-3.24	117.57	122.82
16	M	403	BCL	CHD-C1D-ND	-3.24	120.25	124.80
16	1	102	BCL	CMB-C2B-C1B	3.24	130.35	125.42
16	M	403	BCL	C1D-CHD-C4C	-3.24	118.81	126.62
16	A	102	BCL	C3C-C4C-CHD	-3.24	116.57	123.39
11	C	401	HEM	C3B-C4B-NB	-3.23	107.15	109.47
16	9	104	BCL	C1-O2A-CGA	3.23	124.47	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	104	BCL	C6-C5-C3	-3.23	105.60	113.47
16	9	104	BCL	C3C-C4C-CHD	-3.23	116.58	123.39
23	K	103	H4X	C24-C23-C25	3.22	123.01	118.09
16	J	101	BCL	CHD-C1D-ND	-3.22	120.27	124.80
24	8	102	LMT	C1B-O5B-C5B	3.22	120.01	113.72
16	5	104	BCL	C4-C3-C2	-3.22	115.36	123.63
16	Y	102	BCL	O2A-CGA-O1A	-3.22	115.57	123.63
24	G	102	LMT	C4B-C3B-C2B	-3.22	105.18	110.83
16	3	104	BCL	O2D-CGD-O1D	-3.21	117.59	123.85
16	K	105	BCL	C3B-C4B-NB	3.21	114.00	109.76
16	9	103	BCL	C1C-NC-C4C	-3.21	105.22	106.68
23	O	106	H4X	C2-C1-C4	3.21	116.82	111.12
24	8	102	LMT	O5B-C5B-C6B	3.20	114.38	106.44
23	G	101	H4X	C29-C28-C30	3.20	122.98	118.09
16	3	104	BCL	CHC-C4B-NB	-3.20	119.25	124.05
16	K	108	BCL	C1-C2-C3	-3.20	120.96	126.20
16	J	101	BCL	O2D-CGD-O1D	-3.19	117.63	123.85
23	Q	105	H4X	C13-C12-C14	3.19	127.98	122.82
11	C	403	HEM	CAD-C3D-C4D	3.19	130.25	124.70
16	T	101	BCL	C1-O2A-CGA	3.19	124.36	116.65
15	5	101	PGV	O03-C19-C20	3.18	121.54	111.83
23	7	104	H4X	C14-C15-C16	-3.18	113.98	123.20
15	9	101	PGV	O03-C19-C20	3.18	121.53	111.83
16	Q	104	BCL	C4-C3-C2	-3.18	115.46	123.63
17	M	404	BPH	C2B-C1B-NB	-3.17	107.14	109.43
16	T	101	BCL	O2D-CGD-O1D	-3.17	117.67	123.85
16	Y	102	BCL	CMB-C2B-C1B	3.17	130.25	125.42
16	U	102	BCL	C4-C3-C5	3.17	120.73	115.23
16	O	104	BCL	CMB-C2B-C1B	3.17	130.24	125.42
24	P	102	LMT	C1'-C2'-C3'	3.17	116.67	110.01
16	X	101	BCL	CHD-C1D-ND	-3.17	120.35	124.80
16	T	101	BCL	C4-C3-C5	3.16	120.71	115.23
17	L	302	BPH	C2B-C1B-NB	-3.16	107.15	109.43
18	L	303	UQ8	C1M-C1-C6	-3.16	119.26	124.45
23	Q	105	H4X	C3-C1-C4	-3.15	105.52	111.12
16	L	301	BCL	CAC-C3C-C4C	-3.15	105.59	112.58
23	B	101	H4X	C13-C12-C11	-3.15	113.28	118.09
16	F	105	BCL	CHD-C1D-ND	-3.15	120.38	124.80
11	C	401	HEM	CBD-CAD-C3D	-3.14	103.84	112.53
15	O	102	PGV	C03-C02-C01	-3.14	104.46	111.78
16	J	101	BCL	C6-C5-C3	-3.14	105.82	113.47
16	L	301	BCL	C1D-CHD-C4C	-3.14	119.05	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	108	BCL	C4-C3-C5	3.14	120.68	115.23
23	G	101	H4X	C9-C10-C11	-3.14	114.11	123.20
23	K	107	H4X	C32-C31-C30	-3.14	114.11	123.20
16	5	103	BCL	CAA-C2A-C3A	-3.14	104.53	113.00
18	L	306	UQ8	C1M-C1-C6	-3.13	119.30	124.45
23	7	104	H4X	C39-C38-C37	-3.13	105.56	111.12
23	5	105	H4X	C2-C1-C4	-3.13	105.56	111.12
16	9	103	BCL	C3D-C4D-ND	3.13	115.07	109.99
15	F	101	PGV	C02-O01-C1	-3.13	110.31	117.80
16	D	103	BCL	C1D-ND-C4D	-3.12	104.12	106.31
23	B	101	H4X	C14-C15-C16	-3.12	114.15	123.20
16	L	304	BCL	C3D-C4D-ND	3.12	115.06	109.99
16	F	103	BCL	C4A-NA-C1A	-3.12	105.25	106.68
15	1	103	PGV	O03-C19-C20	3.12	121.34	111.83
16	2	102	BCL	OBB-CAB-CBB	3.12	126.75	119.77
16	Y	104	BCL	CAC-C3C-C4C	-3.11	105.68	112.58
23	G	101	H4X	C20-C21-C22	-3.11	117.16	123.52
15	H	301	PGV	C02-O01-C1	-3.11	110.36	117.80
23	P	101	H4X	C20-C19-C17	-3.11	122.92	127.28
16	U	103	BCL	C3B-C4B-NB	3.11	113.86	109.76
23	B	101	H4X	C21-C22-C23	-3.10	122.93	127.28
24	2	103	LMT	C12-C11-C10	3.10	134.31	113.36
16	U	103	BCL	CHD-C1D-ND	-3.10	120.44	124.80
15	I	103	PGV	O01-C1-C2	3.10	118.19	111.48
18	L	303	UQ8	C16-C14-C13	-3.10	114.21	121.17
16	F	105	BCL	CAA-C2A-C3A	-3.10	104.62	113.00
15	5	101	PGV	O01-C1-C2	3.10	118.18	111.48
15	1	103	PGV	O12-P-O11	-3.09	98.60	106.67
23	E	101	H4X	C18-C17-C16	3.08	122.79	118.09
16	3	103	BCL	C6-C5-C3	-3.07	105.99	113.47
16	F	103	BCL	CHD-C1D-C2D	3.07	131.87	125.49
16	A	102	BCL	C2D-C1D-ND	3.07	113.16	110.13
23	O	101	H4X	C27-C26-C25	-3.06	114.33	123.20
11	C	402	HEM	CAD-CBD-CGD	-3.06	105.54	113.67
23	V	101	H4X	C34-C33-C35	3.06	120.54	115.23
16	O	104	BCL	C3D-C4D-ND	3.06	114.96	109.99
16	I	102	BCL	C3B-C4B-NB	3.06	113.80	109.76
23	B	101	H4X	C13-C12-C14	3.05	127.76	122.82
16	9	104	BCL	O2D-CGD-O1D	-3.05	117.91	123.85
16	L	304	BCL	C2D-C1D-ND	3.05	113.14	110.13
16	K	108	BCL	C3B-C4B-NB	3.04	113.77	109.76
23	V	101	H4X	C36-C35-C33	3.04	120.87	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	303	UQ8	C3M-O3-C3	3.04	127.15	116.47
15	Q	101	PGV	C21-C20-C19	-3.04	102.56	113.69
11	C	401	HEM	CHB-C1B-NB	3.04	128.12	124.37
15	Q	101	PGV	C22-C21-C20	3.04	124.28	113.13
24	O	101	LMT	C1'-C2'-C3'	3.03	116.39	110.01
16	L	301	BCL	CAA-C2A-C3A	-3.03	104.81	113.00
16	U	102	BCL	C4A-NA-C1A	-3.02	105.30	106.68
16	J	101	BCL	C1-O2A-CGA	3.02	123.97	116.65
16	K	105	BCL	O2A-CGA-CBA	3.02	121.04	111.83
23	O	101	H4X	C2-C1-C4	-3.01	105.76	111.12
11	C	402	HEM	CAA-C2A-C3A	-3.01	120.32	127.07
11	C	404	HEM	CHC-C1C-NC	3.01	127.73	124.45
16	K	105	BCL	CAA-C2A-C3A	-3.00	104.88	113.00
16	U	102	BCL	C3D-C4D-ND	3.00	114.87	109.99
16	J	101	BCL	CAA-C2A-C3A	-3.00	104.89	113.00
16	U	102	BCL	C2D-C1D-ND	3.00	113.09	110.13
16	Q	103	BCL	O2A-CGA-CBA	3.00	120.98	111.83
16	Y	102	BCL	C3D-C2D-C1D	-3.00	101.74	105.83
16	K	105	BCL	CHC-C4B-NB	-2.99	119.56	124.05
16	F	103	BCL	CBA-CAA-C2A	-2.99	104.89	113.79
16	A	102	BCL	C1D-ND-C4D	-2.99	104.21	106.31
23	4	101	H4X	C36-C35-C33	2.99	120.75	113.47
16	Q	104	BCL	CAC-C3C-C4C	-2.99	105.96	112.58
24	N	101	LMT	O5'-C5'-C6'	-2.98	99.04	106.44
16	A	102	BCL	O2A-CGA-CBA	2.98	120.94	111.83
16	7	103	BCL	CAA-C2A-C3A	-2.98	104.94	113.00
16	O	105	BCL	C3B-C4B-NB	2.98	113.69	109.76
24	B	104	LMT	O5B-C5B-C6B	2.98	113.82	106.44
16	5	104	BCL	CMB-C2B-C1B	2.98	129.95	125.42
24	B	102	LMT	O5B-C5B-C4B	2.97	115.06	109.70
16	X	101	BCL	C3B-C4B-NB	2.97	113.68	109.76
16	J	101	BCL	CHC-C1C-NC	2.97	128.69	124.40
16	O	105	BCL	CHD-C1D-ND	-2.97	120.62	124.80
23	Q	105	H4X	C31-C32-C33	-2.97	123.51	127.69
16	I	102	BCL	C3D-C2D-C1D	-2.97	101.78	105.83
24	2	103	LMT	C4B-C3B-C2B	-2.97	105.62	110.83
16	K	108	BCL	C1D-CHD-C4C	-2.97	119.47	126.62
24	4	102	LMT	C4B-C3B-C2B	-2.97	105.62	110.83
15	Y	105	PGV	O01-C1-C2	2.96	117.89	111.48
16	A	102	BCL	C3B-C4B-NB	2.96	113.67	109.76
16	F	105	BCL	C3B-C4B-NB	2.96	113.67	109.76
23	4	101	H4X	C14-C15-C16	-2.96	114.63	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	V	101	H4X	C9-C10-C11	-2.96	114.63	123.20
16	K	108	BCL	CAC-C3C-C4C	-2.96	106.02	112.58
11	C	403	HEM	CHD-C1D-ND	2.96	127.60	124.42
16	3	103	BCL	C1C-NC-C4C	-2.95	105.33	106.68
16	D	104	BCL	CHC-C4B-NB	-2.95	119.62	124.05
16	M	403	BCL	C1-O2A-CGA	2.95	123.80	116.65
23	Z	101	H4X	C36-C35-C33	2.95	120.66	113.47
16	L	304	BCL	CMA-C3A-C4A	-2.95	103.84	111.77
16	2	102	BCL	C3B-C4B-NB	2.95	113.65	109.76
16	O	104	BCL	CBB-CAB-C3B	2.95	126.62	120.40
15	K	102	PGV	O01-C1-C2	2.95	120.83	111.83
16	K	108	BCL	O2D-CGD-CBD	2.95	116.39	111.23
18	L	306	UQ8	C20-C19-C21	2.95	120.35	115.23
23	6	101	H4X	C31-C32-C33	-2.94	123.55	127.69
16	3	104	BCL	C1D-CHD-C4C	-2.94	119.52	126.62
23	O	101	H4X	C16-C17-C19	-2.94	114.38	119.01
16	O	105	BCL	O2D-CGD-O1D	-2.94	118.12	123.85
23	P	101	H4X	C39-C38-C37	-2.94	105.90	111.12
16	L	301	BCL	CHB-C4A-NA	2.94	128.64	124.40
16	O	105	BCL	C1-O2A-CGA	2.93	123.75	116.65
24	6	102	LMT	C4B-C3B-C2B	-2.92	105.70	110.83
23	5	105	H4X	C15-C14-C12	-2.92	123.18	127.28
16	O	105	BCL	C2A-C1A-CHA	-2.92	118.80	123.87
23	2	101	H4X	C34-C33-C35	2.92	120.30	115.23
11	C	404	HEM	C4C-CHD-C1D	-2.91	119.83	126.02
18	L	303	UQ8	C7-C8-C9	-2.91	121.81	126.83
16	5	104	BCL	C1-O2A-CGA	2.91	123.69	116.65
16	F	105	BCL	C6-C5-C3	-2.91	106.38	113.47
15	O	102	PGV	C02-O01-C1	-2.91	110.84	117.80
16	D	104	BCL	C1D-CHD-C4C	-2.91	119.61	126.62
23	Q	105	H4X	C29-C28-C30	2.91	122.53	118.09
16	5	103	BCL	C1C-NC-C4C	-2.90	105.35	106.68
16	3	104	BCL	C3B-C4B-NB	2.90	113.59	109.76
23	2	101	H4X	C4-C5-C6	2.90	119.30	112.33
23	B	101	H4X	C8-C7-C6	2.90	120.26	115.23
23	G	101	H4X	C26-C27-C28	-2.90	123.22	127.28
15	F	104	PGV	O03-C19-C20	2.89	120.66	111.83
16	A	102	BCL	C3D-C4D-ND	2.89	114.69	109.99
15	A	101	PGV	O11-P-O13	2.89	120.41	108.94
23	2	101	H4X	C5-C6-C7	2.89	120.51	113.47
24	6	102	LMT	O5'-C5'-C6'	-2.89	99.28	106.44
16	M	403	BCL	CBB-CAB-C3B	-2.89	114.31	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2	101	H4X	C9-C10-C11	-2.89	114.83	123.20
16	K	108	BCL	C2A-C1A-CHA	-2.89	118.85	123.87
16	Y	104	BCL	CMB-C2B-C1B	2.89	129.81	125.42
16	M	403	BCL	O2A-CGA-CBA	2.88	120.63	111.83
16	3	103	BCL	CMC-C2C-C3C	-2.88	102.84	113.98
16	J	101	BCL	C4-C3-C5	2.88	120.23	115.23
16	L	304	BCL	C1D-ND-C4D	-2.88	104.29	106.31
16	T	101	BCL	C1D-CHD-C4C	-2.88	119.68	126.62
23	B	101	H4X	C2-C1-C3	-2.88	105.17	110.43
15	M	406	PGV	O03-C19-C20	2.87	120.60	111.83
23	7	104	H4X	C24-C23-C25	2.87	122.47	118.09
16	M	402	BCL	OBb-CAB-CBB	2.87	126.19	119.77
16	3	103	BCL	C3D-C4D-ND	2.87	114.64	109.99
16	K	108	BCL	C1C-NC-C4C	-2.86	105.37	106.68
16	M	402	BCL	CHD-C1D-C2D	2.86	131.44	125.49
16	9	104	BCL	CAA-C2A-C3A	-2.86	105.26	113.00
16	Q	104	BCL	CED-O2D-CGD	2.86	122.41	115.92
24	J	102	LMT	C4B-C3B-C2B	-2.86	105.81	110.83
24	6	102	LMT	C1B-O1B-C4'	2.86	124.76	117.98
23	B	101	H4X	C40-C38-C37	2.86	116.20	111.12
23	Q	105	H4X	C40-C38-C39	-2.86	105.20	110.43
16	Y	102	BCL	O2A-CGA-CBA	2.86	120.55	111.83
11	C	402	HEM	CHD-C4C-NC	2.86	127.56	124.45
14	C	407	DGA	OG2-CG2-CG3	2.85	114.35	107.96
23	O	106	H4X	C14-C15-C16	-2.85	114.93	123.20
16	Y	102	BCL	C3D-C4D-ND	2.85	114.62	109.99
23	B	101	H4X	C5-C6-C7	2.85	120.41	113.47
11	C	402	HEM	C3C-C2C-C1C	2.85	109.74	107.05
24	Z	102	LMT	C4B-C3B-C2B	-2.85	105.83	110.83
24	6	102	LMT	O1B-C1B-C2B	2.85	115.10	108.09
16	3	103	BCL	CAC-C3C-C4C	-2.85	106.26	112.58
16	Y	102	BCL	O2D-CGD-O1D	-2.85	118.31	123.85
23	B	101	H4X	C2-C1-C4	2.85	116.18	111.12
24	0	101	LMT	C1'-O5'-C5'	2.84	119.27	113.72
16	S	103	BCL	C3B-C4B-NB	2.84	113.51	109.76
23	U	104	H4X	C5-C6-C7	2.84	120.38	113.47
23	6	101	H4X	C3-C1-C4	-2.83	106.08	111.12
23	5	105	H4X	C14-C15-C16	-2.83	114.99	123.20
11	C	403	HEM	C1C-CHC-C4B	-2.83	120.01	126.02
23	2	101	H4X	C24-C23-C22	-2.83	118.23	122.82
23	O	106	H4X	C2-C1-C3	-2.83	105.26	110.43
24	X	102	LMT	C1B-O5B-C5B	2.83	119.24	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	105	BCL	C1D-CHD-C4C	-2.83	119.81	126.62
16	M	403	BCL	C3A-C2A-C1A	2.82	105.56	101.34
16	2	102	BCL	C1D-CHD-C4C	-2.82	119.82	126.62
23	7	104	H4X	C5-C6-C7	2.82	120.34	113.47
16	3	104	BCL	CMC-C2C-C3C	-2.82	103.08	113.98
16	W	102	BCL	OBB-CAB-C3B	-2.82	115.45	120.43
16	5	103	BCL	C6-C5-C3	-2.82	106.61	113.47
16	D	104	BCL	CAA-C2A-C3A	-2.82	105.39	113.00
16	3	104	BCL	C1-C2-C3	-2.81	121.59	126.20
16	X	101	BCL	CBB-CAB-C3B	-2.81	114.48	120.40
23	O	106	H4X	C9-C10-C11	-2.81	115.06	123.20
23	G	101	H4X	C10-C9-C7	-2.81	123.74	127.69
16	5	103	BCL	C3D-C4D-ND	2.80	114.55	109.99
16	D	103	BCL	CHB-C1B-C2B	-2.80	119.29	127.43
23	4	101	H4X	C10-C9-C7	-2.79	123.76	127.69
23	B	101	H4X	C36-C35-C33	2.79	120.27	113.47
23	V	101	H4X	C10-C9-C7	-2.79	123.76	127.69
16	O	105	BCL	C4-C3-C2	-2.79	116.46	123.63
23	Q	105	H4X	C29-C28-C27	-2.79	118.30	122.82
16	Q	104	BCL	C4D-CHA-C1A	-2.79	117.92	121.24
23	U	104	H4X	C29-C28-C30	2.78	122.34	118.09
16	I	102	BCL	CMC-C2C-C3C	-2.78	103.22	113.98
16	9	104	BCL	C1D-CHD-C4C	-2.78	119.91	126.62
16	U	102	BCL	CHB-C1B-C2B	-2.78	119.36	127.43
15	I	103	PGV	O03-C19-C20	2.78	120.31	111.83
23	O	106	H4X	C24-C23-C22	-2.77	118.32	122.82
16	K	105	BCL	C11-C12-C13	-2.77	106.76	115.97
16	5	103	BCL	C3B-C4B-NB	2.77	113.41	109.76
16	B	103	BCL	C3D-C4D-ND	2.76	114.48	109.99
18	L	306	UQ8	C12-C13-C14	-2.76	121.30	127.62
16	B	103	BCL	C7-C6-C5	2.76	120.62	113.26
23	2	101	H4X	C13-C12-C11	2.76	122.31	118.09
16	F	105	BCL	CHC-C1C-NC	2.76	128.39	124.40
16	L	301	BCL	O2A-CGA-O1A	-2.76	116.72	123.63
16	1	102	BCL	C3B-C4B-NB	2.76	113.40	109.76
23	6	101	H4X	C36-C35-C33	2.76	120.18	113.47
16	I	102	BCL	CBA-CAA-C2A	-2.75	105.60	113.79
16	U	103	BCL	CHC-C4B-NB	-2.75	119.92	124.05
23	E	101	H4X	C32-C31-C30	-2.75	115.23	123.20
16	7	103	BCL	O2D-CGD-O1D	-2.75	118.49	123.85
16	K	108	BCL	C4-C3-C2	-2.75	116.56	123.63
11	C	404	HEM	CHA-C4D-ND	2.75	127.77	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	104	BCL	OBD-CAD-C3D	-2.75	121.99	128.42
23	K	103	H4X	C20-C21-C22	-2.75	117.89	123.52
23	V	101	H4X	C27-C26-C25	-2.75	115.24	123.20
16	3	104	BCL	CAC-C3C-C4C	-2.75	106.49	112.58
16	9	104	BCL	C3B-C4B-NB	2.75	113.38	109.76
23	4	101	H4X	C8-C7-C6	2.74	119.99	115.23
16	1	102	BCL	C4-C3-C5	2.74	119.99	115.23
16	F	105	BCL	C6-C7-C8	-2.74	106.86	115.97
15	Y	105	PGV	O03-C19-C20	2.74	120.19	111.83
23	6	101	H4X	C14-C15-C16	-2.74	115.27	123.20
23	K	103	H4X	C26-C27-C28	-2.74	123.44	127.28
16	B	103	BCL	CAA-C2A-C3A	-2.74	105.60	113.00
23	K	103	H4X	C18-C17-C16	2.74	122.27	118.09
23	V	101	H4X	C5-C6-C7	2.73	120.13	113.47
16	T	101	BCL	CED-O2D-CGD	2.73	122.12	115.92
16	O	104	BCL	C2A-C3A-C4A	-2.73	97.45	101.87
15	I	103	PGV	O12-P-O11	-2.73	99.55	106.67
16	J	101	BCL	C4-C3-C2	-2.73	116.62	123.63
24	8	102	LMT	C1'-C2'-C3'	2.73	115.75	110.01
16	A	102	BCL	C5-C3-C2	-2.73	115.05	121.17
16	5	104	BCL	CHC-C1C-NC	2.73	128.34	124.40
11	C	401	HEM	O2D-CGD-CBD	2.73	122.61	114.00
16	7	102	BCL	C1D-ND-C4D	-2.72	104.40	106.31
16	2	102	BCL	CHC-C1C-NC	2.72	128.33	124.40
15	K	106	PGV	O01-C1-C2	2.72	117.37	111.48
16	Q	104	BCL	CAA-C2A-C3A	-2.72	105.64	113.00
16	Q	104	BCL	C3D-C4D-ND	2.72	114.41	109.99
11	C	402	HEM	CMD-C2D-C1D	2.72	129.29	125.03
16	L	301	BCL	C5-C3-C2	-2.72	115.06	121.17
23	Q	105	H4X	C21-C20-C19	-2.72	117.95	123.52
16	U	102	BCL	C3B-C4B-NB	2.72	113.35	109.76
16	K	105	BCL	C6-C5-C3	-2.72	106.85	113.47
15	F	104	PGV	C02-O01-C1	-2.72	111.30	117.80
16	9	103	BCL	OBB-CAB-C3B	-2.71	115.63	120.43
16	D	103	BCL	CBA-CAA-C2A	-2.71	105.72	113.79
18	L	303	UQ8	C20-C19-C21	2.71	119.93	115.23
23	4	101	H4X	C2-C1-C4	-2.71	106.31	111.12
23	K	107	H4X	C13-C12-C14	2.70	127.19	122.82
23	B	101	H4X	C4-C5-C6	2.70	118.82	112.33
11	C	404	HEM	C4B-C3B-C2B	2.70	109.76	107.28
23	B	101	H4X	C32-C31-C30	-2.70	115.38	123.20
11	C	403	HEM	O2D-CGD-CBD	2.70	122.53	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	102	LMT	O5'-C5'-C6'	-2.70	99.75	106.44
23	E	101	H4X	C31-C32-C33	-2.70	123.90	127.69
16	K	108	BCL	CHD-C1D-ND	-2.70	121.01	124.80
16	Q	103	BCL	CMC-C2C-C1C	2.69	119.01	111.77
22	H	302	CDL	OA6-CA5-OA7	-2.69	117.42	123.70
23	K	103	H4X	C14-C15-C16	-2.68	115.42	123.20
11	C	404	HEM	CMA-C3A-C2A	2.68	131.31	125.62
16	B	103	BCL	O2A-CGA-CBA	2.68	120.01	111.83
23	O	106	H4X	C36-C35-C33	2.68	119.99	113.47
16	7	102	BCL	C5-C3-C2	-2.68	115.16	121.17
23	P	101	H4X	C2-C1-C4	-2.68	106.36	111.12
23	O	106	H4X	C18-C17-C16	2.68	122.18	118.09
23	U	104	H4X	C14-C15-C16	-2.68	115.45	123.20
16	F	105	BCL	CHC-C4B-NB	-2.68	120.04	124.05
16	5	104	BCL	C2A-C1A-CHA	-2.67	119.22	123.87
16	D	103	BCL	OBb-CAB-C3B	-2.67	115.70	120.43
23	5	105	H4X	C27-C26-C25	-2.67	115.45	123.20
11	C	402	HEM	C4C-CHD-C1D	-2.67	120.34	126.02
16	Q	104	BCL	C1D-CHD-C4C	-2.67	120.18	126.62
18	L	306	UQ8	C11-C9-C8	-2.67	115.17	121.17
16	X	101	BCL	C1D-CHD-C4C	-2.67	120.18	126.62
16	B	103	BCL	CHC-C4B-NB	-2.67	120.04	124.05
16	D	104	BCL	C4-C3-C5	2.67	119.86	115.23
16	9	103	BCL	C11-C12-C13	-2.67	107.10	115.97
18	L	303	UQ8	O3-C3-C2	2.67	125.63	116.64
16	Y	104	BCL	CMC-C2C-C3C	-2.67	103.68	113.98
16	5	104	BCL	CMC-C2C-C3C	-2.66	103.69	113.98
16	U	102	BCL	O2A-CGA-CBA	2.66	119.95	111.83
16	L	301	BCL	C2D-C1D-ND	2.66	112.76	110.13
16	O	105	BCL	CHC-C4B-NB	-2.66	120.07	124.05
16	Q	104	BCL	C2D-C1D-ND	2.65	112.75	110.13
23	B	101	H4X	C26-C25-C23	-2.65	119.09	126.36
16	J	101	BCL	C1D-CHD-C4C	-2.65	120.22	126.62
16	2	102	BCL	CHC-C4B-NB	-2.65	120.07	124.05
16	T	101	BCL	CAA-C2A-C3A	-2.65	105.83	113.00
15	L	305	PGV	O04-C19-C20	-2.65	113.42	123.78
16	X	101	BCL	CHC-C4B-NB	-2.65	120.08	124.05
22	Y	103	CDL	OA6-CA5-C11	2.65	119.18	111.15
16	I	102	BCL	CAA-C2A-C3A	-2.65	105.85	113.00
16	Y	102	BCL	C5-C3-C2	-2.65	115.23	121.17
16	M	403	BCL	CGD-CBD-CAD	-2.64	102.28	110.85
23	4	101	H4X	C34-C33-C35	2.64	119.81	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	5	103	BCL	C2D-C1D-ND	2.64	112.74	110.13
16	7	102	BCL	OBB-CAB-CBB	-2.64	113.85	119.77
24	Z	102	LMT	O5'-C1'-O1'	-2.64	103.81	110.04
16	D	104	BCL	C4-C3-C2	-2.64	116.85	123.63
23	Q	105	H4X	C18-C17-C16	2.64	122.12	118.09
16	L	301	BCL	CHD-C1D-ND	-2.64	121.09	124.80
11	C	402	HEM	C4C-C3C-C2C	-2.64	104.53	106.81
16	J	101	BCL	C2A-C1A-CHA	-2.64	119.29	123.87
11	C	403	HEM	C4C-C3C-C2C	2.64	109.10	106.81
16	F	103	BCL	CMA-C3A-C2A	-2.64	103.79	113.98
16	Q	104	BCL	C2A-C1A-CHA	-2.63	119.30	123.87
16	M	403	BCL	C16-C15-C13	-2.63	107.21	115.97
15	3	101	PGV	O04-C19-C20	-2.63	113.49	123.78
23	6	101	H4X	C29-C28-C27	2.63	127.08	122.82
16	T	101	BCL	C2D-C1D-ND	2.63	112.73	110.13
16	X	101	BCL	CAA-C2A-C3A	-2.63	105.89	113.00
16	T	101	BCL	CHC-C1C-NC	2.63	128.19	124.40
15	3	101	PGV	C03-C02-C01	-2.63	105.66	111.78
16	O	105	BCL	C7-C6-C5	2.63	120.26	113.26
23	2	101	H4X	C31-C32-C33	-2.63	124.00	127.69
16	K	108	BCL	O2A-CGA-CBA	2.63	119.84	111.83
23	V	101	H4X	C40-C38-C37	2.63	115.79	111.12
16	X	101	BCL	O2A-CGA-CBA	2.62	119.83	111.83
16	O	104	BCL	C3B-C4B-NB	2.62	113.22	109.76
16	2	102	BCL	C1-C2-C3	-2.62	121.90	126.20
23	K	103	H4X	C2-C1-C4	-2.62	106.46	111.12
16	7	102	BCL	C3B-C4B-NB	2.62	113.22	109.76
15	3	101	PGV	C02-O01-C1	-2.62	111.53	117.80
15	L	305	PGV	C21-C20-C19	-2.62	104.11	113.69
23	B	101	H4X	C20-C19-C17	-2.62	123.61	127.28
16	5	104	BCL	CHB-C4A-NA	2.62	128.17	124.40
16	L	301	BCL	CED-O2D-CGD	2.61	121.84	115.92
16	Q	104	BCL	OBB-CAB-CBB	2.61	125.62	119.77
16	M	402	BCL	C3D-C4D-ND	2.61	114.23	109.99
24	2	103	LMT	O3B-C3B-C4B	-2.61	104.22	110.38
15	C	408	PGV	O01-C02-C03	2.61	112.21	106.21
15	Y	105	PGV	C02-O01-C1	-2.61	111.55	117.80
16	7	102	BCL	C2D-C1D-ND	2.61	112.71	110.13
16	L	301	BCL	C1-O2A-CGA	2.61	122.97	116.65
23	P	101	H4X	C18-C17-C16	2.60	122.06	118.09
16	5	104	BCL	C1D-CHD-C4C	-2.60	120.34	126.62
16	B	103	BCL	C1D-ND-C4D	-2.60	104.49	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	K	103	H4X	C15-C14-C12	-2.60	123.63	127.28
16	5	104	BCL	C3D-C4D-ND	2.60	114.21	109.99
16	Y	102	BCL	O1D-CGD-CBD	-2.60	119.39	124.52
23	O	101	H4X	C15-C14-C12	-2.60	123.64	127.28
15	3	101	PGV	O01-C1-O02	-2.59	117.64	123.70
16	T	101	BCL	C3B-C4B-NB	2.59	113.18	109.76
23	Z	101	H4X	C14-C15-C16	-2.59	115.69	123.20
11	C	401	HEM	CBC-CAC-C3C	-2.59	114.58	127.53
16	3	104	BCL	CMB-C2B-C1B	2.59	129.36	125.42
15	F	101	PGV	C21-C20-C19	-2.59	104.21	113.69
24	X	102	LMT	C6B-C5B-C4B	-2.59	106.66	113.02
23	K	107	H4X	C9-C10-C11	-2.59	115.70	123.20
15	D	101	PGV	C02-O01-C1	-2.59	111.61	117.80
16	O	104	BCL	CBA-CAA-C2A	-2.59	106.10	113.79
16	S	103	BCL	C1C-NC-C4C	-2.58	105.50	106.68
16	9	104	BCL	C1C-NC-C4C	-2.58	105.50	106.68
16	7	102	BCL	C1D-CHD-C4C	-2.58	120.40	126.62
16	T	101	BCL	CMB-C2B-C1B	2.58	129.35	125.42
24	T	102	LMT	O5B-C5B-C4B	2.58	114.35	109.70
16	B	103	BCL	C3B-C4B-NB	2.58	113.16	109.76
24	P	102	LMT	O5B-C5B-C6B	2.58	112.83	106.44
16	Q	103	BCL	CHB-C1B-C2B	-2.58	119.94	127.43
16	T	101	BCL	C2A-C1A-CHA	-2.58	119.39	123.87
16	M	402	BCL	CHC-C1C-NC	2.58	128.12	124.40
16	Y	102	BCL	CBB-CAB-C3B	2.58	125.83	120.40
16	W	102	BCL	C2D-C1D-ND	2.57	112.67	110.13
11	C	404	HEM	C3B-C2B-C1B	-2.57	104.48	106.41
16	L	304	BCL	C1D-CHD-C4C	-2.57	120.41	126.62
16	Y	102	BCL	C3B-C4B-NB	2.57	113.16	109.76
24	P	102	LMT	C6B-C5B-C4B	-2.57	106.71	113.02
23	7	104	H4X	C32-C31-C30	-2.57	115.76	123.20
16	F	105	BCL	C2A-C1A-CHA	-2.57	119.41	123.87
16	I	102	BCL	CHD-C1D-C2D	2.57	130.82	125.49
16	F	105	BCL	C7-C6-C5	2.56	120.09	113.26
15	I	103	PGV	O14-P-O13	2.56	120.82	110.83
23	E	101	H4X	C14-C15-C16	-2.56	115.77	123.20
24	E	102	LMT	C4B-C3B-C2B	-2.56	106.33	110.83
23	Q	105	H4X	C24-C23-C25	2.56	122.00	118.09
24	0	101	LMT	C12-C11-C10	2.56	130.65	113.36
16	7	102	BCL	CAA-C2A-C3A	-2.56	106.08	113.00
11	C	404	HEM	C1C-CHC-C4B	-2.56	120.58	126.02
16	5	103	BCL	CHB-C1B-C2B	-2.56	120.00	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	104	BCL	O2A-CGA-CBA	2.56	119.63	111.83
16	K	108	BCL	C1-O2A-CGA	2.55	122.83	116.65
16	7	102	BCL	C4-C3-C5	2.55	119.66	115.23
16	Q	103	BCL	C3D-C4D-ND	2.55	114.13	109.99
16	Y	102	BCL	CMA-C3A-C2A	-2.55	104.12	113.98
24	2	103	LMT	C3B-C4B-C5B	-2.55	105.62	110.23
16	O	105	BCL	CHC-C1C-NC	2.55	128.07	124.40
16	9	104	BCL	CHC-C4B-NB	-2.54	120.23	124.05
16	U	103	BCL	C3D-C4D-ND	2.54	114.12	109.99
23	O	101	H4X	C9-C10-C11	-2.54	115.83	123.20
23	5	105	H4X	C32-C31-C30	-2.54	115.83	123.20
16	D	104	BCL	CHC-C1C-NC	2.54	128.07	124.40
16	L	304	BCL	O2A-CGA-O1A	-2.54	117.27	123.63
16	J	101	BCL	C3D-C4D-ND	2.54	114.12	109.99
22	S	101	CDL	OA6-CA5-C11	2.54	116.97	111.48
16	I	102	BCL	C5-C3-C2	-2.54	115.47	121.17
16	2	102	BCL	C1-O2A-CGA	2.54	122.79	116.65
11	C	402	HEM	CAA-C2A-C1A	2.54	129.89	124.94
16	1	102	BCL	CBA-CAA-C2A	-2.54	106.25	113.79
16	Q	103	BCL	CMB-C2B-C1B	2.54	129.28	125.42
16	X	101	BCL	CHB-C1B-C2B	-2.53	120.07	127.43
16	I	102	BCL	CHB-C1B-C2B	-2.53	120.07	127.43
23	U	104	H4X	C9-C10-C11	-2.53	115.86	123.20
16	B	103	BCL	C2A-C1A-CHA	-2.53	119.47	123.87
16	2	102	BCL	CHD-C1D-ND	-2.53	121.24	124.80
16	3	103	BCL	CBA-CAA-C2A	-2.53	106.27	113.79
15	A	101	PGV	O05-C05-C04	-2.53	100.96	109.70
24	B	104	LMT	C3B-C4B-C5B	-2.53	105.65	110.23
17	M	404	BPH	O2D-CGD-CBD	2.52	113.72	110.95
23	K	107	H4X	C14-C15-C16	-2.52	115.90	123.20
24	J	102	LMT	O5'-C1'-O1'	-2.52	104.09	110.04
16	O	104	BCL	C1D-ND-C4D	-2.52	104.55	106.31
16	2	102	BCL	C19-C18-C17	2.52	126.44	111.55
23	Z	101	H4X	C27-C26-C25	-2.52	115.91	123.20
16	U	103	BCL	CMB-C2B-C1B	2.51	129.24	125.42
16	9	103	BCL	C1D-CHD-C4C	-2.51	120.57	126.62
16	2	102	BCL	CHB-C1B-C2B	-2.51	120.15	127.43
16	B	103	BCL	C4-C3-C5	2.50	119.58	115.23
16	1	102	BCL	C1D-ND-C4D	-2.50	104.56	106.31
23	7	104	H4X	C2-C1-C4	2.50	115.57	111.12
24	T	102	LMT	C6B-C5B-C4B	-2.50	106.88	113.02
16	S	103	BCL	C3D-C4D-ND	2.50	114.05	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	106	H4X	C10-C9-C7	-2.50	124.18	127.69
16	1	102	BCL	CHD-C1D-C2D	2.49	130.67	125.49
24	B	104	LMT	O5'-C5'-C6'	-2.49	100.26	106.44
11	C	403	HEM	CAD-C3D-C2D	-2.49	123.20	127.87
15	L	305	PGV	O14-P-O13	2.49	124.02	112.44
23	K	103	H4X	C36-C35-C33	2.49	119.53	113.47
24	Z	102	LMT	C1B-O5B-C5B	2.48	118.57	113.72
23	4	101	H4X	C5-C6-C7	2.48	119.52	113.47
23	B	101	H4X	C21-C20-C19	-2.48	118.44	123.52
11	C	403	HEM	CHB-C1B-C2B	-2.48	119.89	126.95
24	8	102	LMT	C6B-C5B-C4B	-2.48	106.93	113.02
16	D	104	BCL	C4A-NA-C1A	-2.48	105.55	106.68
23	P	101	H4X	C9-C10-C11	-2.48	116.02	123.20
23	O	106	H4X	C31-C32-C33	-2.48	124.21	127.69
16	M	403	BCL	CMC-C2C-C3C	-2.48	104.41	113.98
23	Z	101	H4X	C32-C31-C30	-2.48	116.02	123.20
16	Q	104	BCL	CHB-C1B-C2B	-2.48	120.24	127.43
21	M	405	MQ8	C11-C3-C2	-2.47	120.65	124.89
16	L	304	BCL	CHC-C1C-NC	2.47	127.97	124.40
16	S	103	BCL	CBA-CAA-C2A	-2.47	106.45	113.79
16	O	105	BCL	C3D-C4D-ND	2.46	113.99	109.99
24	V	102	LMT	C6B-C5B-C4B	-2.46	106.97	113.02
11	C	402	HEM	CHB-C1B-C2B	-2.46	119.95	126.95
23	K	103	H4X	C16-C17-C19	-2.46	115.14	119.01
24	R	101	LMT	O5B-C5B-C6B	2.46	112.53	106.44
16	F	103	BCL	C1C-NC-C4C	-2.46	105.56	106.68
16	M	403	BCL	C3D-C4D-ND	2.46	113.98	109.99
15	F	101	PGV	C01-O03-C19	2.45	126.07	117.12
23	6	101	H4X	C8-C7-C6	2.45	119.48	115.23
16	M	402	BCL	CHB-C1B-C2B	-2.45	120.32	127.43
16	L	301	BCL	O1D-CGD-CBD	-2.45	119.69	124.52
16	L	301	BCL	OB B-CAB-C3B	-2.45	116.11	120.43
16	U	103	BCL	C1D-CHD-C4C	-2.44	120.73	126.62
16	5	104	BCL	C3B-C4B-NB	2.44	112.98	109.76
16	X	101	BCL	C4A-NA-C1A	-2.44	105.56	106.68
24	T	102	LMT	C1B-O5B-C5B	2.44	118.49	113.72
16	D	104	BCL	CHB-C1B-C2B	-2.44	120.34	127.43
16	M	402	BCL	C1-O2A-CGA	2.44	122.56	116.65
11	C	403	HEM	CAC-C3C-C4C	-2.44	119.00	124.82
16	L	301	BCL	CMA-C3A-C4A	-2.43	105.23	111.77
24	J	102	LMT	O1B-C4'-C5'	2.43	115.86	109.48
23	6	101	H4X	C40-C38-C37	-2.43	106.80	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	101	LMT	C3B-C4B-C5B	-2.43	105.82	110.23
24	R	101	LMT	C1B-O5B-C5B	2.43	118.47	113.72
24	R	101	LMT	C4B-C3B-C2B	-2.43	106.57	110.83
16	3	104	BCL	O2A-CGA-CBA	2.43	119.23	111.83
16	B	103	BCL	C1-O2A-CGA	2.42	122.52	116.65
11	C	403	HEM	C4C-CHD-C1D	-2.42	120.87	126.02
16	U	102	BCL	CBA-CAA-C2A	-2.42	106.58	113.79
24	E	102	LMT	C12-C11-C10	2.42	129.72	113.36
16	9	104	BCL	CHC-C1C-NC	2.42	127.89	124.40
16	1	102	BCL	C3A-C2A-C1A	2.42	104.96	101.34
16	F	103	BCL	C3D-C4D-ND	2.42	113.92	109.99
16	J	101	BCL	C6-C7-C8	-2.42	107.93	115.97
23	B	101	H4X	C24-C23-C22	-2.42	118.90	122.82
23	E	101	H4X	C2-C1-C4	-2.42	106.83	111.12
16	L	301	BCL	CAA-CBA-CGA	-2.41	106.35	113.21
24	P	102	LMT	C12-C11-C10	2.41	129.66	113.36
16	F	105	BCL	CMB-C2B-C1B	2.41	129.09	125.42
16	U	103	BCL	C2A-C1A-CHA	-2.41	119.69	123.87
18	L	306	UQ8	C21-C19-C18	-2.40	115.77	121.17
16	9	104	BCL	C4A-NA-C1A	-2.40	105.58	106.68
16	D	103	BCL	C3A-C2A-C1A	2.40	104.94	101.34
16	7	103	BCL	CMA-C3A-C2A	-2.40	104.70	113.98
24	J	102	LMT	O1B-C1B-C2B	2.40	113.99	108.09
15	A	101	PGV	O05-C05-C06	-2.40	99.25	109.18
24	4	102	LMT	O5'-C1'-O1'	-2.40	104.38	110.04
23	G	101	H4X	C26-C25-C23	-2.40	119.80	126.36
24	2	103	LMT	O5'-C1'-C2'	2.39	115.29	110.37
23	V	101	H4X	C13-C12-C14	2.39	126.69	122.82
16	M	403	BCL	CMC-C2C-C1C	-2.39	105.34	111.77
24	N	101	LMT	O1B-C1B-C2B	2.39	113.98	108.09
23	U	104	H4X	C26-C25-C23	-2.39	119.80	126.36
11	C	403	HEM	C4A-CHB-C1B	-2.39	120.63	126.25
22	H	302	CDL	OA4-PA1-OA3	2.39	123.56	112.44
16	M	403	BCL	O2A-CGA-O1A	-2.39	117.65	123.63
23	6	101	H4X	C40-C38-C39	2.39	114.79	110.43
16	5	103	BCL	C1-O2A-CGA	2.39	122.43	116.65
16	O	105	BCL	CMB-C2B-C1B	2.39	129.05	125.42
16	9	104	BCL	C3D-C4D-ND	2.39	113.86	109.99
16	L	304	BCL	C3B-C4B-NB	2.39	112.91	109.76
16	L	301	BCL	CHB-C1B-C2B	-2.38	120.50	127.43
15	D	101	PGV	C03-C02-C01	-2.38	106.23	111.78
11	C	404	HEM	CHB-C1B-C2B	-2.38	120.18	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	U	104	H4X	C16-C17-C19	-2.38	115.27	119.01
23	5	105	H4X	C18-C17-C16	2.38	121.72	118.09
16	2	102	BCL	CAC-C3C-C4C	-2.38	107.30	112.58
24	T	102	LMT	C12-C11-C10	2.38	129.43	113.36
16	J	101	BCL	O2A-CGA-CBA	2.38	119.09	111.83
16	B	103	BCL	C2D-C1D-ND	2.38	112.48	110.13
16	L	301	BCL	C7-C6-C5	-2.38	106.92	113.26
16	3	104	BCL	CMA-C3A-C2A	-2.38	104.79	113.98
15	D	101	PGV	O03-C19-O04	-2.37	117.69	123.63
16	K	105	BCL	O2A-C1-C2	2.37	117.24	108.11
16	B	103	BCL	CHC-C1C-NC	2.37	127.82	124.40
23	6	101	H4X	C29-C28-C30	-2.37	114.47	118.09
16	K	108	BCL	C7-C6-C5	2.37	119.57	113.26
16	L	304	BCL	O2A-CGA-CBA	2.37	119.05	111.83
16	T	101	BCL	OB B-CAB-C3B	-2.37	116.25	120.43
11	C	401	HEM	C3B-C2B-C1B	2.37	108.19	106.41
16	O	104	BCL	C3A-C2A-C1A	2.36	104.88	101.34
24	6	102	LMT	O5'-C1'-O1'	-2.36	104.46	110.04
16	J	101	BCL	CHC-C4B-NB	-2.36	120.51	124.05
16	M	403	BCL	C7-C6-C5	-2.36	106.97	113.26
23	Q	105	H4X	C32-C31-C30	-2.36	116.36	123.20
18	L	306	UQ8	C8-C7-C6	-2.36	106.27	112.08
18	L	303	UQ8	C6-C1-C2	2.36	121.03	119.17
24	2	103	LMT	O5B-C5B-C4B	2.36	113.95	109.70
16	T	101	BCL	C6-C5-C3	-2.36	107.73	113.47
16	D	103	BCL	C3D-C4D-ND	2.36	113.82	109.99
24	0	101	LMT	O1B-C1B-C2B	2.36	113.89	108.09
16	Y	102	BCL	C2D-C1D-ND	2.36	112.46	110.13
16	A	102	BCL	C4A-NA-C1A	-2.35	105.61	106.68
18	L	306	UQ8	C16-C14-C13	-2.35	115.89	121.17
16	9	104	BCL	CHB-C1B-C2B	-2.35	120.60	127.43
16	D	104	BCL	O2D-CGD-O1D	-2.35	119.27	123.85
23	2	101	H4X	C3-C1-C4	-2.35	106.94	111.12
16	A	102	BCL	CHC-C4B-NB	-2.35	120.53	124.05
16	O	105	BCL	CAA-C2A-C3A	-2.35	106.66	113.00
11	C	401	HEM	CAD-CBD-CGD	-2.34	107.45	113.67
16	L	301	BCL	C17-C16-C15	-2.34	102.78	113.28
16	B	103	BCL	CHD-C1D-ND	-2.34	121.51	124.80
11	C	401	HEM	CHD-C1D-C2D	-2.34	121.33	125.03
24	2	103	LMT	C1B-O1B-C4'	2.34	123.53	117.98
16	Q	104	BCL	CMA-C3A-C2A	-2.34	104.94	113.98
23	2	101	H4X	C36-C35-C33	2.34	119.16	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	104	LMT	C4-C3-C2	2.34	126.18	114.37
23	G	101	H4X	C13-C12-C11	2.34	121.66	118.09
11	C	403	HEM	C3B-C2B-C1B	-2.33	104.66	106.41
21	M	405	MQ8	C36-C35-C33	2.33	120.92	113.19
24	V	102	LMT	C4B-C3B-C2B	-2.33	106.73	110.83
16	Q	104	BCL	C7-C6-C5	2.33	119.48	113.26
15	H	301	PGV	O04-C19-C20	-2.33	114.66	123.78
18	L	306	UQ8	C12-C11-C9	-2.33	105.46	113.19
16	7	102	BCL	C3D-C4D-ND	2.33	113.77	109.99
16	3	103	BCL	C1D-CHD-C4C	-2.33	121.01	126.62
16	U	103	BCL	O2D-CGD-O1D	-2.33	119.32	123.85
16	1	102	BCL	C1C-NC-C4C	2.33	107.74	106.68
23	O	106	H4X	C39-C38-C37	-2.33	106.99	111.12
16	K	105	BCL	C3A-C2A-C1A	2.32	104.81	101.34
16	1	102	BCL	C1D-CHD-C4C	-2.32	121.02	126.62
15	3	101	PGV	O01-C02-C03	2.32	116.67	108.34
16	5	104	BCL	CAC-C3C-C4C	-2.32	107.44	112.58
24	2	103	LMT	O3'-C3'-C2'	-2.32	104.91	110.38
23	4	101	H4X	C9-C10-C11	-2.32	116.48	123.20
23	P	101	H4X	C4-C5-C6	2.32	117.90	112.33
16	X	101	BCL	CMB-C2B-C3B	2.32	132.97	125.67
24	4	102	LMT	O1B-C1B-C2B	2.32	113.79	108.09
23	O	106	H4X	C3-C1-C4	-2.31	107.01	111.12
16	Q	103	BCL	C3B-C4B-NB	2.31	112.81	109.76
16	O	105	BCL	CHB-C1B-C2B	-2.31	120.72	127.43
24	4	102	LMT	C1B-O1B-C4'	2.31	123.45	117.98
11	C	402	HEM	C4B-C3B-C2B	-2.31	105.16	107.28
16	5	104	BCL	CHC-C4B-NB	-2.31	120.59	124.05
16	5	103	BCL	C1D-CHD-C4C	-2.31	121.05	126.62
24	T	102	LMT	O1B-C1B-C2B	2.31	113.76	108.09
16	Q	104	BCL	C1D-ND-C4D	-2.31	104.69	106.31
24	G	102	LMT	O5'-C1'-O1'	-2.30	104.60	110.04
23	Q	105	H4X	C27-C26-C25	-2.30	116.52	123.20
16	L	301	BCL	C11-C10-C8	-2.30	108.31	115.97
23	E	101	H4X	C24-C23-C22	-2.30	119.09	122.82
23	V	101	H4X	C26-C27-C28	-2.30	124.05	127.28
16	S	103	BCL	C2D-C1D-ND	2.30	112.40	110.13
24	V	102	LMT	O1B-C4'-C5'	2.30	115.50	109.48
15	D	101	PGV	C25-C24-C23	-2.30	102.75	114.37
16	O	104	BCL	OBB-CAB-C3B	-2.30	116.37	120.43
16	3	104	BCL	C7-C6-C5	2.29	119.38	113.26
16	M	402	BCL	C1D-CHD-C4C	-2.29	121.09	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	401	HEM	CMB-C2B-C1B	2.29	128.61	125.03
15	F	104	PGV	C01-O03-C19	2.29	125.47	117.12
11	C	403	HEM	O2A-CGA-CBA	2.28	121.22	114.00
24	Z	102	LMT	O1B-C1B-C2B	2.28	113.71	108.09
24	R	101	LMT	C1B-O1B-C4'	2.28	123.39	117.98
16	B	103	BCL	C4-C3-C2	-2.28	117.77	123.63
16	L	304	BCL	CHB-C1B-C2B	-2.28	120.81	127.43
16	3	104	BCL	OB B-CAB-CBB	2.28	124.87	119.77
16	1	102	BCL	C3D-C4D-ND	2.28	113.69	109.99
23	O	101	H4X	C18-C17-C19	2.28	126.51	122.82
16	1	102	BCL	C16-C15-C13	-2.28	108.40	115.97
16	L	304	BCL	CMB-C2B-C1B	2.28	128.89	125.42
11	C	401	HEM	C4C-CHD-C1D	-2.27	121.19	126.02
24	N	101	LMT	O3B-C3B-C4B	-2.27	105.02	110.38
16	Y	104	BCL	C4-C3-C5	2.27	119.17	115.23
15	F	101	PGV	O04-C19-C20	-2.27	114.89	123.78
16	X	101	BCL	C2D-C1D-ND	2.27	112.38	110.13
23	P	101	H4X	C20-C21-C22	-2.27	118.87	123.52
16	W	102	BCL	C4-C3-C5	2.27	119.17	115.23
16	K	108	BCL	CMC-C2C-C3C	-2.27	105.20	113.98
16	I	102	BCL	O2A-CGA-CBA	2.27	118.76	111.83
16	J	101	BCL	CHB-C4A-NA	2.27	127.67	124.40
17	M	404	BPH	C1C-C2C-C3C	2.27	105.00	102.84
16	5	103	BCL	CBA-CAA-C2A	-2.27	107.05	113.79
16	Q	103	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
18	L	303	UQ8	C17-C18-C19	-2.27	122.44	127.62
24	2	103	LMT	O1B-C1B-C2B	2.26	113.66	108.09
16	K	108	BCL	C3D-C4D-ND	2.26	113.66	109.99
16	3	103	BCL	CMC-C2C-C1C	2.26	117.85	111.77
16	F	103	BCL	C2A-C1A-CHA	-2.26	119.94	123.87
16	O	105	BCL	OB D-CAD-C3D	-2.26	123.13	128.42
23	5	105	H4X	C26-C27-C28	-2.26	124.11	127.28
16	L	304	BCL	C1-C2-C3	-2.26	122.50	126.20
16	7	102	BCL	C4A-NA-C1A	-2.26	105.65	106.68
23	P	101	H4X	C27-C26-C25	-2.26	116.66	123.20
23	K	103	H4X	C29-C28-C27	2.26	126.47	122.82
24	R	101	LMT	C1'-O5'-C5'	2.25	118.12	113.72
16	9	104	BCL	O2A-CGA-CBA	2.25	118.70	111.83
24	T	102	LMT	C1'-O5'-C5'	2.25	118.12	113.72
16	K	108	BCL	CHB-C4A-NA	2.25	127.65	124.40
15	9	101	PGV	C02-O01-C1	-2.25	112.41	117.80
16	K	105	BCL	CGD-CBD-CAD	-2.25	103.57	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	102	BCL	C3B-C4B-NB	2.25	112.72	109.76
23	K	103	H4X	C40-C38-C39	-2.25	106.32	110.43
16	Q	103	BCL	OBb-CAB-C3B	-2.25	116.46	120.43
16	5	104	BCL	O2D-CGD-O1D	-2.25	119.48	123.85
16	X	101	BCL	CMA-C3A-C2A	-2.24	105.31	113.98
23	U	104	H4X	C39-C38-C37	-2.24	107.13	111.12
16	I	102	BCL	CHC-C4B-C3B	-2.24	122.81	131.72
11	C	403	HEM	C2A-C1A-NA	-2.24	107.66	110.15
16	Y	102	BCL	C4A-NA-C1A	-2.24	105.66	106.68
16	J	101	BCL	C3B-C4B-NB	2.24	112.72	109.76
16	B	103	BCL	CHB-C4A-NA	2.24	127.63	124.40
16	3	104	BCL	C2A-C1A-CHA	-2.24	119.98	123.87
17	L	302	BPH	O2D-CGD-CBD	2.24	113.40	110.95
16	I	102	BCL	CAC-C3C-C4C	-2.23	107.62	112.58
16	T	101	BCL	ObD-CAD-C3D	-2.23	123.19	128.42
16	F	105	BCL	CHB-C1B-C2B	-2.23	120.95	127.43
16	U	103	BCL	CHB-C1B-C2B	-2.23	120.95	127.43
15	Q	101	PGV	O01-C1-O02	-2.23	118.49	123.70
16	T	101	BCL	CBB-CAB-C3B	2.23	125.10	120.40
16	9	104	BCL	C4D-CHA-C1A	-2.23	118.59	121.24
18	L	303	UQ8	C20-C19-C18	-2.23	117.91	123.63
23	7	104	H4X	C24-C23-C22	-2.23	119.21	122.82
15	F	101	PGV	O14-P-O11	2.23	112.47	106.67
16	U	102	BCL	C6-C5-C3	-2.23	108.05	113.47
11	C	402	HEM	C4D-ND-C1D	2.22	107.84	105.21
16	W	102	BCL	CAC-C3C-C4C	-2.22	107.65	112.58
24	4	102	LMT	C12-C11-C10	2.22	128.36	113.36
16	K	105	BCL	C3D-C4D-ND	2.22	113.60	109.99
16	Y	104	BCL	C3D-C4D-ND	2.22	113.60	109.99
24	P	102	LMT	O5B-C5B-C4B	2.22	113.70	109.70
23	6	101	H4X	C15-C14-C12	-2.22	124.17	127.28
16	X	101	BCL	CAA-CBA-CGA	-2.22	106.91	113.21
16	Q	103	BCL	CHC-C4B-NB	-2.22	120.72	124.05
15	A	101	PGV	O14-P-O11	-2.22	97.52	107.57
16	Y	104	BCL	CHC-C1C-NC	2.22	127.60	124.40
23	4	101	H4X	C20-C21-C22	-2.21	118.99	123.52
24	6	102	LMT	O5B-C5B-C4B	2.21	113.69	109.70
24	2	103	LMT	O1B-C1B-O5B	2.21	116.51	110.69
24	4	102	LMT	O5B-C5B-C4B	2.21	113.68	109.70
16	U	103	BCL	CED-O2D-CGD	2.21	120.92	115.92
23	6	101	H4X	C13-C12-C14	2.21	126.39	122.82
23	G	101	H4X	C5-C6-C7	2.21	118.84	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	7	102	BCL	CBC-CAC-C3C	-2.21	108.73	113.41
23	5	105	H4X	C34-C33-C35	2.21	119.06	115.23
16	Y	102	BCL	CHB-C1B-C2B	-2.21	121.03	127.43
16	3	103	BCL	C1D-ND-C4D	-2.20	104.77	106.31
16	U	102	BCL	C11-C12-C13	-2.20	108.64	115.97
16	S	103	BCL	O2A-CGA-CBA	2.20	118.55	111.83
16	9	104	BCL	CMB-C2B-C1B	2.20	128.77	125.42
16	L	304	BCL	C1C-NC-C4C	-2.20	105.68	106.68
15	D	101	PGV	C04-C05-C06	-2.19	104.38	111.77
11	C	401	HEM	C2A-C1A-NA	-2.19	107.72	110.15
24	T	102	LMT	C1B-O1B-C4'	2.19	123.18	117.98
16	K	105	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
16	B	103	BCL	C6-C7-C8	-2.19	108.67	115.97
16	U	102	BCL	C1D-CHD-C4C	-2.19	121.34	126.62
16	U	102	BCL	CMC-C2C-C3C	-2.19	105.52	113.98
23	Q	105	H4X	O2-C38-C39	2.18	123.99	108.97
16	T	101	BCL	CHB-C4A-NA	2.18	127.55	124.40
16	Q	103	BCL	CBB-CAB-C3B	2.18	125.00	120.40
23	P	101	H4X	C2-C1-C3	-2.18	106.44	110.43
16	3	103	BCL	C3B-C4B-NB	2.18	112.64	109.76
16	Y	104	BCL	CAA-C2A-C3A	-2.18	107.11	113.00
16	7	102	BCL	O2A-CGA-O1A	-2.18	118.18	123.63
24	B	104	LMT	O5'-C1'-O1'	-2.18	104.90	110.04
16	L	304	BCL	CMC-C2C-C3C	-2.18	105.57	113.98
16	F	103	BCL	CMD-C2D-C3D	-2.17	122.70	127.69
16	M	402	BCL	CED-O2D-CGD	-2.17	110.98	115.92
16	S	103	BCL	CMA-C3A-C2A	-2.17	105.58	113.98
23	2	101	H4X	C14-C15-C16	-2.17	116.91	123.20
24	E	102	LMT	C6B-C5B-C4B	-2.17	107.69	113.02
24	0	101	LMT	C3'-C4'-C5'	-2.17	106.12	110.93
15	K	101	PGV	O03-C19-O04	-2.17	118.20	123.63
23	6	101	H4X	C5-C6-C7	2.17	118.75	113.47
23	U	104	H4X	C30-C28-C27	-2.17	115.60	119.01
18	L	303	UQ8	C10-C9-C11	2.17	118.99	115.23
16	9	103	BCL	C1D-ND-C4D	-2.17	104.79	106.31
15	I	103	PGV	O03-C19-O04	-2.17	118.21	123.63
16	Y	104	BCL	C7-C6-C5	2.16	119.03	113.26
23	G	101	H4X	C11-C12-C14	-2.16	115.60	119.01
16	J	101	BCL	O1A-CGA-CBA	-2.16	115.32	123.78
23	Z	101	H4X	C34-C33-C35	2.16	118.98	115.23
16	7	103	BCL	C3B-C4B-NB	2.16	112.61	109.76
16	3	103	BCL	O2A-CGA-CBA	2.16	118.42	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	401	HEM	CMB-C2B-C3B	-2.16	123.20	128.43
16	9	104	BCL	C2A-C1A-CHA	-2.16	120.12	123.87
16	Y	104	BCL	CHB-C1B-C2B	-2.16	121.16	127.43
15	D	101	PGV	O01-C1-O02	-2.16	118.66	123.70
11	C	403	HEM	CMC-C2C-C3C	-2.16	123.21	128.43
15	K	106	PGV	C01-O03-C19	2.16	125.00	117.12
16	7	103	BCL	CAC-C3C-C4C	-2.15	107.80	112.58
16	W	102	BCL	C5-C3-C2	-2.15	116.33	121.17
24	Z	102	LMT	C6B-C5B-C4B	-2.15	107.73	113.02
24	X	102	LMT	O3B-C3B-C4B	-2.15	105.30	110.38
16	F	103	BCL	C1D-ND-C4D	-2.15	104.80	106.31
15	Y	105	PGV	O12-P-O11	-2.15	101.06	106.67
23	E	101	H4X	C8-C7-C6	2.15	118.96	115.23
23	G	101	H4X	C27-C26-C25	-2.15	116.97	123.20
24	J	102	LMT	O1B-C1B-O5B	2.15	116.34	110.69
16	O	105	BCL	C2D-C1D-ND	2.15	112.25	110.13
16	Q	104	BCL	CHC-C1C-NC	2.14	127.50	124.40
24	V	102	LMT	O1B-C1B-C2B	2.14	113.36	108.09
23	7	104	H4X	C9-C10-C11	-2.14	116.99	123.20
22	H	302	CDL	OB4-PB2-OB5	2.14	117.28	107.57
16	7	103	BCL	C2A-C1A-CHA	-2.14	120.15	123.87
22	S	101	CDL	O1-C1-CB2	2.14	117.09	109.70
23	2	101	H4X	C2-C1-C4	-2.14	107.32	111.12
15	Y	105	PGV	O14-P-O13	2.14	119.17	110.83
23	P	101	H4X	C31-C32-C33	-2.14	124.68	127.69
16	O	104	BCL	CHC-C4B-NB	-2.14	120.84	124.05
23	Q	105	H4X	C24-C23-C22	-2.14	119.36	122.82
24	G	102	LMT	O3'-C3'-C2'	-2.14	105.34	110.38
24	E	102	LMT	O5'-C1'-O1'	-2.14	105.00	110.04
24	B	104	LMT	C3'-C4'-C5'	-2.14	106.20	110.93
23	K	107	H4X	C39-C38-C37	-2.13	107.33	111.12
16	7	102	BCL	CBB-CAB-C3B	2.13	124.90	120.40
23	6	101	H4X	C4-C5-C6	2.13	117.45	112.33
24	J	102	LMT	O3B-C3B-C4B	-2.13	105.35	110.38
23	7	104	H4X	C20-C21-C22	-2.13	119.16	123.52
15	K	101	PGV	O03-C19-C20	2.12	118.31	111.83
23	K	107	H4X	C13-C12-C11	-2.12	114.84	118.09
23	4	101	H4X	C27-C26-C25	-2.12	117.05	123.20
16	D	104	BCL	C3D-C4D-ND	2.12	113.44	109.99
15	L	305	PGV	C02-O01-C1	-2.12	112.72	117.80
16	9	103	BCL	C1-O2A-CGA	2.12	121.79	116.65
16	3	104	BCL	C3D-C4D-ND	2.12	113.43	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	101	H4X	C21-C20-C19	-2.12	119.18	123.52
16	K	105	BCL	CHD-C1D-C2D	2.12	129.89	125.49
16	K	105	BCL	CHC-C1C-NC	2.12	127.45	124.40
16	2	102	BCL	C2A-C1A-CHA	-2.12	120.19	123.87
16	W	102	BCL	C3D-C4D-ND	2.12	113.42	109.99
16	2	102	BCL	C3D-C4D-ND	2.11	113.42	109.99
16	F	103	BCL	CED-O2D-CGD	2.11	120.71	115.92
11	C	404	HEM	CMA-C3A-C4A	-2.11	122.20	125.42
11	C	402	HEM	CHC-C1C-NC	2.11	126.75	124.45
16	K	108	BCL	CAA-CBA-CGA	-2.11	107.21	113.21
16	S	103	BCL	C1-O2A-CGA	2.11	121.76	116.65
24	4	102	LMT	C1-O1'-C1'	2.11	117.29	113.68
11	C	403	HEM	CHA-C4D-ND	2.11	126.98	124.37
16	M	402	BCL	CMA-C3A-C2A	-2.11	105.83	113.98
23	Q	105	H4X	C13-C12-C11	-2.11	114.87	118.09
24	J	102	LMT	O3'-C3'-C2'	-2.11	105.41	110.38
24	Z	102	LMT	O5B-C5B-C4B	2.11	113.50	109.70
18	L	303	UQ8	C7-C6-C1	-2.11	121.28	124.89
16	7	103	BCL	OBD-CAD-C3D	-2.11	123.49	128.42
15	K	106	PGV	O12-P-O11	-2.10	101.18	106.67
16	3	104	BCL	CAA-CBA-CGA	-2.10	107.23	113.21
16	X	101	BCL	CHC-C1C-NC	2.10	127.44	124.40
15	9	101	PGV	O01-C1-O02	-2.10	118.79	123.70
23	Q	105	H4X	C40-C38-C37	2.10	114.86	111.12
16	F	105	BCL	C3D-C4D-ND	2.10	113.40	109.99
16	9	104	BCL	OBB-CAB-C3B	-2.10	116.72	120.43
15	K	101	PGV	O01-C1-O02	-2.10	118.80	123.70
16	D	103	BCL	CMA-C3A-C2A	-2.10	105.86	113.98
23	O	101	H4X	C26-C25-C23	-2.10	120.61	126.36
16	Q	103	BCL	OBD-CAD-C3D	-2.10	123.51	128.42
15	3	101	PGV	O03-C01-C02	2.10	114.44	108.40
15	I	103	PGV	O01-C1-O02	-2.10	118.81	123.70
23	K	103	H4X	C26-C25-C23	-2.09	120.62	126.36
24	R	101	LMT	C3'-C4'-C5'	-2.09	106.29	110.93
23	6	101	H4X	C39-C38-C37	-2.09	107.40	111.12
11	C	401	HEM	C1A-CHA-C4D	-2.09	121.32	126.25
23	K	103	H4X	C27-C26-C25	-2.09	117.13	123.20
16	2	102	BCL	C6-C7-C8	-2.09	109.01	115.97
16	F	103	BCL	C1-C2-C3	-2.09	122.77	126.20
16	F	103	BCL	CMC-C2C-C3C	-2.09	105.90	113.98
15	F	101	PGV	O14-P-O12	-2.09	99.97	107.80
23	2	101	H4X	C24-C23-C25	2.09	121.28	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	103	BCL	CMA-C3A-C2A	-2.09	105.92	113.98
16	2	102	BCL	O2A-CGA-CBA	2.08	118.19	111.83
15	K	101	PGV	C02-O01-C1	-2.08	112.81	117.80
16	3	103	BCL	CHB-C1B-C2B	-2.08	121.38	127.43
16	K	105	BCL	CED-O2D-CGD	2.08	120.64	115.92
23	6	101	H4X	C2-C1-C3	-2.08	106.62	110.43
24	8	102	LMT	C1-O1'-C1'	-2.08	110.12	113.68
16	A	102	BCL	CHB-C1B-C2B	-2.08	121.39	127.43
16	T	101	BCL	C4D-CHA-C1A	-2.08	118.76	121.24
23	O	101	H4X	C24-C23-C22	2.08	126.18	122.82
16	W	102	BCL	CHB-C1B-C2B	-2.08	121.40	127.43
16	S	103	BCL	CHB-C1B-C2B	-2.08	121.40	127.43
16	2	102	BCL	OBb-CAB-C3B	-2.08	116.76	120.43
16	7	103	BCL	CHA-C4D-ND	2.08	136.83	132.55
23	6	101	H4X	C32-C31-C30	-2.08	117.19	123.20
16	F	103	BCL	OBb-CAB-C3B	-2.07	116.77	120.43
11	C	402	HEM	CBD-CAD-C3D	-2.07	106.81	112.53
24	Z	102	LMT	O4'-C4B-C5B	2.07	114.42	109.32
16	1	102	BCL	CHB-C1B-C2B	-2.07	121.42	127.43
16	U	103	BCL	CHC-C1C-NC	2.07	127.38	124.40
24	Z	102	LMT	C1B-O1B-C4'	2.07	122.88	117.98
16	M	402	BCL	C6-C5-C3	-2.06	108.44	113.47
16	K	105	BCL	CHB-C1B-C2B	-2.06	121.44	127.43
18	L	303	UQ8	C15-C14-C13	-2.06	118.33	123.63
23	K	103	H4X	C10-C9-C7	-2.06	124.79	127.69
24	G	102	LMT	O3B-C3B-C4B	-2.06	105.52	110.38
16	7	103	BCL	CHD-C1D-ND	-2.06	121.91	124.80
16	L	301	BCL	C3B-C4B-NB	2.06	112.48	109.76
16	3	104	BCL	CHB-C1B-C2B	-2.06	121.45	127.43
15	C	408	PGV	O12-P-O11	-2.06	101.30	106.67
16	I	102	BCL	C1C-NC-C4C	-2.06	105.74	106.68
16	1	102	BCL	CED-O2D-CGD	2.06	120.58	115.92
16	9	104	BCL	C4-C3-C2	-2.06	118.34	123.63
17	L	302	BPH	C7-C6-C5	2.06	118.74	113.26
16	L	304	BCL	CHA-C1A-NA	-2.06	121.73	126.39
16	B	103	BCL	CHB-C1B-C2B	-2.06	121.46	127.43
23	K	103	H4X	C34-C33-C35	2.06	118.80	115.23
16	B	103	BCL	OBd-CAD-C3D	-2.05	123.61	128.42
15	Q	101	PGV	O04-C19-C20	-2.05	115.75	123.78
24	Z	102	LMT	O1B-C1B-O5B	2.05	116.09	110.69
23	4	101	H4X	C26-C25-C23	-2.05	120.75	126.36
16	B	103	BCL	CMA-C3A-C2A	-2.05	106.06	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	E	102	LMT	O5B-C5B-C4B	2.05	113.39	109.70
15	K	102	PGV	O14-P-O13	2.05	121.96	112.44
16	Y	102	BCL	CMC-C2C-C3C	-2.05	106.07	113.98
23	4	101	H4X	C26-C27-C28	-2.04	124.41	127.28
23	E	101	H4X	C16-C17-C19	-2.04	115.79	119.01
23	K	103	H4X	C21-C20-C19	-2.04	119.34	123.52
24	0	101	LMT	O5B-C5B-C6B	2.04	111.50	106.44
16	F	105	BCL	CMC-C2C-C3C	-2.04	106.09	113.98
16	J	101	BCL	C2D-C1D-ND	2.04	112.15	110.13
16	O	105	BCL	CHB-C4A-NA	2.04	127.34	124.40
18	L	306	UQ8	C15-C14-C13	-2.04	118.39	123.63
16	1	102	BCL	C2A-C3A-C4A	-2.04	98.57	101.87
24	R	101	LMT	O1B-C1B-C2B	2.04	113.11	108.09
16	O	104	BCL	O2A-CGA-CBA	2.04	118.05	111.83
23	K	103	H4X	C2M-O2-C38	-2.04	104.36	117.25
24	J	102	LMT	O6'-C6'-C5'	2.04	118.27	111.33
11	C	402	HEM	CMB-C2B-C1B	2.04	128.22	125.03
24	0	101	LMT	O1'-C1-C2	2.04	116.28	109.37
16	M	402	BCL	C9-C8-C7	2.03	118.53	111.27
18	L	303	UQ8	O3-C3-C4	-2.03	115.95	123.64
24	2	103	LMT	O1B-C4'-C5'	2.03	114.81	109.48
15	M	406	PGV	C7-C6-C5	2.03	124.64	114.37
16	M	402	BCL	C2D-C1D-ND	2.03	112.14	110.13
16	1	102	BCL	C1-C2-C3	-2.03	122.87	126.20
24	T	102	LMT	O5'-C1'-O1'	-2.03	105.25	110.04
16	M	402	BCL	CHC-C4B-C3B	-2.03	123.66	131.72
23	K	107	H4X	C5-C6-C7	2.03	118.41	113.47
24	V	102	LMT	O1B-C1B-O5B	2.03	116.03	110.69
11	C	404	HEM	O2D-CGD-CBD	2.03	120.41	114.00
16	7	102	BCL	CGD-CBD-CAD	-2.03	104.28	110.85
16	O	104	BCL	C4A-NA-C1A	-2.03	105.75	106.68
16	O	105	BCL	CMC-C2C-C3C	-2.03	106.14	113.98
24	6	102	LMT	O5'-C5'-C4'	2.03	113.91	109.72
11	C	402	HEM	C4A-CHB-C1B	-2.03	121.48	126.25
23	U	104	H4X	C32-C31-C30	-2.02	117.33	123.20
16	I	102	BCL	C3D-C4D-ND	2.02	113.28	109.99
15	1	103	PGV	O03-C19-O04	-2.02	118.57	123.63
24	N	101	LMT	C6B-C5B-C4B	-2.02	108.05	113.02
16	L	304	BCL	C9-C8-C10	2.02	118.48	111.27
23	7	104	H4X	C29-C28-C30	2.02	121.17	118.09
16	O	104	BCL	C1D-CHD-C4C	-2.02	121.75	126.62
16	L	301	BCL	C3D-C4D-ND	2.02	113.27	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	104	BCL	CMB-C2B-C1B	2.02	128.49	125.42
16	1	102	BCL	O1D-CGD-CBD	-2.02	120.54	124.52
16	F	103	BCL	CHC-C1C-NC	2.02	127.31	124.40
16	Q	104	BCL	C3B-C4B-NB	2.02	112.42	109.76
23	V	101	H4X	C15-C14-C12	2.02	130.10	127.28
16	Q	104	BCL	CHD-C1D-ND	-2.01	121.97	124.80
24	G	102	LMT	O4'-C4B-C5B	2.01	114.28	109.32
23	B	101	H4X	C24-C23-C25	2.01	121.16	118.09
24	E	102	LMT	O3B-C3B-C4B	-2.01	105.63	110.38
16	5	103	BCL	OBB-CAB-C3B	-2.01	116.88	120.43
16	M	403	BCL	CHA-C1A-NA	-2.01	121.84	126.39
16	M	403	BCL	C3B-C4B-NB	2.01	112.41	109.76
15	O	102	PGV	O01-C1-O02	-2.01	119.01	123.70
24	B	104	LMT	C1B-C2B-C3B	-2.01	105.79	110.01
16	7	103	BCL	C4D-CHA-C1A	-2.00	118.85	121.24
24	V	102	LMT	O4'-C4B-C5B	2.00	114.26	109.32
24	8	102	LMT	O3B-C3B-C4B	-2.00	105.66	110.38
11	C	401	HEM	C1C-CHC-C4B	-2.00	121.76	126.02
23	V	101	H4X	C31-C30-C28	-2.00	120.87	126.36
16	Y	104	BCL	C4-C3-C2	-2.00	118.48	123.63
24	J	102	LMT	O5'-C1'-C2'	2.00	114.48	110.37
16	F	103	BCL	C3B-C4B-NB	2.00	112.40	109.76
24	B	104	LMT	O5B-C5B-C4B	2.00	113.31	109.70

