



Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 01:07 AM JST

PDB ID : 9M8M / pdb_00009m8m
EMDB ID : EMD-63714
Title : Structure of photosynthetic LH1-RC complex the Halophilic Nonsulfur Purple Bacterium, Rhodothalassium salexigens
Authors : Tani, K.; Kanno, R.; Inami, M.; Ooya, T.; Matsushita, R.; Minamino, A.; Takenaka, S.; Takaichi, S.; Purba, E.R.; Hall, M.; Mochizuki, T.; Yu, L.-J.; Mizoguchi, A.; Humbel, B.M.; Madigan, M.T.; Kimura, Y.; Wang-Otomo, Z.-Y.
Deposited on : 2025-03-12
Resolution : 2.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

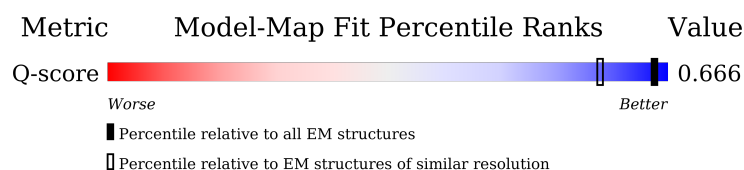
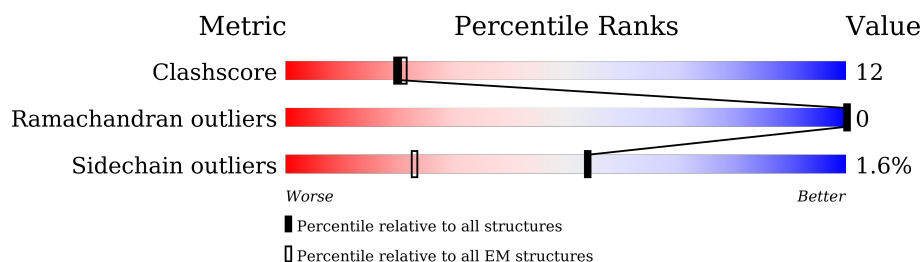
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	385	 71% 18% 11%
2	L	275	 76% 23%
3	M	323	 72% 25% ..

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Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
4	H	324	
5	1	59	
5	3	59	
5	5	59	
5	7	59	
5	9	59	
5	A	59	
5	D	59	
5	F	59	
5	I	59	
5	K	59	
5	O	59	
5	Q	59	
5	S	59	
5	U	59	
5	W	59	
5	Y	59	
6	0	67	
6	2	67	
6	4	67	
6	6	67	
6	8	67	
6	B	67	
6	E	67	
6	G	67	

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Mol	Chain	Length	Quality of chain
6	J	67	
6	N	67	
6	P	67	
6	R	67	
6	T	67	
6	V	67	
6	X	67	
6	Z	67	

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

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

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 27731 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	344	Total	C	N	O	S	0	0
			2675	1663	465	523	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	274	Total	C	N	O	S	0	0
			2175	1469	347	351	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
			2518	1679	412	418	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	268	Total	C	N	O	S	0	0
			2109	1350	351	402	6		

- Molecule 5 is a protein called Light-harvesting complex 1 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	47	Total	C	N	O	S	0	0
			414	283	66	62	3		
5	D	47	Total	C	N	O	S	0	0
			414	283	66	62	3		
5	F	47	Total	C	N	O	S	0	0
			414	283	66	62	3		
5	I	47	Total	C	N	O	S	0	0
			414	283	66	62	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	47	Total 414	C 283	N 66	O 62	S 3	0	0
5	O	47	Total 414	C 283	N 66	O 62	S 3	0	0
5	Q	47	Total 414	C 283	N 66	O 62	S 3	0	0
5	S	47	Total 414	C 283	N 66	O 62	S 3	0	0
5	U	47	Total 414	C 283	N 66	O 62	S 3	0	0
5	W	47	Total 414	C 283	N 66	O 62	S 3	0	0
5	Y	46	Total 405	C 278	N 65	O 59	S 3	0	0
5	1	47	Total 414	C 283	N 66	O 62	S 3	0	0
5	3	46	Total 405	C 278	N 65	O 59	S 3	0	0
5	5	47	Total 414	C 283	N 66	O 62	S 3	0	0
5	7	47	Total 414	C 283	N 66	O 62	S 3	0	0
5	9	47	Total 414	C 283	N 66	O 62	S 3	0	0

- Molecule 6 is a protein called Light-harvesting complex 1 beta chain.