There are no chirality outliers.

All (1300) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	401	HEM	C2B-C3B-CAB-CBB
11	C	401	HEM	C4B-C3B-CAB-CBB
11	C	402	HEM	C2C-C3C-CAC-CBC
11	C	402	HEM	C4C-C3C-CAC-CBC
11	C	404	HEM	C2B-C3B-CAB-CBB
14	C	407	DGA	CA2-CA1-OG1-CG1
14	C	407	DGA	OA1-CA1-OG1-CG1
14	C	407	DGA	CB2-CB1-OG2-CG2
14	C	407	DGA	CG1-CG2-OG2-CB1
15	C	408	PGV	C03-O11-P-O12
15	C	408	PGV	C03-O11-P-O14
15	C	408	PGV	C01-C02-C03-O11
15	C	408	PGV	C2-C1-O01-C02
15	L	305	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
15	L	305	PGV	C03-O11-P-O14
15	M	406	PGV	C03-O11-P-O12
15	M	406	PGV	C03-O11-P-O13
15	M	406	PGV	C04-O12-P-O11
15	M	406	PGV	C04-O12-P-O13
15	M	406	PGV	C04-O12-P-O14
15	H	301	PGV	C03-O11-P-O14
15	H	301	PGV	C04-O12-P-O11
15	H	301	PGV	C04-O12-P-O13
15	H	301	PGV	C04-O12-P-O14
15	H	301	PGV	O12-C04-C05-C06
15	H	301	PGV	O12-C04-C05-O05
15	F	101	PGV	C03-O11-P-O12
15	F	104	PGV	C03-O11-P-O12
15	F	104	PGV	C03-O11-P-O14
15	F	104	PGV	C05-C04-O12-P
15	F	104	PGV	O02-C1-O01-C02
15	I	103	PGV	C03-O11-P-O14
15	K	101	PGV	O12-C04-C05-C06
15	K	101	PGV	O02-C1-O01-C02
15	K	102	PGV	C03-O11-P-O12
15	K	102	PGV	C03-O11-P-O13
15	K	102	PGV	O01-C02-C03-O11
15	K	106	PGV	C03-O11-P-O12
15	O	102	PGV	C03-O11-P-O12
15	O	102	PGV	C03-O11-P-O13
15	O	102	PGV	C04-O12-P-O11
15	O	102	PGV	C04-O12-P-O14
15	Q	101	PGV	C03-O11-P-O12
15	Q	101	PGV	C03-O11-P-O13
15	Q	101	PGV	C03-O11-P-O14
15	Q	101	PGV	C04-O12-P-O11
15	Q	101	PGV	O03-C01-C02-O01
15	Q	101	PGV	C04-C05-C06-O06
15	Y	105	PGV	O02-C1-O01-C02
15	Y	105	PGV	C2-C1-O01-C02
15	1	103	PGV	C03-O11-P-O12
15	1	103	PGV	C03-O11-P-O14
15	5	101	PGV	C03-O11-P-O14
15	9	101	PGV	C03-O11-P-O12
15	9	101	PGV	C03-O11-P-O14
15	9	101	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
15	9	101	PGV	C04-O12-P-O13
15	9	101	PGV	C04-O12-P-O14
15	9	101	PGV	O01-C02-C03-O11
15	9	101	PGV	O12-C04-C05-O05
16	L	304	BCL	C11-C10-C8-C9
16	M	402	BCL	C6-C7-C8-C9
16	M	403	BCL	CAD-CBD-CGD-O1D
16	M	403	BCL	CAD-CBD-CGD-O2D
16	B	103	BCL	C1A-C2A-CAA-CBA
16	F	105	BCL	C1A-C2A-CAA-CBA
16	J	101	BCL	C1A-C2A-CAA-CBA
16	K	105	BCL	C2-C3-C5-C6
16	K	105	BCL	C4-C3-C5-C6
16	K	108	BCL	C1A-C2A-CAA-CBA
16	O	105	BCL	C1A-C2A-CAA-CBA
16	Q	103	BCL	C11-C10-C8-C7
16	T	101	BCL	C1A-C2A-CAA-CBA
16	2	102	BCL	C1A-C2A-CAA-CBA
16	3	104	BCL	C1A-C2A-CAA-CBA
16	5	103	BCL	C2C-C3C-CAC-CBC
16	5	104	BCL	C1A-C2A-CAA-CBA
16	9	104	BCL	C1A-C2A-CAA-CBA
17	L	302	BPH	C4C-C3C-CAC-CBC
17	M	404	BPH	C1-C2-C3-C4
17	M	404	BPH	C1-C2-C3-C5
18	L	303	UQ8	C15-C14-C16-C17
22	H	302	CDL	CA2-OA2-PA1-OA4
22	H	302	CDL	CA2-OA2-PA1-OA5
22	H	302	CDL	CA3-OA5-PA1-OA2
22	H	302	CDL	CA3-OA5-PA1-OA3
22	H	302	CDL	CB2-OB2-PB2-OB3
22	H	302	CDL	CB3-OB5-PB2-OB2
22	H	302	CDL	CB3-OB5-PB2-OB3
22	S	101	CDL	CA2-C1-CB2-OB2
22	S	101	CDL	CA2-OA2-PA1-OA4
22	S	101	CDL	CA2-OA2-PA1-OA5
22	S	101	CDL	CB2-OB2-PB2-OB3
22	S	101	CDL	CB2-OB2-PB2-OB4
22	S	101	CDL	CB2-OB2-PB2-OB5
22	Y	103	CDL	CA3-OA5-PA1-OA3
22	Y	103	CDL	CB3-OB5-PB2-OB2
22	Y	103	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
22	Y	103	CDL	CB3-OB5-PB2-OB4
22	Y	103	CDL	OB5-CB3-CB4-OB6
23	B	101	H4X	C36-C37-C38-O2
23	B	101	H4X	C36-C37-C38-C39
23	B	101	H4X	C36-C37-C38-C40
23	E	101	H4X	C4-C1-O1-C1M
23	G	101	H4X	C29-C28-C30-C31
23	G	101	H4X	C27-C28-C30-C31
23	G	101	H4X	C2-C1-O1-C1M
23	K	103	H4X	C37-C38-O2-C2M
23	K	103	H4X	C36-C37-C38-O2
23	K	103	H4X	C36-C37-C38-C39
23	K	103	H4X	C36-C37-C38-C40
23	K	103	H4X	C3-C1-C4-C5
23	K	103	H4X	O1-C1-C4-C5
23	K	107	H4X	C27-C28-C30-C31
23	K	107	H4X	C3-C1-C4-C5
23	K	107	H4X	C2-C1-C4-C5
23	K	107	H4X	O1-C1-C4-C5
23	K	107	H4X	C2-C1-O1-C1M
23	O	101	H4X	C36-C37-C38-C39
23	O	101	H4X	C15-C16-C17-C19
23	O	101	H4X	C15-C16-C17-C18
23	O	101	H4X	C3-C1-C4-C5
23	O	101	H4X	C2-C1-C4-C5
23	O	101	H4X	O1-C1-C4-C5
23	O	106	H4X	C15-C16-C17-C19
23	O	106	H4X	C4-C1-O1-C1M
23	P	101	H4X	C3-C1-C4-C5
23	P	101	H4X	C2-C1-C4-C5
23	P	101	H4X	O1-C1-C4-C5
23	Q	105	H4X	C40-C38-O2-C2M
23	Q	105	H4X	C36-C37-C38-O2
23	Q	105	H4X	C36-C37-C38-C40
23	Q	105	H4X	C27-C28-C30-C31
23	U	104	H4X	C27-C28-C30-C31
23	V	101	H4X	C36-C37-C38-C39
23	V	101	H4X	C36-C37-C38-C40
23	V	101	H4X	C27-C28-C30-C31
23	V	101	H4X	C4-C1-O1-C1M
23	Z	101	H4X	C27-C28-C30-C31
23	2	101	H4X	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
23	2	101	H4X	C27-C28-C30-C31
23	2	101	H4X	C3-C1-C4-C5
23	2	101	H4X	C2-C1-C4-C5
23	4	101	H4X	C15-C16-C17-C19
23	4	101	H4X	C15-C16-C17-C18
23	4	101	H4X	C3-C1-C4-C5
23	4	101	H4X	C2-C1-C4-C5
23	5	105	H4X	C3-C1-C4-C5
23	5	105	H4X	O1-C1-C4-C5
23	5	105	H4X	C4-C1-O1-C1M
23	5	105	H4X	C3-C1-O1-C1M
23	6	101	H4X	C27-C28-C30-C31
23	7	104	H4X	C27-C28-C30-C31
23	7	104	H4X	C3-C1-C4-C5
24	E	102	LMT	O5'-C1'-O1'-C1
24	G	102	LMT	O5'-C1'-O1'-C1
24	J	102	LMT	O5'-C1'-O1'-C1
24	N	101	LMT	O5'-C1'-O1'-C1
24	R	101	LMT	O5'-C1'-O1'-C1
24	2	103	LMT	O5'-C1'-O1'-C1
24	4	102	LMT	O5'-C1'-O1'-C1
24	6	102	LMT	O5'-C1'-O1'-C1
24	0	101	LMT	O5'-C1'-O1'-C1
24	E	102	LMT	O5B-C1B-O1B-C4'
24	G	102	LMT	O5B-C1B-O1B-C4'
24	R	101	LMT	O5B-C1B-O1B-C4'
24	V	102	LMT	O5B-C1B-O1B-C4'
24	B	104	LMT	O5B-C1B-O1B-C4'
24	J	102	LMT	O5B-C1B-O1B-C4'
24	N	101	LMT	O5B-C1B-O1B-C4'
24	P	102	LMT	O5B-C1B-O1B-C4'
24	T	102	LMT	O5B-C1B-O1B-C4'
24	X	102	LMT	O5B-C1B-O1B-C4'
24	2	103	LMT	O5B-C1B-O1B-C4'
24	4	102	LMT	O5B-C1B-O1B-C4'
24	8	102	LMT	O5B-C1B-O1B-C4'
24	0	101	LMT	O5B-C1B-O1B-C4'
24	Z	102	LMT	O5B-C1B-O1B-C4'
24	6	102	LMT	O5B-C1B-O1B-C4'
16	A	102	BCL	C5-C6-C7-C8
14	C	407	DGA	OB1-CB1-OG2-CG2
15	C	408	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
16	O	105	BCL	C3-C5-C6-C7
16	Q	104	BCL	C3-C5-C6-C7
16	U	103	BCL	C3-C5-C6-C7
16	7	103	BCL	C3-C5-C6-C7
16	9	104	BCL	C3-C5-C6-C7
17	L	302	BPH	C3-C5-C6-C7
15	F	104	PGV	C2-C1-O01-C02
15	K	101	PGV	C2-C1-O01-C02
16	A	102	BCL	C4-C3-C5-C6
16	O	104	BCL	C4-C3-C5-C6
16	U	102	BCL	C4-C3-C5-C6
18	L	306	UQ8	C20-C19-C21-C22
18	L	306	UQ8	C12-C11-C9-C10
23	O	101	H4X	C5-C6-C7-C8
23	4	101	H4X	C5-C6-C7-C8
16	A	102	BCL	C2-C3-C5-C6
16	O	104	BCL	C2-C3-C5-C6
18	L	303	UQ8	C13-C14-C16-C17
23	O	101	H4X	C5-C6-C7-C9
16	K	108	BCL	C3-C5-C6-C7
21	M	405	MQ8	C41-C42-C43-C45
21	M	405	MQ8	C41-C42-C43-C44
16	Q	103	BCL	O1A-CGA-O2A-C1
16	A	102	BCL	C3-C5-C6-C7
16	U	102	BCL	C3-C5-C6-C7
15	5	101	PGV	O12-C04-C05-O05
22	H	302	CDL	O1-C1-CA2-OA2
15	F	104	PGV	C20-C19-O03-C01
16	Q	103	BCL	CBA-CGA-O2A-C1
15	K	106	PGV	C2-C1-O01-C02
24	B	102	LMT	O5B-C5B-C6B-O6B
16	X	101	BCL	C3-C5-C6-C7
16	Y	104	BCL	C3-C5-C6-C7
16	9	103	BCL	CBD-CGD-O2D-CED
24	R	101	LMT	O5'-C5'-C6'-O6'
24	T	102	LMT	O5'-C5'-C6'-O6'
24	X	102	LMT	O5'-C5'-C6'-O6'
16	M	402	BCL	C4-C3-C5-C6
17	M	404	BPH	C4-C3-C5-C6
21	M	405	MQ8	C29-C28-C30-C31
23	5	105	H4X	C5-C6-C7-C8
16	M	402	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	U	102	BCL	C2-C3-C5-C6
17	M	404	BPH	C2-C3-C5-C6
18	L	306	UQ8	C18-C19-C21-C22
18	L	306	UQ8	C12-C11-C9-C8
21	M	405	MQ8	C27-C28-C30-C31
23	4	101	H4X	C5-C6-C7-C9
15	K	106	PGV	O02-C1-O01-C02
24	4	102	LMT	O5'-C5'-C6'-O6'
18	L	303	UQ8	C19-C21-C22-C23
18	L	303	UQ8	C14-C16-C17-C18
18	L	306	UQ8	C14-C16-C17-C18
21	M	405	MQ8	C28-C30-C31-C32
21	M	405	MQ8	C33-C35-C36-C37
21	M	405	MQ8	C38-C40-C41-C42
21	M	405	MQ8	C43-C44-C46-C47
24	8	101	LMT	C4'-C5'-C6'-O6'
24	G	102	LMT	O5B-C5B-C6B-O6B
24	2	103	LMT	O5B-C5B-C6B-O6B
24	4	102	LMT	O5B-C5B-C6B-O6B
24	8	101	LMT	O5B-C5B-C6B-O6B
11	C	402	HEM	C3D-CAD-CBD-CGD
24	B	104	LMT	O5'-C1'-O1'-C1
24	T	102	LMT	O5'-C1'-O1'-C1
24	X	102	LMT	O5'-C1'-O1'-C1
24	Z	102	LMT	O5'-C1'-O1'-C1
16	9	103	BCL	CBA-CGA-O2A-C1
23	K	107	H4X	C1-C4-C5-C6
23	O	101	H4X	C1-C4-C5-C6
23	4	101	H4X	C1-C4-C5-C6
16	A	102	BCL	CBD-CGD-O2D-CED
16	F	103	BCL	CBD-CGD-O2D-CED
16	K	105	BCL	CBD-CGD-O2D-CED
17	M	404	BPH	CBD-CGD-O2D-CED
24	J	102	LMT	O5B-C5B-C6B-O6B
24	N	101	LMT	O5'-C5'-C6'-O6'
24	2	103	LMT	O5'-C5'-C6'-O6'
15	F	104	PGV	O04-C19-O03-C01
16	I	102	BCL	CBD-CGD-O2D-CED
16	U	102	BCL	CBD-CGD-O2D-CED
16	B	103	BCL	C3-C5-C6-C7
24	V	102	LMT	O5'-C5'-C6'-O6'
15	A	101	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
15	3	101	PGV	O12-C04-C05-C06
15	9	101	PGV	O12-C04-C05-C06
22	H	302	CDL	CB2-C1-CA2-OA2
15	Q	101	PGV	C20-C19-O03-C01
15	3	101	PGV	C20-C19-O03-C01
24	G	102	LMT	O5'-C5'-C6'-O6'
24	8	102	LMT	O5'-C5'-C6'-O6'
24	6	102	LMT	O5'-C5'-C6'-O6'
16	M	403	BCL	C11-C10-C8-C9
16	M	403	BCL	C11-C12-C13-C14
16	B	103	BCL	C11-C10-C8-C9
16	D	104	BCL	C11-C10-C8-C9
16	F	105	BCL	C11-C10-C8-C9
16	J	101	BCL	C11-C10-C8-C9
16	K	108	BCL	C11-C10-C8-C9
16	T	101	BCL	C11-C10-C8-C9
16	U	102	BCL	C6-C7-C8-C9
16	U	103	BCL	C11-C10-C8-C9
16	X	101	BCL	C11-C10-C8-C9
16	Y	104	BCL	C11-C10-C8-C9
16	2	102	BCL	C11-C10-C8-C9
16	3	103	BCL	C6-C7-C8-C9
16	3	104	BCL	C11-C10-C8-C9
16	5	104	BCL	C11-C10-C8-C9
16	7	103	BCL	C11-C10-C8-C9
16	9	103	BCL	C11-C10-C8-C9
16	9	104	BCL	C11-C10-C8-C9
17	L	302	BPH	C6-C7-C8-C9
17	L	302	BPH	C11-C10-C8-C9
17	M	404	BPH	C11-C12-C13-C14
17	M	404	BPH	C14-C13-C15-C16
22	Y	103	CDL	CB3-CB4-CB6-OB8
24	0	101	LMT	O5'-C5'-C6'-O6'
24	4	102	LMT	C4'-C5'-C6'-O6'
14	C	407	DGA	CA1-CA2-CA3-CA4
15	K	101	PGV	O12-C04-C05-O05
22	S	101	CDL	O1-C1-CB2-OB2
24	J	102	LMT	O5'-C5'-C6'-O6'
15	9	101	PGV	C29-C30-C31-C32
23	O	106	H4X	C15-C16-C17-C18
23	Q	105	H4X	C29-C28-C30-C31
23	U	104	H4X	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
23	U	104	H4X	C15-C16-C17-C18
23	V	101	H4X	C29-C28-C30-C31
23	Z	101	H4X	C29-C28-C30-C31
23	6	101	H4X	C29-C28-C30-C31
23	7	104	H4X	C29-C28-C30-C31
24	E	102	LMT	O5B-C5B-C6B-O6B
24	8	101	LMT	O5'-C5'-C6'-O6'
24	G	102	LMT	C4'-C5'-C6'-O6'
22	Y	103	CDL	OB6-CB4-CB6-OB8
24	R	101	LMT	O5B-C5B-C6B-O6B
24	V	102	LMT	C4'-C5'-C6'-O6'
16	M	402	BCL	C8-C10-C11-C12
24	X	102	LMT	C4'-C5'-C6'-O6'
16	Q	103	BCL	C8-C10-C11-C12
16	5	104	BCL	C15-C16-C17-C18
16	9	104	BCL	C15-C16-C17-C18
17	L	302	BPH	C10-C11-C12-C13
24	Z	102	LMT	O5B-C5B-C6B-O6B
24	Z	102	LMT	O5'-C5'-C6'-O6'
16	K	105	BCL	C3-C5-C6-C7
24	2	103	LMT	C4'-C5'-C6'-O6'
15	M	406	PGV	C1-C2-C3-C4
24	R	101	LMT	C4'-C5'-C6'-O6'
16	B	103	BCL	C11-C12-C13-C15
16	D	103	BCL	C11-C10-C8-C7
16	D	104	BCL	C11-C12-C13-C15
16	F	103	BCL	C11-C10-C8-C7
16	I	102	BCL	C11-C10-C8-C7
16	J	101	BCL	C11-C12-C13-C15
16	K	105	BCL	C11-C10-C8-C7
16	K	108	BCL	C11-C12-C13-C15
16	T	101	BCL	C11-C12-C13-C15
16	W	102	BCL	C11-C10-C8-C7
16	Y	102	BCL	C11-C10-C8-C7
16	Y	104	BCL	C11-C12-C13-C15
16	1	102	BCL	C11-C10-C8-C7
16	3	103	BCL	C11-C10-C8-C7
16	3	104	BCL	C11-C12-C13-C15
16	7	102	BCL	C11-C10-C8-C7
16	7	103	BCL	C11-C12-C13-C15
16	M	402	BCL	CBA-CGA-O2A-C1
24	P	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
24	V	102	LMT	O5B-C5B-C6B-O6B
16	2	102	BCL	C15-C16-C17-C18
15	O	102	PGV	C1-C2-C3-C4
22	H	302	CDL	CB7-C71-C72-C73
18	L	306	UQ8	C9-C11-C12-C13
24	J	102	LMT	C4'-C5'-C6'-O6'
24	N	101	LMT	C4'-C5'-C6'-O6'
24	T	102	LMT	C4'-C5'-C6'-O6'
24	8	102	LMT	C4'-C5'-C6'-O6'
17	M	404	BPH	C3-C5-C6-C7
24	B	102	LMT	O5'-C5'-C6'-O6'
24	6	102	LMT	O5B-C5B-C6B-O6B
15	K	101	PGV	C19-C20-C21-C22
15	1	103	PGV	C19-C20-C21-C22
15	3	101	PGV	C1-C2-C3-C4
15	Q	101	PGV	O04-C19-O03-C01
16	L	304	BCL	C13-C15-C16-C17
16	B	103	BCL	C15-C16-C17-C18
16	D	104	BCL	C15-C16-C17-C18
16	K	108	BCL	C15-C16-C17-C18
16	U	103	BCL	C15-C16-C17-C18
16	X	101	BCL	C15-C16-C17-C18
16	1	102	BCL	C10-C11-C12-C13
16	7	103	BCL	C15-C16-C17-C18
17	L	302	BPH	C13-C15-C16-C17
17	M	404	BPH	C8-C10-C11-C12
16	M	402	BCL	C2A-CAA-CBA-CGA
16	I	102	BCL	C10-C11-C12-C13
16	K	105	BCL	C13-C15-C16-C17
16	O	104	BCL	C15-C16-C17-C18
16	Q	104	BCL	C15-C16-C17-C18
16	T	101	BCL	C15-C16-C17-C18
15	K	106	PGV	C19-C20-C21-C22
15	3	101	PGV	O04-C19-O03-C01
16	9	103	BCL	O1A-CGA-O2A-C1
14	C	407	DGA	CB2-CB3-CB4-CB5
16	F	105	BCL	C15-C16-C17-C18
16	Y	104	BCL	C15-C16-C17-C18
16	1	102	BCL	C8-C10-C11-C12
16	3	104	BCL	C15-C16-C17-C18
15	3	101	PGV	O12-C04-C05-O05
23	2	101	H4X	C1-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
15	M	406	PGV	C19-C20-C21-C22
24	6	102	LMT	C2B-C1B-O1B-C4'
16	J	101	BCL	C15-C16-C17-C18
24	B	104	LMT	O5'-C5'-C6'-O6'
19	L	307	8K6	C12-C13-C14-C15
24	4	102	LMT	C9-C10-C11-C12
24	E	102	LMT	O5'-C5'-C6'-O6'
15	I	103	PGV	C19-C20-C21-C22
16	M	403	BCL	C15-C16-C17-C18
16	7	102	BCL	C8-C10-C11-C12
15	M	406	PGV	C2-C1-O01-C02
24	Z	102	LMT	C2B-C1B-O1B-C4'
15	F	101	PGV	C1-C2-C3-C4
16	J	101	BCL	C3-C5-C6-C7
23	O	101	H4X	C30-C31-C32-C33
15	M	406	PGV	O02-C1-O01-C02
15	5	101	PGV	O12-C04-C05-C06
22	Y	103	CDL	OB5-CB3-CB4-CB6
16	F	103	BCL	C8-C10-C11-C12
16	F	103	BCL	C10-C11-C12-C13
17	L	302	BPH	C5-C6-C7-C8
16	3	103	BCL	C8-C10-C11-C12
17	M	404	BPH	C13-C15-C16-C17
24	B	104	LMT	C4'-C5'-C6'-O6'
24	6	102	LMT	C4'-C5'-C6'-O6'
16	M	402	BCL	C15-C16-C17-C18
16	F	103	BCL	C15-C16-C17-C18
16	Q	103	BCL	C10-C11-C12-C13
16	F	103	BCL	C13-C15-C16-C17
23	V	101	H4X	C33-C35-C36-C37
16	O	105	BCL	C14-C13-C15-C16
24	B	102	LMT	C5'-C4'-O1B-C1B
22	S	101	CDL	CA7-C31-C32-C33
16	7	103	BCL	CBA-CGA-O2A-C1
16	M	402	BCL	O1A-CGA-O2A-C1
24	Z	102	LMT	C4'-C5'-C6'-O6'
24	0	101	LMT	C4'-C5'-C6'-O6'
16	W	102	BCL	C10-C11-C12-C13
16	7	102	BCL	C10-C11-C12-C13
23	K	107	H4X	C29-C28-C30-C31
23	U	104	H4X	C15-C16-C17-C19
15	A	101	PGV	C04-C05-C06-O06

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Mol	Chain	Res	Type	Atoms
15	9	101	PGV	C04-C05-C06-O06
17	L	302	BPH	O2A-C1-C2-C3
16	A	102	BCL	C16-C17-C18-C19
16	3	103	BCL	C16-C17-C18-C19
15	M	406	PGV	C21-C22-C23-C24
15	K	106	PGV	C6-C7-C8-C9
16	F	105	BCL	C3-C5-C6-C7
16	T	101	BCL	C3-C5-C6-C7
24	4	102	LMT	C2B-C1B-O1B-C4'
16	J	101	BCL	C10-C11-C12-C13
24	B	102	LMT	C1-C2-C3-C4
24	G	102	LMT	C1-C2-C3-C4
24	J	102	LMT	C1-C2-C3-C4
24	6	102	LMT	C1-C2-C3-C4
24	P	102	LMT	O5'-C1'-O1'-C1
24	8	102	LMT	O5'-C1'-O1'-C1
24	2	103	LMT	C2B-C1B-O1B-C4'
16	5	103	BCL	C8-C10-C11-C12
16	Y	104	BCL	CBA-CGA-O2A-C1
15	Q	101	PGV	C19-C20-C21-C22
24	N	101	LMT	O5B-C5B-C6B-O6B
24	T	102	LMT	O5B-C5B-C6B-O6B
16	A	102	BCL	C16-C17-C18-C20
16	K	105	BCL	C16-C17-C18-C20
16	Q	103	BCL	C16-C17-C18-C19
16	1	102	BCL	C16-C17-C18-C20
16	9	103	BCL	C16-C17-C18-C20
24	G	102	LMT	C2B-C1B-O1B-C4'
24	B	104	LMT	C1-C2-C3-C4
15	M	406	PGV	C3-C4-C5-C6
15	F	104	PGV	C3-C4-C5-C6
15	I	103	PGV	C24-C25-C26-C27
24	2	103	LMT	C1-C2-C3-C4
15	5	101	PGV	C7-C8-C9-C10
19	L	307	8K6	C4-C5-C6-C7
15	Q	101	PGV	O05-C05-C06-O06
15	I	103	PGV	C26-C27-C28-C29
15	3	101	PGV	C19-C20-C21-C22
24	V	102	LMT	C1-C2-C3-C4
15	I	103	PGV	C22-C23-C24-C25
19	L	307	8K6	C7-C8-C9-C10
16	K	105	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	1	102	BCL	C16-C17-C18-C19
16	F	103	BCL	O1D-CGD-O2D-CED
17	M	404	BPH	O1D-CGD-O2D-CED
16	7	103	BCL	O1A-CGA-O2A-C1
16	Q	103	BCL	C5-C6-C7-C8
24	Z	102	LMT	C1-C2-C3-C4
16	K	105	BCL	O1D-CGD-O2D-CED
16	F	105	BCL	C11-C12-C13-C15
16	O	105	BCL	C11-C12-C13-C15
16	U	103	BCL	C11-C12-C13-C15
16	X	101	BCL	C11-C12-C13-C15
16	9	104	BCL	C11-C12-C13-C15
14	C	407	DGA	CA7-CA8-CA9-CAA
16	S	103	BCL	C5-C6-C7-C8
15	M	406	PGV	C4-C5-C6-C7
15	F	101	PGV	C3-C4-C5-C6
19	L	307	8K6	C10-C11-C12-C13
16	B	103	BCL	C3A-C2A-CAA-CBA
16	D	104	BCL	C3A-C2A-CAA-CBA
16	F	105	BCL	C3A-C2A-CAA-CBA
16	J	101	BCL	C3A-C2A-CAA-CBA
16	K	108	BCL	C3A-C2A-CAA-CBA
16	O	105	BCL	C3A-C2A-CAA-CBA
16	Q	103	BCL	C3A-C2A-CAA-CBA
16	Q	104	BCL	C3A-C2A-CAA-CBA
16	T	101	BCL	C3A-C2A-CAA-CBA
16	U	102	BCL	C3A-C2A-CAA-CBA
16	U	103	BCL	C3A-C2A-CAA-CBA
16	X	101	BCL	C3A-C2A-CAA-CBA
16	Y	104	BCL	C3A-C2A-CAA-CBA
16	2	102	BCL	C3A-C2A-CAA-CBA
16	3	104	BCL	C3A-C2A-CAA-CBA
16	5	104	BCL	C3A-C2A-CAA-CBA
16	7	103	BCL	C3A-C2A-CAA-CBA
16	9	103	BCL	C3A-C2A-CAA-CBA
16	9	104	BCL	C3A-C2A-CAA-CBA
15	M	406	PGV	C6-C7-C8-C9
24	4	102	LMT	C1-C2-C3-C4
24	V	102	LMT	C2B-C1B-O1B-C4'
16	O	105	BCL	C15-C16-C17-C18
16	Y	102	BCL	C13-C15-C16-C17
16	Y	104	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	B	103	BCL	CBA-CGA-O2A-C1
15	K	106	PGV	O03-C01-C02-C03
15	9	101	PGV	C30-C31-C32-C33
16	5	104	BCL	C3-C5-C6-C7
15	Q	101	PGV	C1-C2-C3-C4
15	F	104	PGV	C25-C26-C27-C28
15	I	103	PGV	C27-C28-C29-C30
15	Q	101	PGV	C23-C24-C25-C26
24	B	104	LMT	C2-C3-C4-C5
22	S	101	CDL	C73-C74-C75-C76
15	O	102	PGV	C4-C5-C6-C7
15	D	101	PGV	C28-C29-C30-C31
15	F	104	PGV	C5-C6-C7-C8
24	P	102	LMT	C4'-C5'-C6'-O6'
16	X	101	BCL	CBA-CGA-O2A-C1
16	L	304	BCL	C10-C11-C12-C13
16	K	108	BCL	C10-C11-C12-C13
15	K	101	PGV	C22-C23-C24-C25
15	5	101	PGV	C23-C24-C25-C26
24	T	102	LMT	C1-C2-C3-C4
22	H	302	CDL	C12-C13-C14-C15
15	O	102	PGV	C24-C25-C26-C27
19	5	106	8K6	C6-C7-C8-C9
24	0	101	LMT	C2B-C1B-O1B-C4'
16	F	103	BCL	C16-C17-C18-C19
15	3	101	PGV	C29-C30-C31-C32
24	B	102	LMT	C3'-C4'-O1B-C1B
22	S	101	CDL	C15-C16-C17-C18
16	D	104	BCL	C10-C11-C12-C13
24	J	102	LMT	C2B-C1B-O1B-C4'
24	N	101	LMT	C2B-C1B-O1B-C4'
19	L	307	8K6	C11-C12-C13-C14
16	K	108	BCL	C5-C6-C7-C8
16	Q	103	BCL	C15-C16-C17-C18
15	Q	101	PGV	C22-C23-C24-C25
15	3	101	PGV	C11-C12-C13-C14
15	9	101	PGV	C11-C12-C13-C14
22	H	302	CDL	C11-C12-C13-C14
22	S	101	CDL	C18-C19-C20-C21
23	G	101	H4X	C33-C35-C36-C37
24	6	102	LMT	C9-C10-C11-C12
24	0	101	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
16	3	103	BCL	C16-C17-C18-C20
15	I	103	PGV	C2-C1-O01-C02
15	5	101	PGV	C2-C1-O01-C02
22	H	302	CDL	C51-CB5-OB6-CB4
22	S	101	CDL	C11-CA5-OA6-CA4
24	B	104	LMT	C9-C10-C11-C12
15	Q	101	PGV	C2-C3-C4-C5
24	N	101	LMT	C9-C10-C11-C12
15	9	101	PGV	C25-C26-C27-C28
24	2	103	LMT	C9-C10-C11-C12
23	Q	105	H4X	C10-C11-C12-C13
16	M	402	BCL	C16-C17-C18-C19
16	M	402	BCL	C16-C17-C18-C20
16	9	103	BCL	C16-C17-C18-C19
21	M	405	MQ8	C39-C38-C40-C41
24	Z	102	LMT	C9-C10-C11-C12
24	E	102	LMT	C1-C2-C3-C4
16	B	103	BCL	O1A-CGA-O2A-C1
11	C	401	HEM	C2C-C3C-CAC-CBC
11	C	403	HEM	C2B-C3B-CAB-CBB
23	5	105	H4X	C5-C6-C7-C9
15	L	305	PGV	C29-C30-C31-C32
15	I	103	PGV	C4-C5-C6-C7
16	D	103	BCL	C8-C10-C11-C12
16	Q	104	BCL	C10-C11-C12-C13
15	D	101	PGV	C3-C4-C5-C6
15	5	101	PGV	O02-C1-O01-C02
15	A	101	PGV	O01-C02-C03-O11
22	H	302	CDL	OA5-CA3-CA4-OA6
24	P	102	LMT	O5B-C5B-C6B-O6B
16	O	104	BCL	CBD-CGD-O2D-CED
15	O	102	PGV	C2-C1-O01-C02
16	F	105	BCL	C10-C11-C12-C13
16	Y	102	BCL	C15-C16-C17-C18
16	3	104	BCL	C10-C11-C12-C13
11	C	404	HEM	C4B-C3B-CAB-CBB
15	Q	101	PGV	C21-C22-C23-C24
15	M	406	PGV	C2-C3-C4-C5
15	5	101	PGV	C25-C26-C27-C28
24	T	102	LMT	C2B-C1B-O1B-C4'
16	B	103	BCL	C10-C11-C12-C13
16	9	104	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	0	101	LMT	C2-C3-C4-C5
15	K	106	PGV	O03-C01-C02-O01
24	E	102	LMT	C2B-C1B-O1B-C4'
24	R	101	LMT	C2B-C1B-O1B-C4'
15	K	106	PGV	C25-C26-C27-C28
15	K	106	PGV	C4-C5-C6-C7
15	9	101	PGV	C23-C24-C25-C26
24	T	102	LMT	C2-C3-C4-C5
22	H	302	CDL	C58-C59-C60-C61
17	L	302	BPH	C2C-C3C-CAC-CBC
15	Y	105	PGV	C2-C3-C4-C5
23	O	101	H4X	C4-C5-C6-C7
15	I	103	PGV	O02-C1-O01-C02
22	H	302	CDL	OB7-CB5-OB6-CB4
16	U	103	BCL	C10-C11-C12-C13
16	9	103	BCL	C10-C11-C12-C13
24	8	101	LMT	C7-C8-C9-C10
24	J	102	LMT	C9-C10-C11-C12
16	A	102	BCL	O1D-CGD-O2D-CED
16	Q	104	BCL	O1A-CGA-O2A-C1
16	X	101	BCL	O1A-CGA-O2A-C1
16	3	103	BCL	C3-C5-C6-C7
15	Y	105	PGV	C3-C4-C5-C6
16	D	104	BCL	C1A-C2A-CAA-CBA
16	Q	104	BCL	C1A-C2A-CAA-CBA
16	U	103	BCL	C1A-C2A-CAA-CBA
16	X	101	BCL	C1A-C2A-CAA-CBA
16	Y	104	BCL	C1A-C2A-CAA-CBA
16	7	103	BCL	C1A-C2A-CAA-CBA
16	J	101	BCL	CBA-CGA-O2A-C1
16	K	108	BCL	CBA-CGA-O2A-C1
16	K	105	BCL	C15-C16-C17-C18
24	E	102	LMT	C4'-C5'-C6'-O6'
15	5	101	PGV	C11-C10-C9-C8
22	H	302	CDL	OA5-CA3-CA4-CA6
22	S	101	CDL	C81-C82-C83-C84
16	A	102	BCL	C6-C7-C8-C10
16	D	104	BCL	C11-C10-C8-C7
16	Y	102	BCL	C12-C13-C15-C16
16	2	102	BCL	C11-C10-C8-C7
16	3	103	BCL	C6-C7-C8-C10
16	3	104	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	5	103	BCL	C11-C10-C8-C7
17	L	302	BPH	C6-C7-C8-C10
16	X	101	BCL	C8-C10-C11-C12
24	P	102	LMT	C9-C10-C11-C12
24	8	102	LMT	C9-C10-C11-C12
16	I	102	BCL	C2C-C3C-CAC-CBC
16	Y	104	BCL	C2C-C3C-CAC-CBC
16	O	104	BCL	C10-C11-C12-C13
16	3	103	BCL	C15-C16-C17-C18
24	T	102	LMT	C9-C10-C11-C12
16	A	102	BCL	C6-C7-C8-C9
16	I	102	BCL	C11-C10-C8-C9
16	Q	104	BCL	C11-C10-C8-C9
16	W	102	BCL	C11-C10-C8-C9
16	Y	102	BCL	C14-C13-C15-C16
16	7	102	BCL	C11-C10-C8-C9
22	H	302	CDL	C77-C78-C79-C80
16	D	104	BCL	CBA-CGA-O2A-C1
16	Q	104	BCL	CBA-CGA-O2A-C1
16	9	104	BCL	CBA-CGA-O2A-C1
14	C	407	DGA	CG3-CG2-OG2-CB1
24	X	102	LMT	O5B-C5B-C6B-O6B
15	F	104	PGV	O03-C01-C02-C03
16	L	301	BCL	C3-C5-C6-C7
24	B	102	LMT	C4B-C5B-C6B-O6B
15	F	101	PGV	C4-C5-C6-C7
15	L	305	PGV	C20-C19-O03-C01
22	H	302	CDL	CA7-C31-C32-C33
16	L	304	BCL	C16-C17-C18-C19
16	F	103	BCL	C16-C17-C18-C20
15	M	406	PGV	C7-C8-C9-C10
15	I	103	PGV	C7-C8-C9-C10
15	O	102	PGV	C2-C3-C4-C5
19	L	307	8K6	C11-C10-C9-C8
15	H	301	PGV	C4-C5-C6-C7
16	U	102	BCL	C15-C16-C17-C18
15	Y	105	PGV	C19-C20-C21-C22
24	8	102	LMT	O5B-C5B-C6B-O6B
16	9	104	BCL	O1A-CGA-O2A-C1
21	M	405	MQ8	C37-C38-C40-C41
23	Z	101	H4X	C10-C11-C12-C13
24	B	104	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
16	J	101	BCL	O1A-CGA-O2A-C1
16	3	104	BCL	O1A-CGA-O2A-C1
16	M	402	BCL	C5-C6-C7-C8
15	C	408	PGV	C03-O11-P-O13
15	F	101	PGV	C03-O11-P-O13
15	K	106	PGV	C03-O11-P-O13
15	1	103	PGV	C03-O11-P-O13
16	1	102	BCL	C15-C16-C17-C18
16	U	103	BCL	CBA-CGA-O2A-C1
24	E	102	LMT	C9-C10-C11-C12
16	2	102	BCL	C10-C11-C12-C13
22	S	101	CDL	C72-C73-C74-C75
16	K	108	BCL	O1A-CGA-O2A-C1
15	M	406	PGV	O01-C02-C03-O11
16	D	104	BCL	O1A-CGA-O2A-C1
24	X	102	LMT	C2B-C1B-O1B-C4'
22	S	101	CDL	C74-C75-C76-C77
24	V	102	LMT	C7-C8-C9-C10
16	2	102	BCL	C16-C17-C18-C20
15	L	305	PGV	C5-C6-C7-C8
15	L	305	PGV	C28-C29-C30-C31
15	5	101	PGV	C26-C27-C28-C29
15	L	305	PGV	O03-C01-C02-O01
15	3	101	PGV	O03-C01-C02-O01
22	S	101	CDL	C76-C77-C78-C79
24	B	102	LMT	C4'-C5'-C6'-O6'
24	X	102	LMT	C2-C3-C4-C5
24	R	101	LMT	C1-C2-C3-C4
15	I	103	PGV	C5-C6-C7-C8
16	U	103	BCL	O1A-CGA-O2A-C1
15	K	106	PGV	C3-C4-C5-C6
15	Y	105	PGV	C20-C21-C22-C23
16	F	105	BCL	CBA-CGA-O2A-C1
16	2	102	BCL	CBA-CGA-O2A-C1
15	3	101	PGV	C27-C28-C29-C30
15	3	101	PGV	C28-C29-C30-C31
23	E	101	H4X	C3-C1-O1-C1M
23	G	101	H4X	C3-C1-O1-C1M
23	K	103	H4X	C40-C38-O2-C2M
23	K	107	H4X	C3-C1-O1-C1M
23	O	106	H4X	C2-C1-O1-C1M
23	Q	105	H4X	C39-C38-O2-C2M

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Mol	Chain	Res	Type	Atoms
23	V	101	H4X	C2-C1-O1-C1M
23	Z	101	H4X	C2-C1-O1-C1M
23	2	101	H4X	C2-C1-O1-C1M
23	5	105	H4X	C2-C1-O1-C1M
23	7	104	H4X	C3-C1-O1-C1M
15	H	301	PGV	C24-C25-C26-C27
22	S	101	CDL	C19-C20-C21-C22
16	5	103	BCL	C3-C5-C6-C7
14	C	407	DGA	CB5-CB6-CB7-CB8
14	C	407	DGA	CB3-CB4-CB5-CB6
16	D	103	BCL	C5-C6-C7-C8
16	Y	104	BCL	C10-C11-C12-C13
16	O	104	BCL	O1D-CGD-O2D-CED
17	L	302	BPH	C4-C3-C5-C6
15	Y	105	PGV	C21-C22-C23-C24
16	3	104	BCL	CBA-CGA-O2A-C1
22	H	302	CDL	C55-C56-C57-C58
22	S	101	CDL	OA7-CA5-OA6-CA4
16	M	402	BCL	C11-C10-C8-C9
16	F	103	BCL	C11-C10-C8-C9
16	Q	103	BCL	C11-C10-C8-C9
16	Y	102	BCL	C11-C10-C8-C9
16	9	103	BCL	C11-C12-C13-C14
16	9	103	BCL	C14-C13-C15-C16
19	5	106	8K6	C7-C8-C9-C10
22	S	101	CDL	C77-C78-C79-C80
24	P	102	LMT	C2-C3-C4-C5
24	T	102	LMT	C5-C6-C7-C8
16	I	102	BCL	C8-C10-C11-C12
16	Y	102	BCL	C10-C11-C12-C13
16	9	103	BCL	C5-C6-C7-C8
15	9	101	PGV	C21-C22-C23-C24
24	V	102	LMT	C5-C6-C7-C8
24	6	102	LMT	C5-C6-C7-C8
22	H	302	CDL	C15-C16-C17-C18
15	A	101	PGV	C01-C02-C03-O11
15	9	101	PGV	C01-C02-C03-O11
22	S	101	CDL	OB5-CB3-CB4-CB6
23	E	101	H4X	C3-C1-C4-C5
23	K	103	H4X	C2-C1-C4-C5
23	O	101	H4X	C36-C37-C38-C40
23	5	105	H4X	C2-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
23	6	101	H4X	C3-C1-C4-C5
23	7	104	H4X	C2-C1-C4-C5
15	9	101	PGV	C31-C32-C33-C34
16	M	402	BCL	C6-C7-C8-C10
16	M	402	BCL	C11-C10-C8-C7
16	B	103	BCL	C11-C10-C8-C7
16	Q	103	BCL	C6-C7-C8-C10
16	3	103	BCL	C11-C12-C13-C15
16	9	103	BCL	C6-C7-C8-C10
16	9	103	BCL	C11-C10-C8-C7
16	9	103	BCL	C11-C12-C13-C15
22	S	101	CDL	C11-C12-C13-C14
16	9	103	BCL	O1D-CGD-O2D-CED
24	V	102	LMT	O5'-C1'-O1'-C1
16	2	102	BCL	O1A-CGA-O2A-C1
17	L	302	BPH	C8-C10-C11-C12
23	2	101	H4X	C30-C31-C32-C33
16	D	104	BCL	C3-C5-C6-C7
16	7	103	BCL	C10-C11-C12-C13
23	V	101	H4X	C15-C16-C17-C18
15	D	101	PGV	C26-C27-C28-C29
22	S	101	CDL	C34-C35-C36-C37
15	K	101	PGV	C6-C7-C8-C9
15	L	305	PGV	O03-C01-C02-C03
15	H	301	PGV	O03-C01-C02-C03
15	O	102	PGV	O03-C01-C02-C03
15	3	101	PGV	O03-C01-C02-C03
23	P	101	H4X	C1-C4-C5-C6
24	E	102	LMT	C7-C8-C9-C10
14	C	407	DGA	CB7-CB8-CB9-CAB
15	C	408	PGV	O01-C02-C03-O11
16	I	102	BCL	C16-C17-C18-C20
16	O	104	BCL	C16-C17-C18-C20
22	S	101	CDL	OB5-CB3-CB4-OB6
15	H	301	PGV	C2-C1-O01-C02
24	8	101	LMT	C6-C7-C8-C9
16	I	102	BCL	C13-C15-C16-C17
16	U	102	BCL	C10-C11-C12-C13
22	S	101	CDL	C80-C81-C82-C83
14	C	407	DGA	CBB-CAB-CB9-CB8
15	K	101	PGV	C4-C5-C6-C7
15	D	101	PGV	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
15	F	104	PGV	O03-C01-C02-O01
15	L	305	PGV	O04-C19-O03-C01
15	K	101	PGV	C20-C21-C22-C23
15	Q	101	PGV	C24-C25-C26-C27
17	L	302	BPH	C2-C3-C5-C6
16	Q	103	BCL	C16-C17-C18-C20
24	N	101	LMT	C2-C3-C4-C5
24	E	102	LMT	C5-C6-C7-C8
16	1	102	BCL	C11-C10-C8-C9
16	3	103	BCL	C11-C10-C8-C9
15	L	305	PGV	C4-C5-C6-C7
16	O	104	BCL	C3-C5-C6-C7
23	K	103	H4X	C4-C5-C6-C7
15	F	104	PGV	C20-C21-C22-C23
24	G	102	LMT	C7-C8-C9-C10
16	5	103	BCL	C4C-C3C-CAC-CBC
16	O	104	BCL	C5-C6-C7-C8
19	L	307	8K6	C3-C4-C5-C6
15	F	101	PGV	O04-C19-O03-C01
23	G	101	H4X	C1-C4-C5-C6
16	X	101	BCL	C10-C11-C12-C13
15	F	104	PGV	O12-C04-C05-C06
15	O	102	PGV	C7-C8-C9-C10
24	Z	102	LMT	C2-C3-C4-C5
16	K	105	BCL	CBA-CGA-O2A-C1
22	H	302	CDL	OB5-CB3-CB4-CB6
24	8	101	LMT	C5-C6-C7-C8
23	P	101	H4X	C15-C16-C17-C18
15	M	406	PGV	C22-C23-C24-C25
16	K	105	BCL	C6-C7-C8-C10
16	K	108	BCL	C11-C10-C8-C7
16	9	103	BCL	C12-C13-C15-C16
17	L	302	BPH	C11-C10-C8-C7
17	M	404	BPH	C6-C7-C8-C10
24	0	101	LMT	C7-C8-C9-C10
15	O	102	PGV	C20-C21-C22-C23
16	Q	103	BCL	C3-C5-C6-C7
24	R	101	LMT	C9-C10-C11-C12
15	F	101	PGV	C03-O11-P-O14
15	I	103	PGV	C03-O11-P-O12
15	9	101	PGV	C1-C2-C3-C4
15	O	102	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
15	O	102	PGV	C30-C31-C32-C33
16	F	105	BCL	O1A-CGA-O2A-C1
16	5	104	BCL	O1A-CGA-O2A-C1
11	C	402	HEM	C2B-C3B-CAB-CBB
11	C	404	HEM	C2C-C3C-CAC-CBC
15	K	101	PGV	C23-C24-C25-C26
16	K	105	BCL	O2A-C1-C2-C3
15	O	102	PGV	C25-C26-C27-C28
16	L	304	BCL	C16-C17-C18-C20
15	L	305	PGV	C24-C25-C26-C27
16	5	103	BCL	C15-C16-C17-C18
16	5	104	BCL	C10-C11-C12-C13
16	9	103	BCL	C15-C16-C17-C18
15	F	104	PGV	C24-C25-C26-C27
19	L	307	8K6	C15-C16-C17-C18
15	Q	101	PGV	O03-C01-C02-C03
15	O	102	PGV	C11-C10-C9-C8
16	I	102	BCL	C16-C17-C18-C19
16	5	104	BCL	C16-C17-C18-C20
15	9	101	PGV	C24-C25-C26-C27
15	H	301	PGV	C22-C23-C24-C25
24	8	101	LMT	C4B-C5B-C6B-O6B
16	W	102	BCL	C13-C15-C16-C17
16	7	102	BCL	C5-C6-C7-C8
15	F	101	PGV	C22-C23-C24-C25
15	9	101	PGV	C28-C29-C30-C31
15	M	406	PGV	O03-C01-C02-O01
15	H	301	PGV	O03-C01-C02-O01
15	A	101	PGV	O03-C01-C02-O01
15	O	102	PGV	O03-C01-C02-O01
16	9	103	BCL	C6-C7-C8-C9
14	C	407	DGA	CA6-CA7-CA8-CA9
24	P	102	LMT	C1-C2-C3-C4
15	K	101	PGV	C2-C3-C4-C5
24	B	102	LMT	C2-C3-C4-C5
24	2	103	LMT	C5-C6-C7-C8
16	T	101	BCL	C8-C10-C11-C12
24	E	102	LMT	C2-C3-C4-C5
22	H	302	CDL	CB5-C51-C52-C53
15	L	305	PGV	C2-C3-C4-C5
15	F	101	PGV	C20-C19-O03-C01
19	L	307	8K6	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
15	O	102	PGV	C19-C20-C21-C22
16	O	105	BCL	CBA-CGA-O2A-C1
24	B	104	LMT	C2B-C1B-O1B-C4'
24	8	102	LMT	C2B-C1B-O1B-C4'
16	Y	102	BCL	C16-C17-C18-C20
24	4	102	LMT	C11-C10-C9-C8
15	F	101	PGV	C20-C21-C22-C23
16	Y	102	BCL	C8-C10-C11-C12
16	Q	103	BCL	C1A-C2A-CAA-CBA
16	D	103	BCL	C13-C15-C16-C17
23	4	101	H4X	C27-C28-C30-C31
16	K	105	BCL	O1A-CGA-O2A-C1
16	L	301	BCL	C2A-CAA-CBA-CGA
15	M	406	PGV	C01-C02-C03-O11
15	5	101	PGV	C01-C02-C03-O11
15	K	106	PGV	C27-C28-C29-C30
16	U	102	BCL	C6-C7-C8-C10
16	Y	104	BCL	C11-C10-C8-C7
16	7	102	BCL	C6-C7-C8-C10
17	L	302	BPH	C12-C13-C15-C16
16	5	104	BCL	C16-C17-C18-C19
15	O	102	PGV	C5-C6-C7-C8
15	5	101	PGV	C21-C22-C23-C24
24	Z	102	LMT	C5-C6-C7-C8
16	O	105	BCL	C10-C11-C12-C13
16	3	104	BCL	C8-C10-C11-C12
16	K	105	BCL	C3A-C2A-CAA-CBA
15	H	301	PGV	O02-C1-O01-C02
15	H	301	PGV	O01-C02-C03-O11
15	5	101	PGV	O01-C02-C03-O11
22	H	302	CDL	OB5-CB3-CB4-OB6
16	K	105	BCL	C6-C7-C8-C9
16	3	103	BCL	C11-C12-C13-C14
23	O	101	H4X	C20-C21-C22-C23
16	F	103	BCL	C5-C6-C7-C8
15	5	101	PGV	C14-C15-C16-C17
16	O	105	BCL	O1A-CGA-O2A-C1
24	8	102	LMT	C2-C3-C4-C5
16	5	103	BCL	C10-C11-C12-C13
24	P	102	LMT	C7-C8-C9-C10
15	5	101	PGV	O03-C01-C02-C03
24	J	102	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	U	103	BCL	CAA-CBA-CGA-O2A
24	R	101	LMT	C7-C8-C9-C10
16	9	104	BCL	C5-C6-C7-C8
15	F	104	PGV	C2-C3-C4-C5
24	X	102	LMT	O1'-C1-C2-C3
16	X	101	BCL	CAA-CBA-CGA-O2A
15	M	406	PGV	C03-O11-P-O14
15	D	101	PGV	C03-O11-P-O13
15	F	104	PGV	C03-O11-P-O13
15	K	101	PGV	C04-O12-P-O13
15	K	102	PGV	C04-O12-P-O13
15	O	102	PGV	C03-O11-P-O14
15	Q	101	PGV	C04-O12-P-O13
15	3	101	PGV	C03-O11-P-O13
15	3	101	PGV	C04-O12-P-O13
15	5	101	PGV	C03-O11-P-O12
23	4	101	H4X	C11-C10-C9-C7
16	3	104	BCL	C3-C5-C6-C7
15	3	101	PGV	C21-C22-C23-C24
15	3	101	PGV	C30-C31-C32-C33
16	D	104	BCL	CAA-CBA-CGA-O2A
16	Y	104	BCL	C8-C10-C11-C12
22	Y	103	CDL	CB4-CB3-OB5-PB2
23	O	106	H4X	C24-C23-C25-C26
24	B	102	LMT	C9-C10-C11-C12
16	M	403	BCL	C16-C17-C18-C19
16	O	105	BCL	CAA-CBA-CGA-O2A
16	T	101	BCL	CAA-CBA-CGA-O2A
16	T	101	BCL	O1A-CGA-O2A-C1
16	M	403	BCL	CBD-CGD-O2D-CED
19	5	106	8K6	C5-C6-C7-C8
24	P	102	LMT	C2B-C1B-O1B-C4'
16	5	103	BCL	C16-C17-C18-C19
24	0	101	LMT	C9-C10-C11-C12
15	5	101	PGV	C03-C02-O01-C1
16	B	103	BCL	CAA-CBA-CGA-O2A
16	Y	104	BCL	C16-C17-C18-C20
15	Q	101	PGV	C01-C02-C03-O11
16	7	103	BCL	CAA-CBA-CGA-O2A
16	O	104	BCL	C11-C10-C8-C9
16	Q	103	BCL	C6-C7-C8-C9
16	L	301	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	J	101	BCL	C11-C10-C8-C7
16	5	104	BCL	C11-C12-C13-C15
15	K	101	PGV	C5-C6-C7-C8
17	M	404	BPH	O1A-CGA-O2A-C1
15	K	106	PGV	O01-C02-C03-O11
15	H	301	PGV	O01-C1-C2-C3
16	5	104	BCL	CAA-CBA-CGA-O2A
16	A	102	BCL	C15-C16-C17-C18
16	5	103	BCL	C4-C3-C5-C6
16	J	101	BCL	CAA-CBA-CGA-O2A
16	3	104	BCL	CAA-CBA-CGA-O2A
16	3	104	BCL	C16-C17-C18-C20
16	K	108	BCL	CAA-CBA-CGA-O2A
16	2	102	BCL	CAA-CBA-CGA-O2A
16	9	104	BCL	CAA-CBA-CGA-O2A
16	5	104	BCL	CBA-CGA-O2A-C1
16	K	108	BCL	C16-C17-C18-C20
16	O	104	BCL	C16-C17-C18-C19
15	5	101	PGV	C15-C16-C17-C18
16	Y	104	BCL	CAA-CBA-CGA-O2A
16	3	103	BCL	C13-C15-C16-C17
15	I	103	PGV	C2-C3-C4-C5
16	F	105	BCL	CAA-CBA-CGA-O2A
16	Q	104	BCL	CAA-CBA-CGA-O2A
14	C	407	DGA	CB4-CB5-CB6-CB7
16	3	103	BCL	C10-C11-C12-C13
23	E	101	H4X	C2-C1-O1-C1M
23	K	103	H4X	C39-C38-O2-C2M
23	O	106	H4X	C3-C1-O1-C1M
23	V	101	H4X	C3-C1-O1-C1M
23	2	101	H4X	C3-C1-O1-C1M
23	7	104	H4X	C2-C1-O1-C1M
22	H	302	CDL	C19-C20-C21-C22
23	E	101	H4X	C17-C19-C20-C21
23	Q	105	H4X	C11-C10-C9-C7
19	L	307	8K6	C9-C10-C11-C12
15	F	104	PGV	C19-C20-C21-C22
24	B	102	LMT	C6-C7-C8-C9
15	C	408	PGV	C2-C3-C4-C5
15	A	101	PGV	C1-C2-C3-C4
16	Y	104	BCL	C11-C12-C13-C14
17	M	404	BPH	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	J	102	LMT	C3-C4-C5-C6
24	B	104	LMT	C5-C6-C7-C8
11	C	401	HEM	C2A-CAA-CBA-CGA
16	2	102	BCL	C16-C17-C18-C19
16	Q	103	BCL	C4-C3-C5-C6
16	7	102	BCL	C4-C3-C5-C6
15	F	101	PGV	C21-C22-C23-C24
11	C	404	HEM	C4C-C3C-CAC-CBC
23	5	105	H4X	C36-C37-C38-C40
23	6	101	H4X	C2-C1-C4-C5
16	K	108	BCL	C16-C17-C18-C19
16	O	104	BCL	C11-C10-C8-C7
16	2	102	BCL	C11-C12-C13-C15
16	T	101	BCL	C10-C11-C12-C13
16	7	103	BCL	C8-C10-C11-C12
16	I	102	BCL	O1D-CGD-O2D-CED
15	A	101	PGV	O12-C04-C05-O05
15	D	101	PGV	C27-C28-C29-C30
15	D	101	PGV	C4-C5-C6-C7
16	A	102	BCL	C10-C11-C12-C13
16	K	105	BCL	C8-C10-C11-C12
15	I	103	PGV	O03-C01-C02-O01
15	I	103	PGV	C11-C10-C9-C8
22	S	101	CDL	C79-C80-C81-C82
15	1	103	PGV	C4-C5-C6-C7
16	5	104	BCL	C8-C10-C11-C12
15	D	101	PGV	C2-C3-C4-C5
24	X	102	LMT	C7-C8-C9-C10
16	K	105	BCL	C2-C1-O2A-CGA
16	2	102	BCL	C2-C1-O2A-CGA
16	3	103	BCL	C2-C1-O2A-CGA
23	U	104	H4X	C30-C31-C32-C33
15	L	305	PGV	C23-C24-C25-C26
16	2	102	BCL	C8-C10-C11-C12
24	8	102	LMT	O1'-C1-C2-C3
16	U	102	BCL	C13-C15-C16-C17
23	P	101	H4X	C15-C16-C17-C19
15	F	104	PGV	C6-C7-C8-C9
15	5	101	PGV	C19-C20-C21-C22
15	D	101	PGV	C7-C8-C9-C10
15	Y	105	PGV	C22-C23-C24-C25
24	X	102	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	9	103	BCL	C3-C5-C6-C7
16	D	103	BCL	C11-C10-C8-C9
16	O	105	BCL	C11-C10-C8-C9
16	5	103	BCL	C11-C10-C8-C9
15	5	101	PGV	C13-C14-C15-C16
24	8	102	LMT	C7-C8-C9-C10
22	S	101	CDL	C12-C13-C14-C15
16	M	403	BCL	O1D-CGD-O2D-CED
16	L	301	BCL	CBD-CGD-O2D-CED
16	3	103	BCL	C4-C3-C5-C6
15	Y	105	PGV	C1-C2-C3-C4
15	9	101	PGV	O05-C05-C06-O06
11	C	401	HEM	CAA-CBA-CGA-O2A
11	C	402	HEM	CAD-CBD-CGD-O1D
24	Z	102	LMT	C7-C8-C9-C10
14	C	407	DGA	OG1-CG1-CG2-OG2
16	K	105	BCL	C1A-C2A-CAA-CBA
16	U	102	BCL	C1A-C2A-CAA-CBA
16	9	103	BCL	C1A-C2A-CAA-CBA
16	U	102	BCL	C16-C17-C18-C20
11	C	401	HEM	CAA-CBA-CGA-O1A
14	C	407	DGA	CB9-CAB-CBB-CCB
15	I	103	PGV	C02-C03-O11-P
11	C	404	HEM	CAD-CBD-CGD-O1D
15	D	101	PGV	C23-C24-C25-C26
24	B	104	LMT	C3-C4-C5-C6
24	N	101	LMT	C5-C6-C7-C8
16	L	301	BCL	C12-C13-C15-C16
16	M	403	BCL	C11-C10-C8-C7
16	9	104	BCL	C11-C10-C8-C7
17	M	404	BPH	C11-C12-C13-C15
15	F	104	PGV	C21-C22-C23-C24
16	J	101	BCL	C16-C17-C18-C20
19	L	307	8K6	C6-C7-C8-C9
16	S	103	BCL	C15-C16-C17-C18
23	Q	105	H4X	C15-C16-C17-C18
23	V	101	H4X	C24-C23-C25-C26
23	Z	101	H4X	C15-C16-C17-C18
23	4	101	H4X	C29-C28-C30-C31
24	6	102	LMT	C2-C3-C4-C5
23	O	106	H4X	C34-C33-C35-C36
16	Q	103	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	Q	104	BCL	C5-C6-C7-C8
23	Q	105	H4X	C10-C11-C12-C14
15	D	101	PGV	C20-C21-C22-C23
22	S	101	CDL	C14-C15-C16-C17
16	L	301	BCL	C11-C10-C8-C9
16	A	102	BCL	C11-C10-C8-C9
17	M	404	BPH	C6-C7-C8-C9
15	K	106	PGV	C28-C29-C30-C31
24	G	102	LMT	C3-C4-C5-C6
16	5	103	BCL	C13-C15-C16-C17
23	Z	101	H4X	C5-C6-C7-C8
11	C	403	HEM	CAA-CBA-CGA-O1A
15	K	101	PGV	O04-C19-O03-C01
24	B	102	LMT	O1'-C1-C2-C3
16	X	101	BCL	C16-C17-C18-C20
11	C	404	HEM	CAD-CBD-CGD-O2D
23	O	101	H4X	C36-C37-C38-O2
22	H	302	CDL	C74-C75-C76-C77
16	T	101	BCL	C2A-CAA-CBA-CGA
23	2	101	H4X	C4-C1-O1-C1M
11	C	403	HEM	CAA-CBA-CGA-O2A
16	7	103	BCL	C5-C6-C7-C8
24	E	102	LMT	C2-C1-O1'-C1'
24	8	101	LMT	C2-C1-O1'-C1'
24	B	104	LMT	C4-C5-C6-C7
11	C	402	HEM	CAD-CBD-CGD-O2D
17	L	302	BPH	CHA-CBD-CGD-O1D
17	M	404	BPH	CHA-CBD-CGD-O1D
22	H	302	CDL	C71-C72-C73-C74
16	D	103	BCL	C4-C3-C5-C6
16	W	102	BCL	C4-C3-C5-C6
23	2	101	H4X	C5-C6-C7-C8
22	S	101	CDL	OB6-CB4-CB6-OB8
17	L	302	BPH	C15-C16-C17-C18
16	L	301	BCL	C11-C10-C8-C7
16	L	304	BCL	C6-C7-C8-C10
16	F	105	BCL	C11-C10-C8-C7
16	T	101	BCL	C11-C10-C8-C7
16	X	101	BCL	C11-C10-C8-C7
15	1	103	PGV	C21-C22-C23-C24
24	8	102	LMT	C1-C2-C3-C4
15	3	101	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
15	K	106	PGV	C03-O11-P-O14
16	X	101	BCL	C2A-CAA-CBA-CGA
16	F	105	BCL	C2-C1-O2A-CGA
16	J	101	BCL	C2-C1-O2A-CGA
16	K	108	BCL	C2-C1-O2A-CGA
16	O	105	BCL	C2-C1-O2A-CGA
16	W	102	BCL	C2-C1-O2A-CGA
16	3	104	BCL	C2-C1-O2A-CGA
16	5	104	BCL	C2-C1-O2A-CGA
16	Q	104	BCL	C16-C17-C18-C20
16	U	103	BCL	C5-C6-C7-C8
16	I	102	BCL	C3A-C2A-CAA-CBA
15	Q	101	PGV	C7-C8-C9-C10
16	S	103	BCL	C10-C11-C12-C13
11	C	401	HEM	C4C-C3C-CAC-CBC
11	C	403	HEM	C4B-C3B-CAB-CBB
24	B	102	LMT	C11-C10-C9-C8
22	S	101	CDL	C83-C84-C85-C86
15	C	408	PGV	C3-C4-C5-C6
15	K	101	PGV	C21-C22-C23-C24
15	F	104	PGV	C4-C5-C6-C7
15	3	101	PGV	C26-C27-C28-C29
16	D	104	BCL	C11-C12-C13-C14
16	K	108	BCL	C14-C13-C15-C16
15	3	101	PGV	C9-C10-C11-C12
15	F	101	PGV	O03-C19-C20-C21
15	3	101	PGV	O01-C1-C2-C3
15	1	103	PGV	O02-C1-O01-C02
19	5	106	8K6	C9-C10-C11-C12
15	9	101	PGV	C19-C20-C21-C22
23	K	107	H4X	C15-C16-C17-C19
23	6	101	H4X	C15-C16-C17-C19
16	D	104	BCL	C4-C3-C5-C6
15	I	103	PGV	O03-C19-C20-C21
16	K	108	BCL	C2A-CAA-CBA-CGA
16	2	102	BCL	C2A-CAA-CBA-CGA
16	5	104	BCL	C2A-CAA-CBA-CGA
15	O	102	PGV	C31-C32-C33-C34
16	L	304	BCL	C11-C10-C8-C7
16	A	102	BCL	C11-C10-C8-C7
16	O	104	BCL	C12-C13-C15-C16
16	Q	104	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	Q	104	BCL	C11-C12-C13-C15
16	U	103	BCL	C11-C10-C8-C7
17	M	404	BPH	C12-C13-C15-C16
15	D	101	PGV	O03-C19-C20-C21
18	L	303	UQ8	C5-C4-O4-C4M
16	D	104	BCL	C2-C1-O2A-CGA
16	F	103	BCL	C2-C1-O2A-CGA
16	T	101	BCL	C2-C1-O2A-CGA
16	X	101	BCL	C2-C1-O2A-CGA
16	9	104	BCL	C2-C1-O2A-CGA
15	3	101	PGV	C25-C26-C27-C28
22	H	302	CDL	CA5-C11-C12-C13
15	3	101	PGV	C3-C4-C5-C6
24	P	102	LMT	O1'-C1-C2-C3
15	K	106	PGV	C7-C8-C9-C10
16	Y	104	BCL	C5-C6-C7-C8
23	5	105	H4X	C39-C38-O2-C2M
16	F	105	BCL	C2A-CAA-CBA-CGA
16	O	105	BCL	C2A-CAA-CBA-CGA
16	O	105	BCL	C5-C6-C7-C8
14	C	407	DGA	CA3-CA4-CA5-CA6
16	Y	102	BCL	C16-C17-C18-C19
22	S	101	CDL	C82-C83-C84-C85
15	O	102	PGV	C23-C24-C25-C26
18	L	303	UQ8	C12-C11-C9-C10
23	7	104	H4X	C5-C6-C7-C8
16	5	103	BCL	C2-C3-C5-C6
24	2	103	LMT	C11-C10-C9-C8
15	O	102	PGV	C3-C4-C5-C6
15	1	103	PGV	O01-C1-C2-C3
24	N	101	LMT	C2-C1-O1'-C1'
24	G	102	LMT	C4-C5-C6-C7
16	Y	104	BCL	C14-C13-C15-C16
15	A	101	PGV	O03-C01-C02-C03
16	D	104	BCL	C16-C17-C18-C20
15	F	104	PGV	C02-C01-O03-C19
16	M	403	BCL	C1A-C2A-CAA-CBA
16	I	102	BCL	C1A-C2A-CAA-CBA
15	Q	101	PGV	C6-C7-C8-C9
24	V	102	LMT	C2-C3-C4-C5
16	J	101	BCL	C4-C3-C5-C6
16	X	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	5	104	BCL	C4-C3-C5-C6
23	G	101	H4X	C5-C6-C7-C8
23	V	101	H4X	C15-C16-C17-C19
23	Z	101	H4X	C30-C31-C32-C33
24	G	102	LMT	C2-C3-C4-C5
15	I	103	PGV	C12-C13-C14-C15
24	4	102	LMT	C7-C8-C9-C10
16	3	104	BCL	C16-C17-C18-C19
15	H	301	PGV	C01-C02-C03-O11
14	C	407	DGA	OG1-CA1-CA2-CA3
15	1	103	PGV	O03-C19-C20-C21
22	S	101	CDL	C75-C76-C77-C78
18	L	306	UQ8	C16-C17-C18-C19
16	B	103	BCL	C2-C1-O2A-CGA
16	U	103	BCL	C2-C1-O2A-CGA
16	5	103	BCL	C2-C1-O2A-CGA
16	7	103	BCL	C2-C1-O2A-CGA
16	I	102	BCL	C6-C7-C8-C10
16	5	104	BCL	C11-C10-C8-C7
16	T	101	BCL	CBA-CGA-O2A-C1
24	B	104	LMT	C5'-C4'-O1B-C1B
22	Y	103	CDL	O1-C1-CB2-OB2
16	O	105	BCL	C8-C10-C11-C12
15	K	101	PGV	C25-C26-C27-C28
16	F	103	BCL	C2C-C3C-CAC-CBC
16	K	108	BCL	C2C-C3C-CAC-CBC
16	5	104	BCL	C2C-C3C-CAC-CBC
16	B	103	BCL	C2A-CAA-CBA-CGA
16	D	104	BCL	C2A-CAA-CBA-CGA
16	U	103	BCL	C2A-CAA-CBA-CGA
16	3	104	BCL	C2A-CAA-CBA-CGA
15	M	406	PGV	C02-C03-O11-P
16	M	403	BCL	C3A-C2A-CAA-CBA
16	U	102	BCL	O1A-CGA-O2A-C1
24	2	103	LMT	C3'-C4'-O1B-C1B
24	N	101	LMT	O1'-C1-C2-C3
11	C	404	HEM	CAA-CBA-CGA-O1A
16	K	108	BCL	C11-C12-C13-C14
16	7	102	BCL	C6-C7-C8-C9
15	F	101	PGV	O04-C19-C20-C21
15	3	101	PGV	O02-C1-C2-C3
24	T	102	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	0	101	LMT	C1-C2-C3-C4
16	5	103	BCL	C16-C17-C18-C20
14	C	407	DGA	OA1-CA1-CA2-CA3
15	D	101	PGV	O04-C19-C20-C21
16	3	103	BCL	C2-C3-C5-C6
23	Z	101	H4X	C5-C6-C7-C9
15	I	103	PGV	O04-C19-C20-C21
16	T	101	BCL	C16-C17-C18-C20
16	M	403	BCL	C8-C10-C11-C12
23	Z	101	H4X	C10-C11-C12-C14
15	1	103	PGV	O04-C19-C20-C21
16	U	103	BCL	C8-C10-C11-C12
24	G	102	LMT	C3'-C4'-O1B-C1B
16	3	103	BCL	CAD-CBD-CGD-O2D
15	9	101	PGV	C7-C8-C9-C10
16	Q	104	BCL	C2-C1-O2A-CGA
16	Y	104	BCL	C2-C1-O2A-CGA
16	9	103	BCL	C2-C1-O2A-CGA
15	1	103	PGV	O02-C1-C2-C3
11	C	401	HEM	CAD-CBD-CGD-O1D
15	M	406	PGV	C5-C6-C7-C8
11	C	401	HEM	CAD-CBD-CGD-O2D
16	Y	104	BCL	C16-C17-C18-C19
11	C	402	HEM	CAA-CBA-CGA-O1A
22	S	101	CDL	C12-C11-CA5-OA7
15	K	106	PGV	C22-C23-C24-C25

There are no ring outliers.

80 monomers are involved in 235 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	3	104	BCL	5	0
16	T	101	BCL	3	0
16	5	104	BCL	2	0
16	9	103	BCL	6	0
24	4	102	LMT	3	0
16	D	104	BCL	1	0
17	L	302	BPH	7	0
14	C	407	DGA	6	0
16	Q	104	BCL	3	0
15	Y	105	PGV	6	0
23	E	101	H4X	1	0

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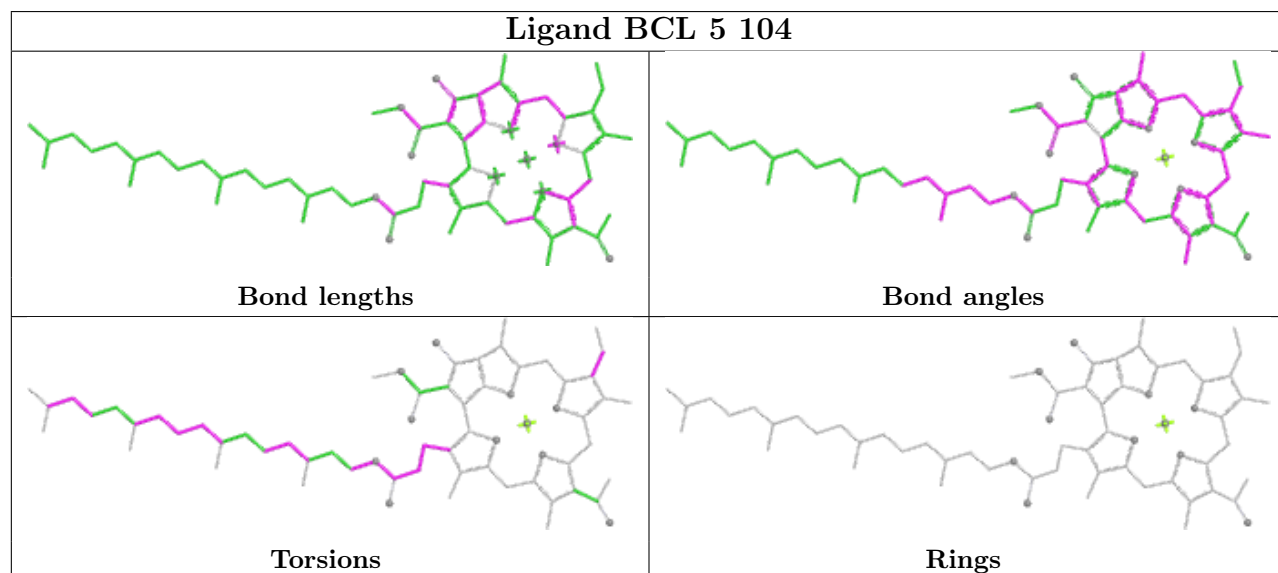
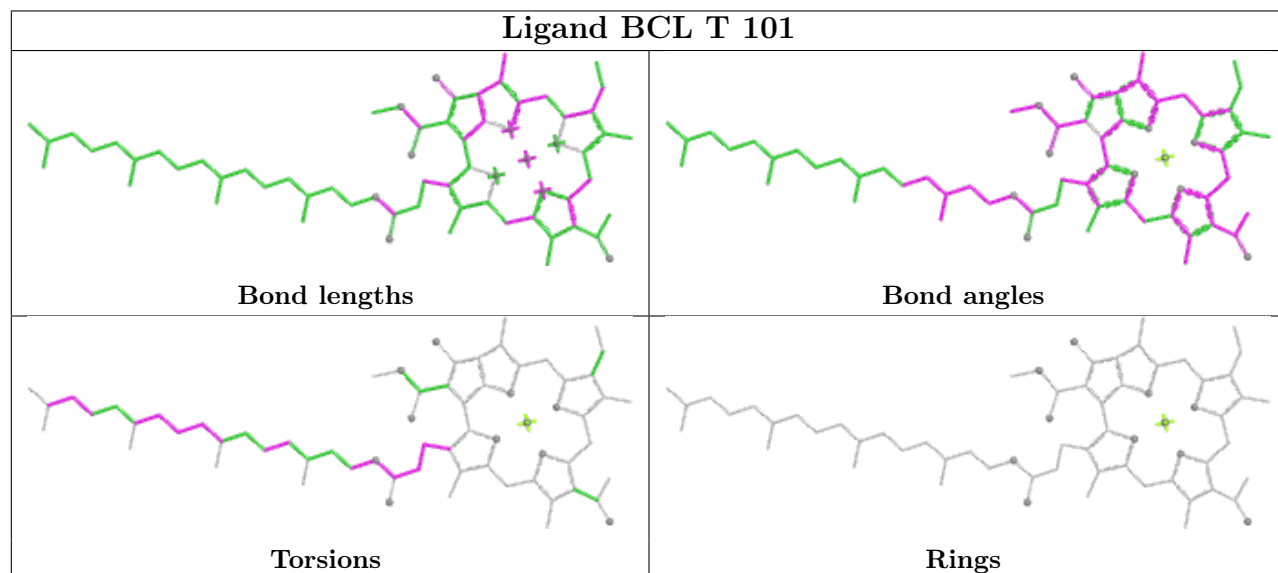
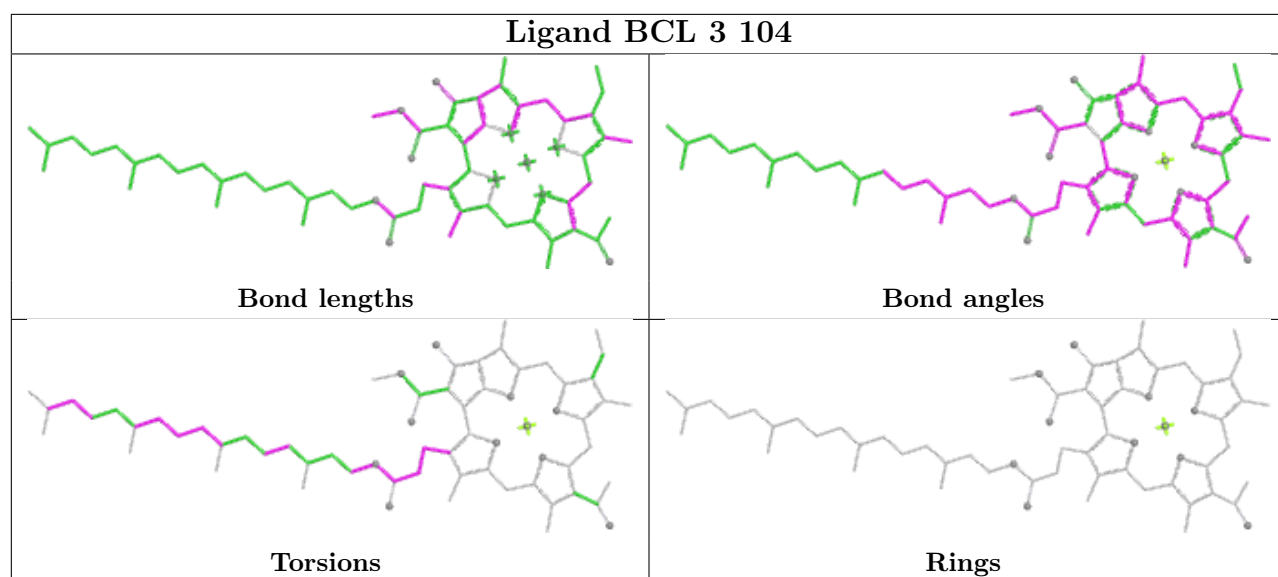
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	S	103	BCL	6	0
17	M	404	BPH	7	0
16	F	103	BCL	3	0
16	J	101	BCL	4	0
24	N	101	LMT	3	0
16	U	103	BCL	2	0
11	C	402	HEM	5	0
15	H	301	PGV	1	0
16	D	103	BCL	4	0
24	B	102	LMT	3	0
24	J	102	LMT	2	0
24	8	101	LMT	2	0
16	W	102	BCL	3	0
22	S	101	CDL	1	0
16	Y	102	BCL	1	0
11	C	403	HEM	9	0
15	O	102	PGV	5	0
16	K	105	BCL	7	0
15	9	101	PGV	2	0
15	K	101	PGV	3	0
24	X	102	LMT	2	0
22	H	302	CDL	3	0
24	8	102	LMT	3	0
16	Y	104	BCL	2	0
24	P	102	LMT	2	0
16	Q	103	BCL	5	0
21	M	405	MQ8	2	0
24	R	101	LMT	2	0
16	K	108	BCL	3	0
19	L	307	8K6	1	0
16	7	103	BCL	3	0
24	6	102	LMT	2	0
16	X	101	BCL	2	0
16	7	102	BCL	4	0
15	5	101	PGV	4	0
24	G	102	LMT	1	0
24	B	104	LMT	2	0
16	M	402	BCL	2	0
15	F	104	PGV	2	0
24	T	102	LMT	2	0
16	F	105	BCL	2	0
16	3	103	BCL	6	0

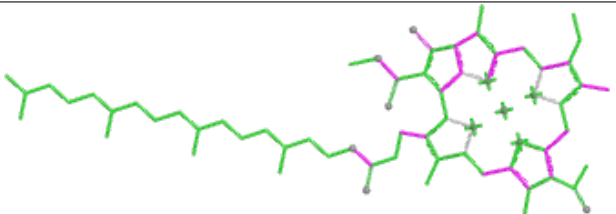
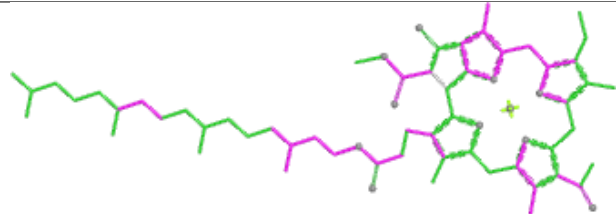
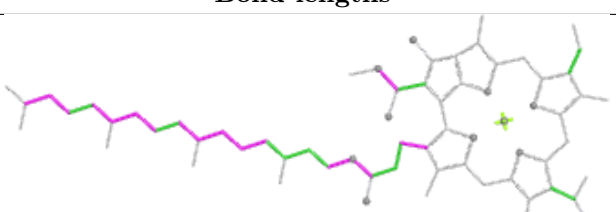
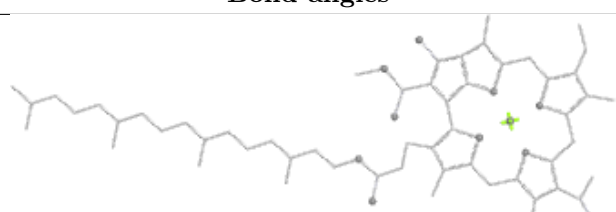
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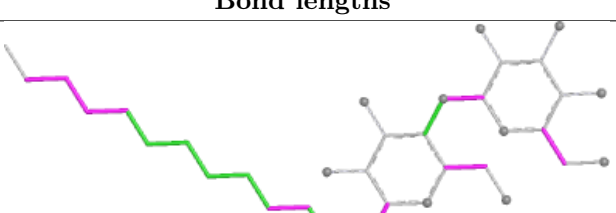
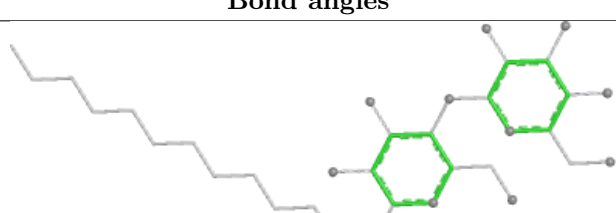
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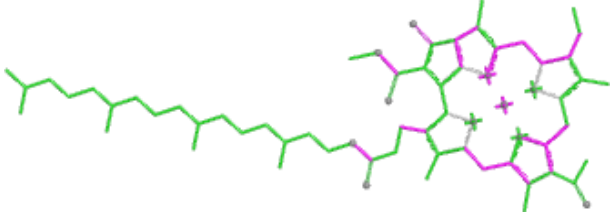
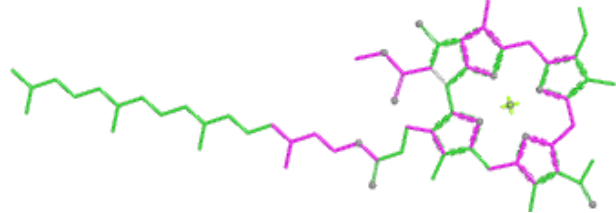
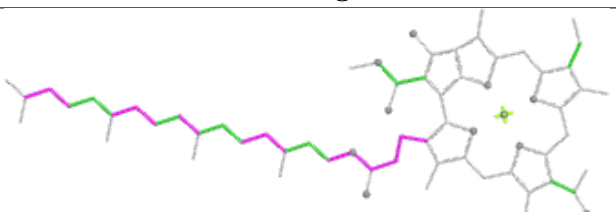
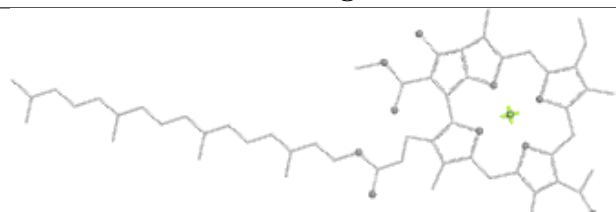
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	102	BCL	7	0
15	L	305	PGV	3	0
23	O	106	H4X	1	0
15	Q	101	PGV	1	0
16	I	102	BCL	4	0
16	5	103	BCL	6	0
16	U	102	BCL	7	0
24	V	102	LMT	1	0
16	9	104	BCL	1	0
11	C	401	HEM	6	0
16	O	104	BCL	2	0
16	M	403	BCL	6	0
11	C	404	HEM	9	0
16	1	102	BCL	4	0
16	2	102	BCL	2	0
16	L	301	BCL	5	0
24	2	103	LMT	2	0
24	E	102	LMT	2	0
15	3	101	PGV	4	0
23	G	101	H4X	1	0
16	L	304	BCL	4	0
15	M	406	PGV	1	0
24	Z	102	LMT	1	0
24	0	101	LMT	1	0
16	O	105	BCL	3	0
16	B	103	BCL	2	0
18	L	306	UQ8	7	0

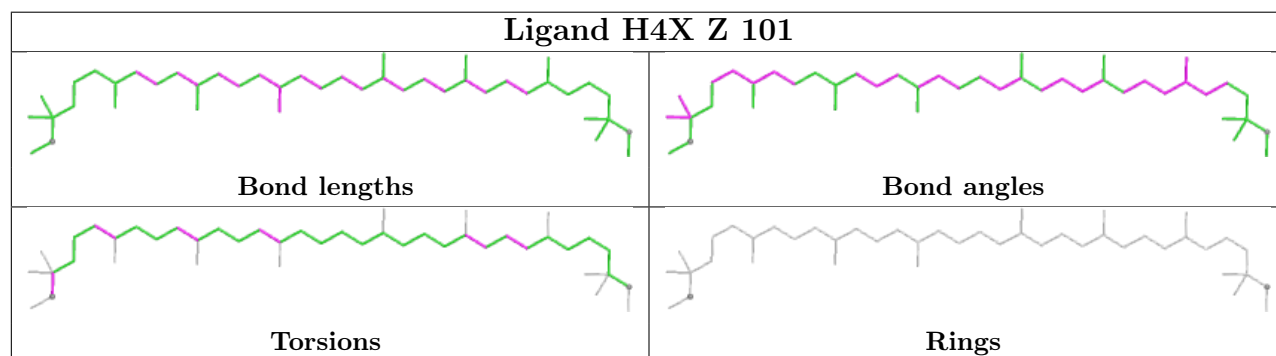
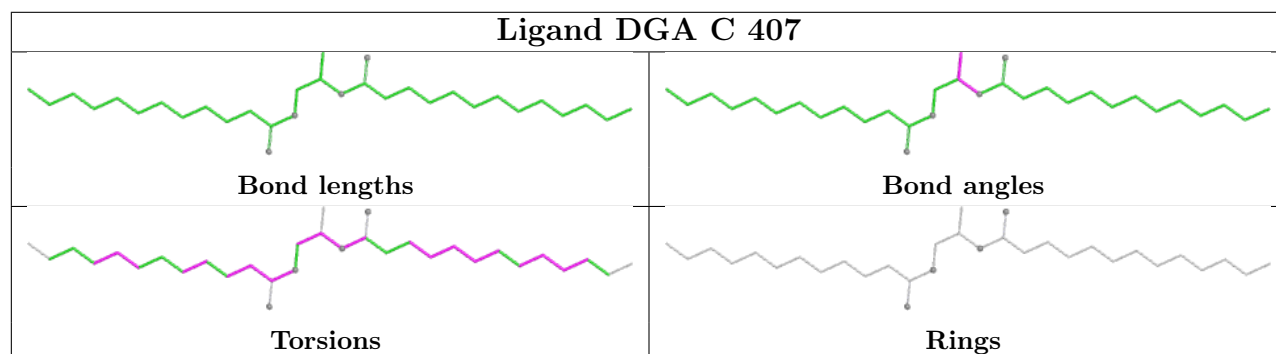
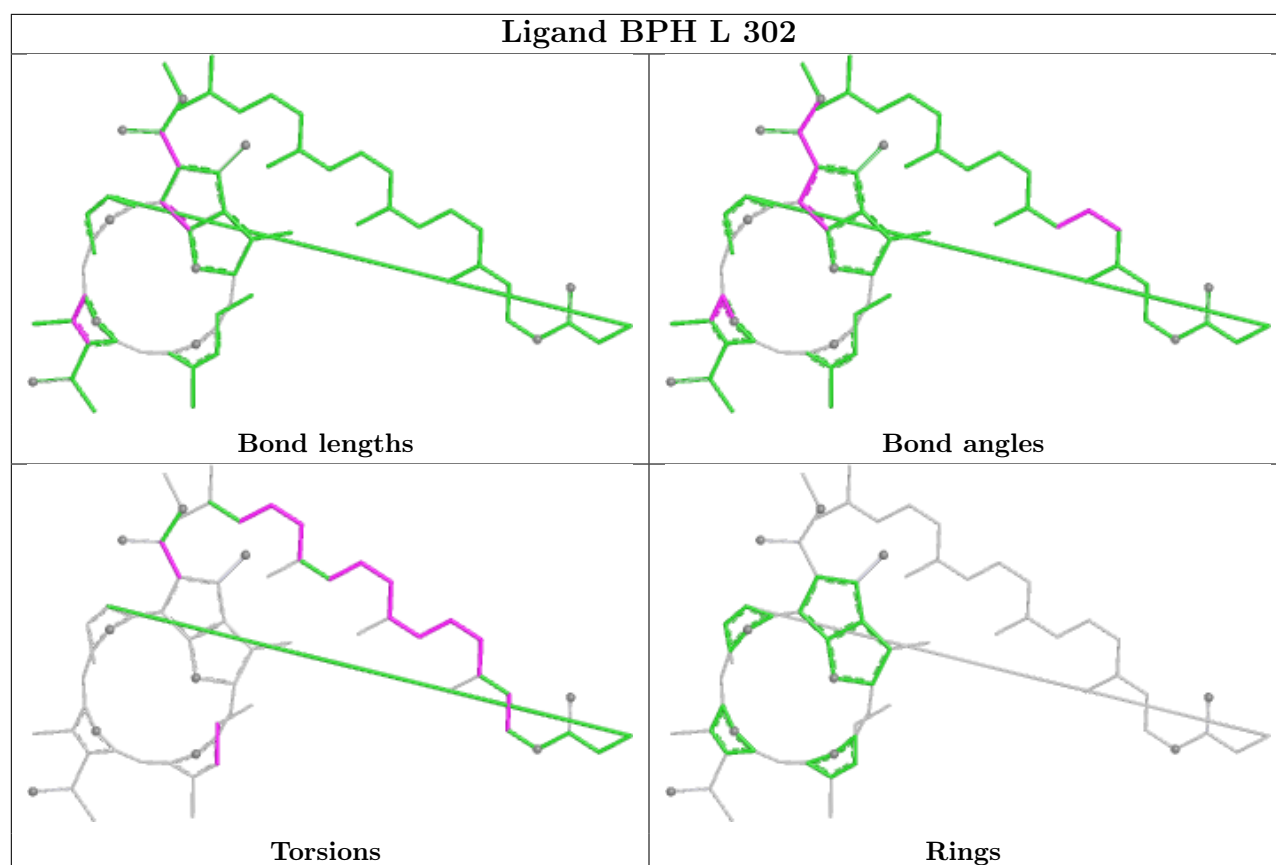
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

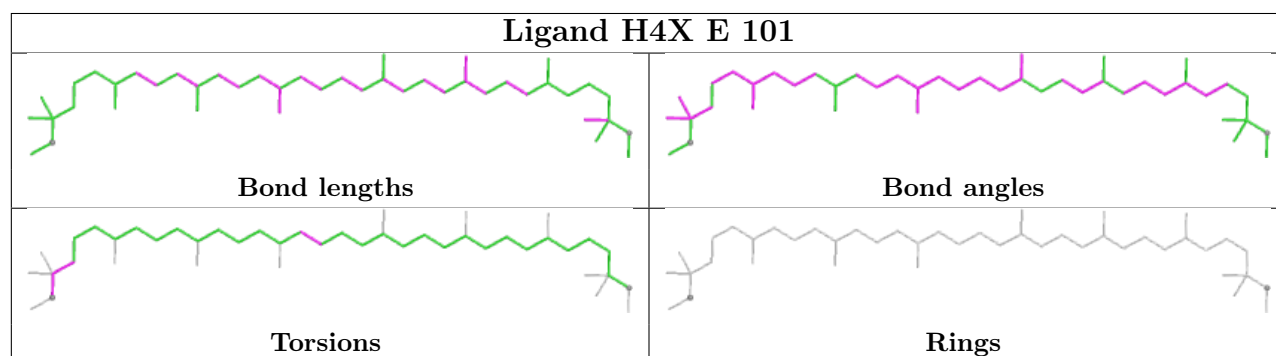
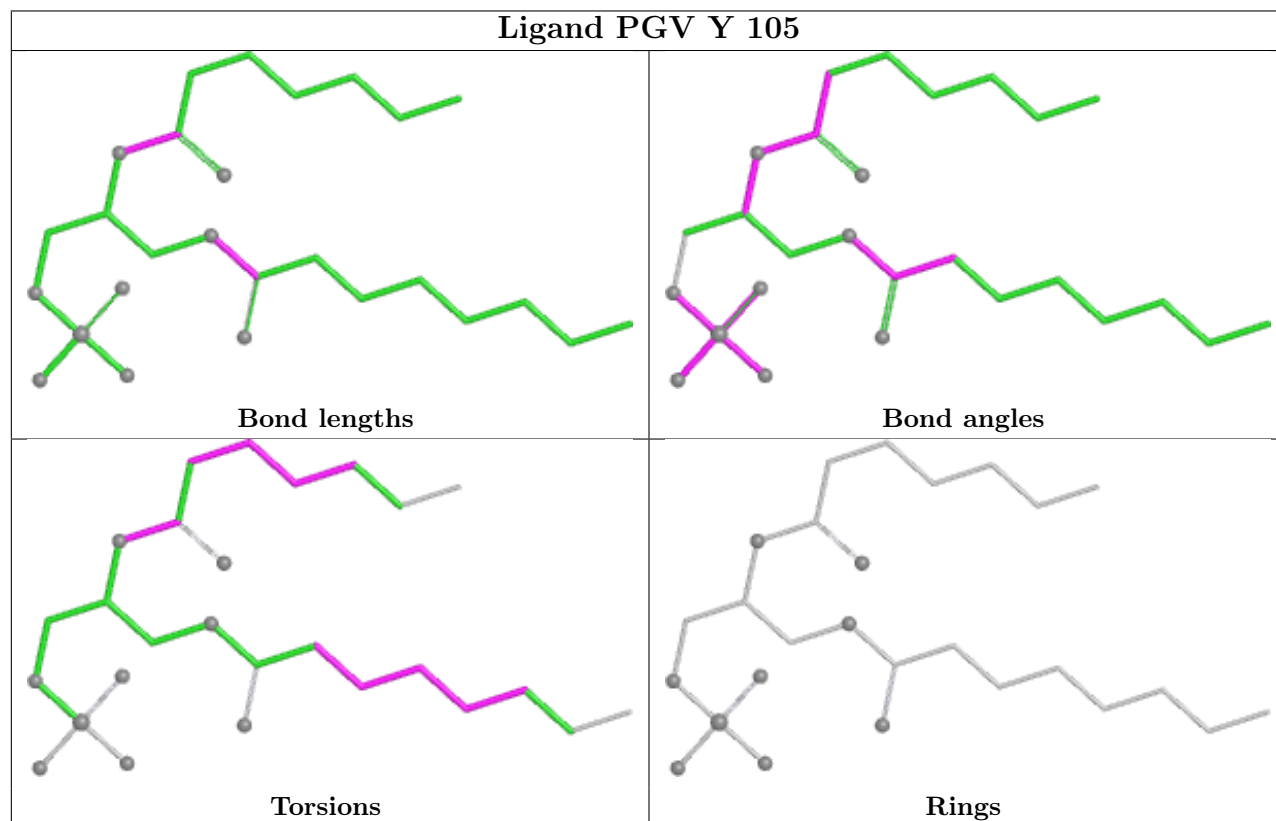
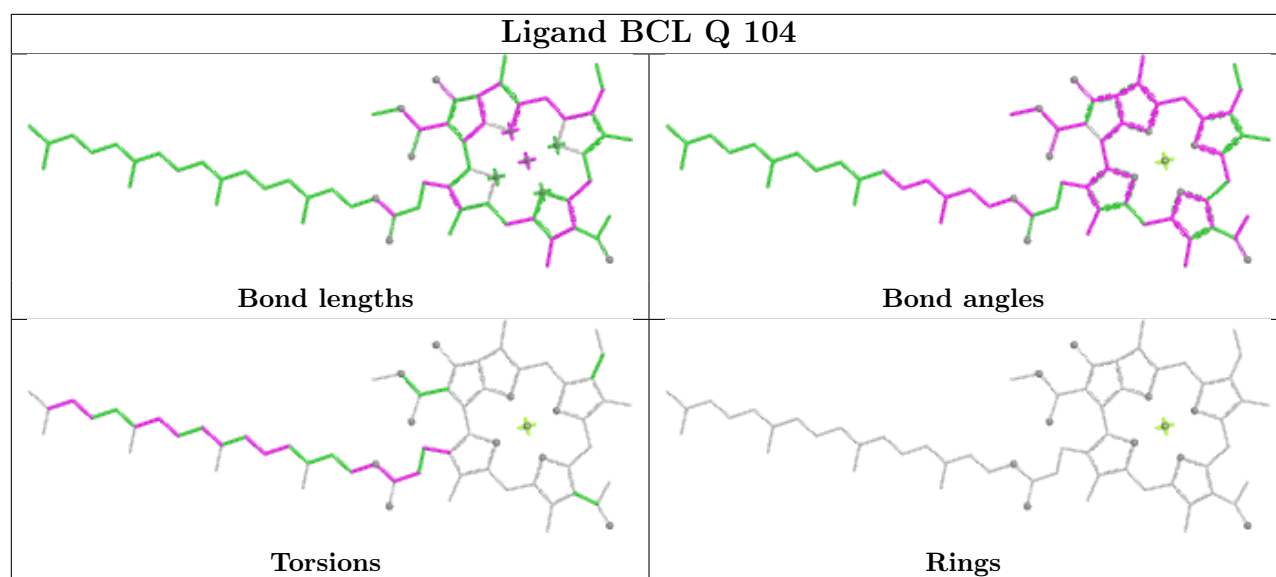


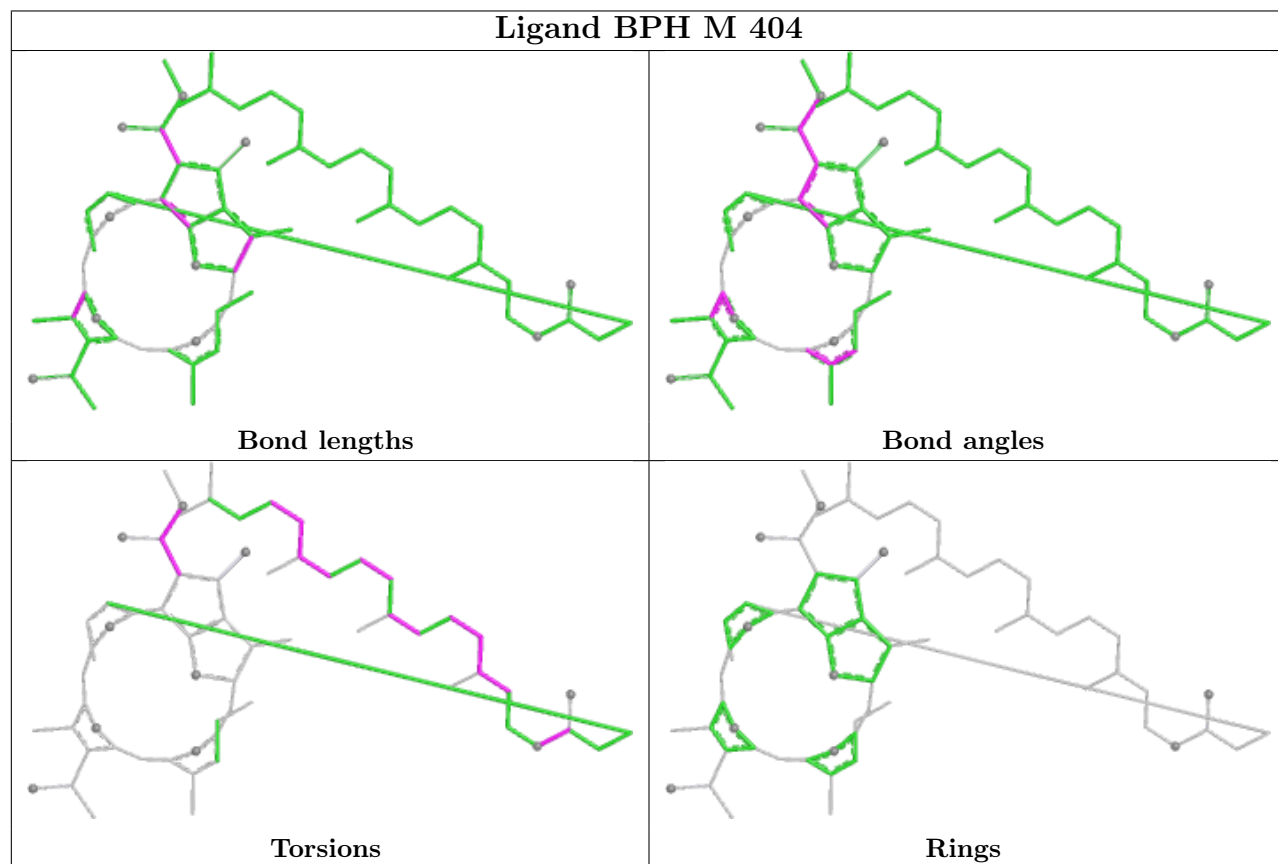
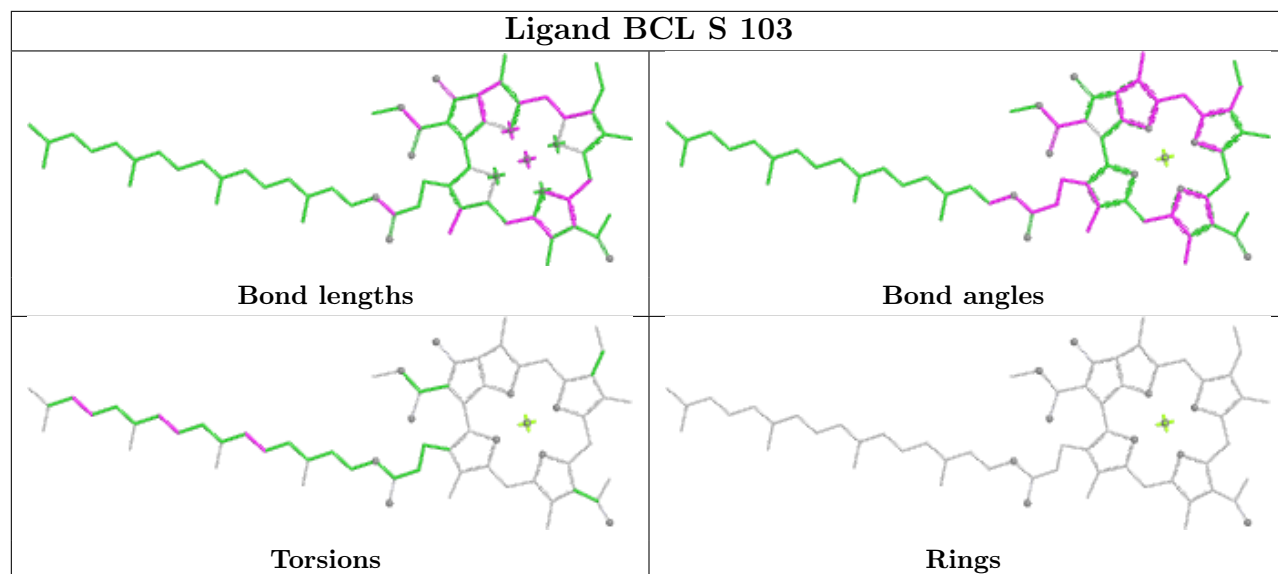
Ligand BCL 9 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

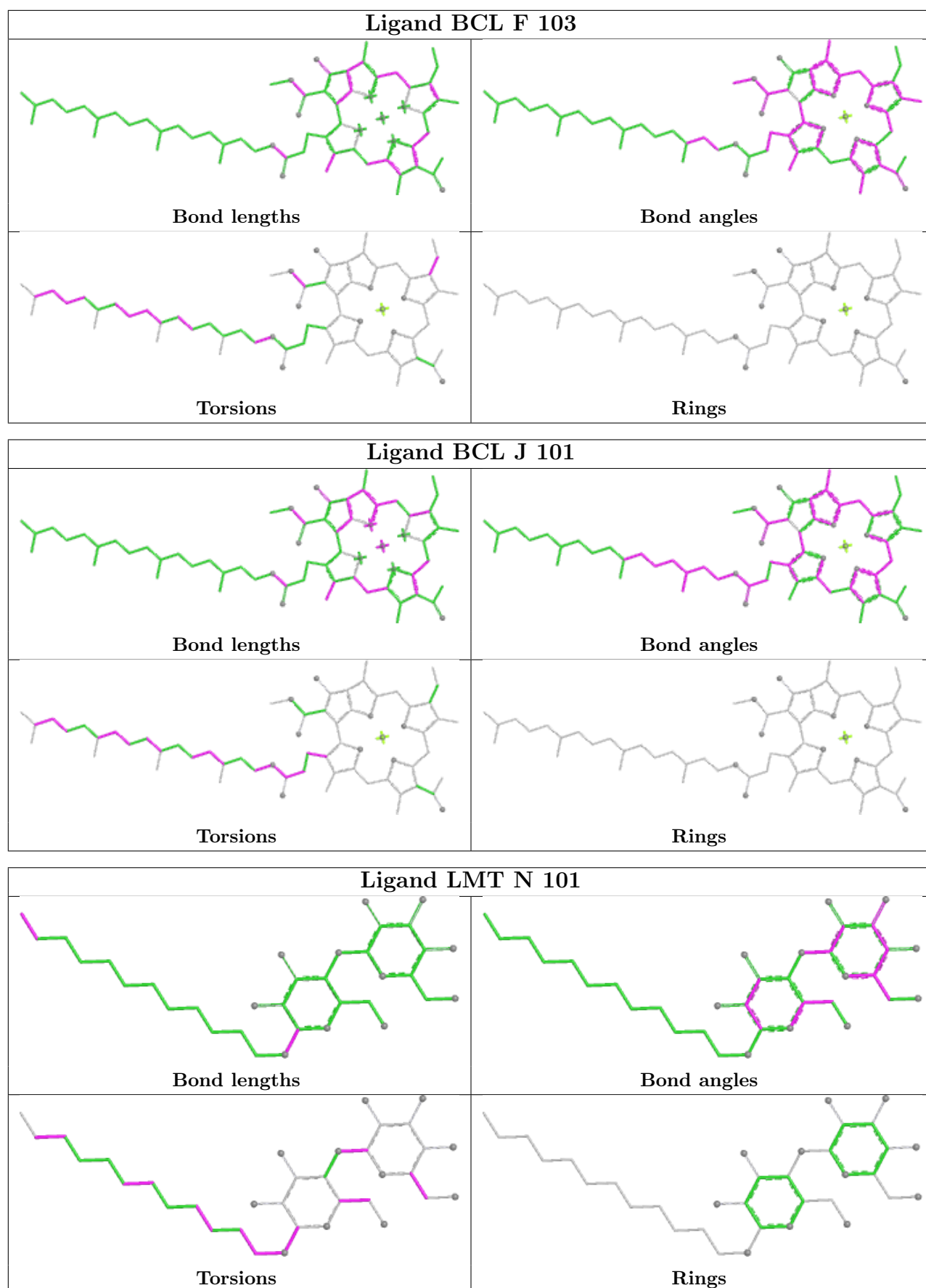
Ligand LMT 4 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL D 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

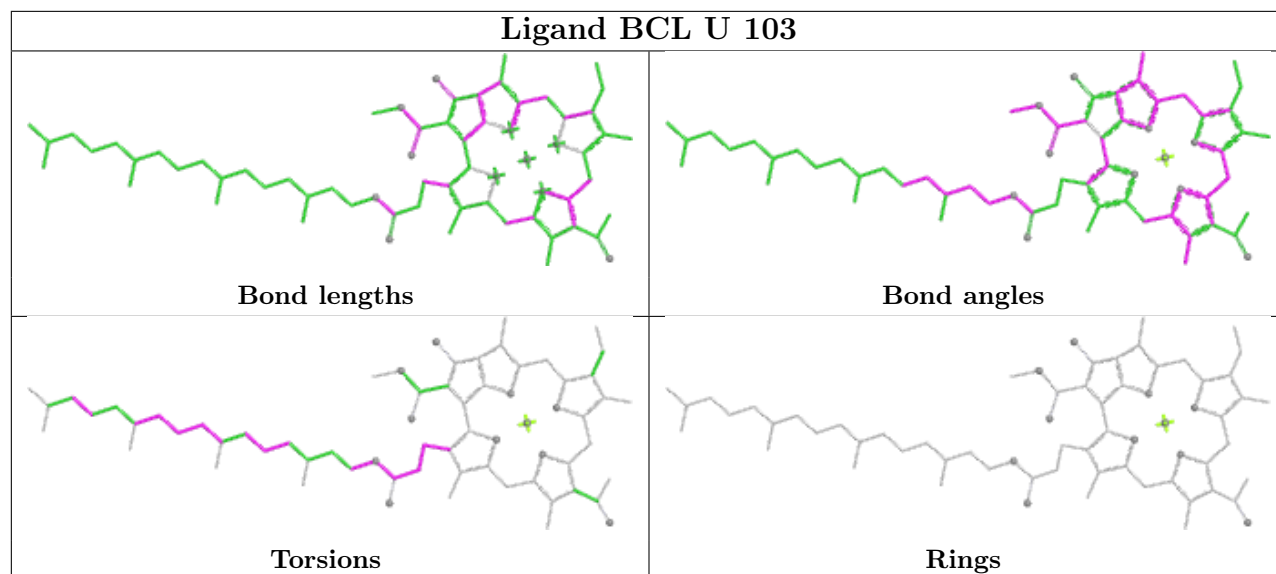




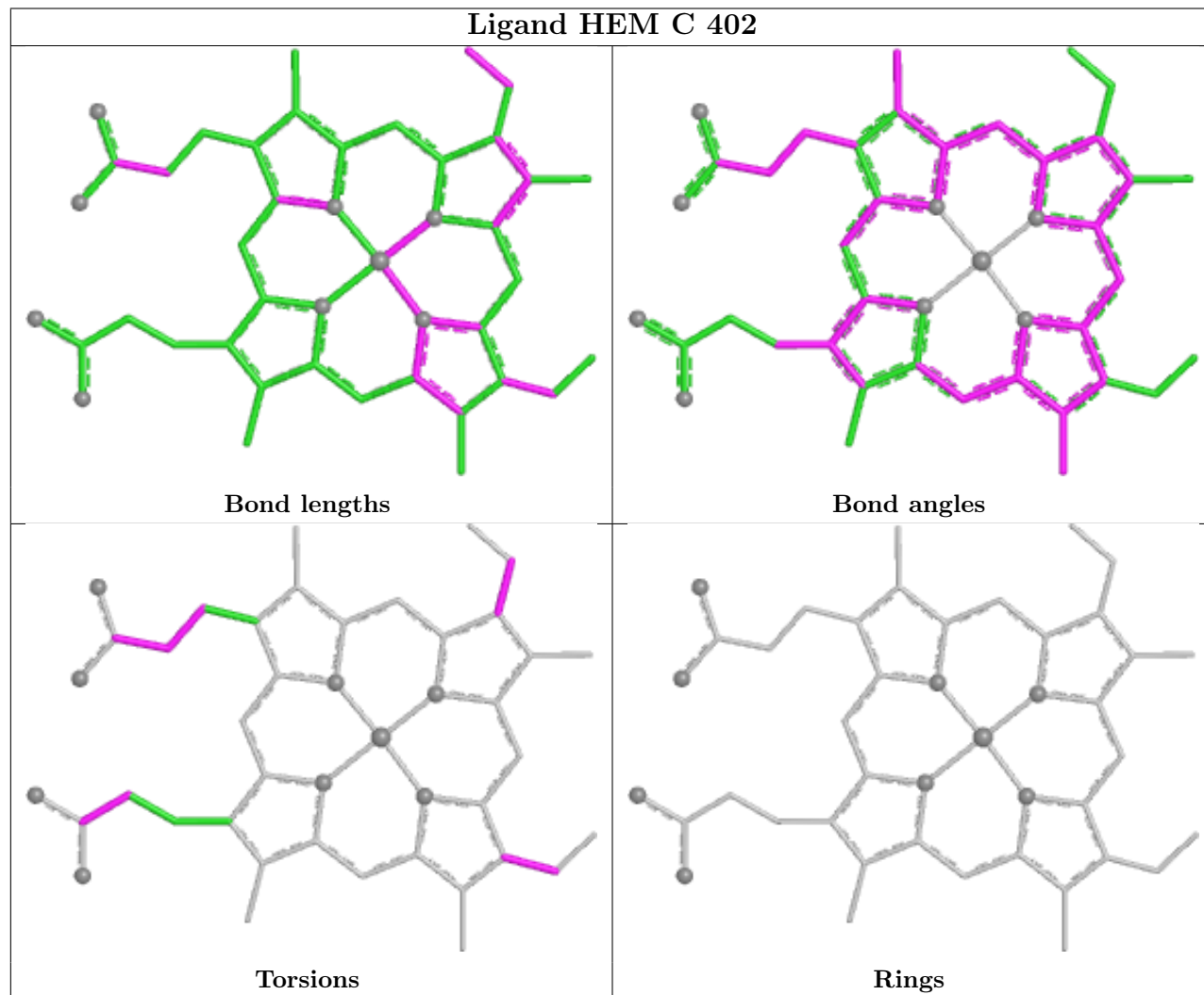


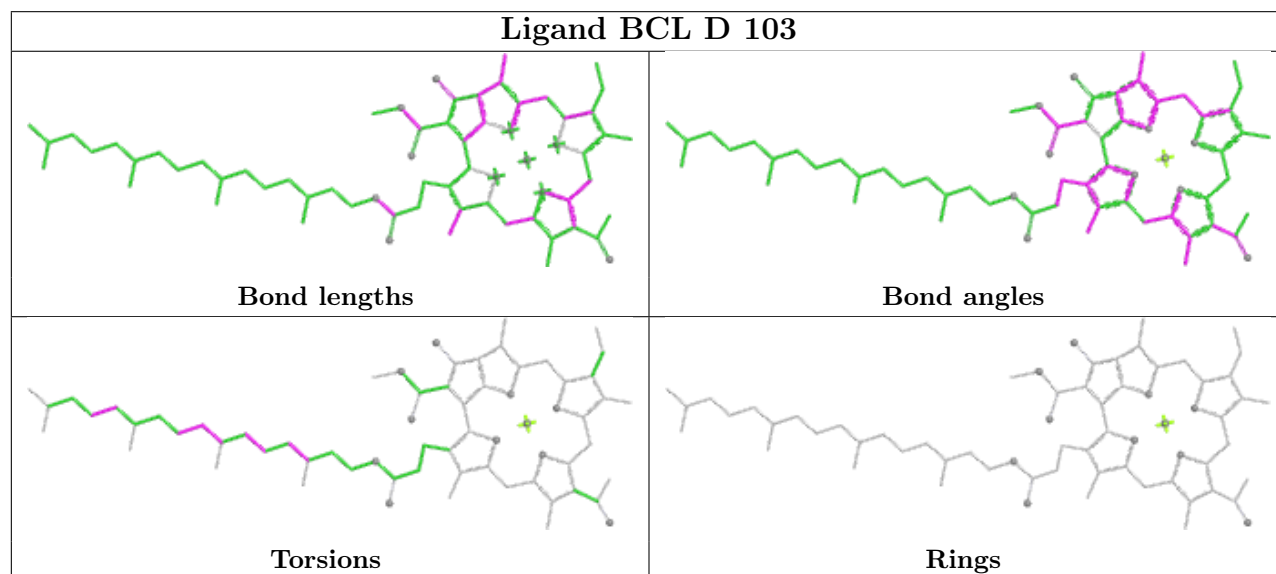
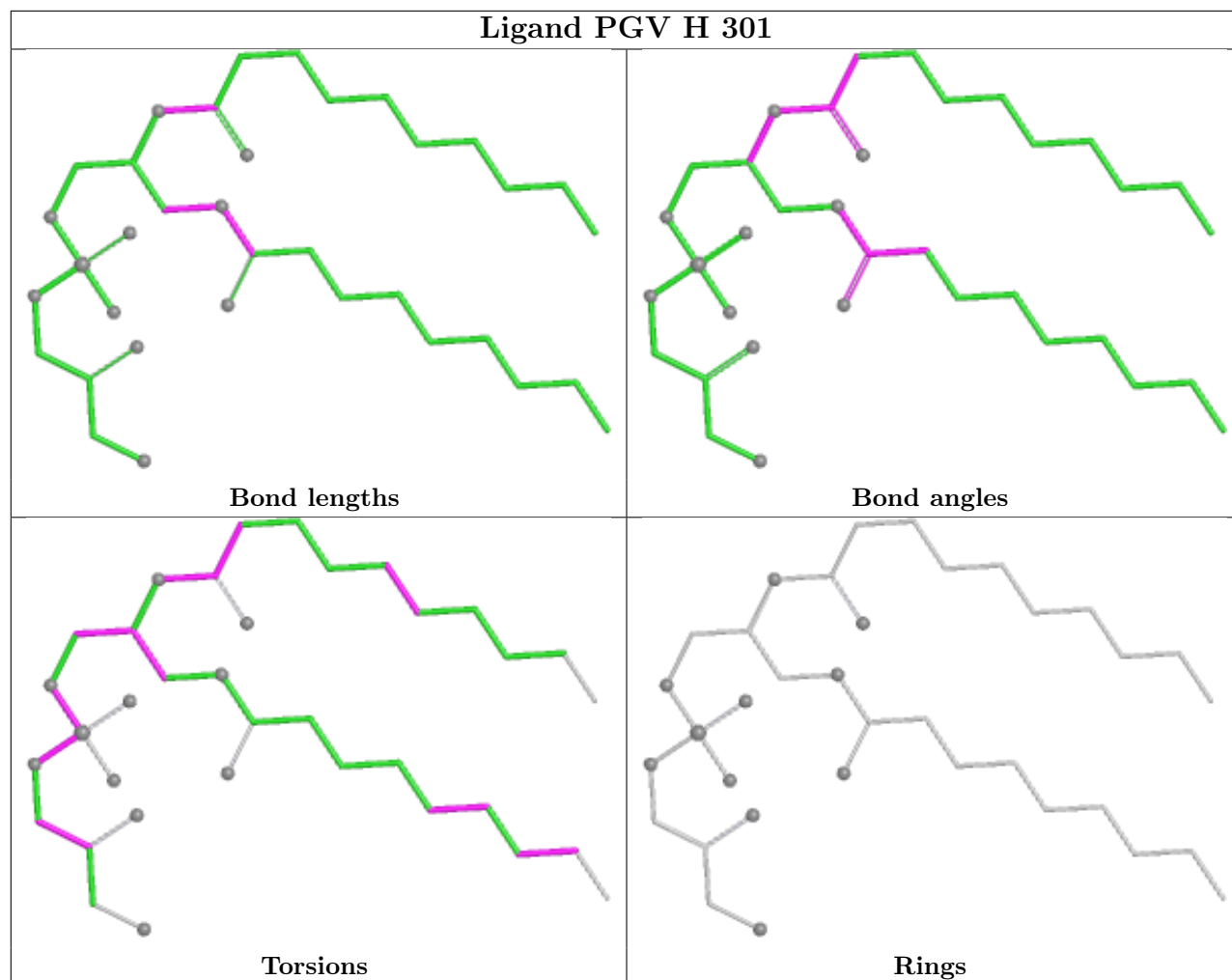


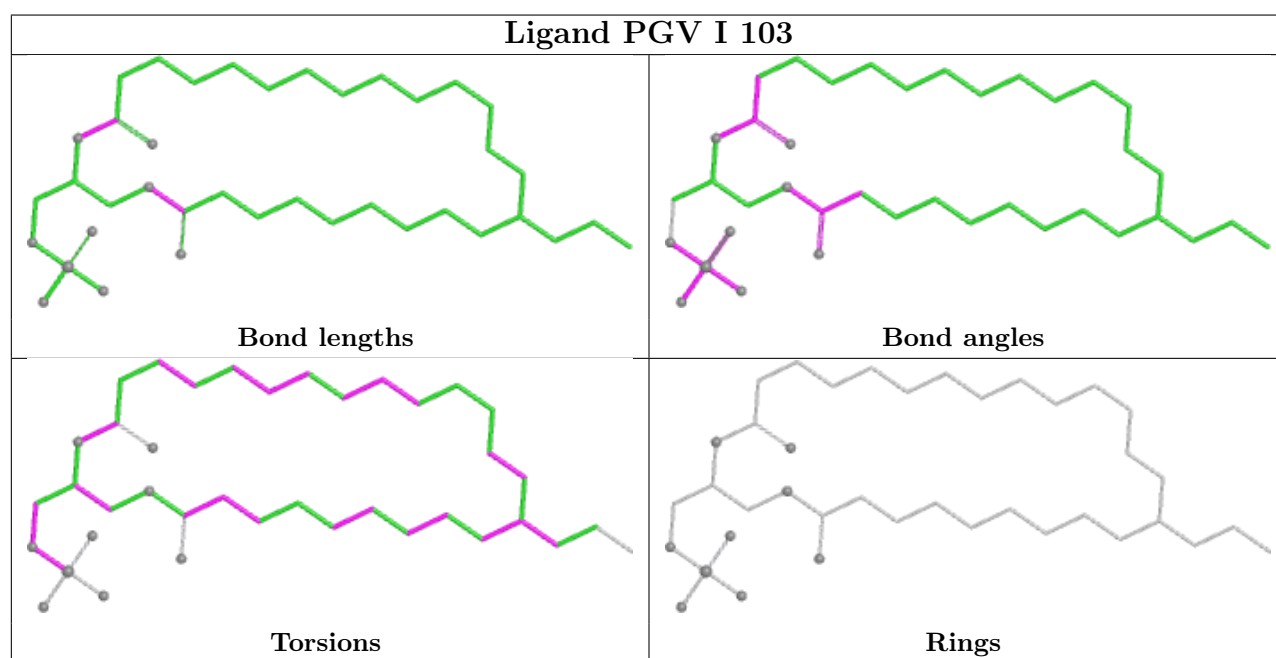
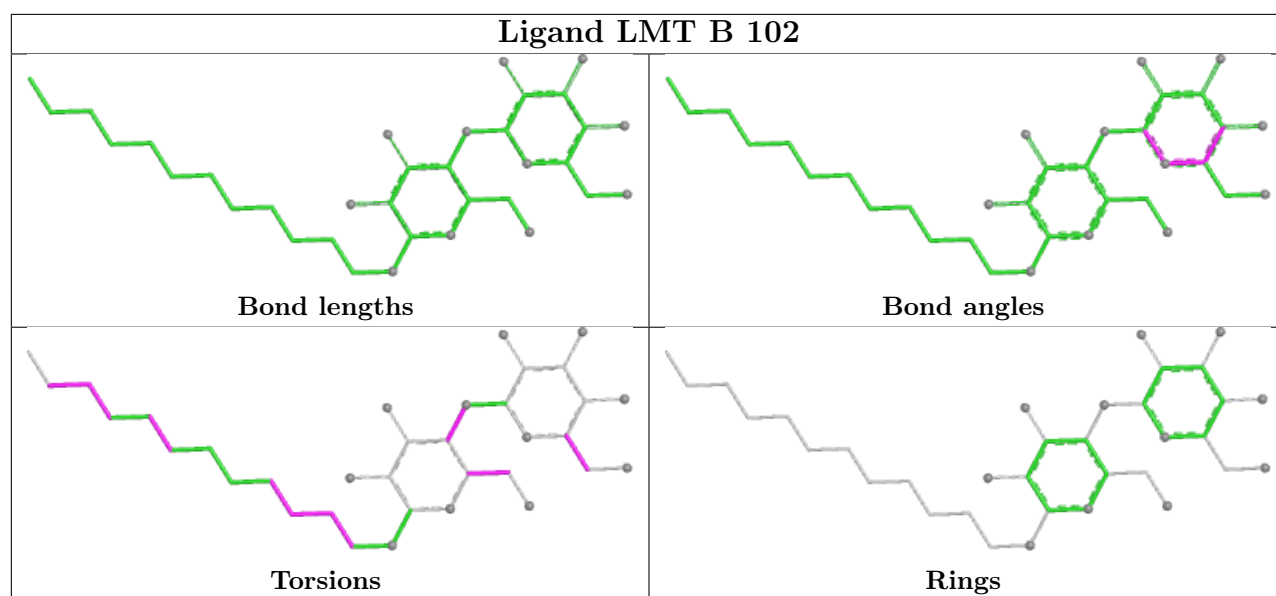
Ligand BCL U 103

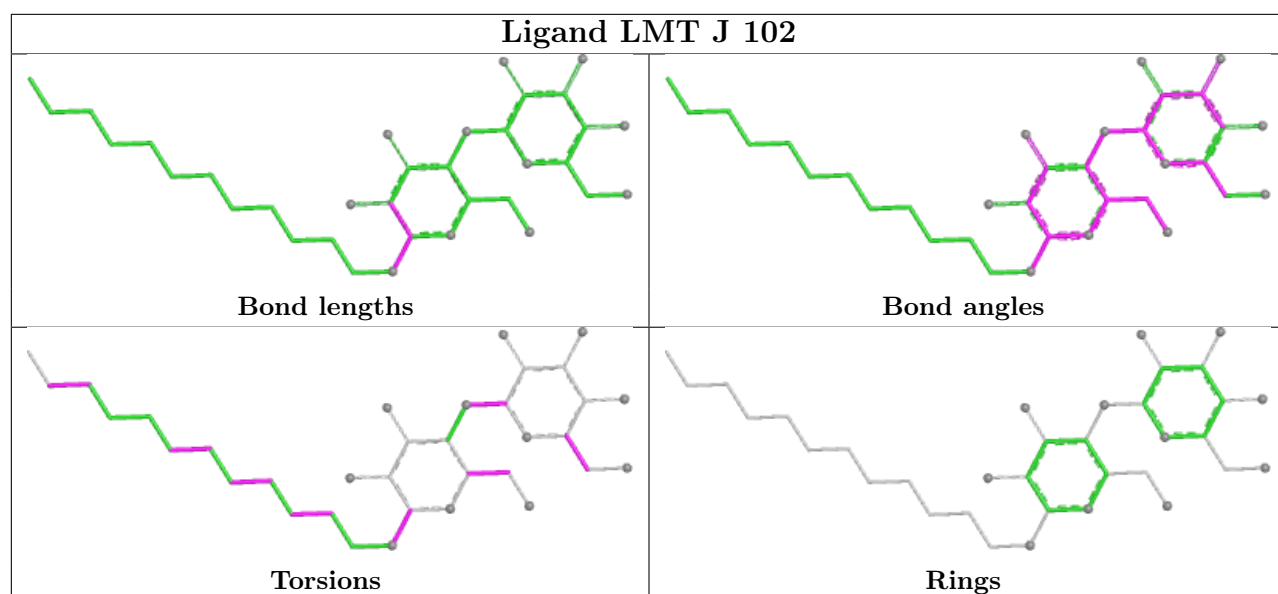
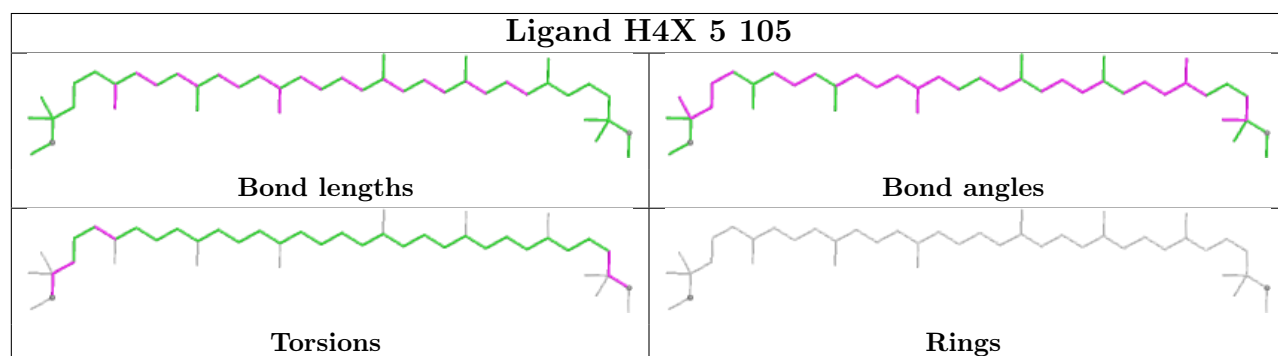
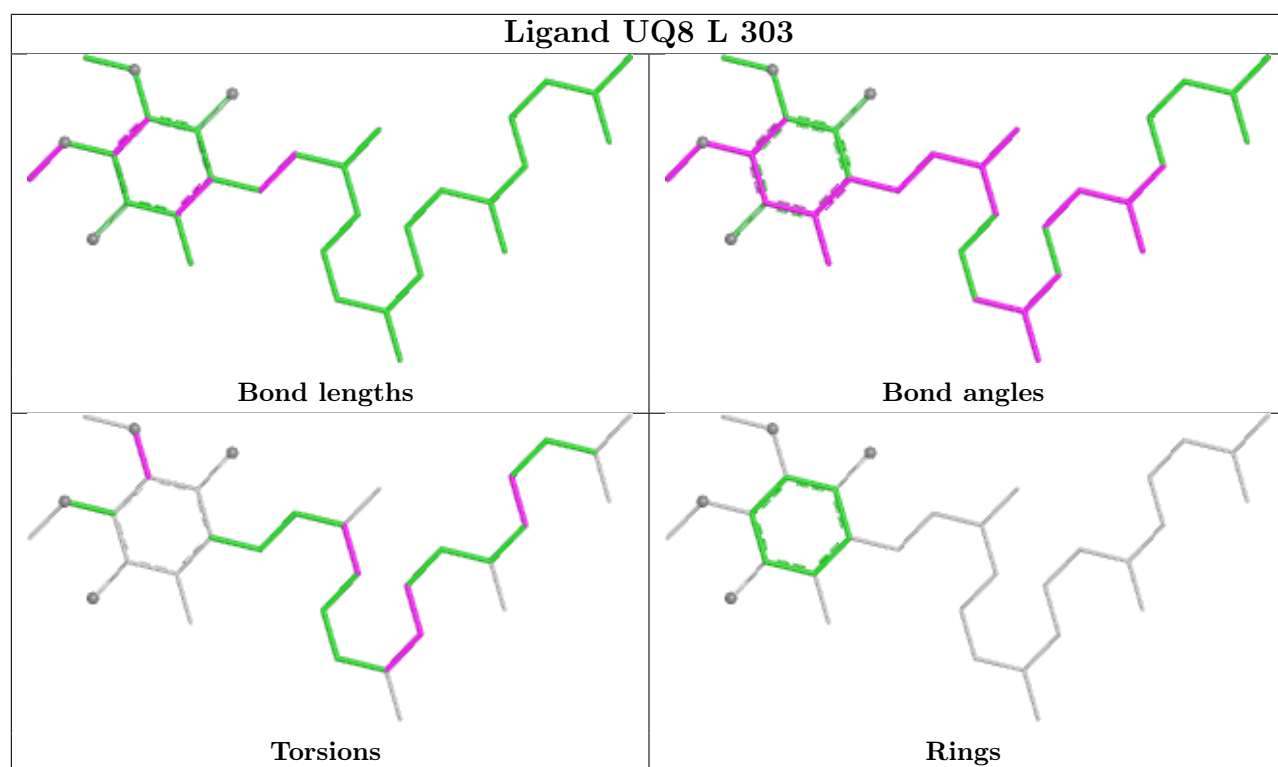


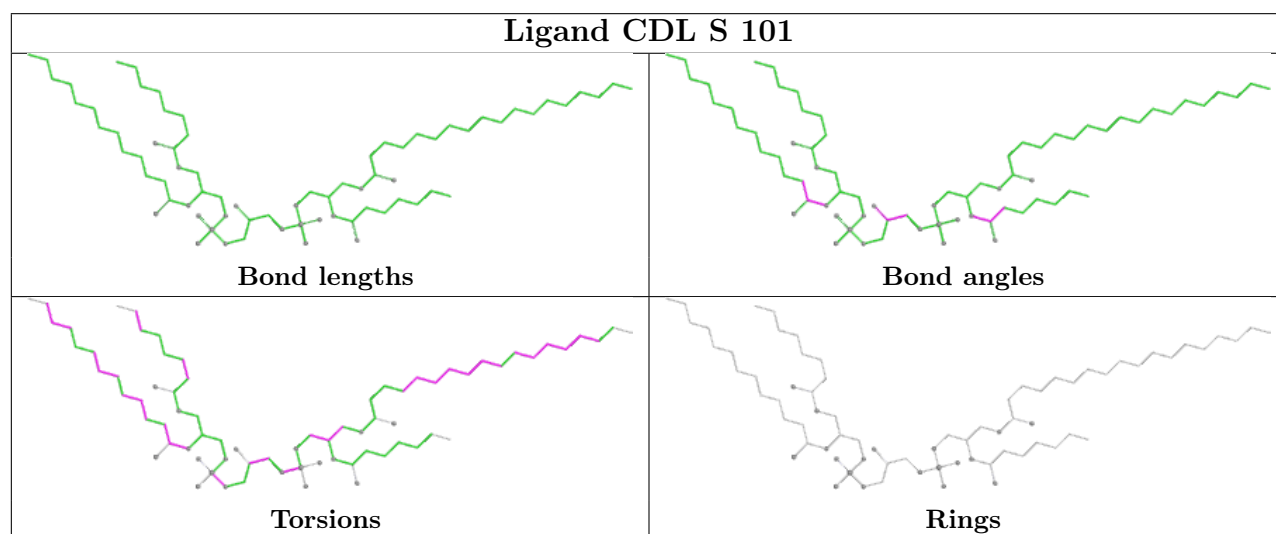
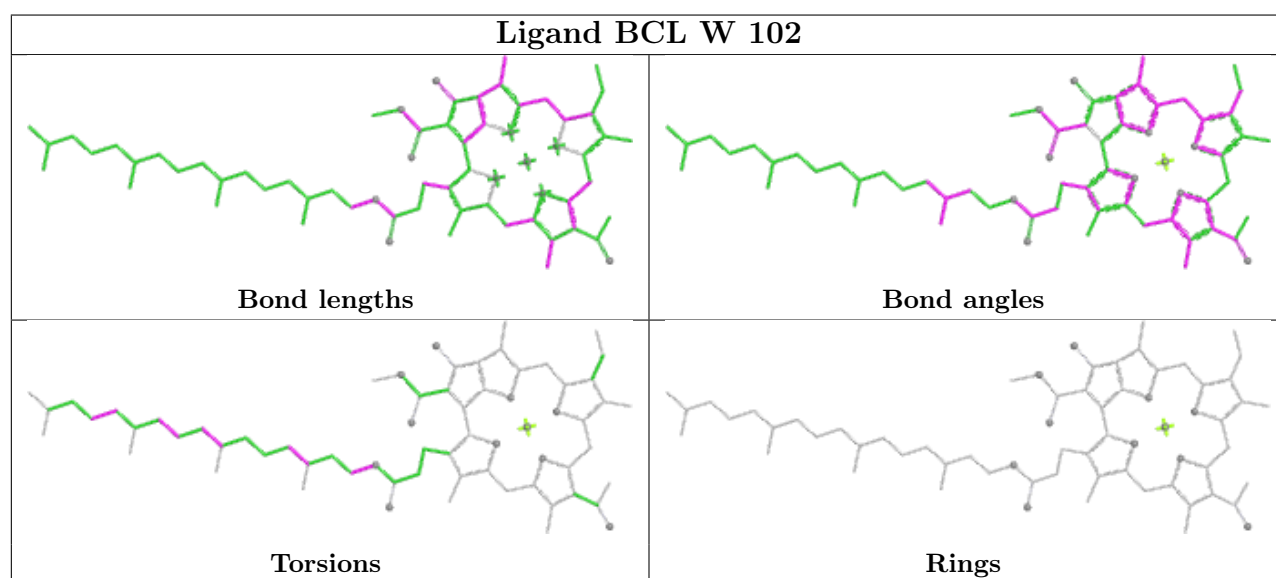
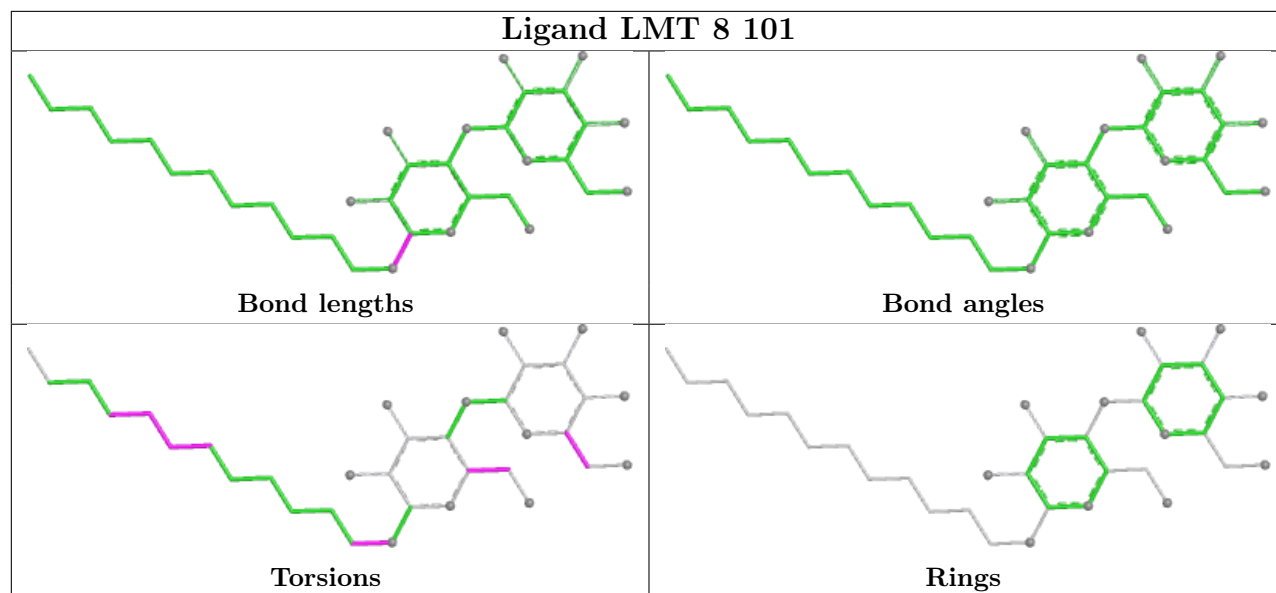
Ligand HEM C 402



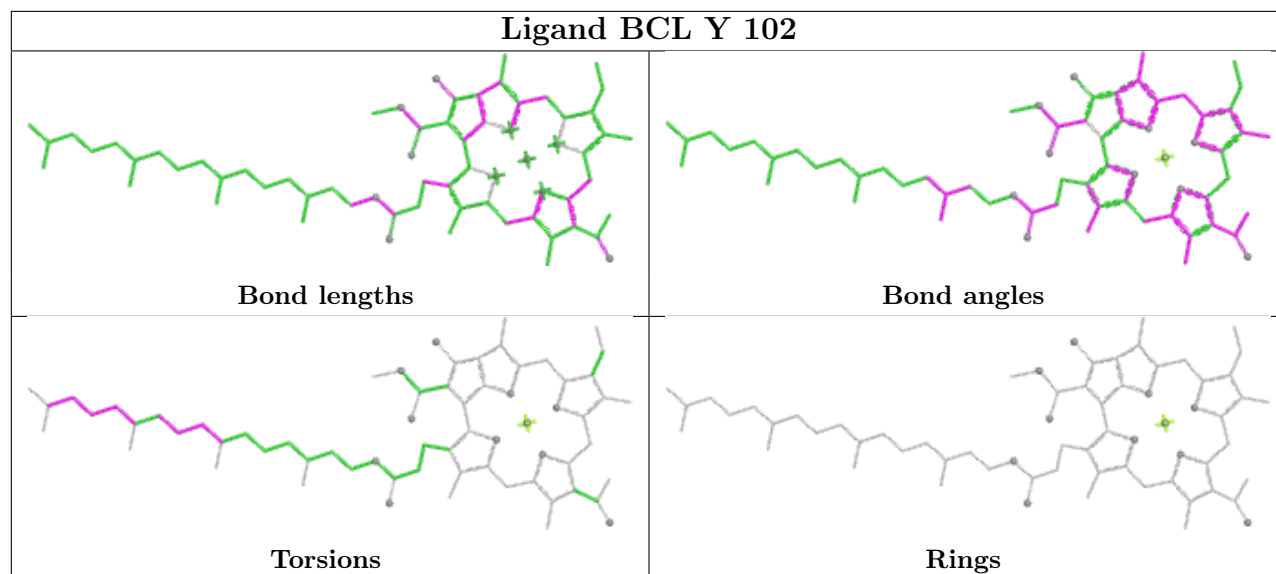




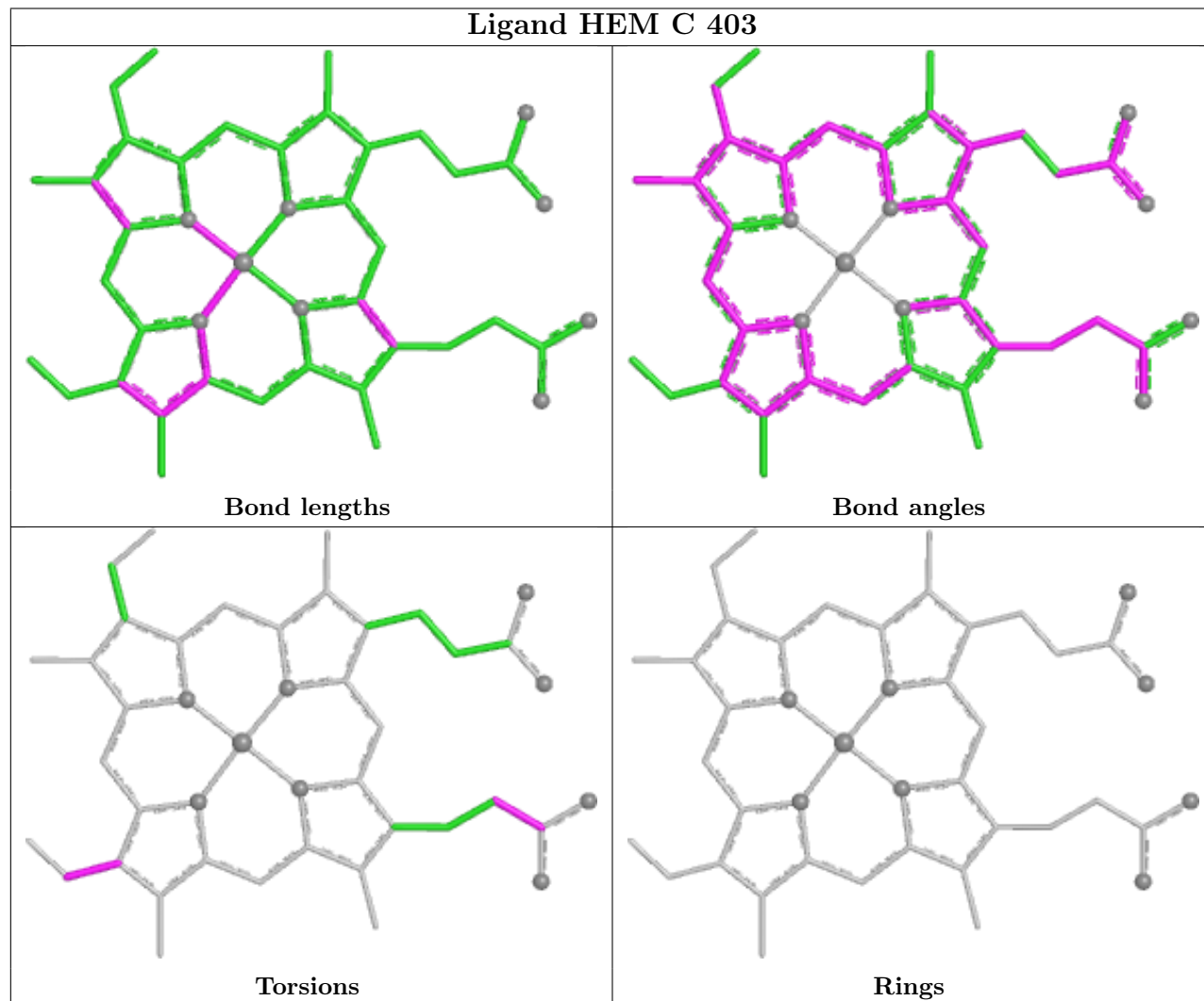


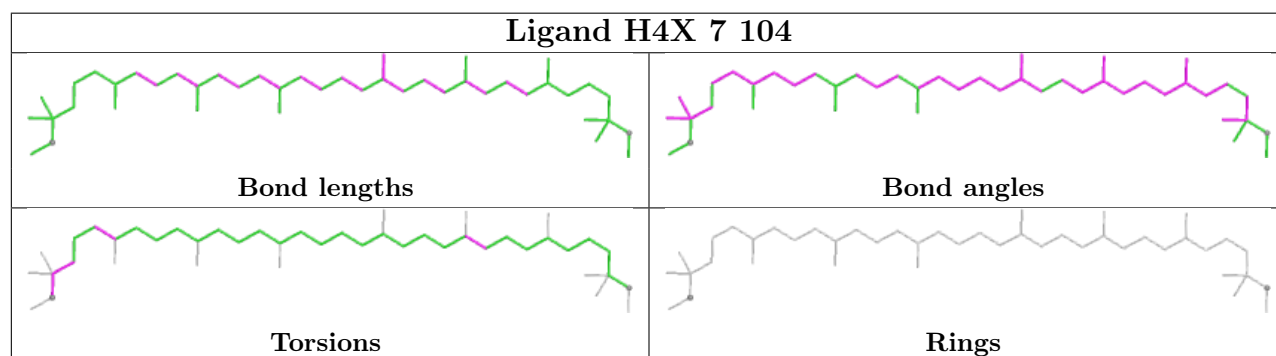
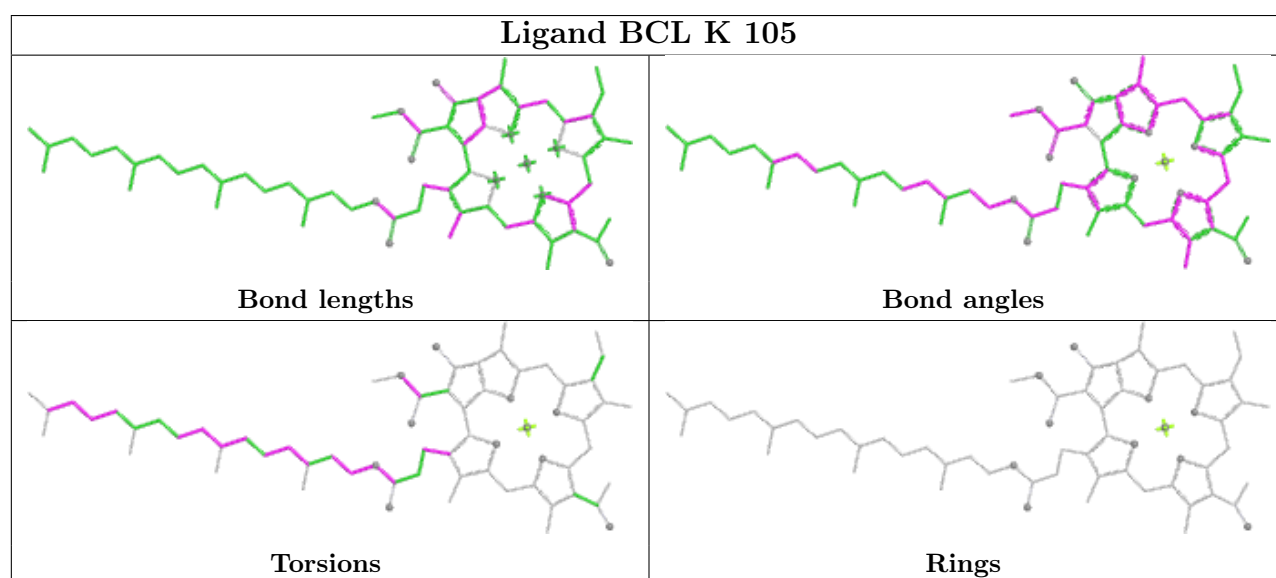
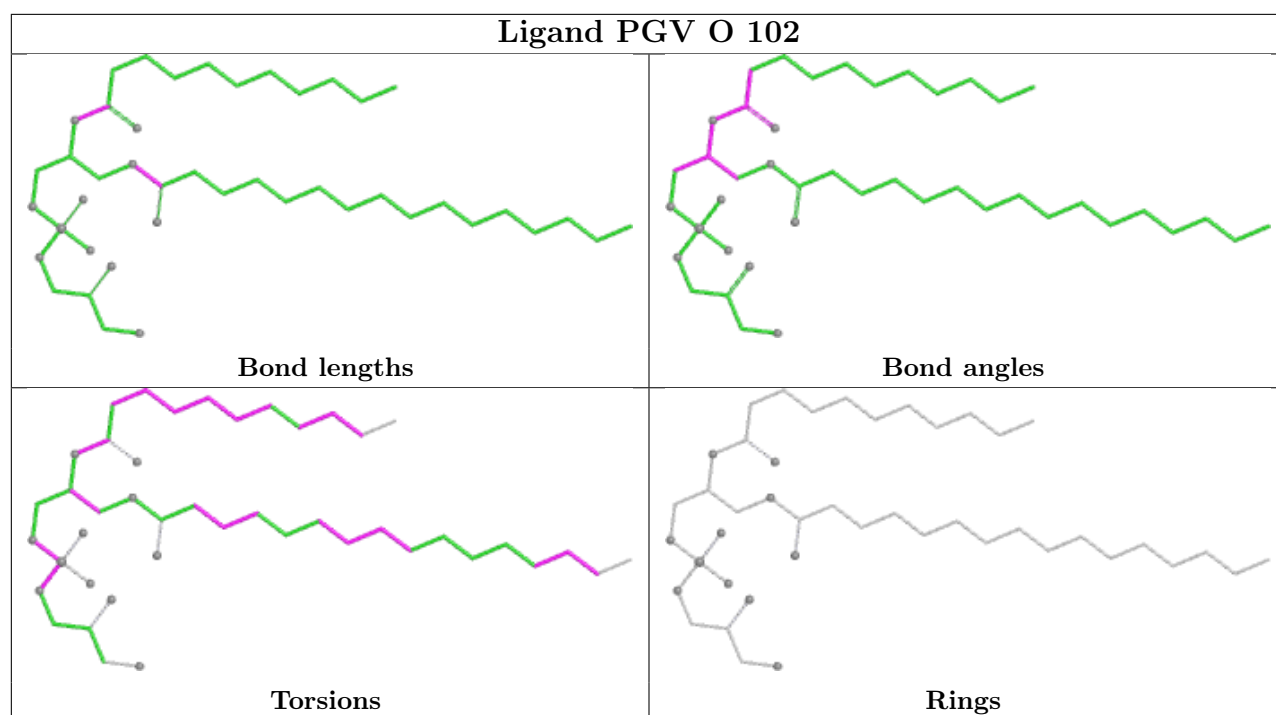


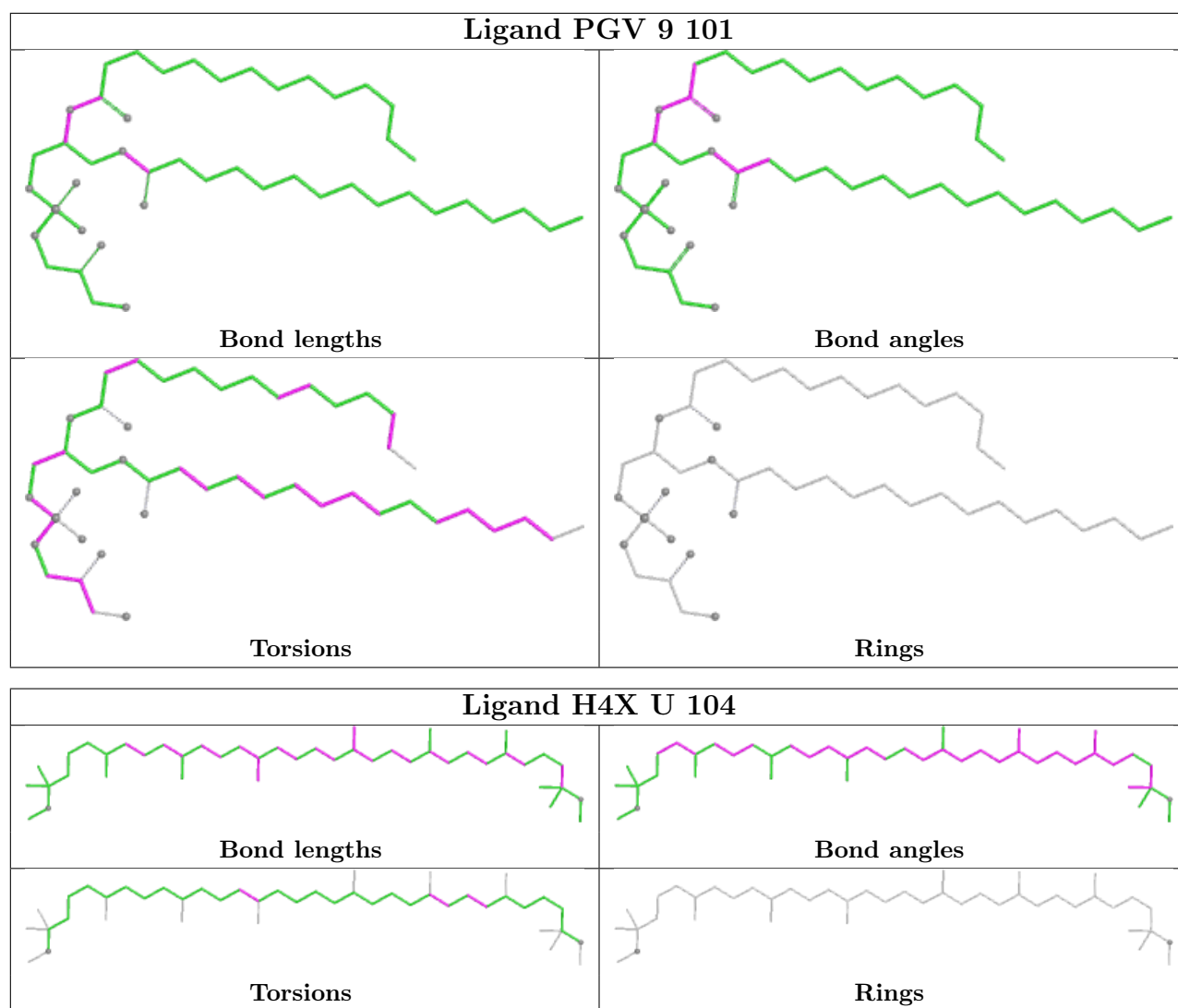
Ligand BCL Y 102

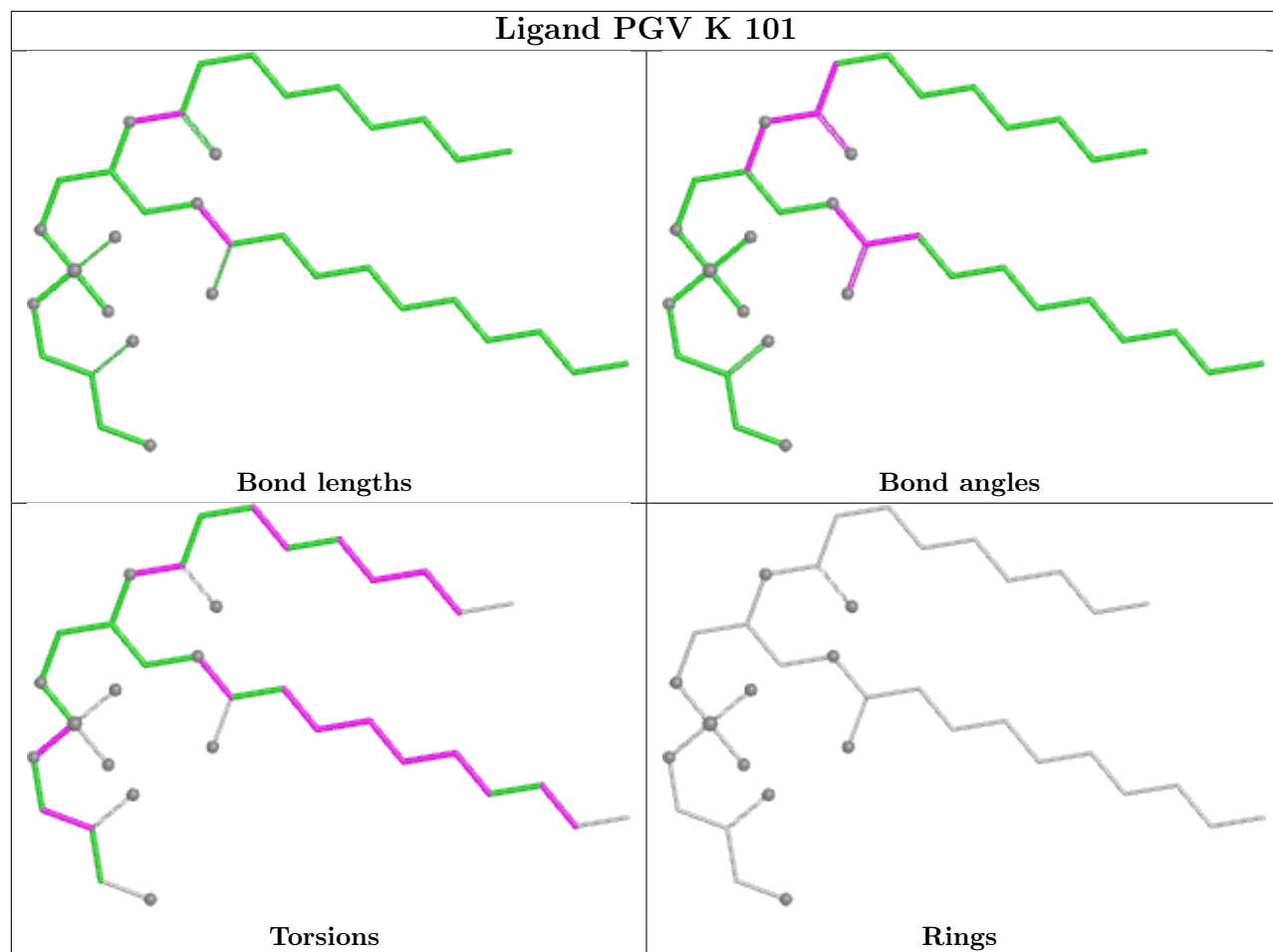


Ligand HEM C 403

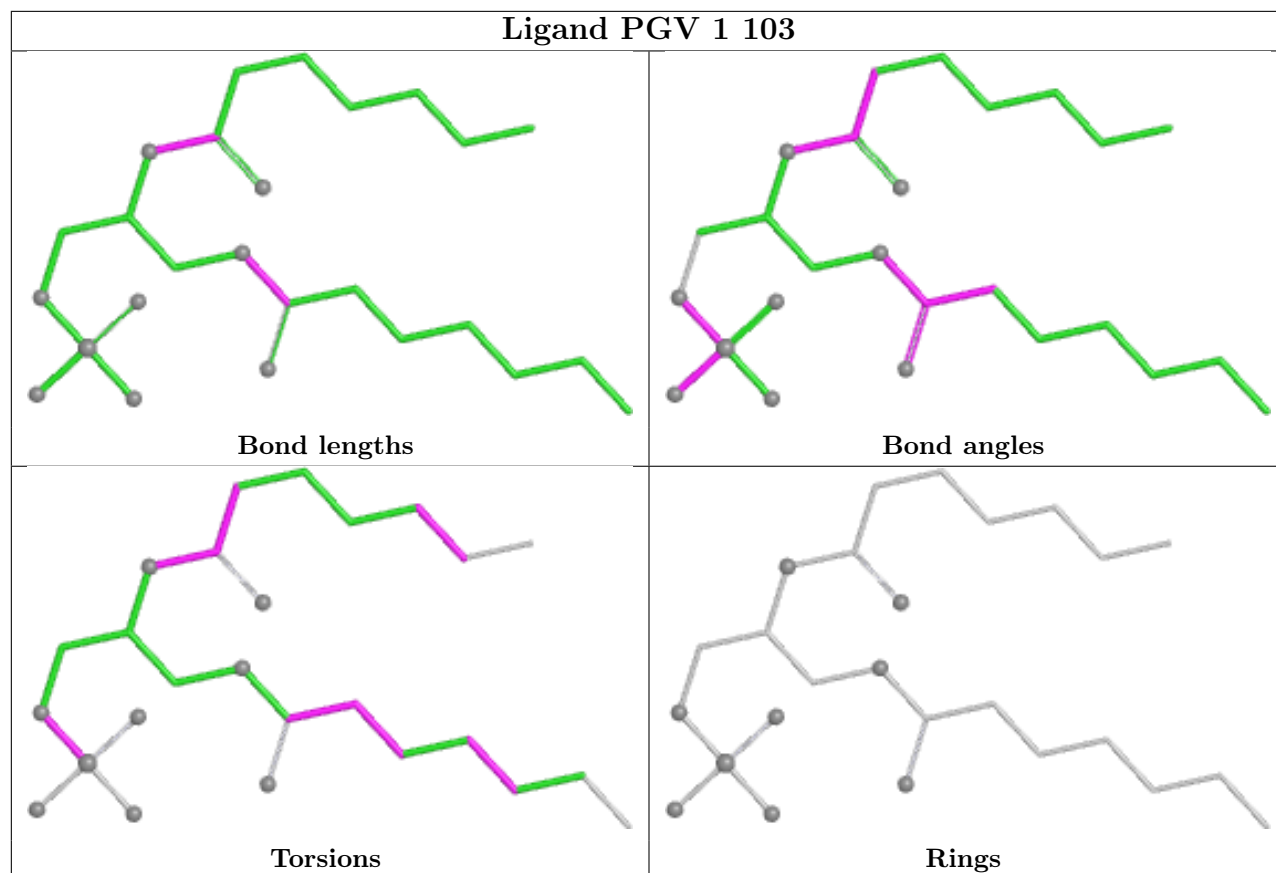




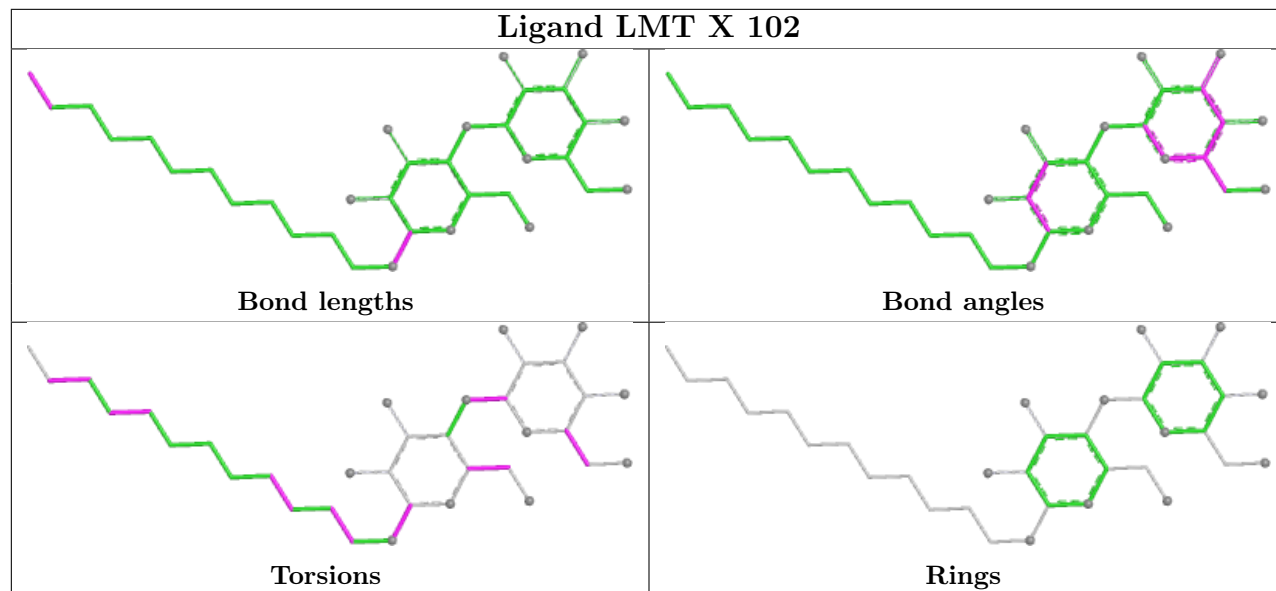


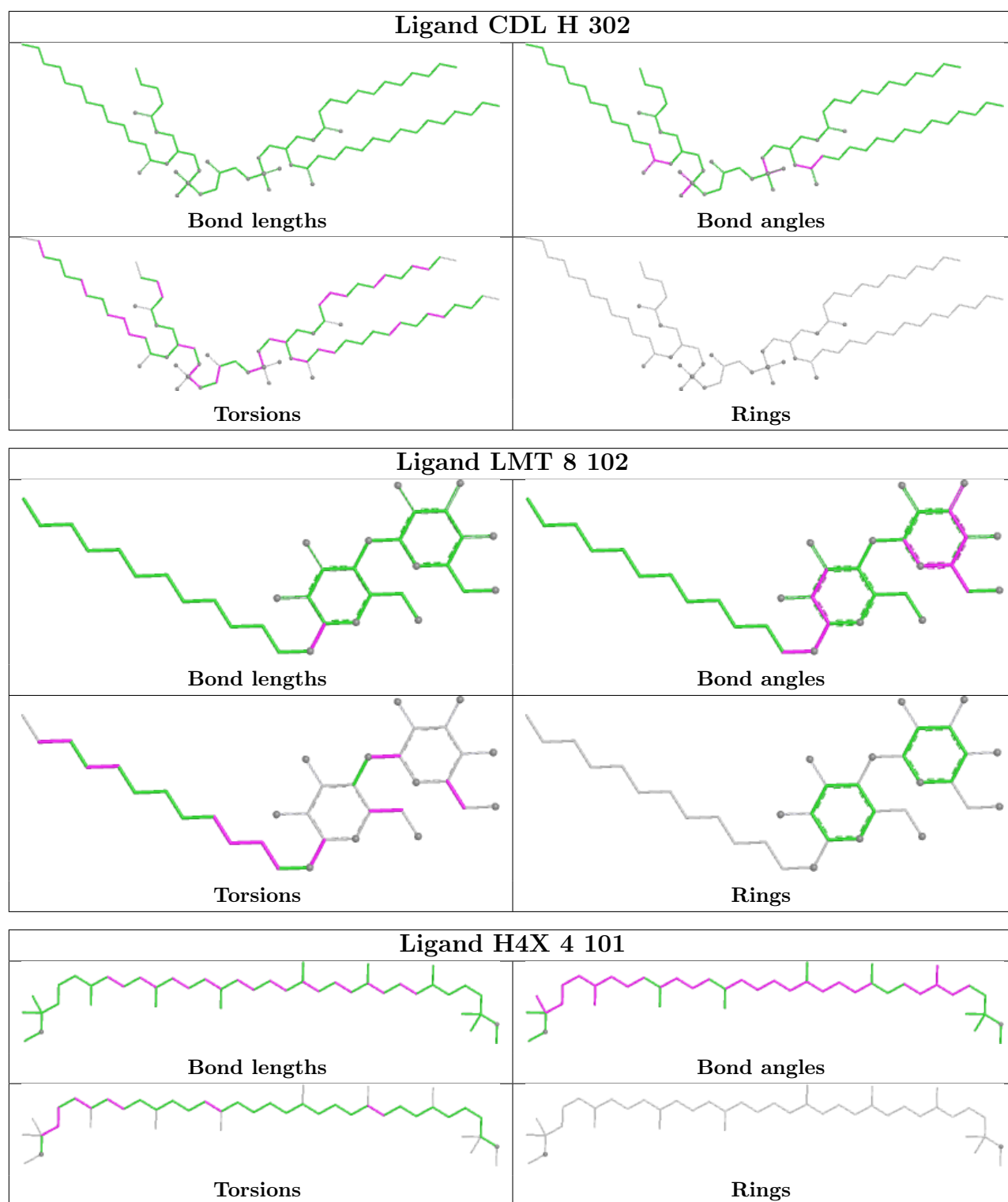


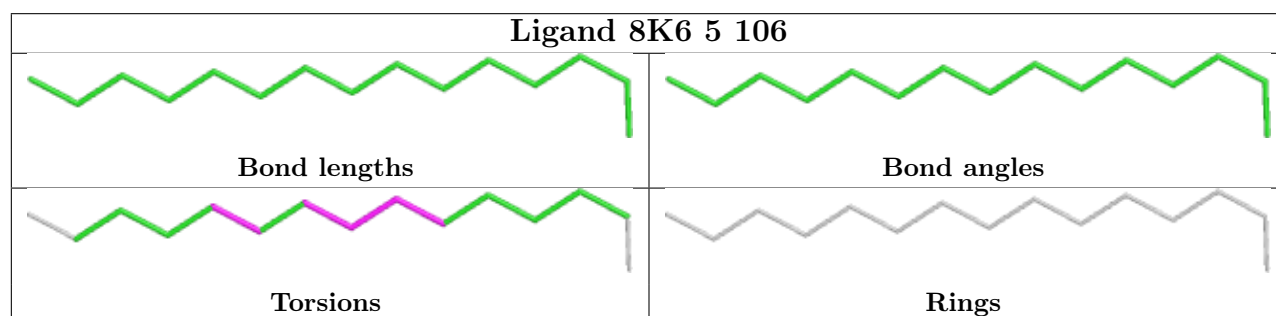
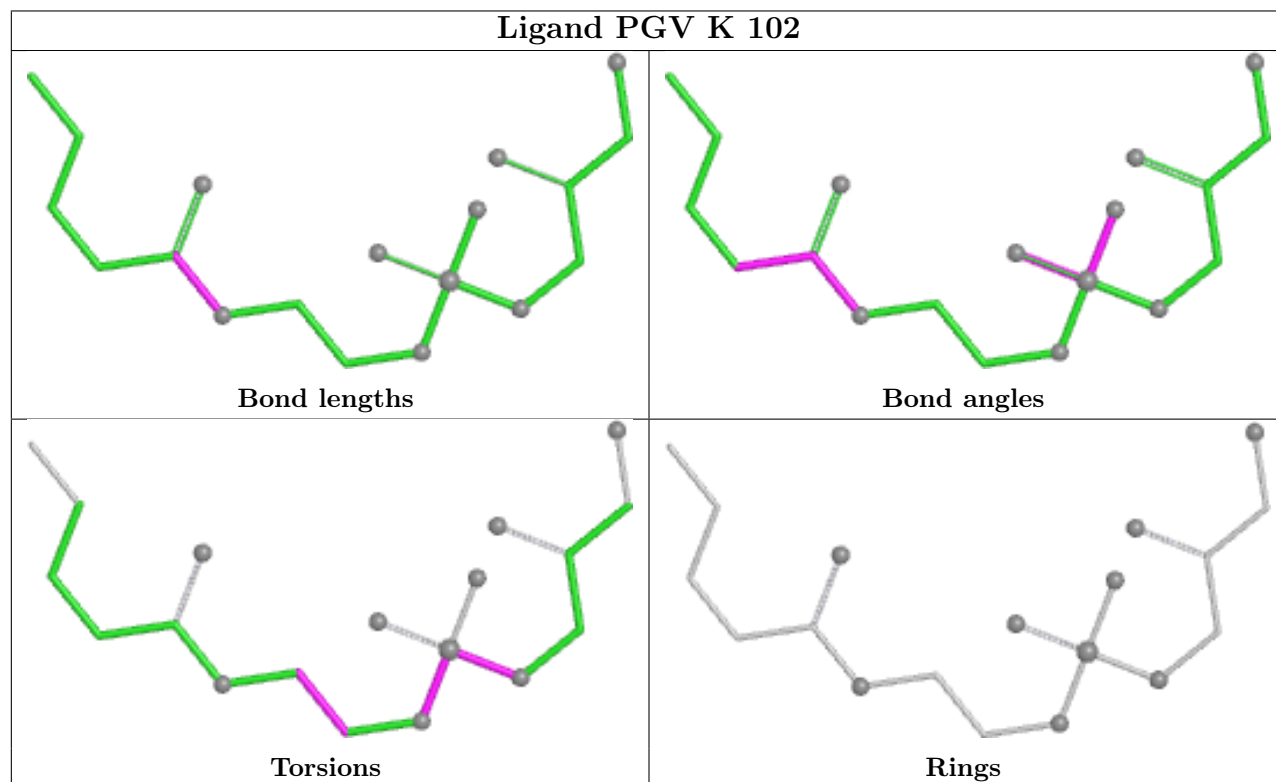
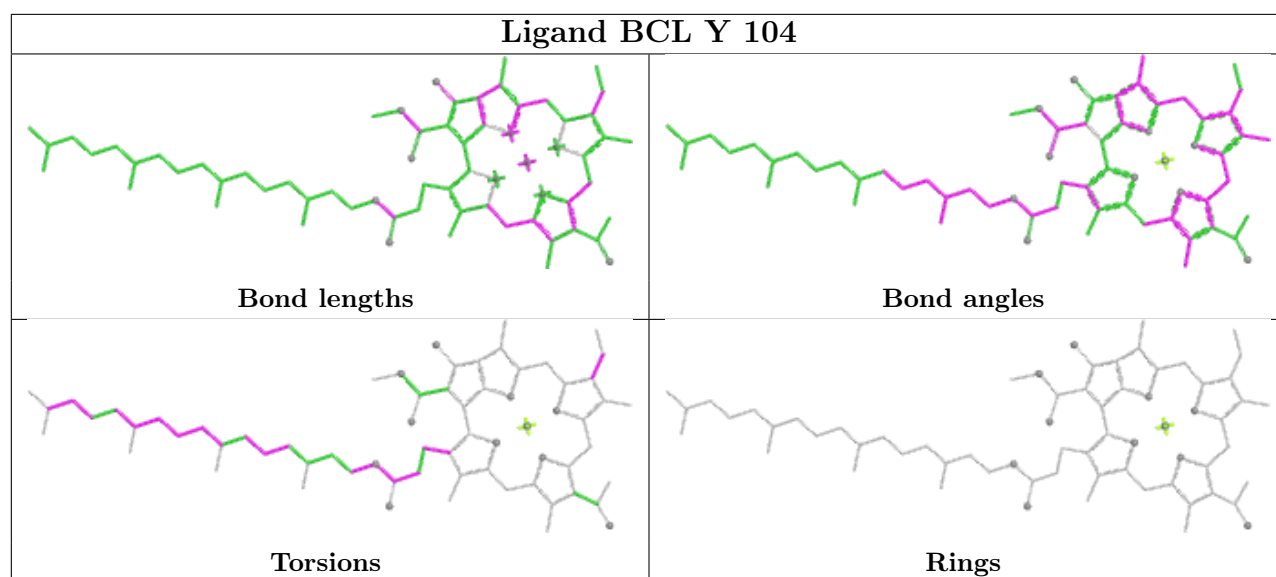
Ligand PGV 1 103

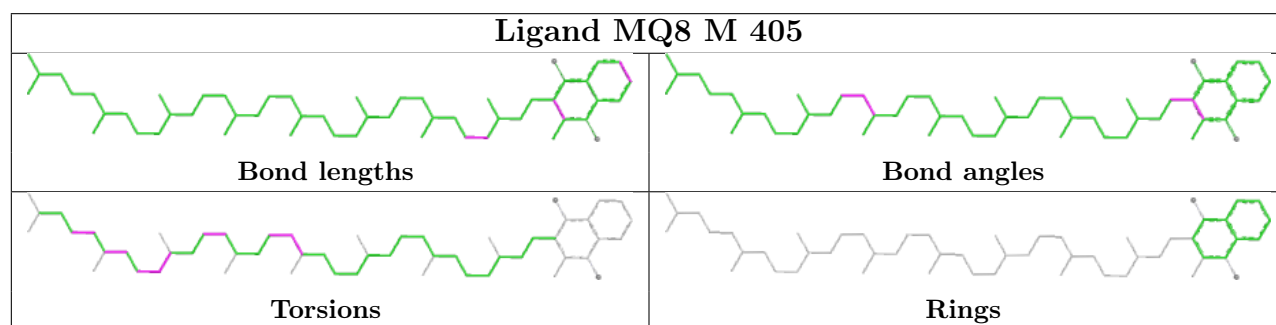
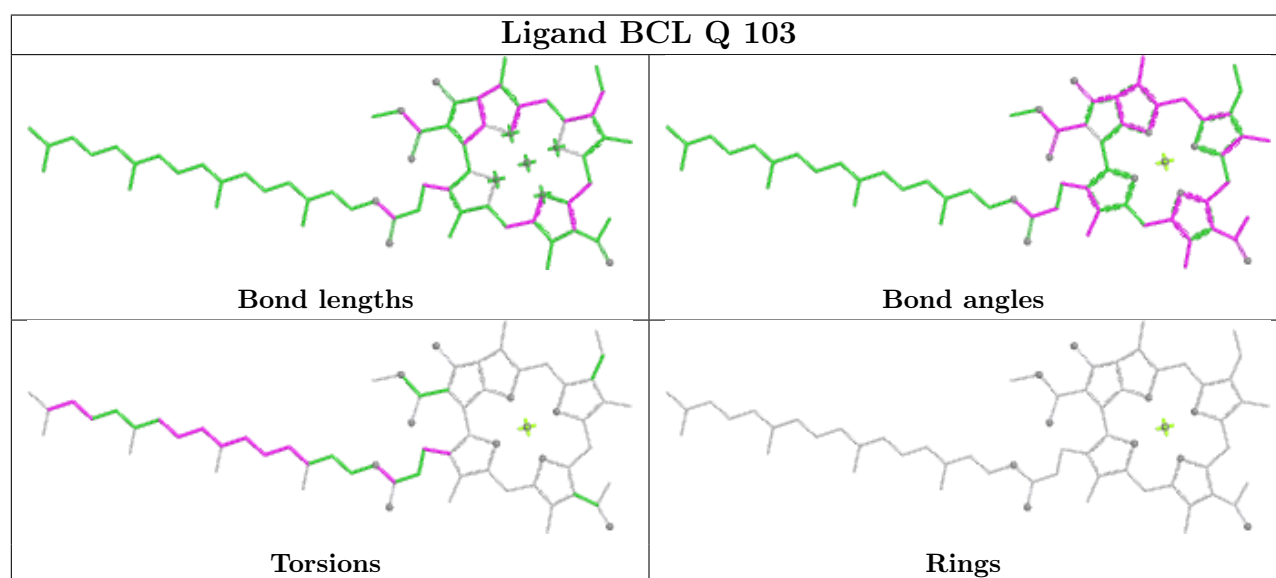
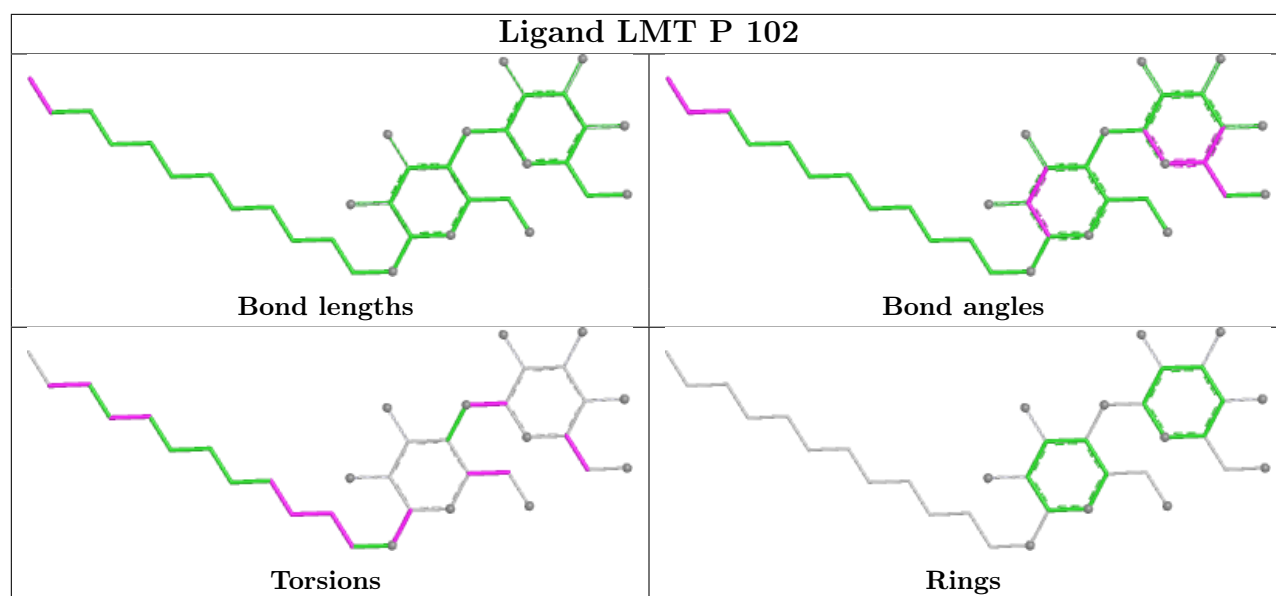


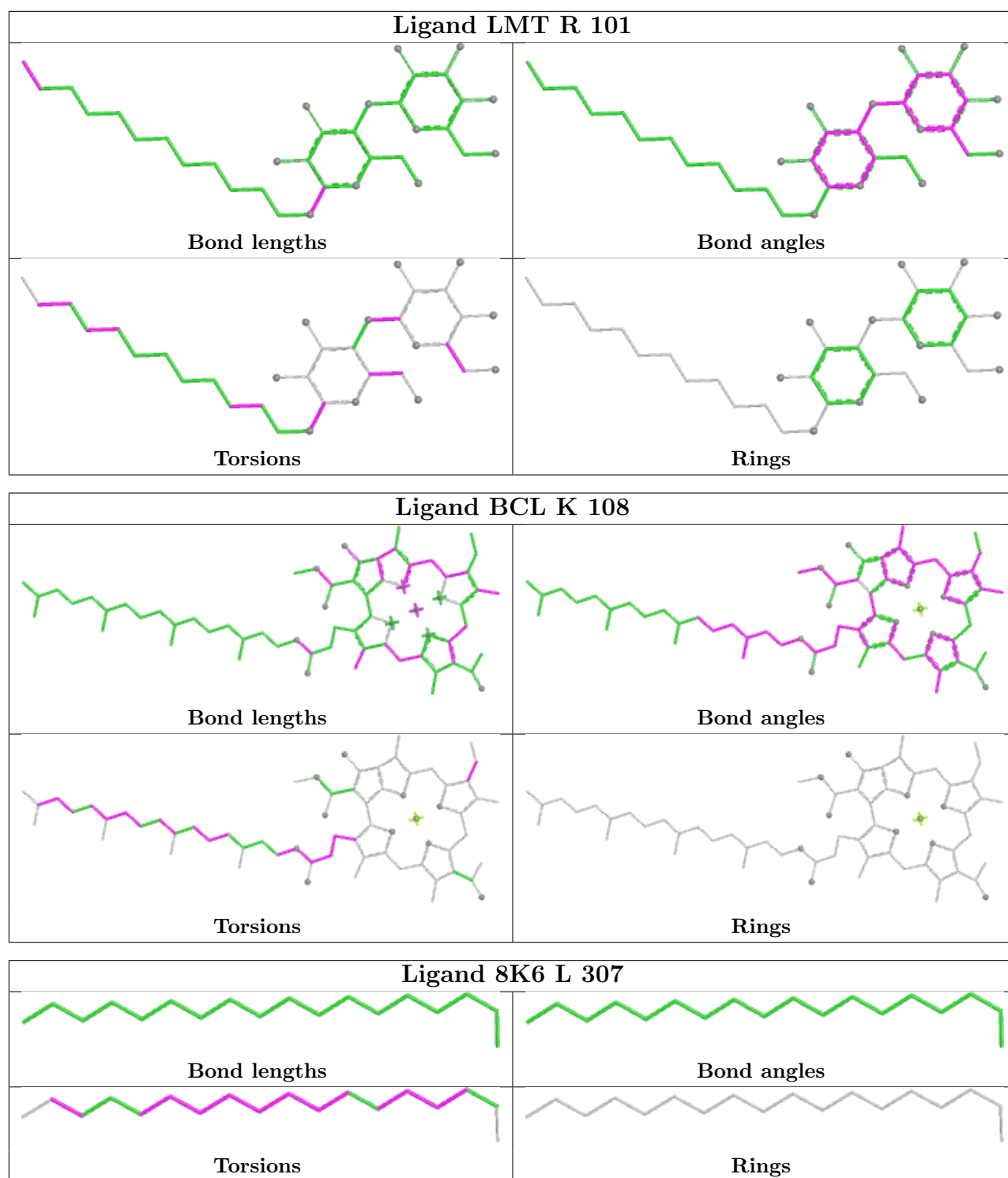
Ligand LMT X 102

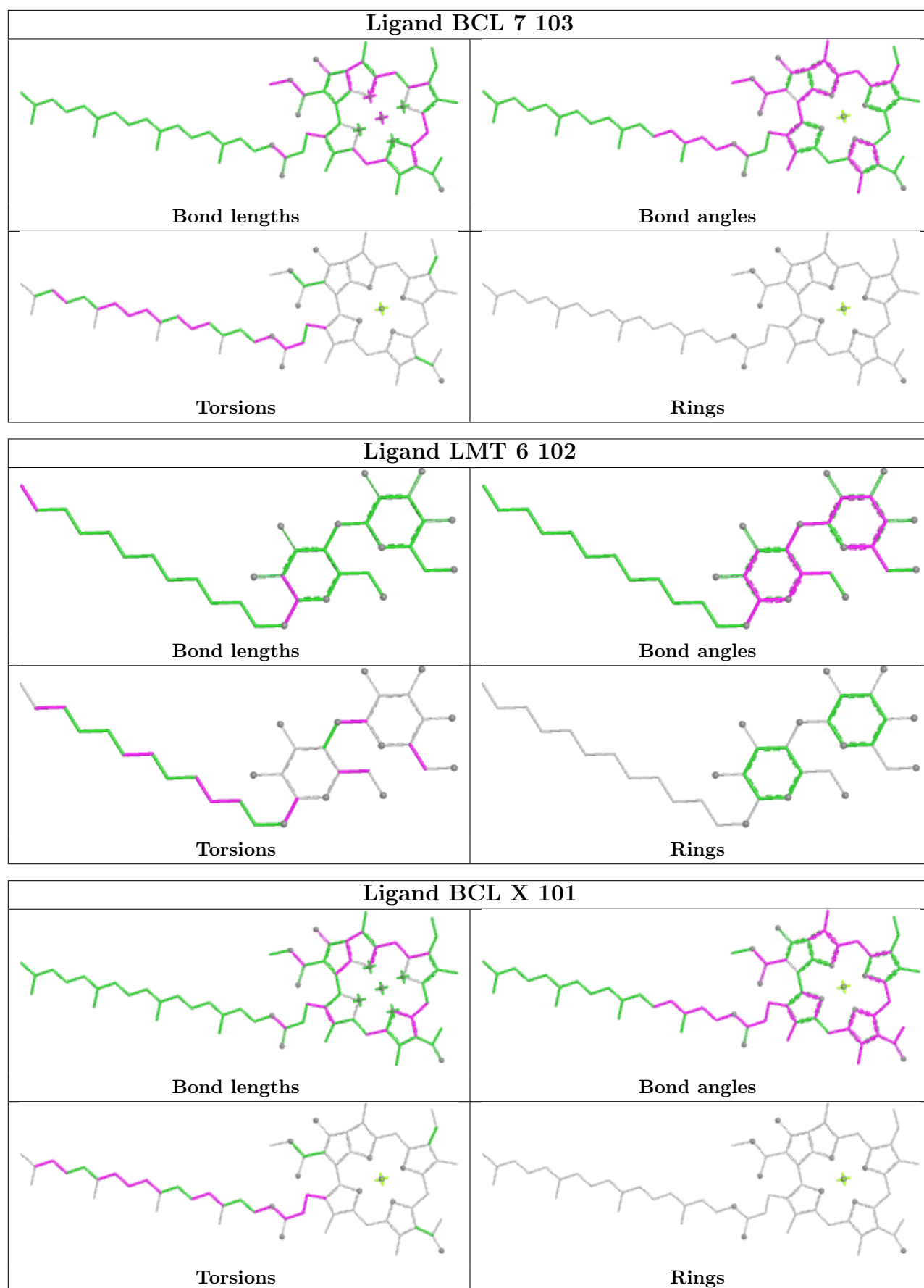




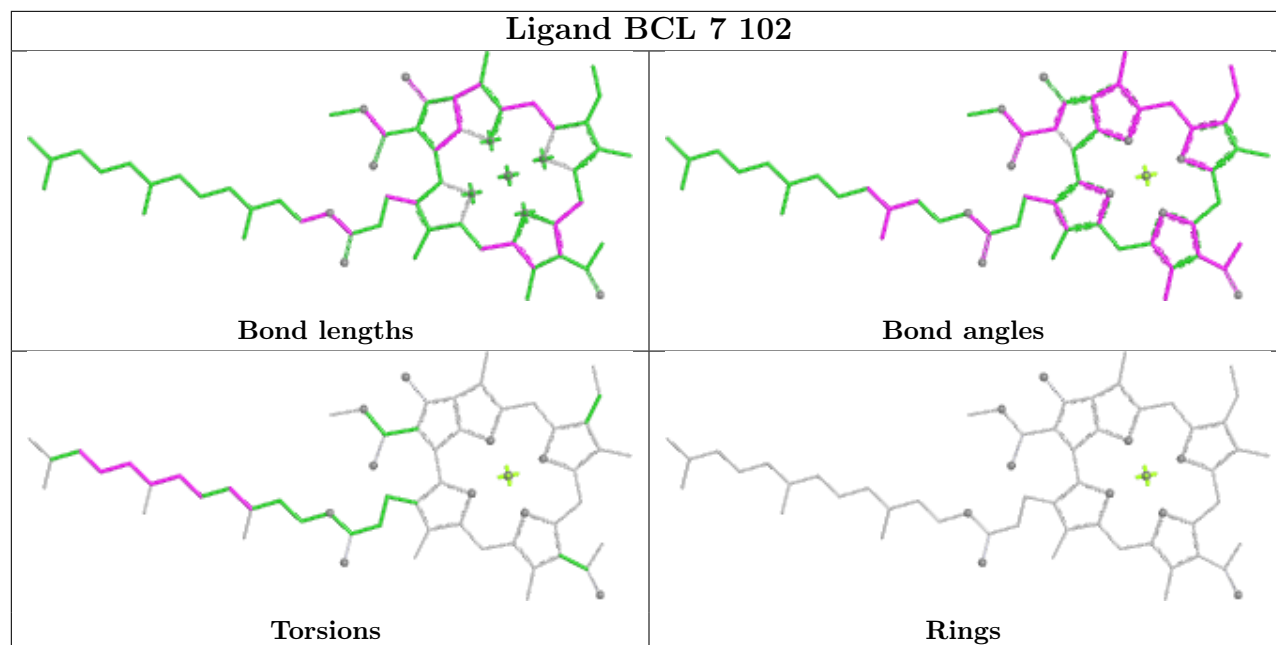




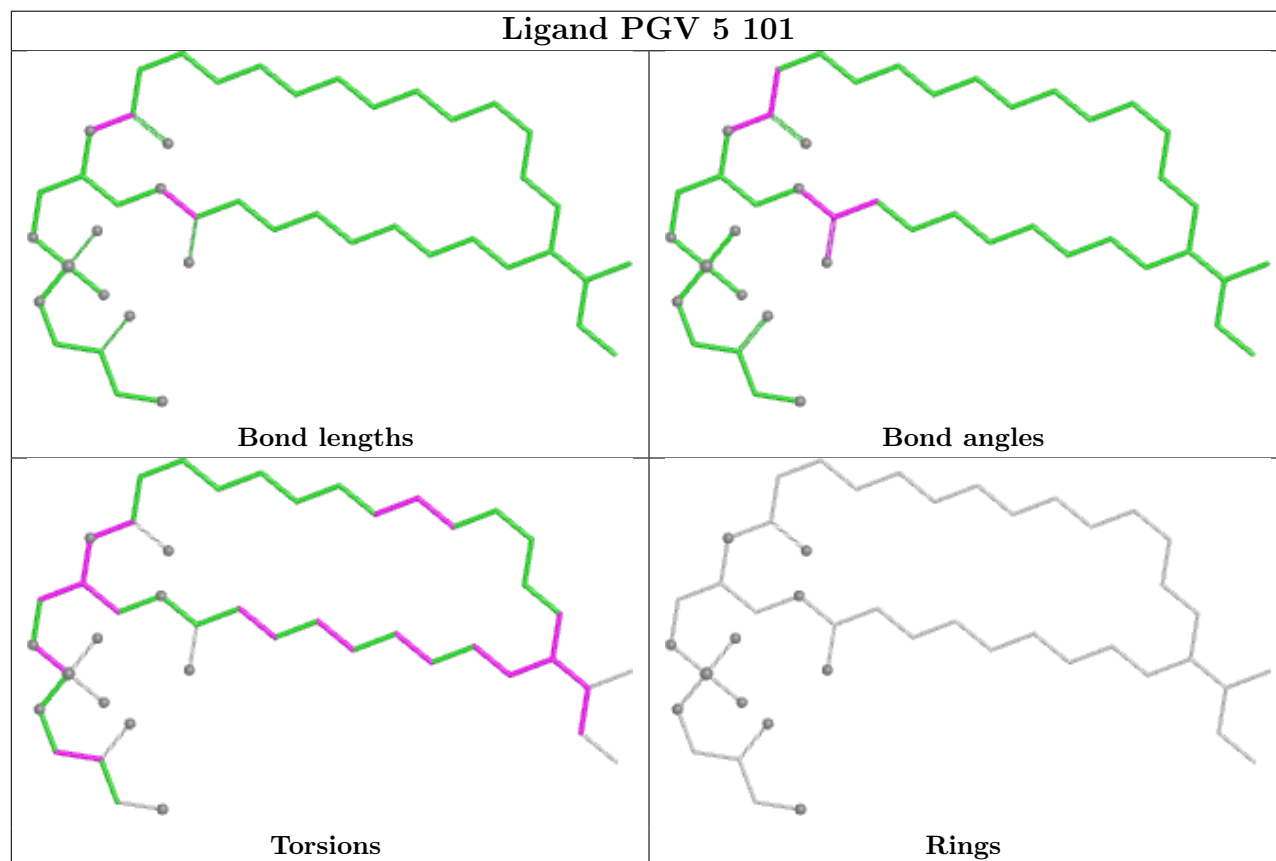


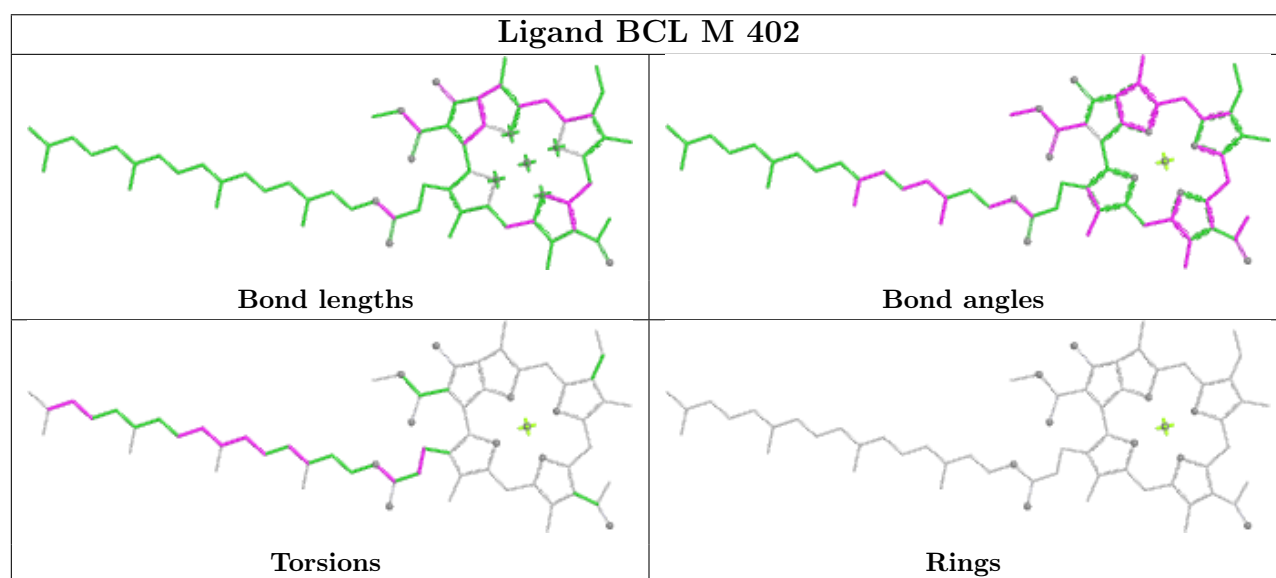
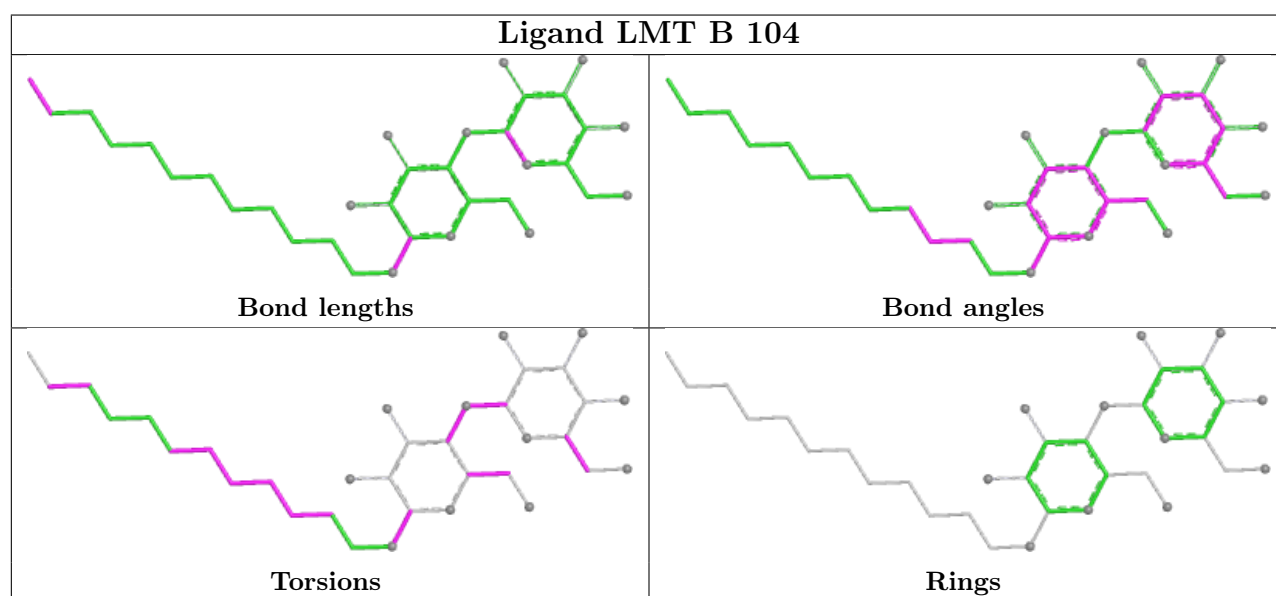
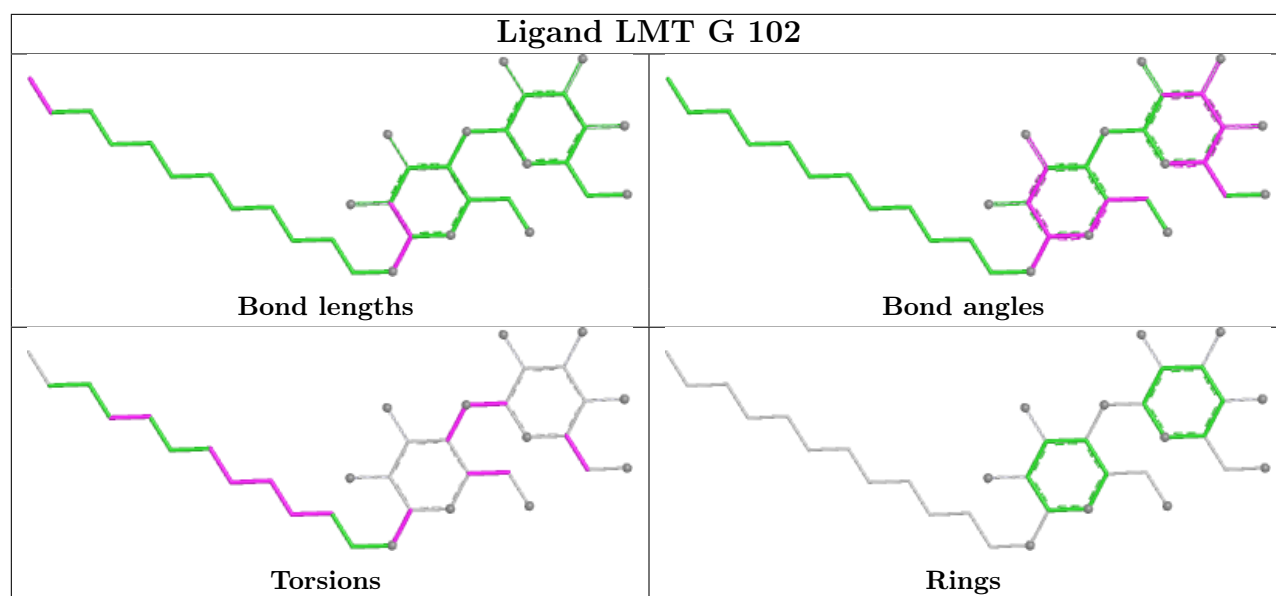


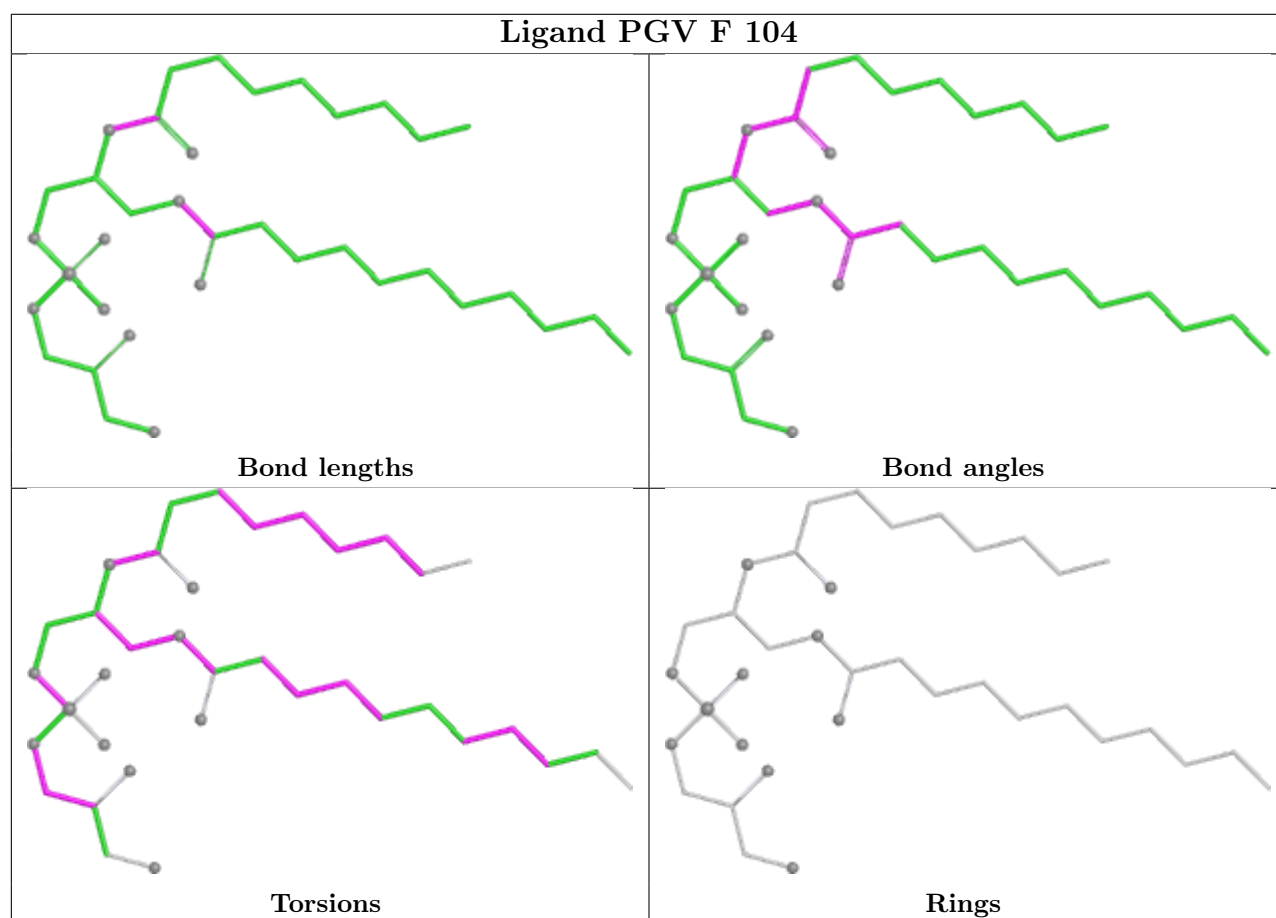
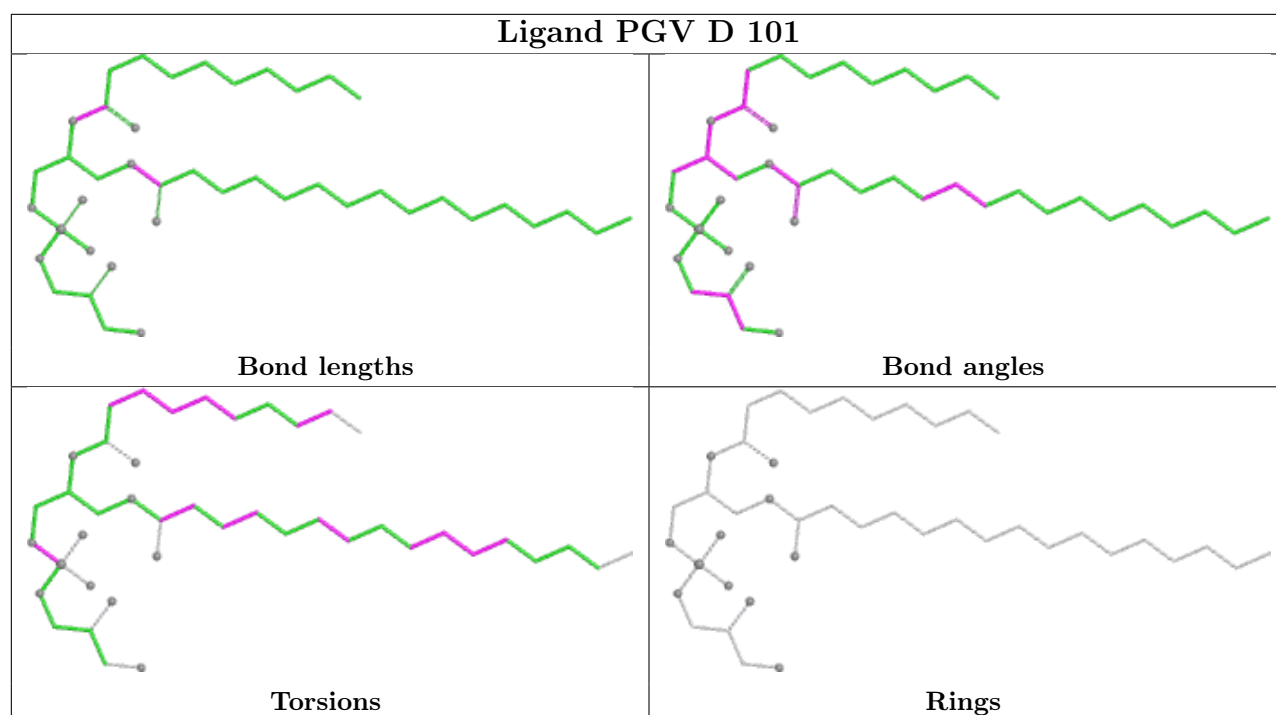
Ligand BCL 7 102

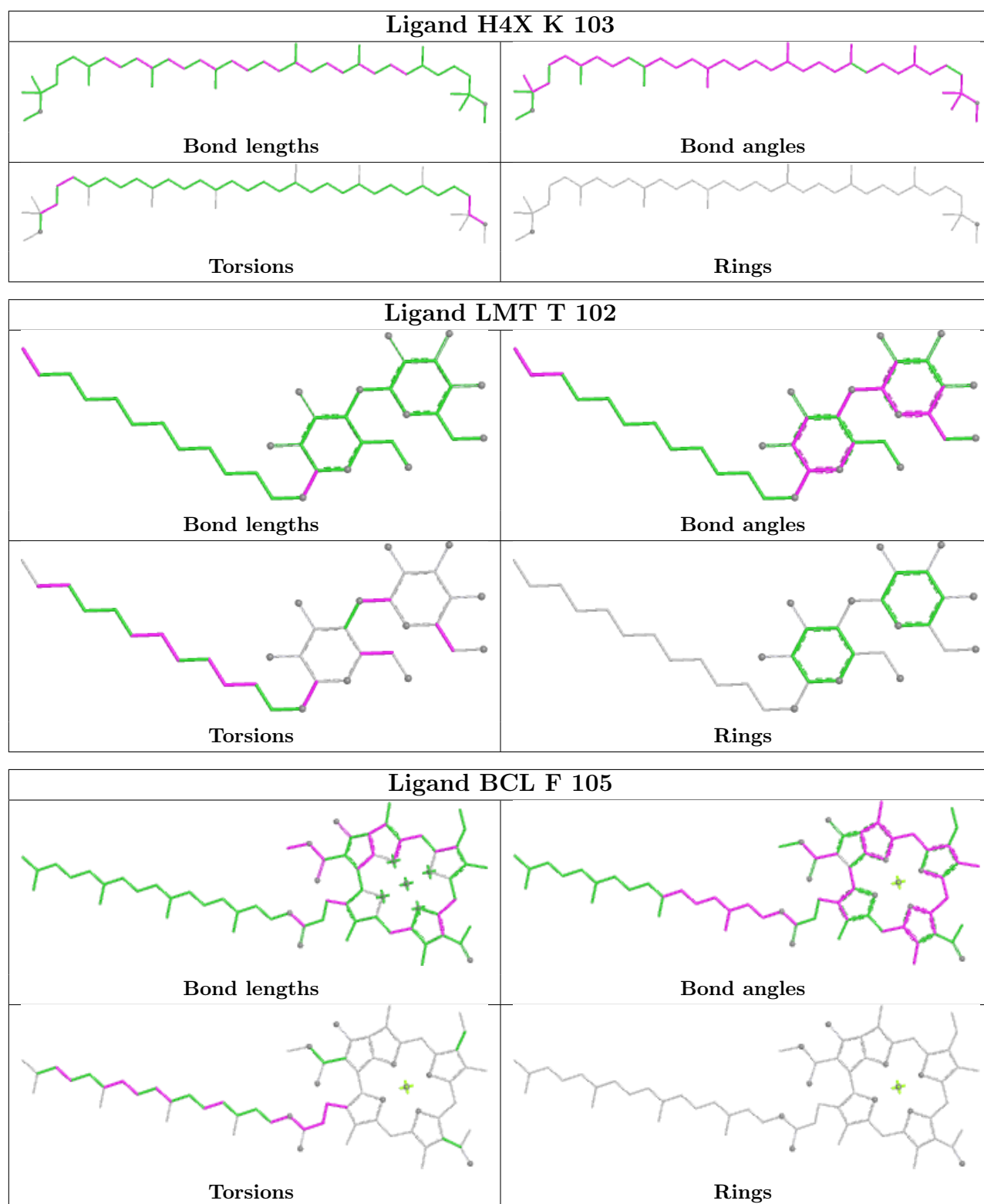


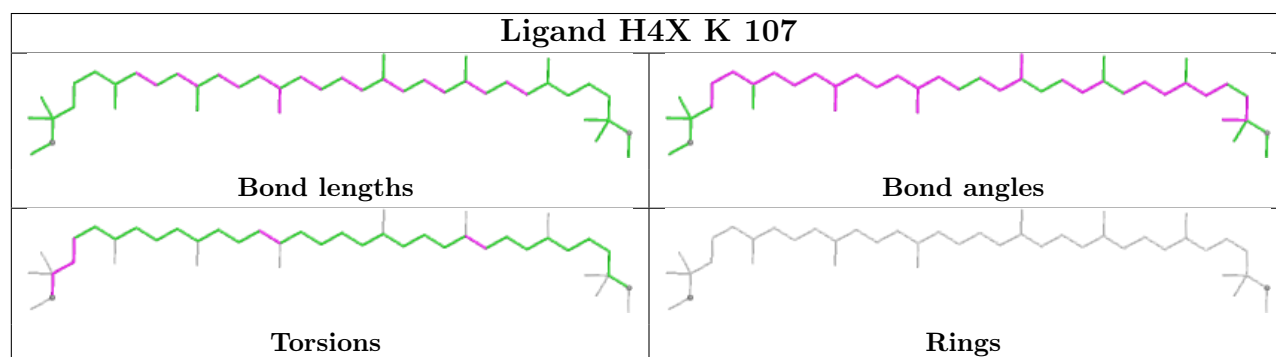
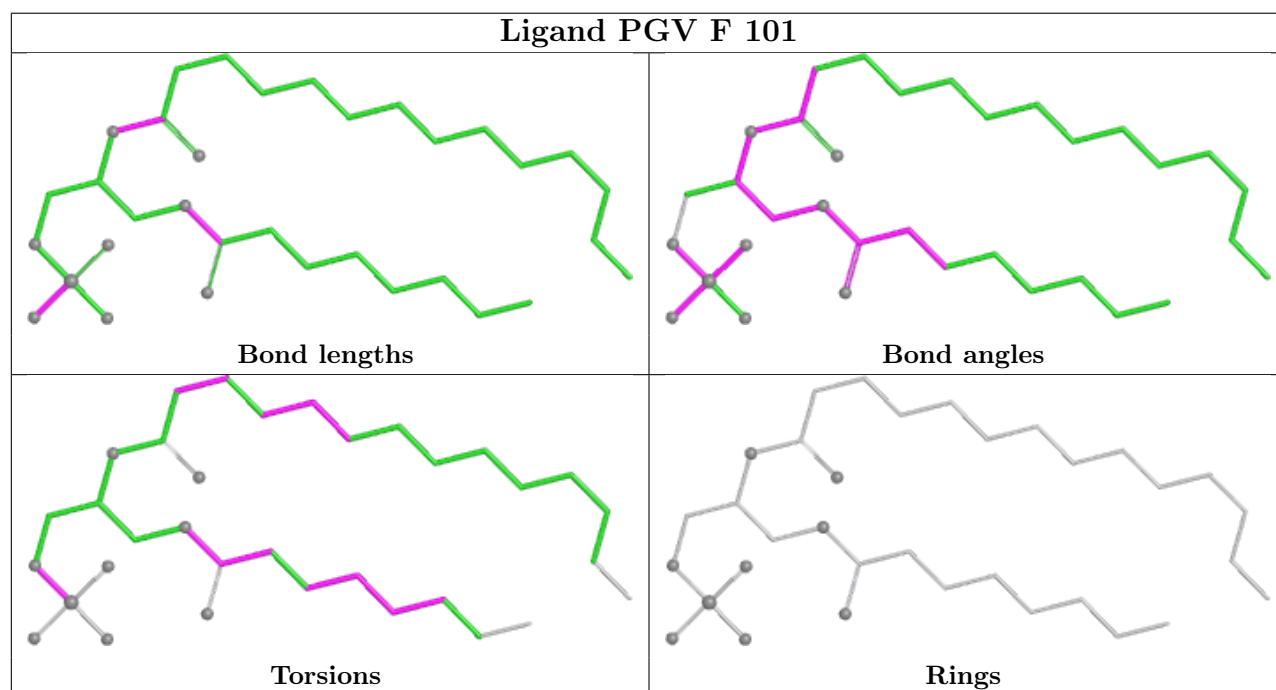
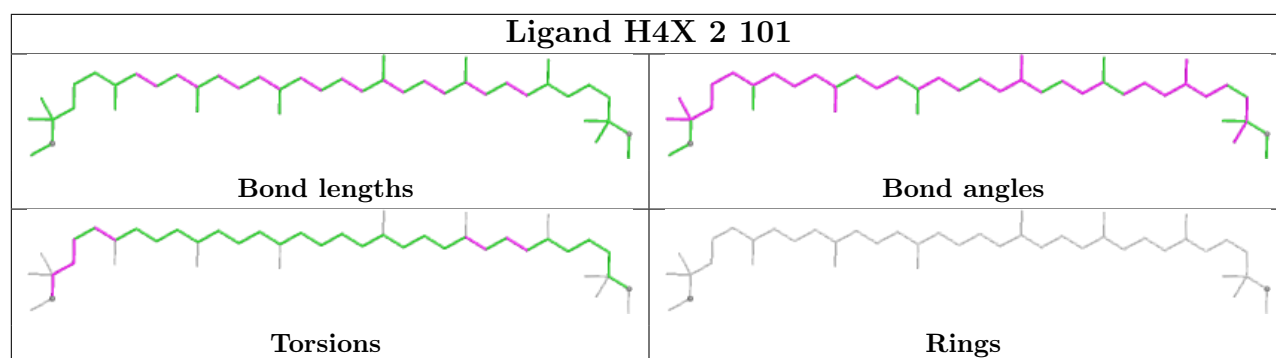
Ligand PGV 5 101

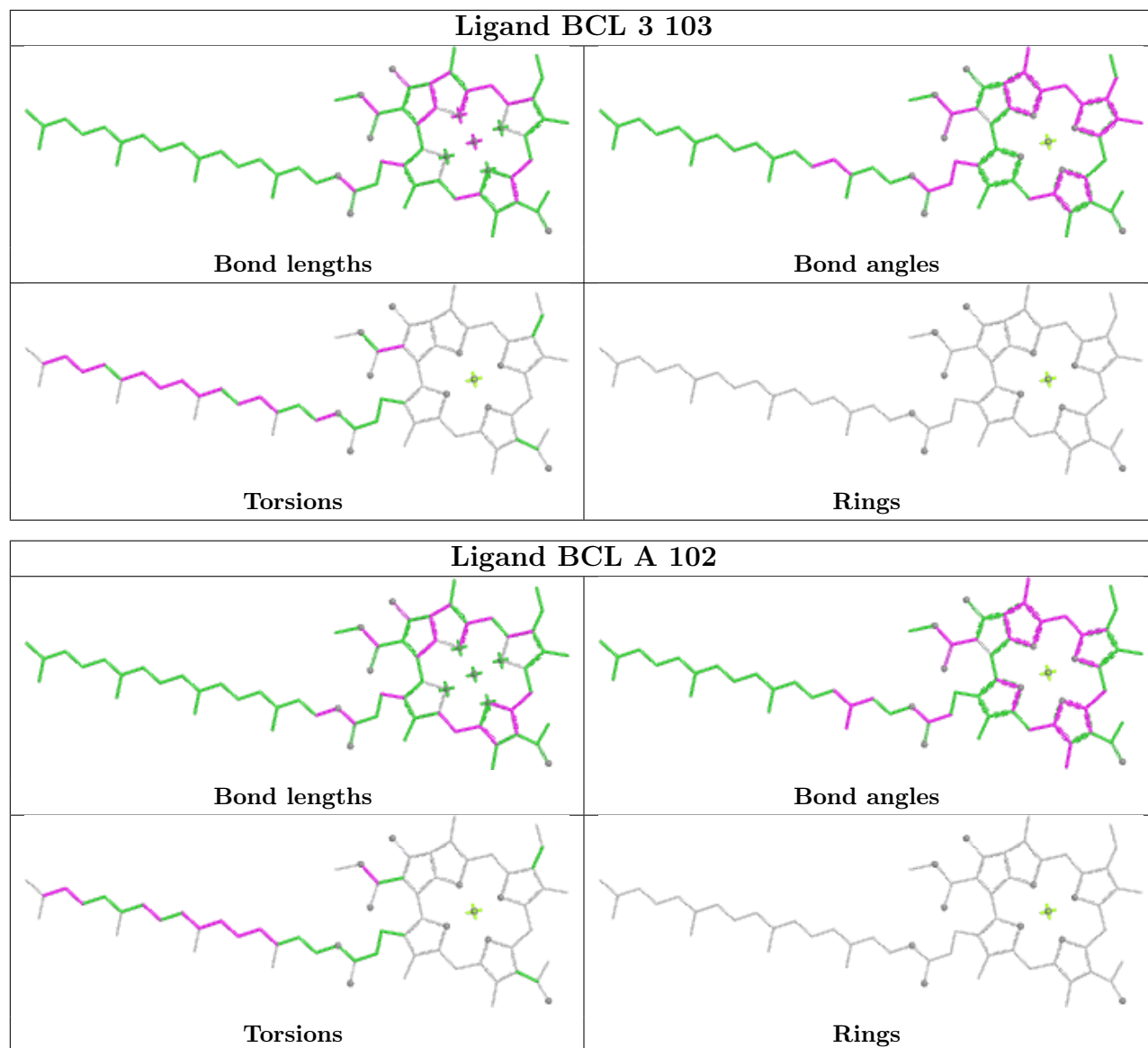


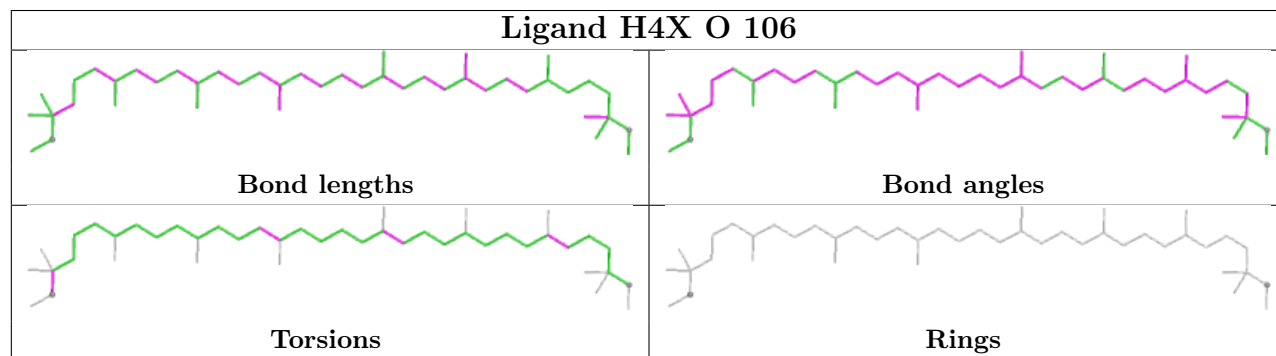
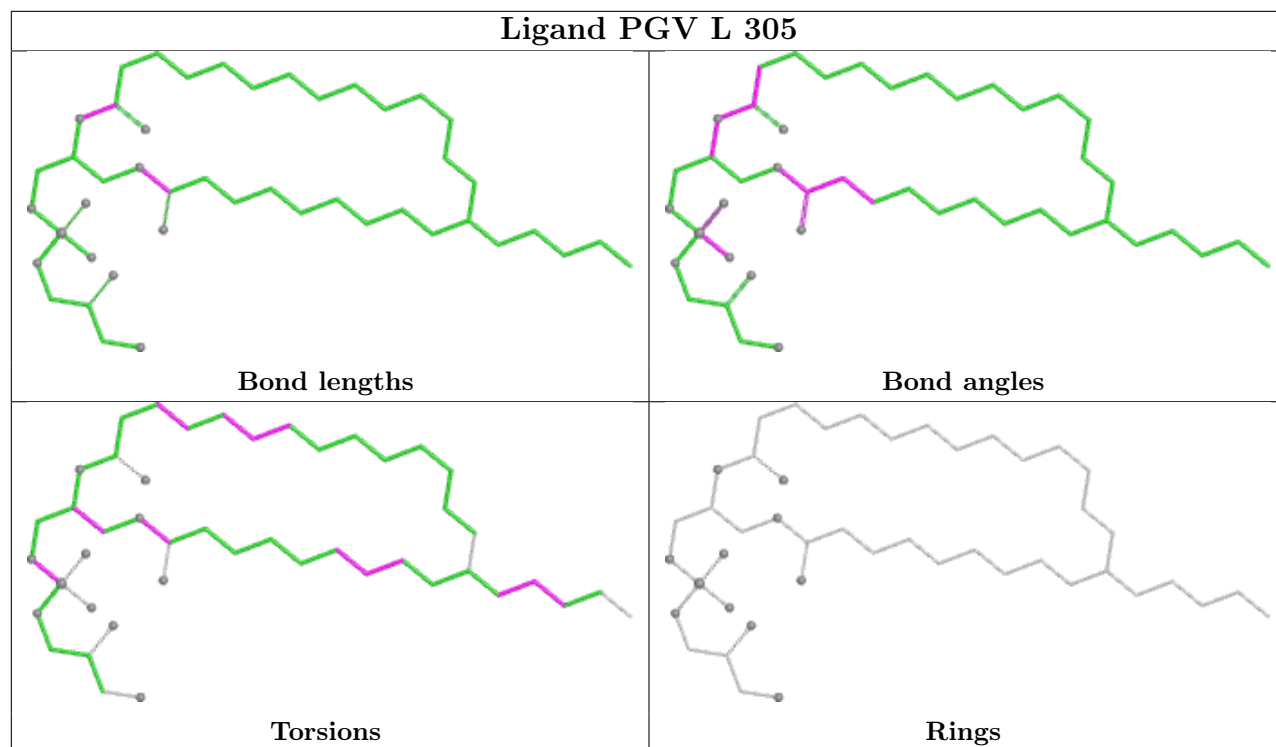


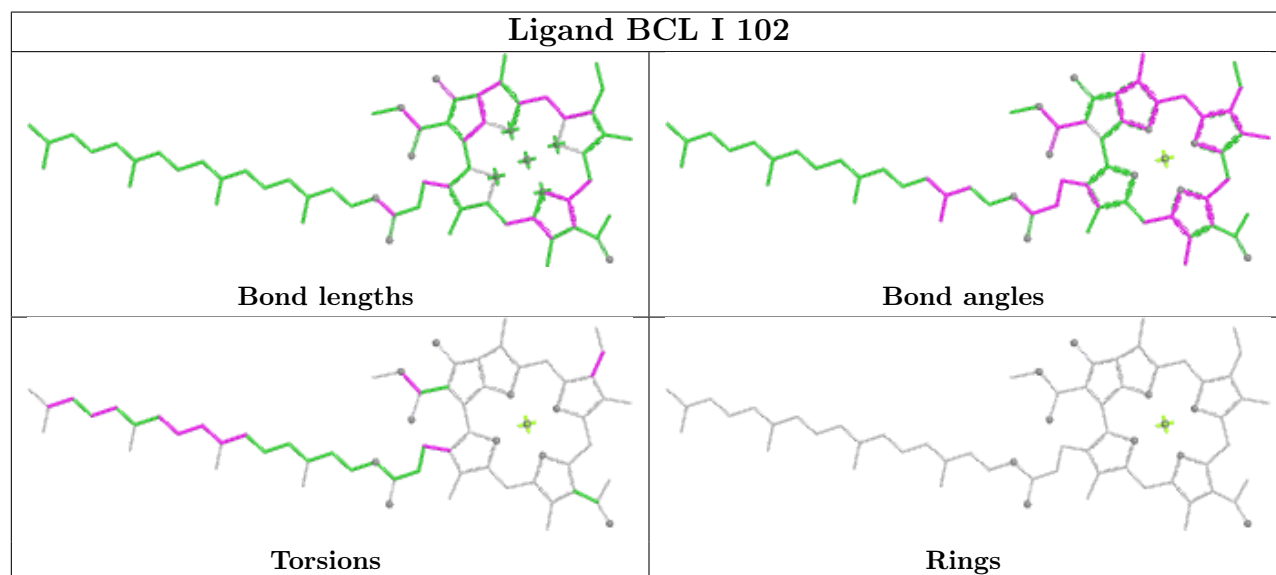
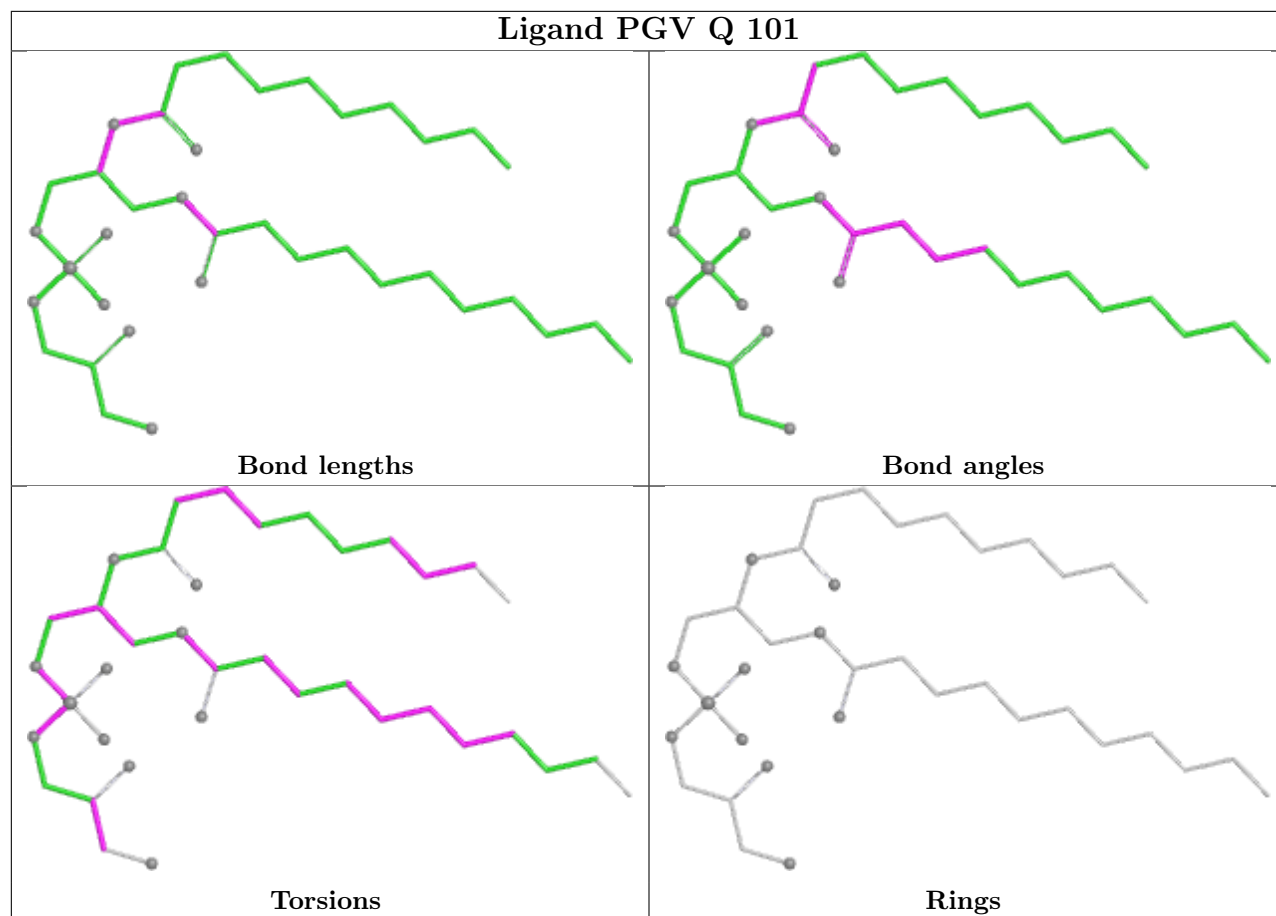


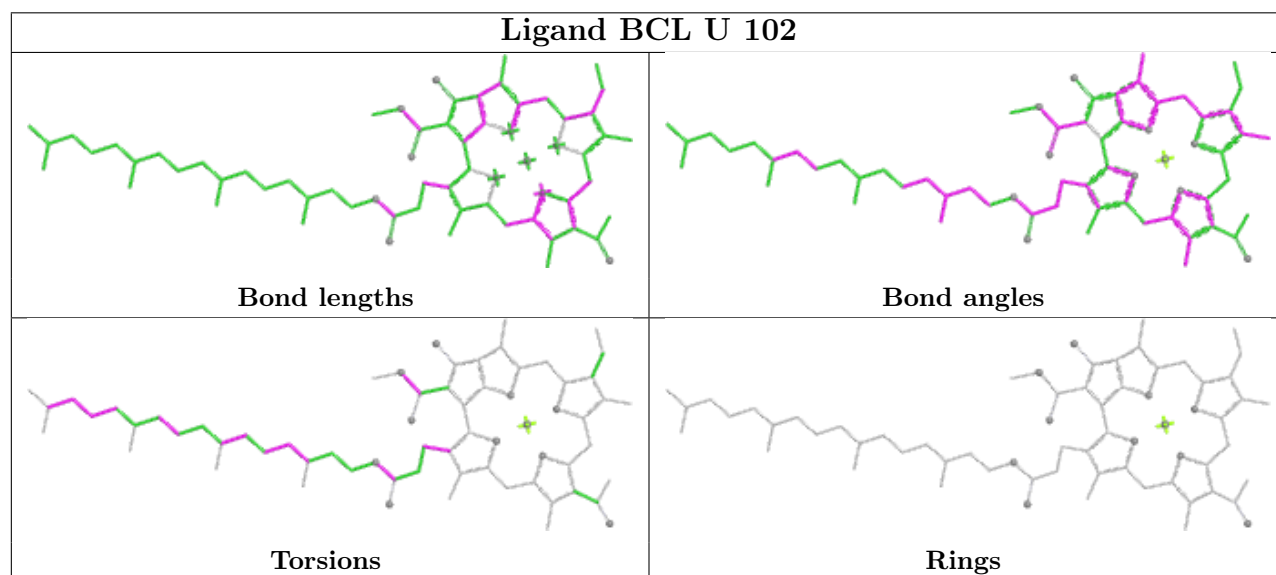
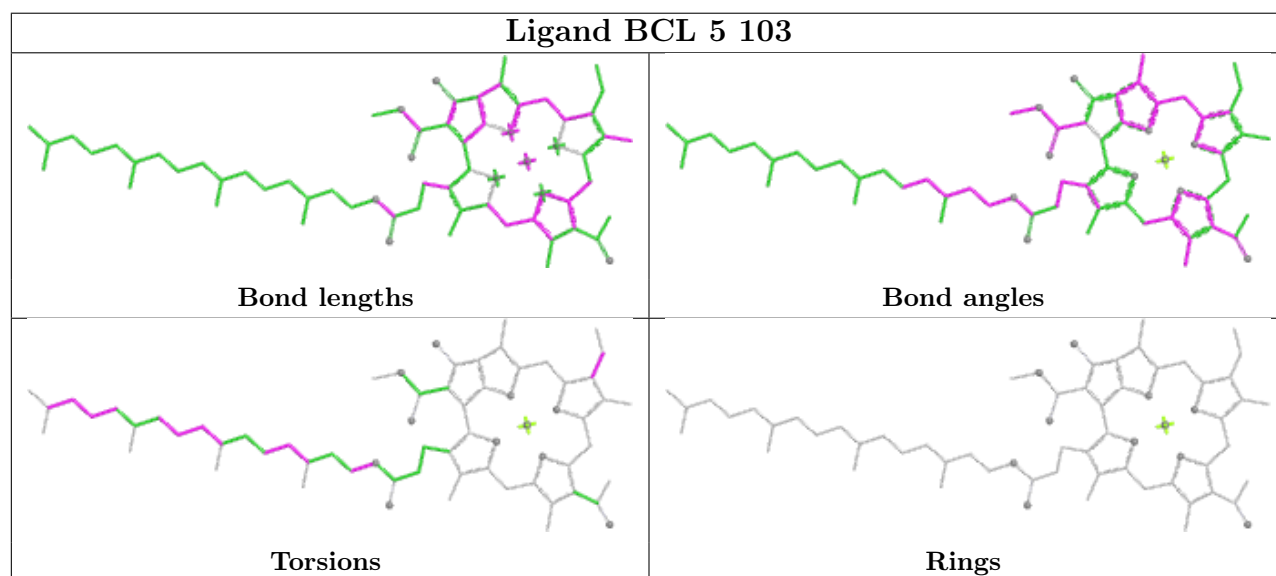
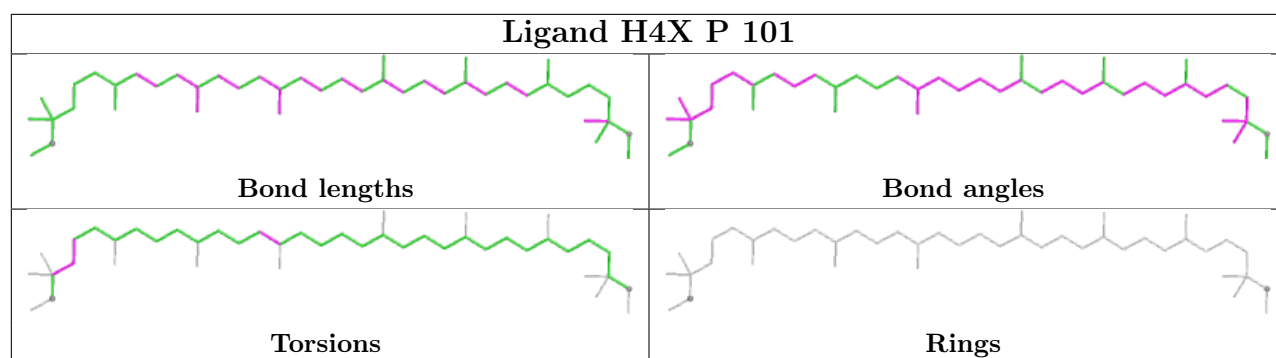


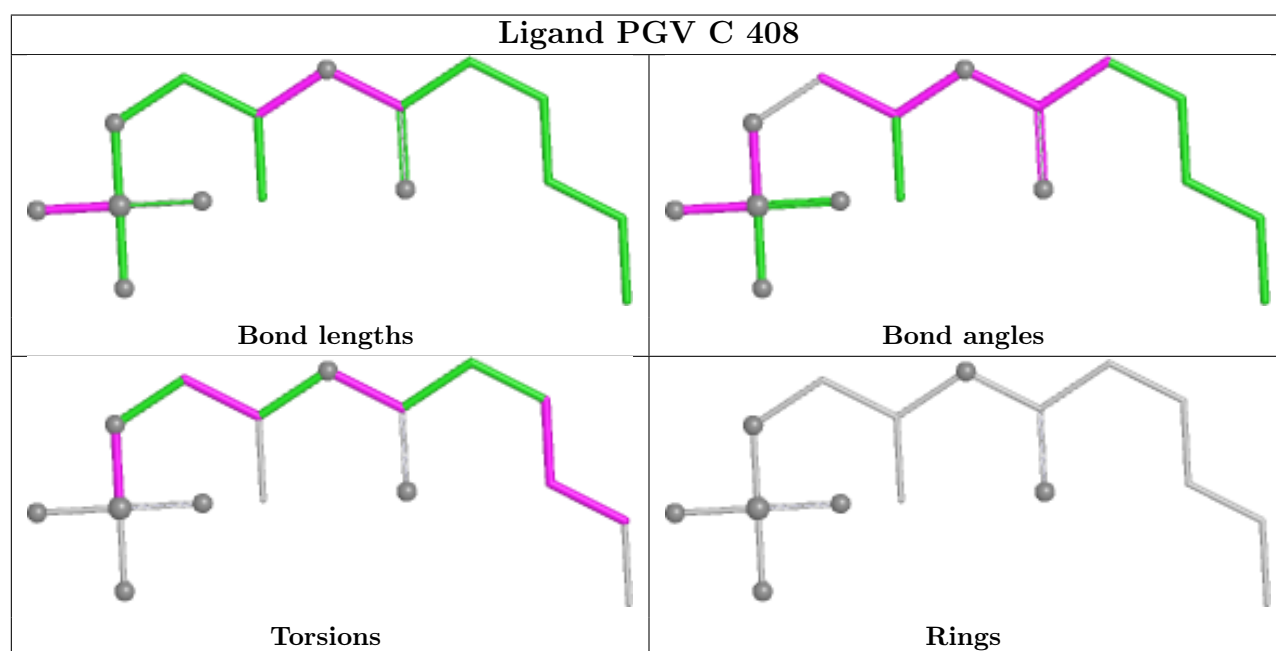
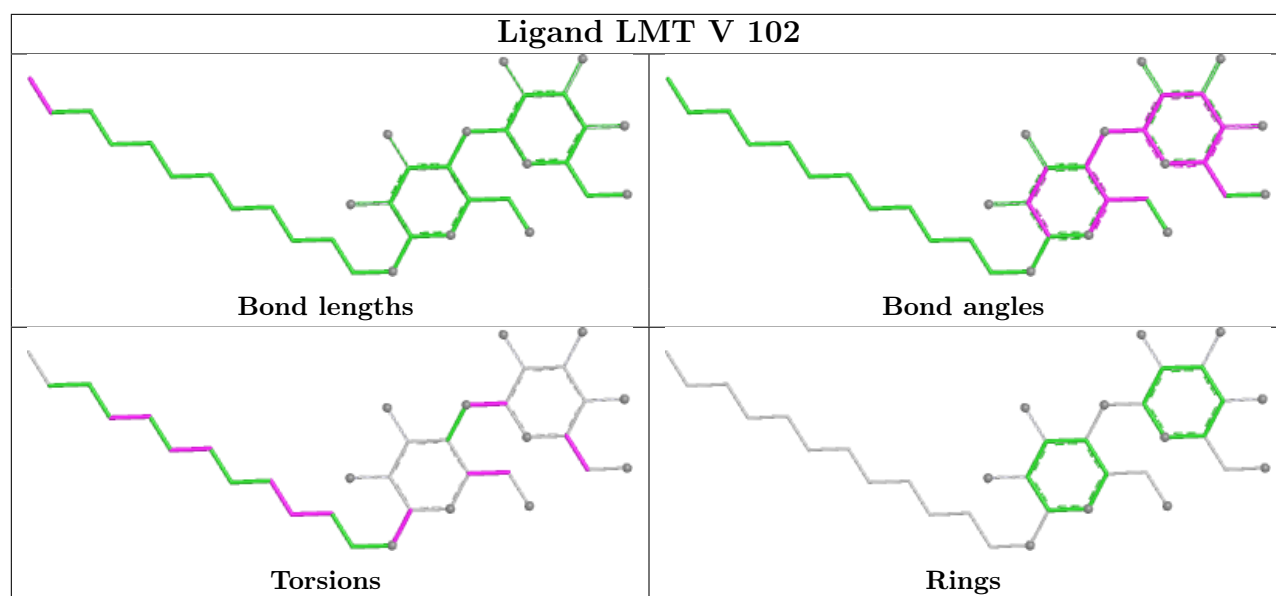




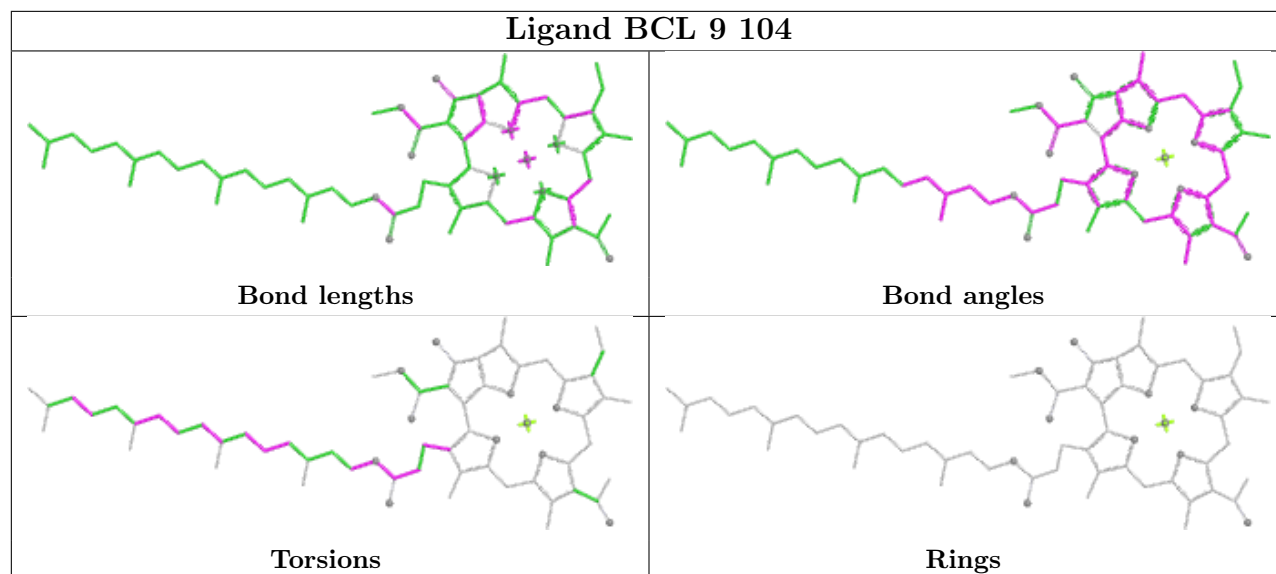




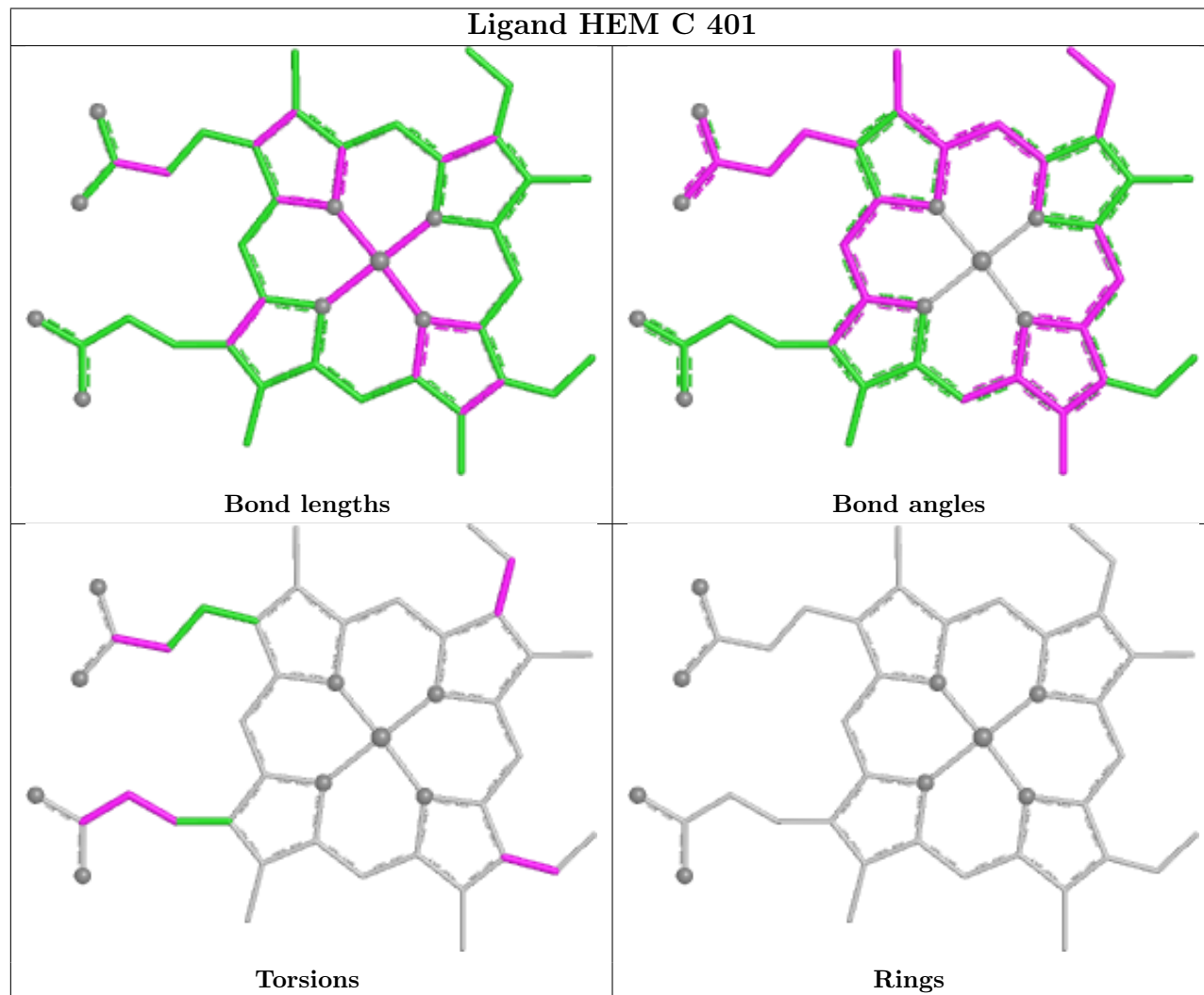


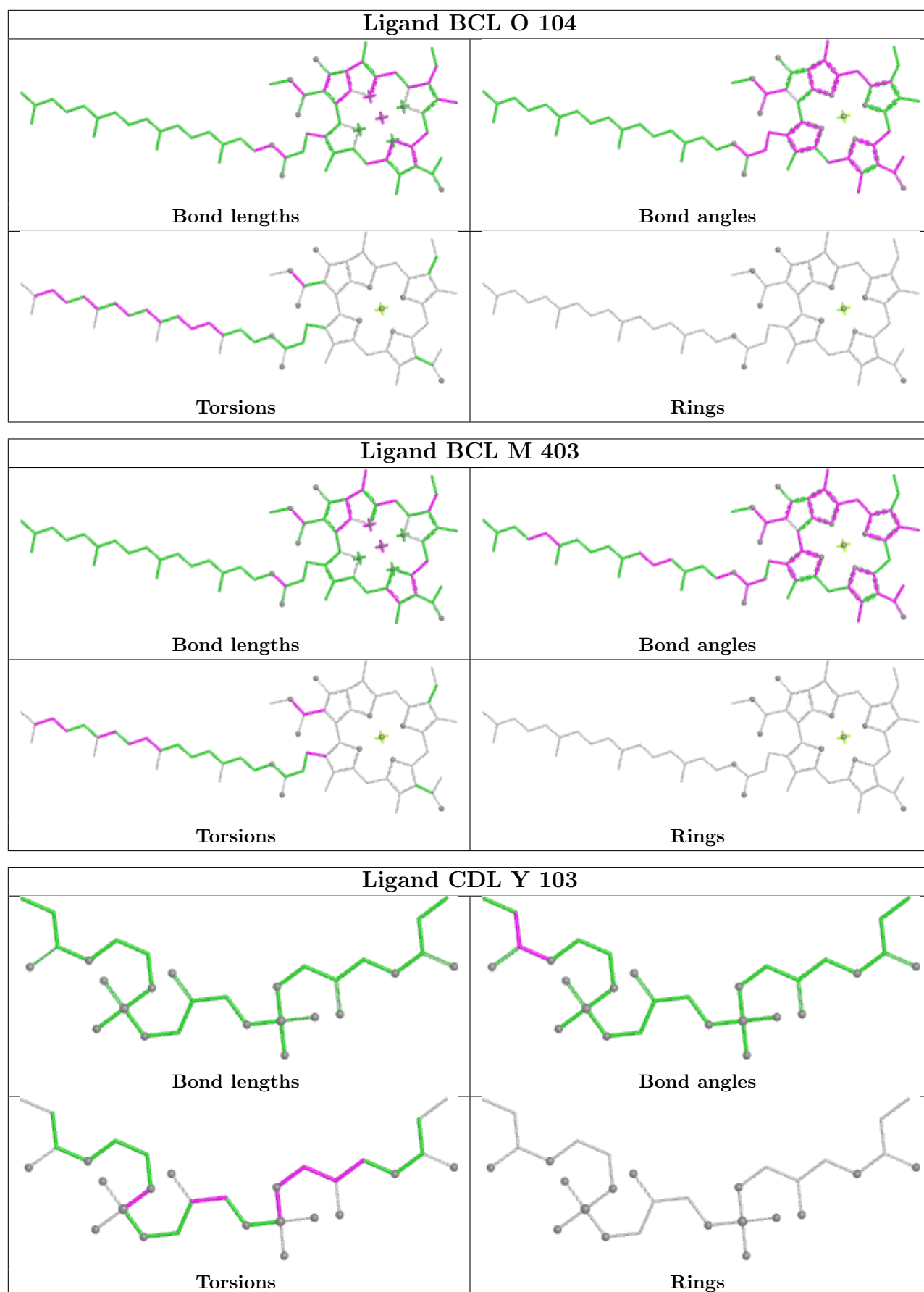


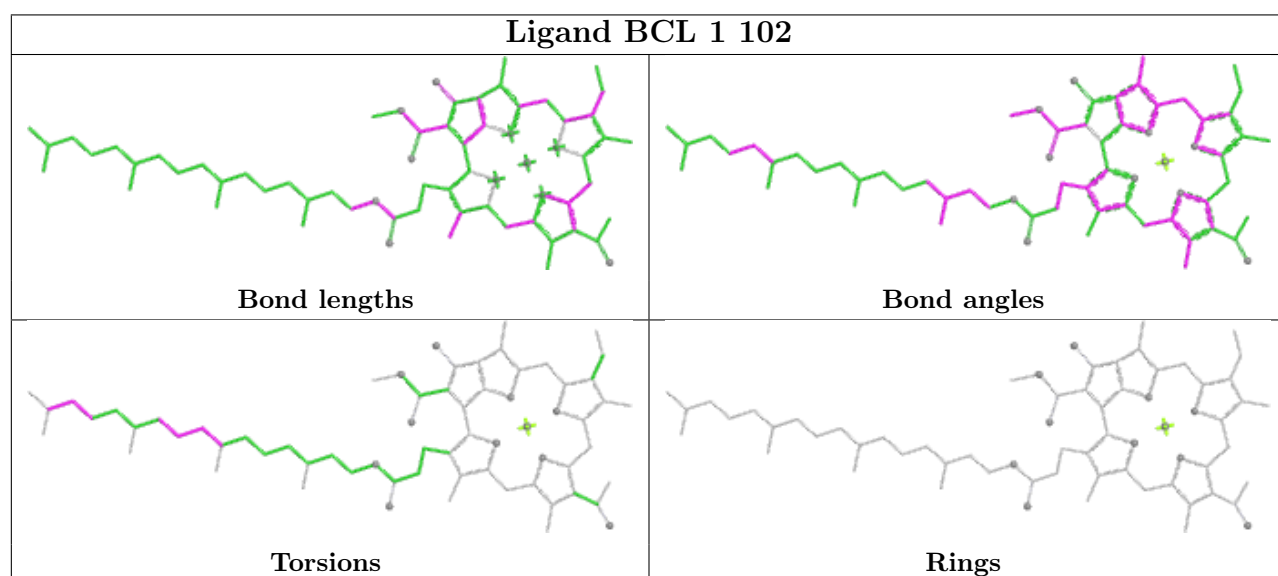
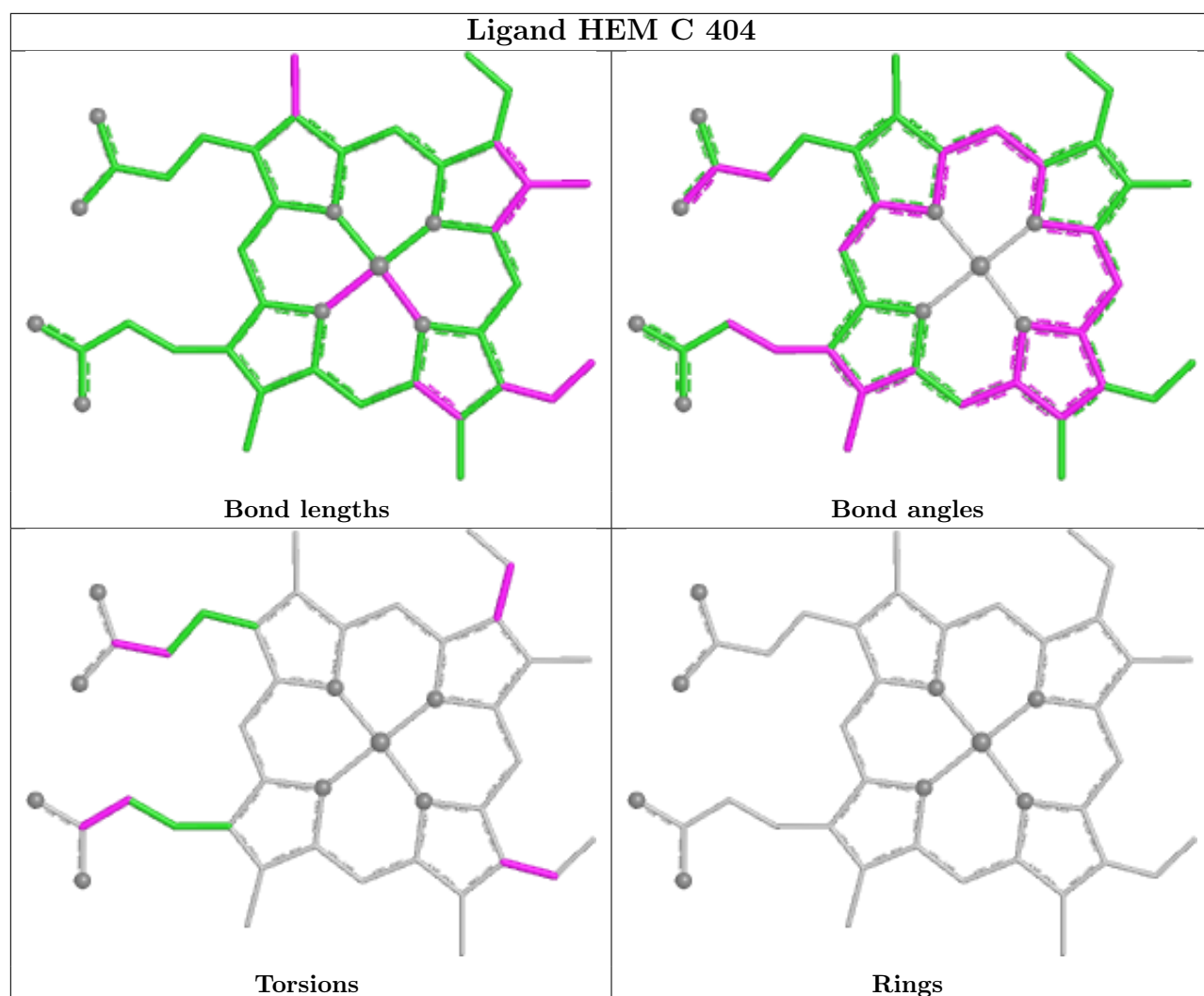
Ligand BCL 9 104

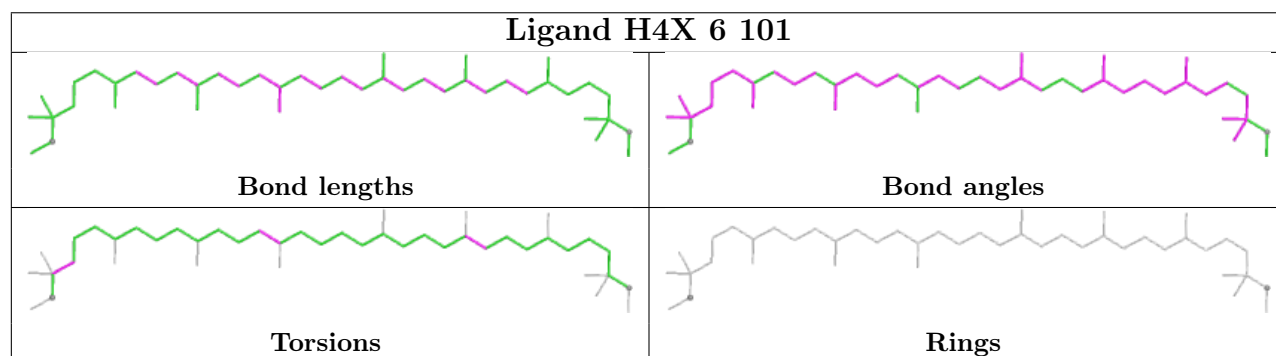
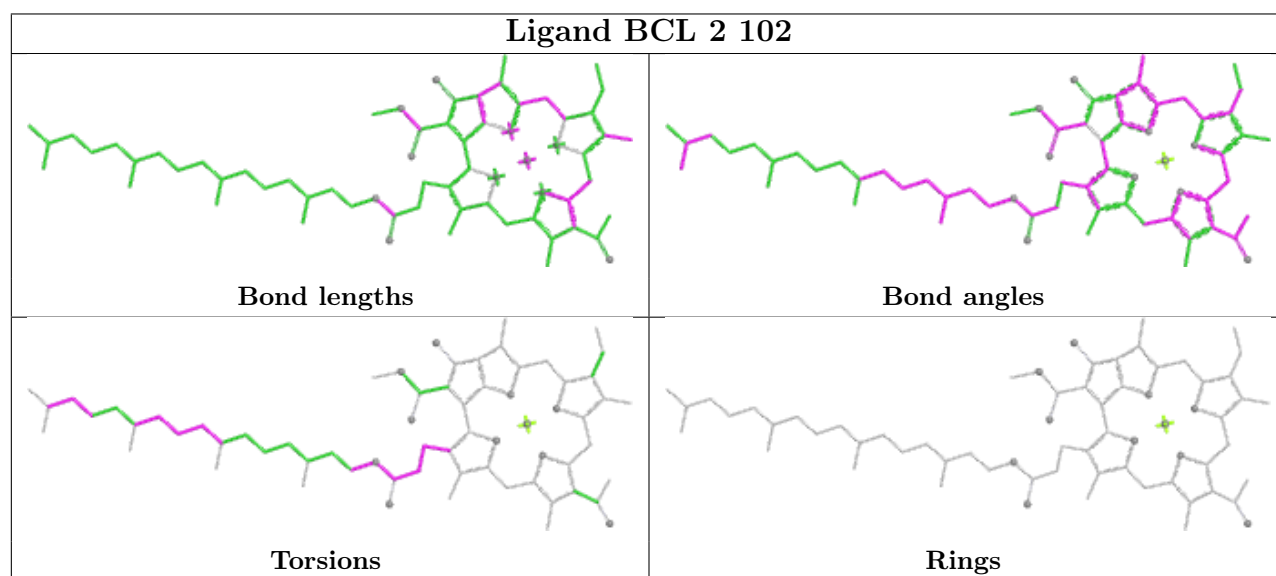
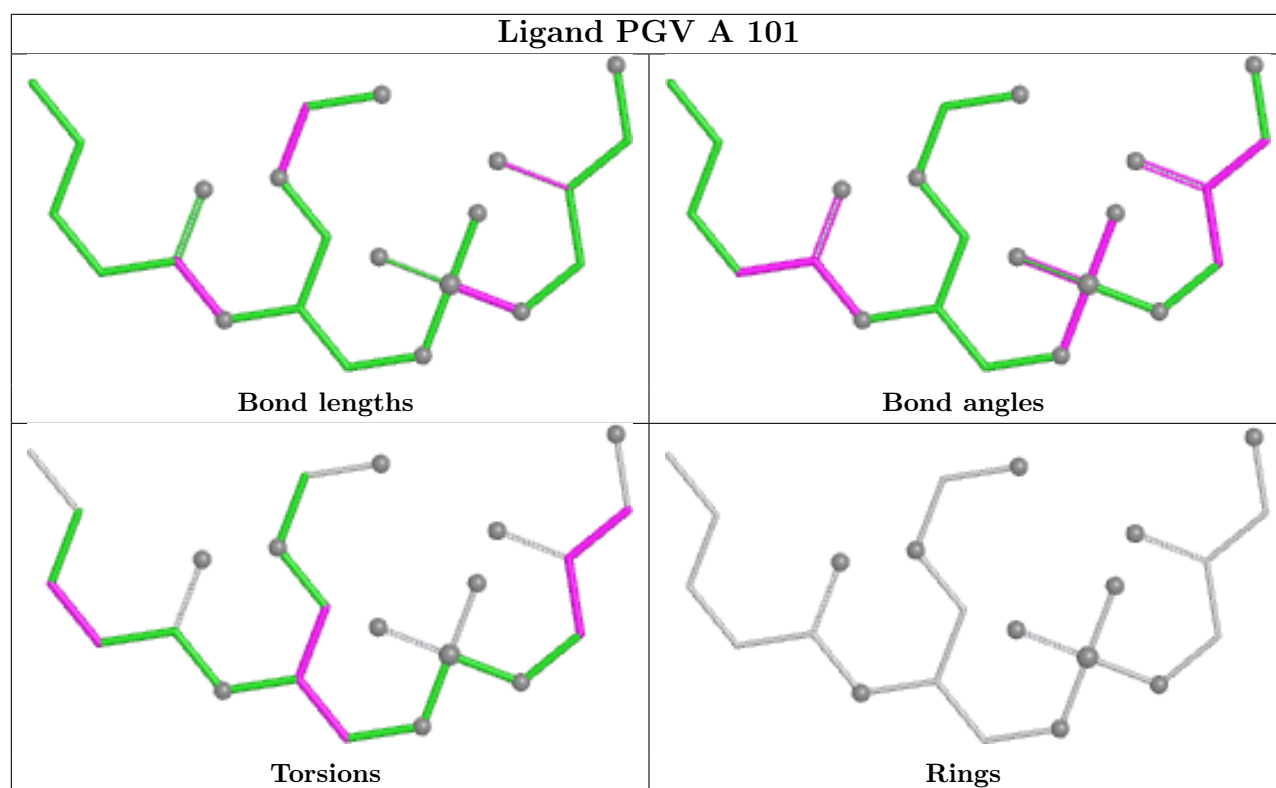


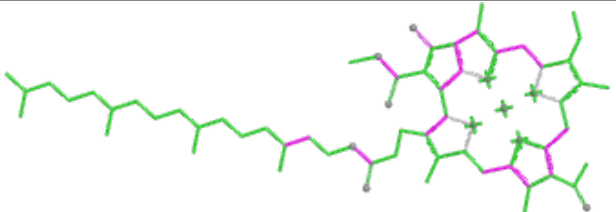
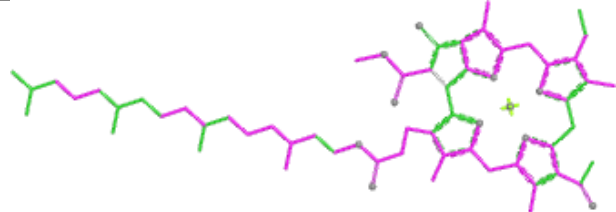
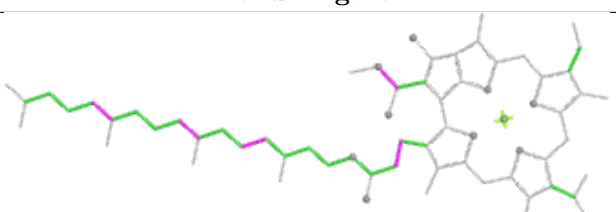
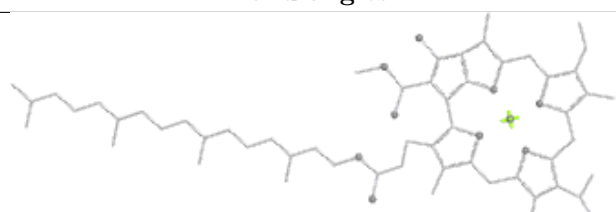
Ligand HEM C 401

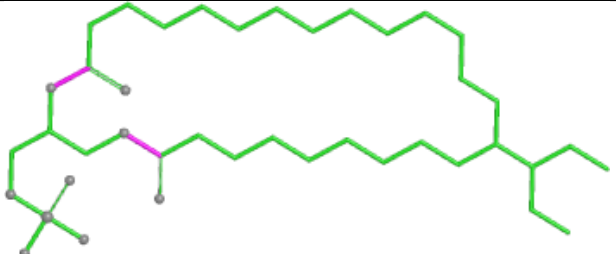
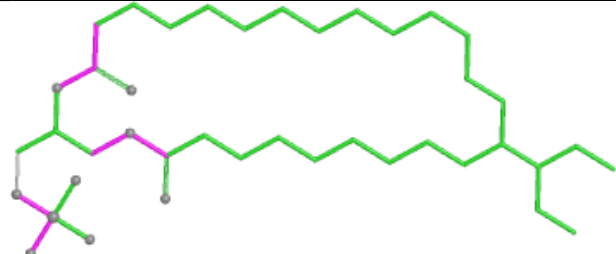
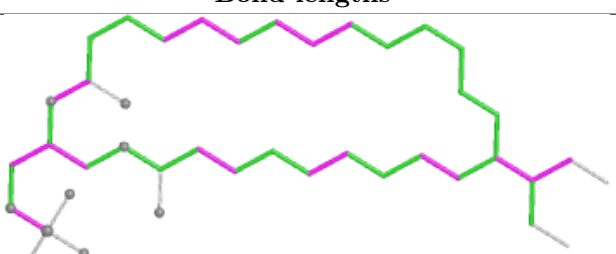
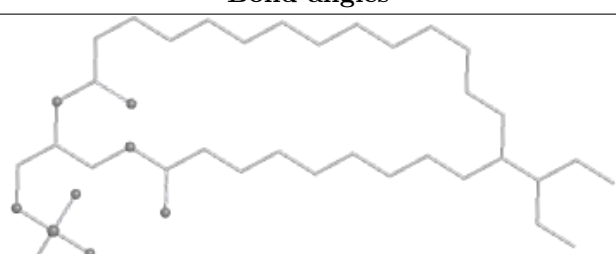


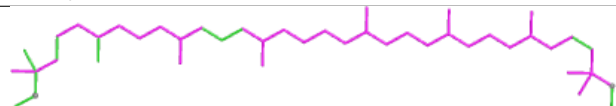
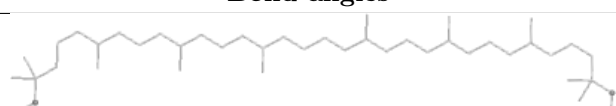


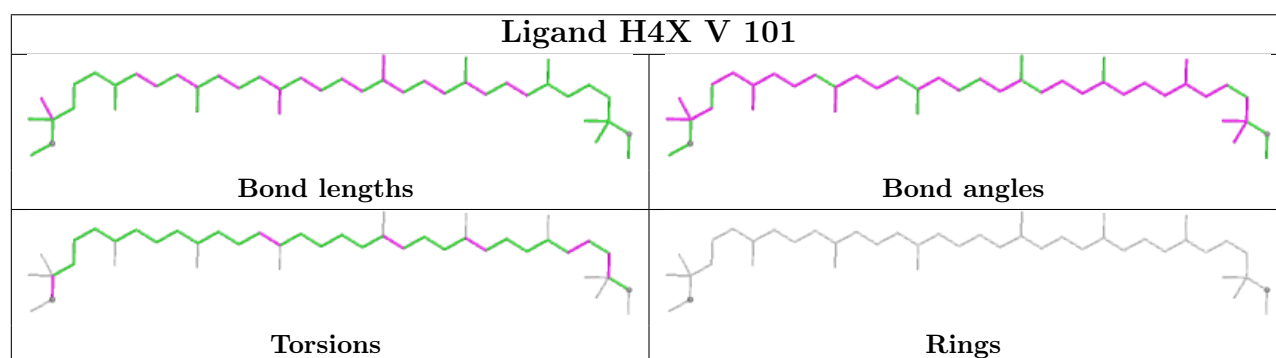
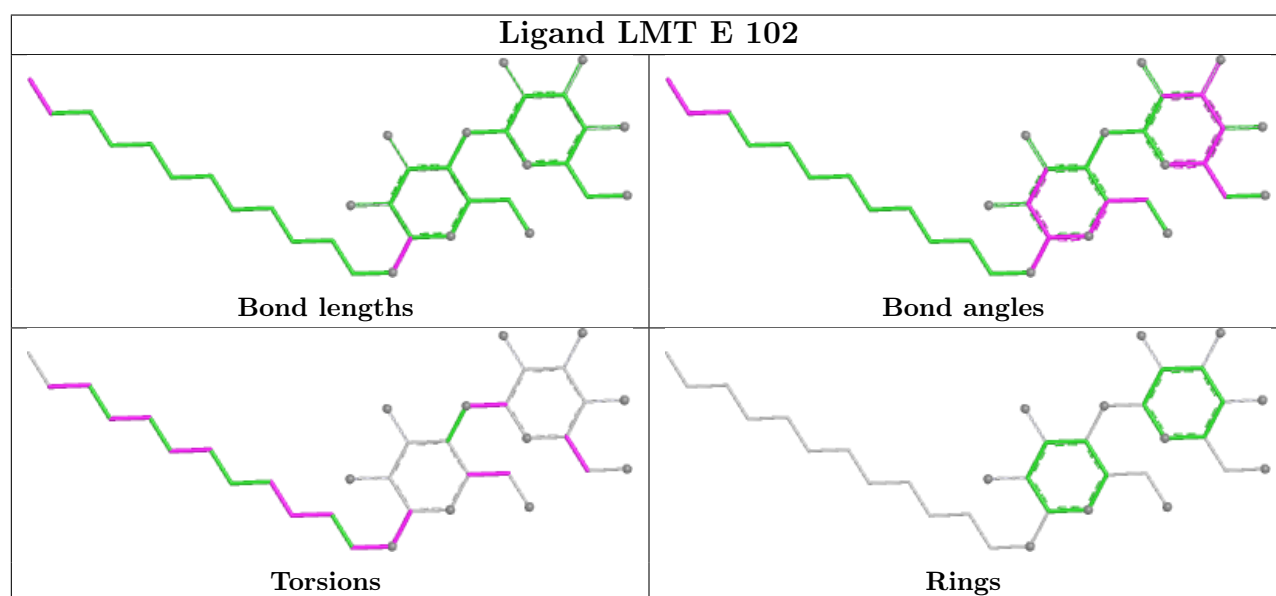
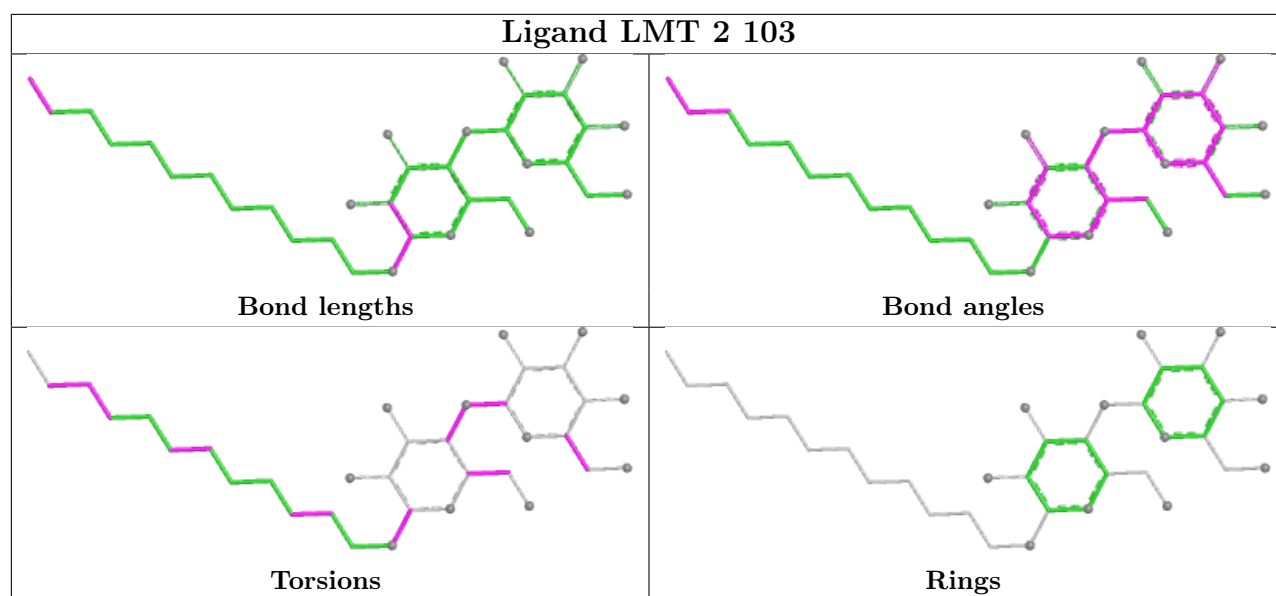


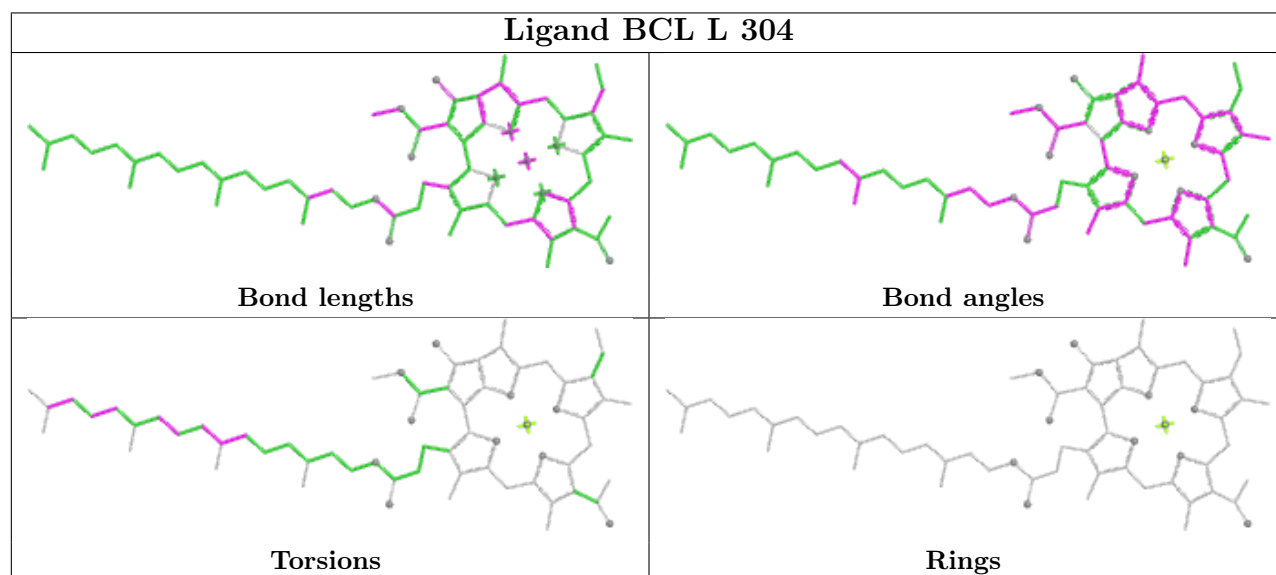
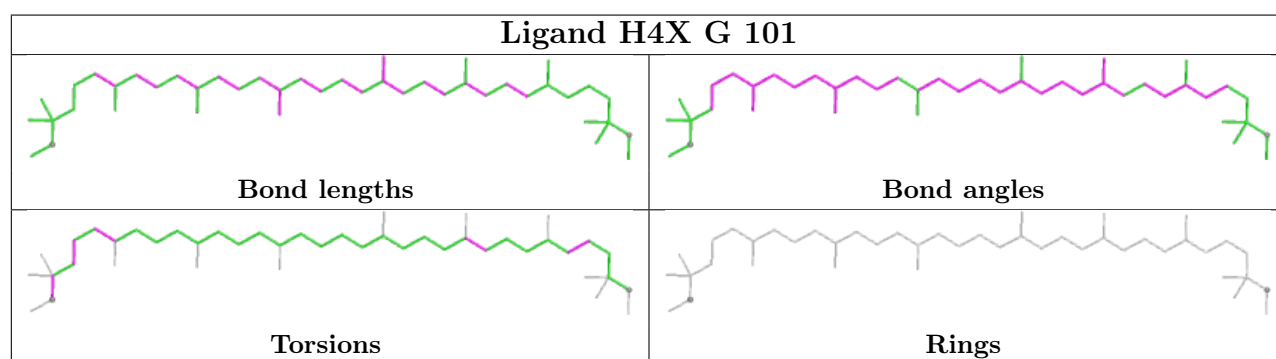
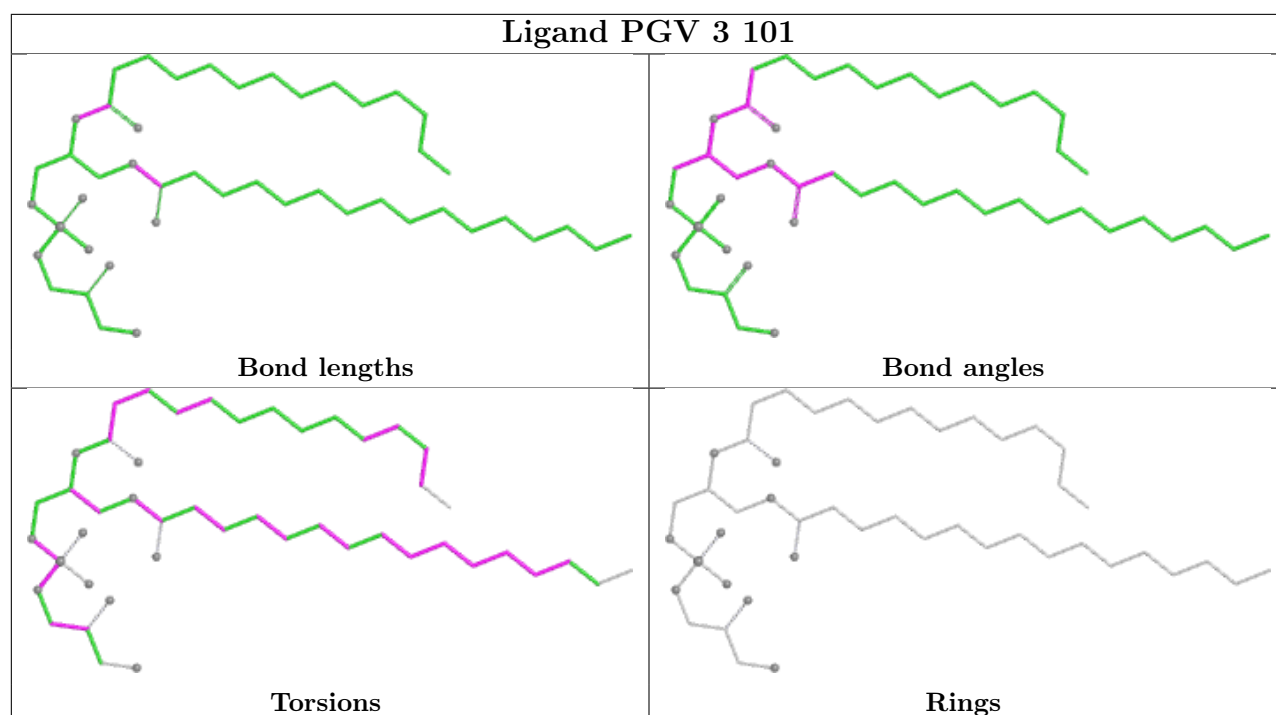


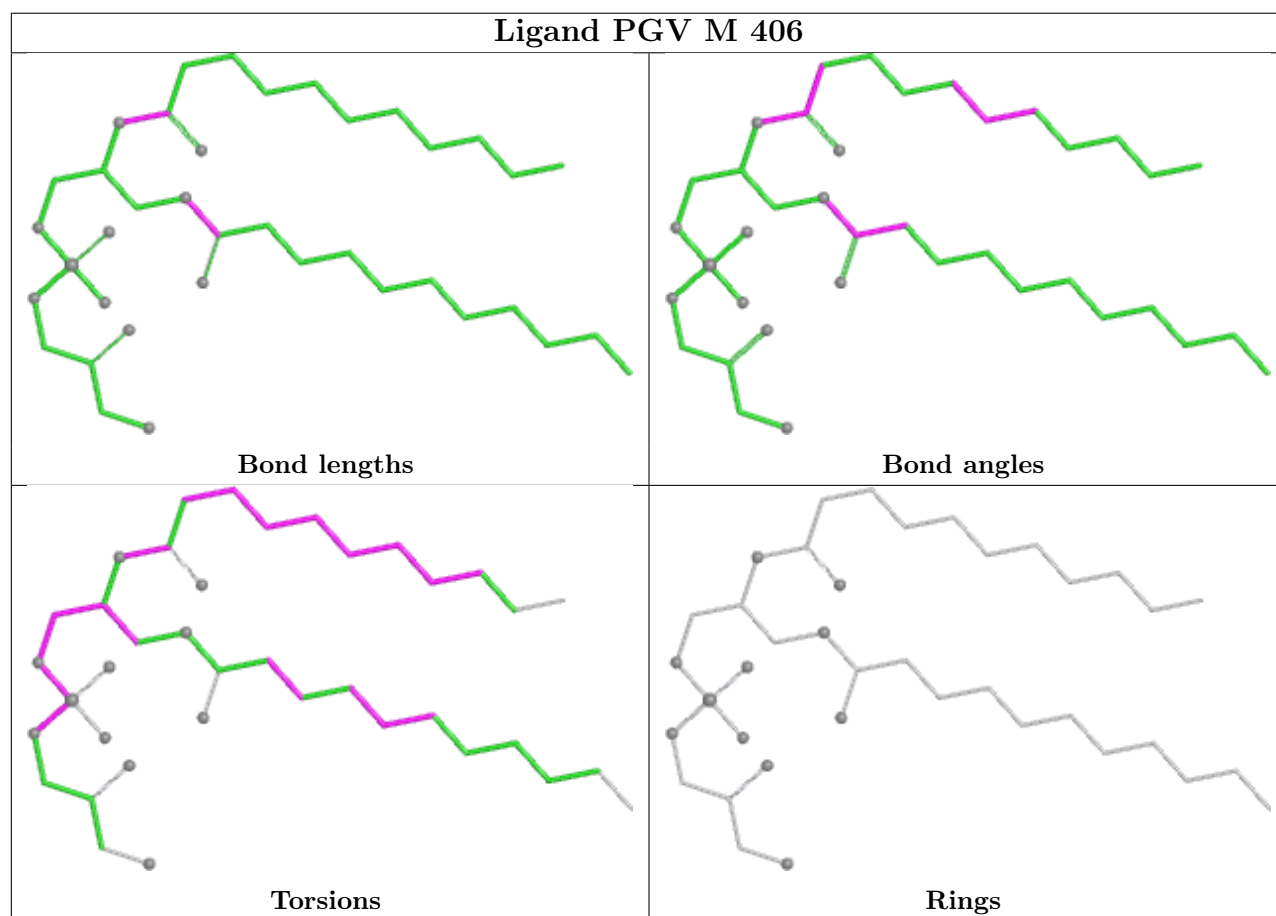
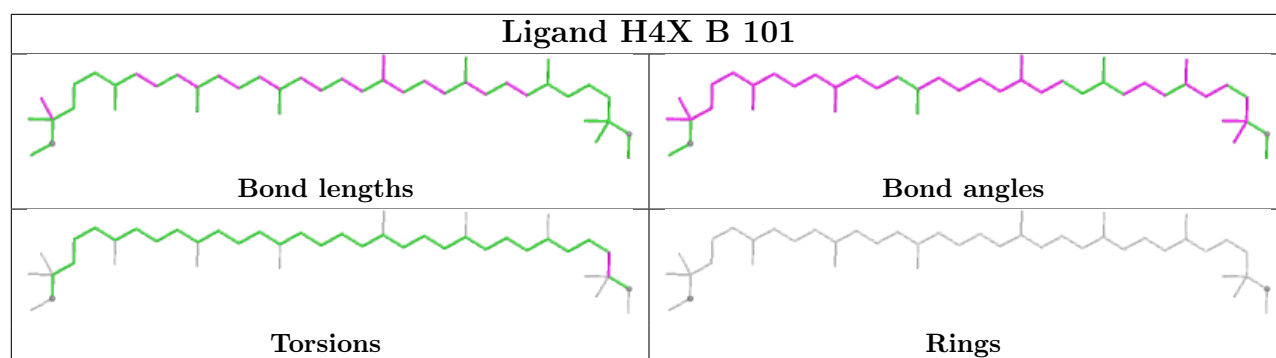
Ligand BCL L 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

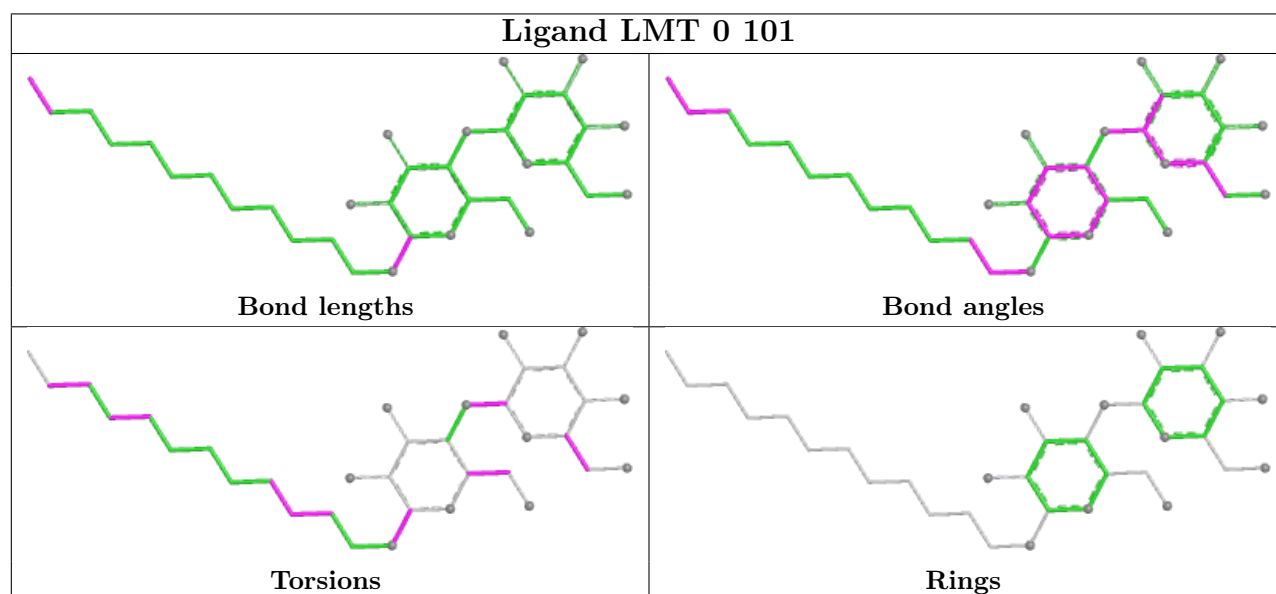
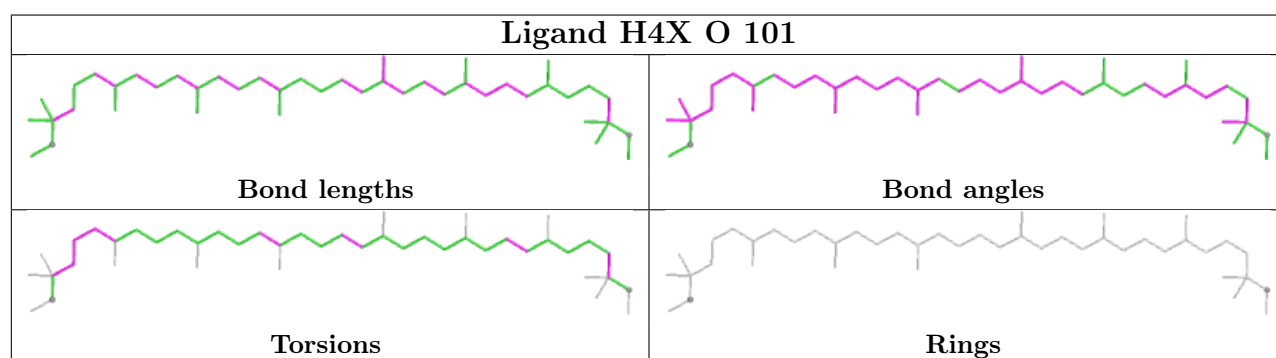
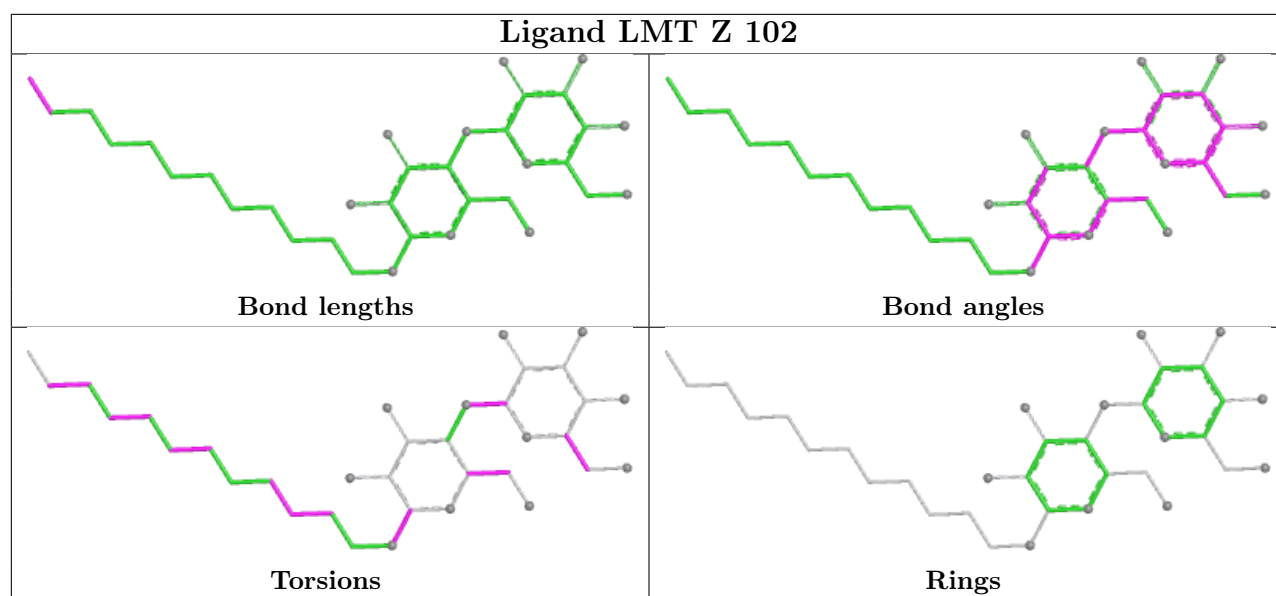
Ligand PGV K 106	
	
Bond lengths	Bond angles
	
Torsions	Rings

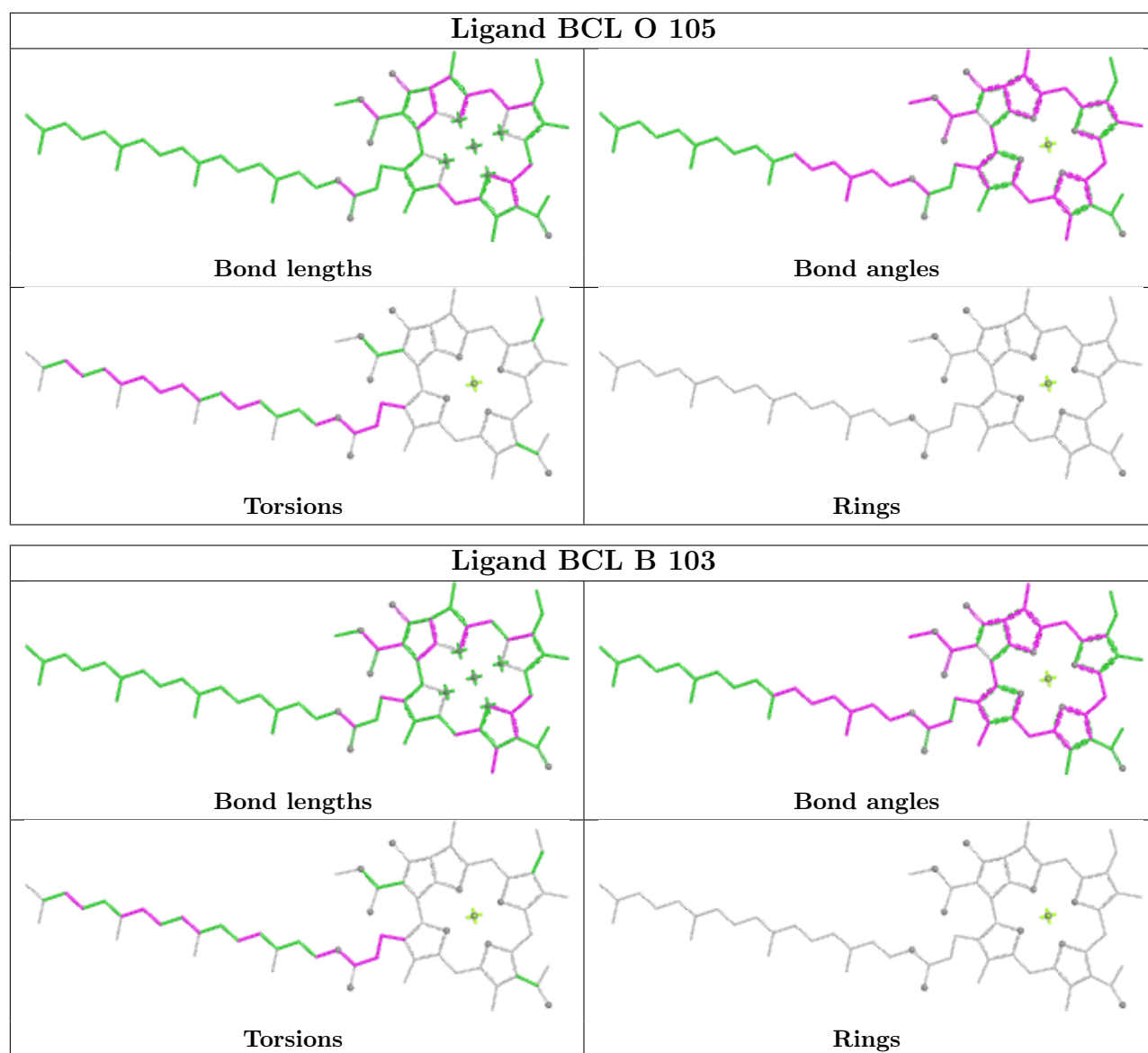
Ligand H4X Q 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

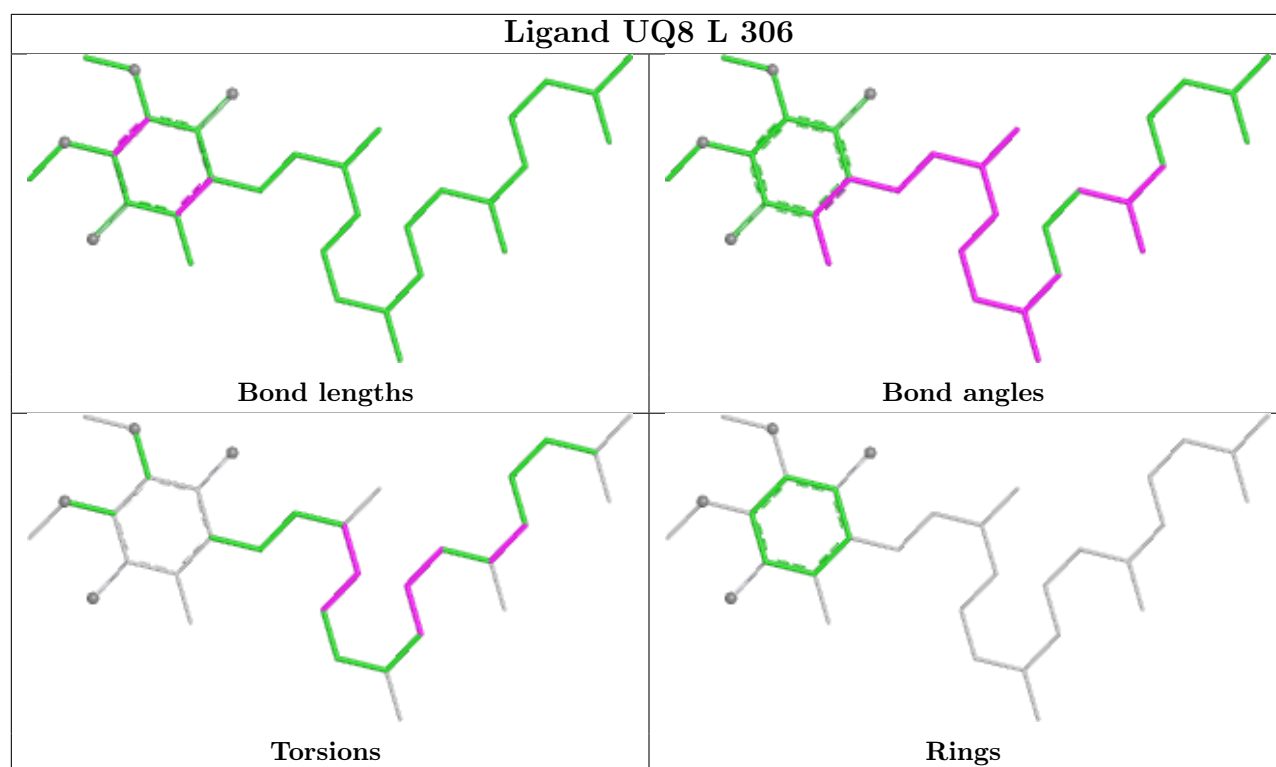












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

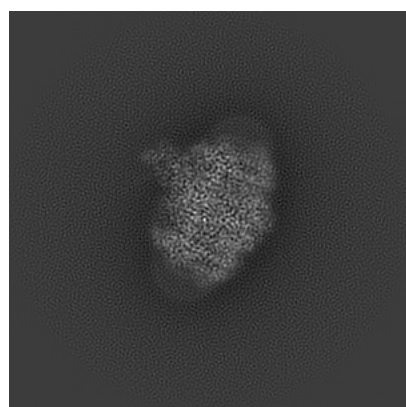
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30314. These allow visual inspection of the internal detail of the map and identification of artifacts.

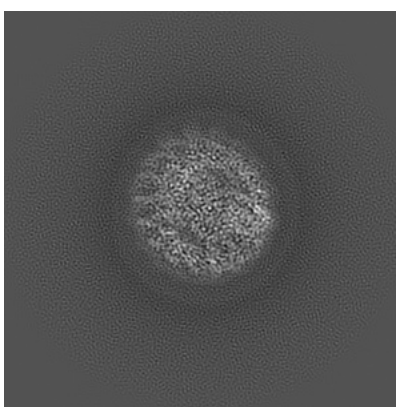
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

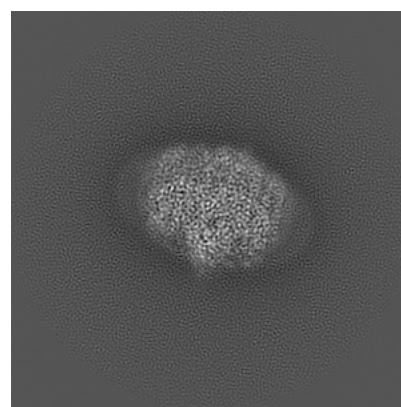
6.1.1 Primary map



X



Y

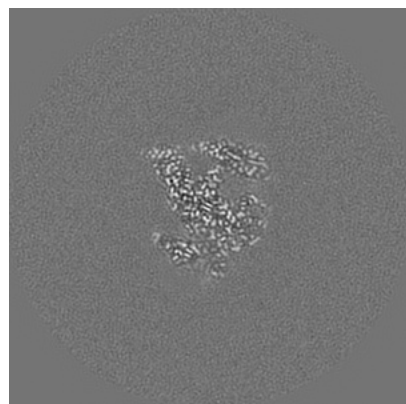


Z

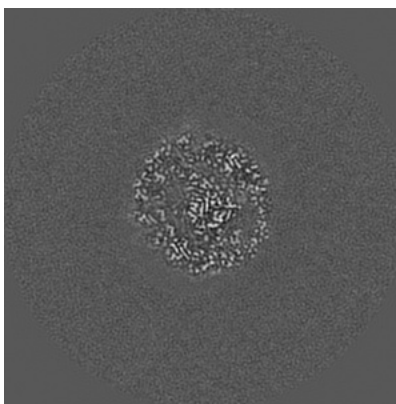
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

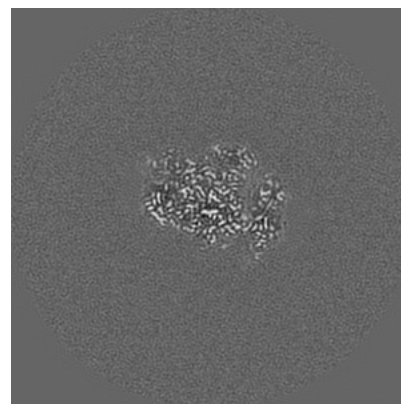
6.2.1 Primary map



X Index: 200



Y Index: 200

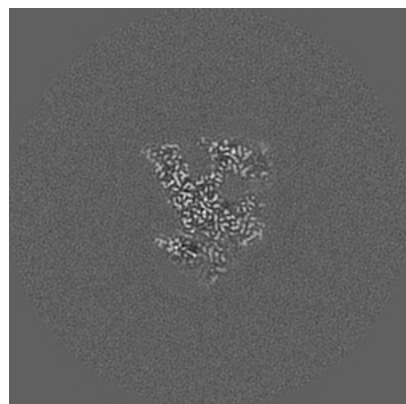


Z Index: 200

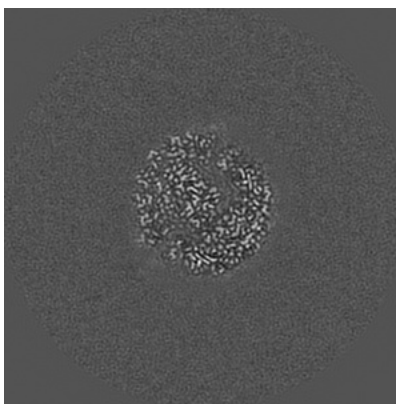
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

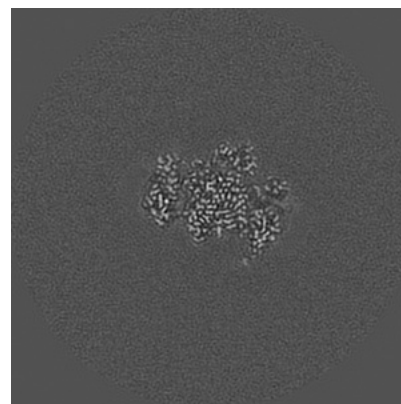
6.3.1 Primary map



X Index: 197



Y Index: 211

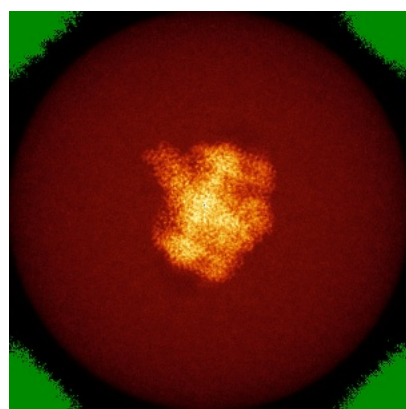


Z Index: 190

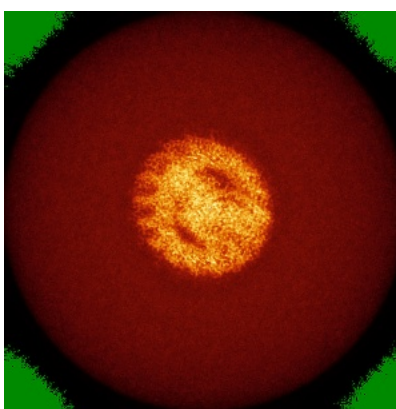
The images above show the largest variance slices of the map in three orthogonal directions.

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

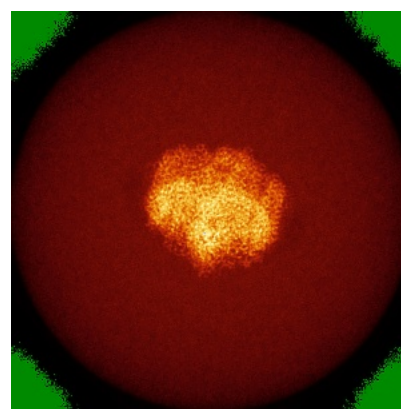
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

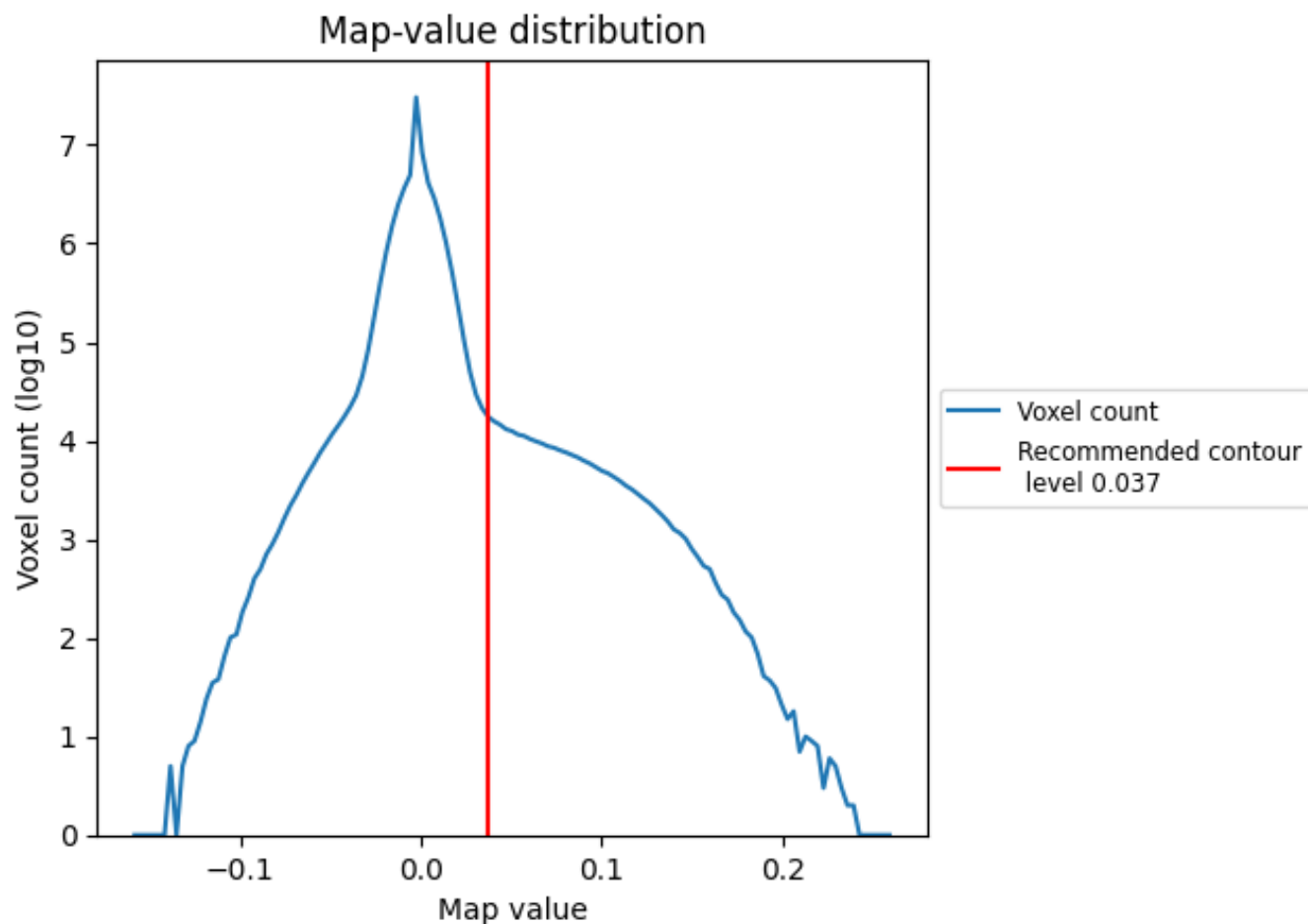
6.6 Mask visualisation

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

7 Map analysis [i](#)

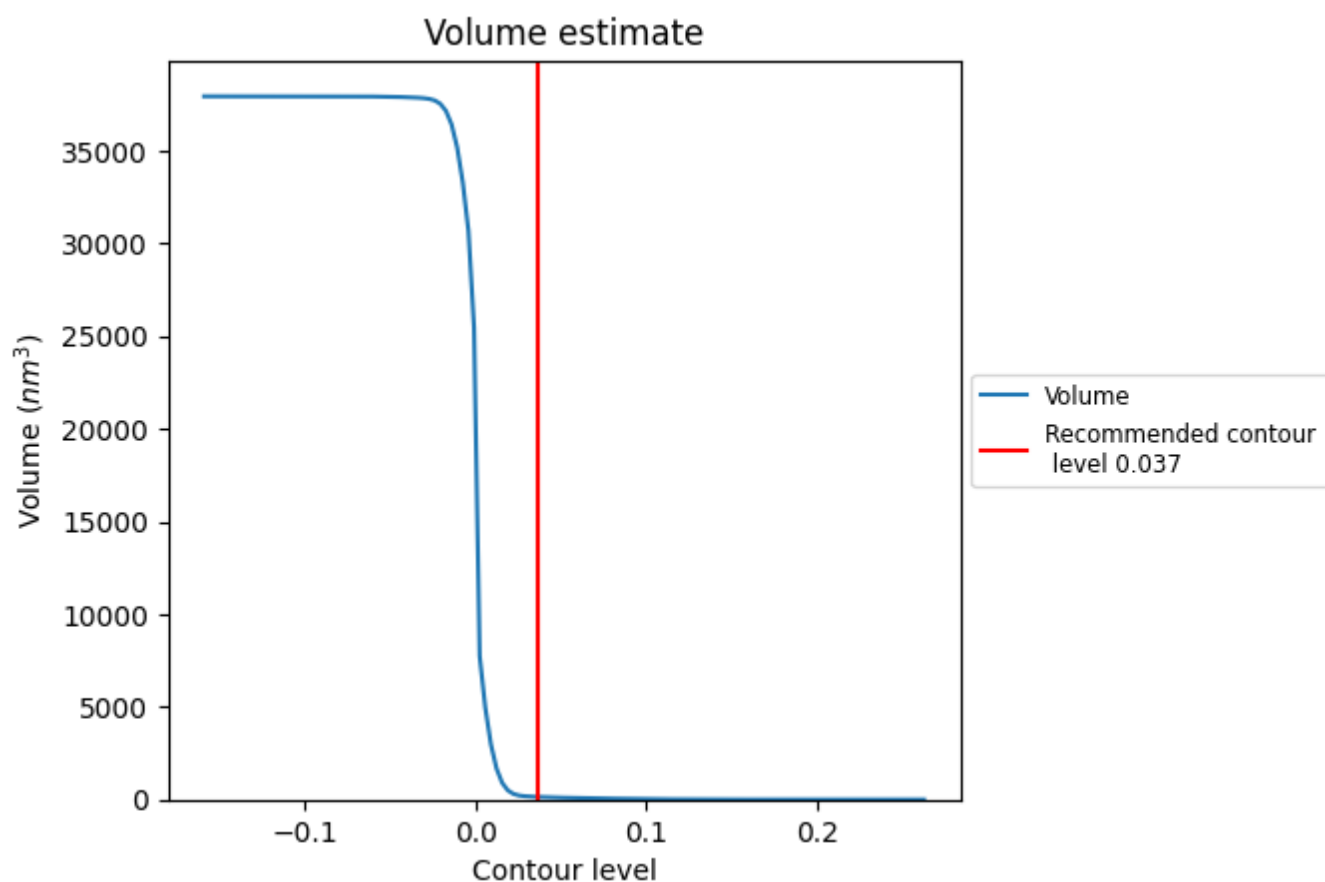
This section contains the results of statistical analysis of the map.

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.

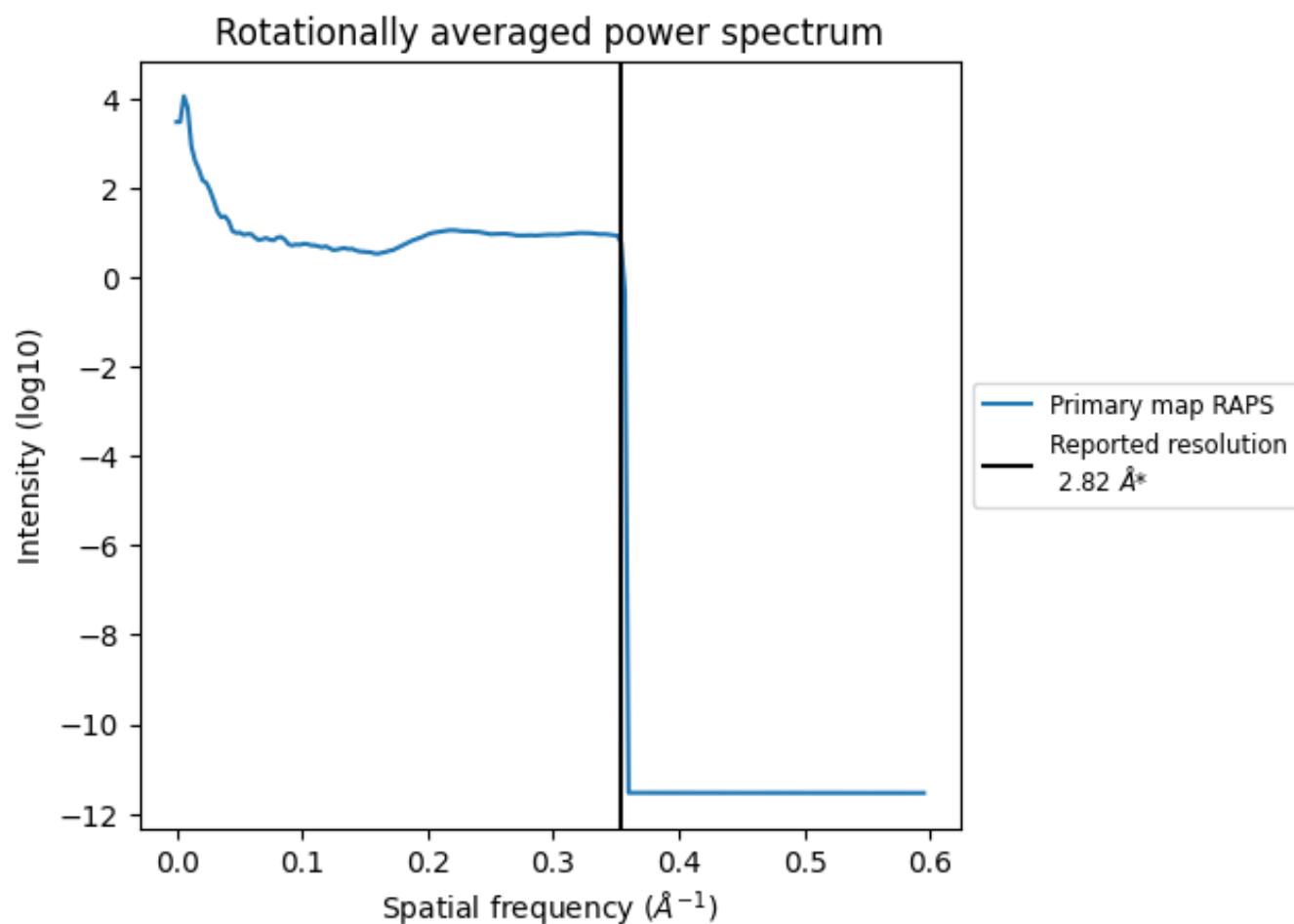
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 140 nm³; this corresponds to an approximate mass of 127 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 ⓘ

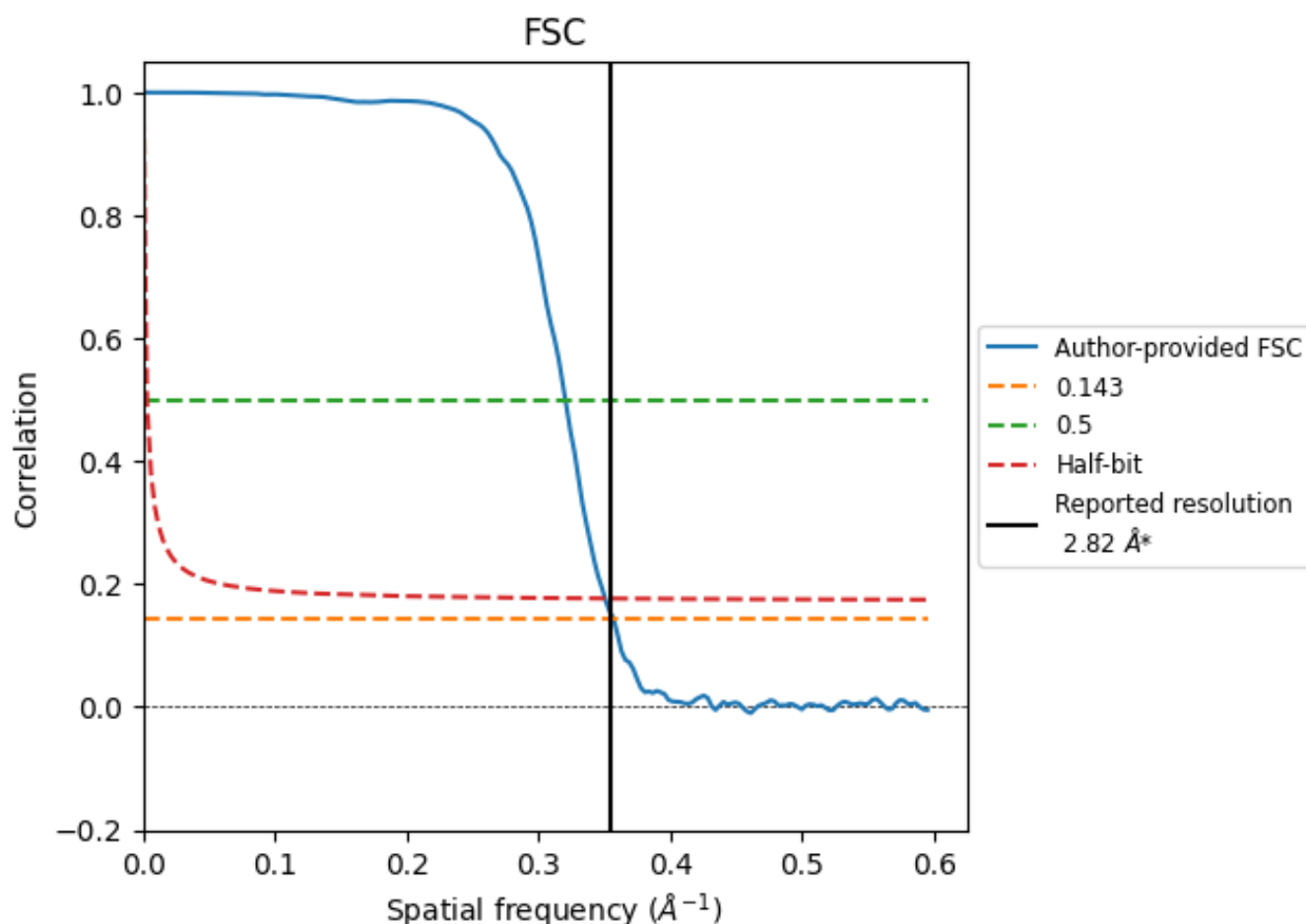


*Reported resolution corresponds to spatial frequency of 0.355 $\text{\AA}^{-1}$

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 0.355 Å⁻¹

8.2 Resolution estimates [i](#)

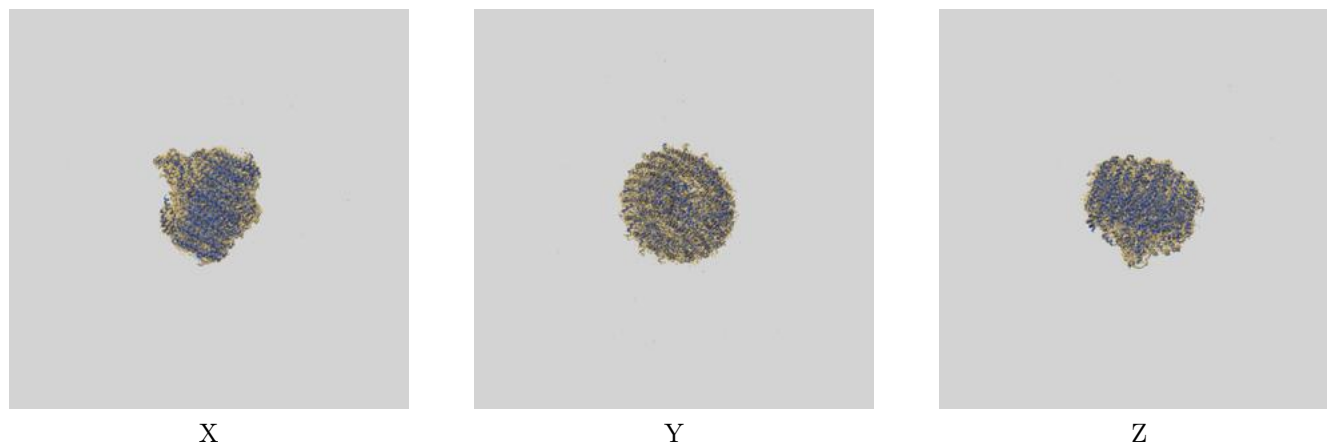
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.80	3.12	2.85
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

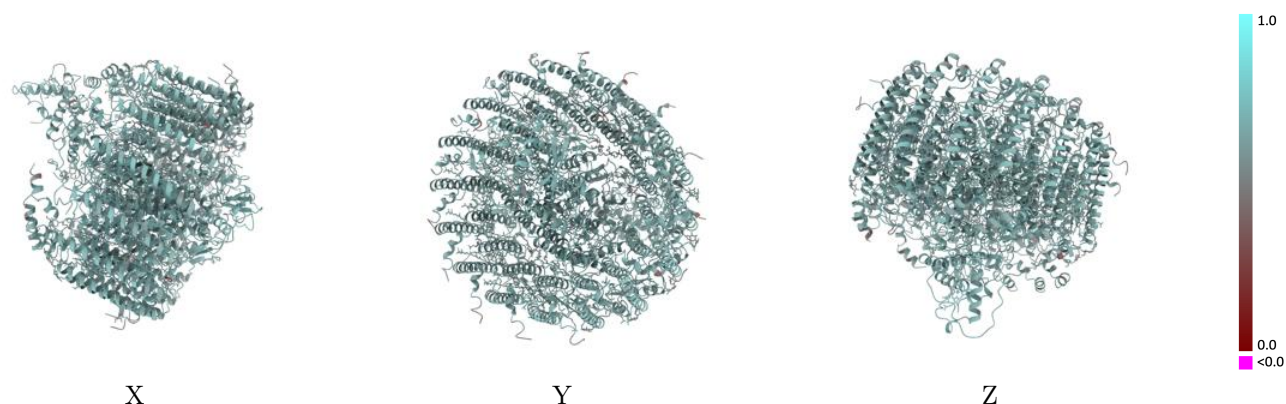
This section contains information regarding the fit between EMDB map EMD-30314 and PDB model 7C9R. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



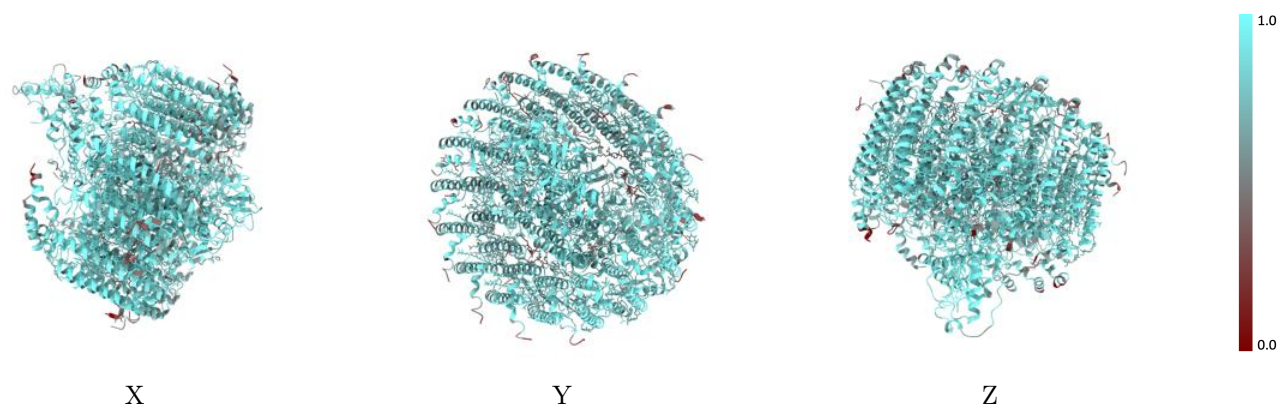
The images above show the 3D surface view of the map at the recommended contour level 0.037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



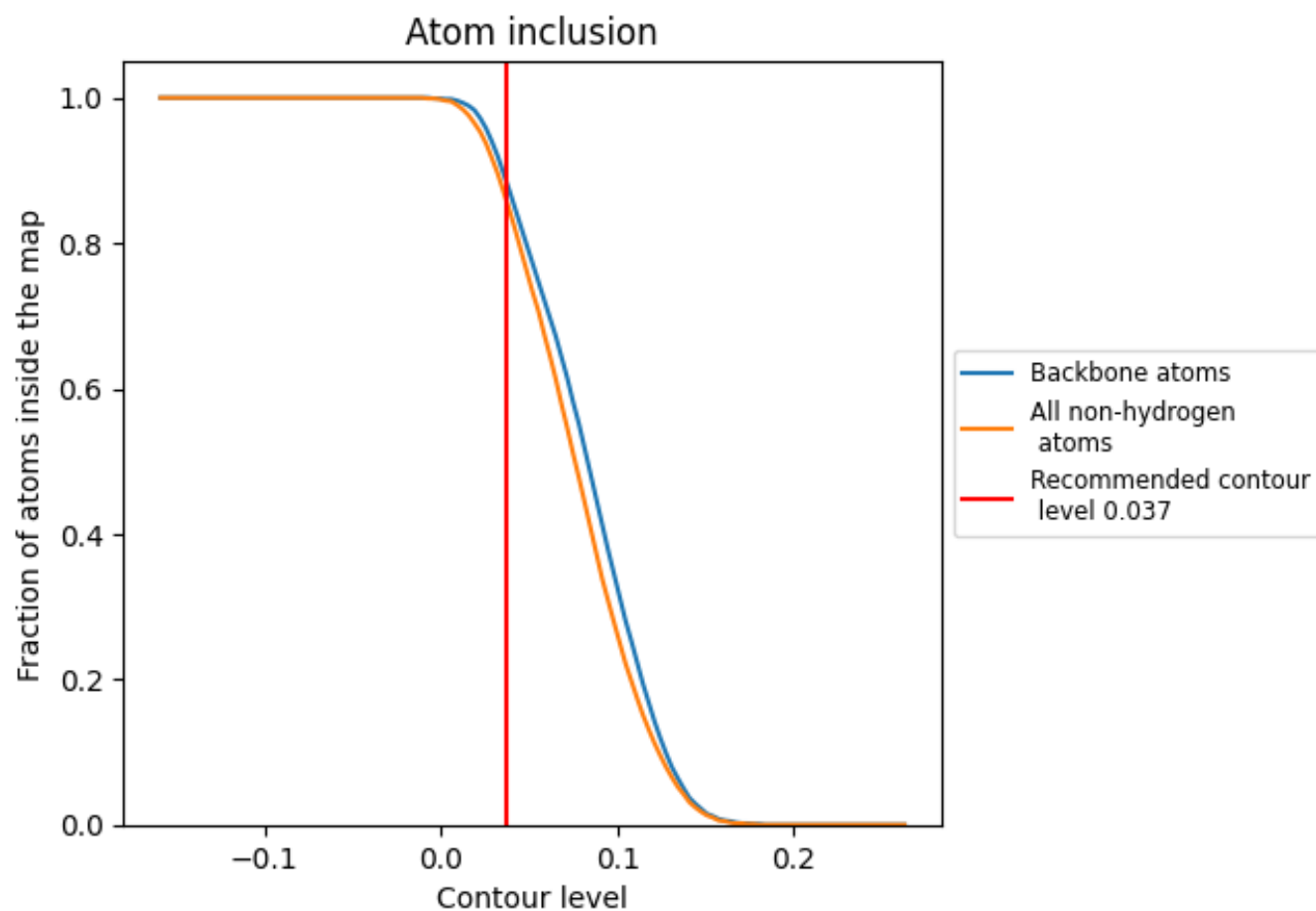
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.037).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.6320
0	 0.8250	 0.6030
1	 0.8120	 0.6140
2	 0.8200	 0.6170
3	 0.7930	 0.6150
4	 0.8500	 0.6250
5	 0.8260	 0.6250
6	 0.8680	 0.6300
7	 0.8500	 0.6270
8	 0.7890	 0.6050
9	 0.8730	 0.6380
A	 0.8540	 0.6280
B	 0.8560	 0.6260
C	 0.9080	 0.6420
D	 0.8430	 0.6300
E	 0.8580	 0.6330
F	 0.8320	 0.6270
G	 0.8610	 0.6300
H	 0.8520	 0.6330
I	 0.8340	 0.6240
J	 0.8780	 0.6320
K	 0.8210	 0.6290
L	 0.9390	 0.6520
M	 0.9220	 0.6520
N	 0.8500	 0.6250
O	 0.8420	 0.6280
P	 0.8610	 0.6310
Q	 0.8810	 0.6350
R	 0.8390	 0.6160
S	 0.7630	 0.6090
T	 0.8490	 0.6300
U	 0.8580	 0.6310
V	 0.8450	 0.6240
W	 0.8350	 0.6180
X	 0.8480	 0.6220



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Chain	Atom inclusion	Q-score
Y	 0.7860	 0.6140
Z	 0.8440	 0.6250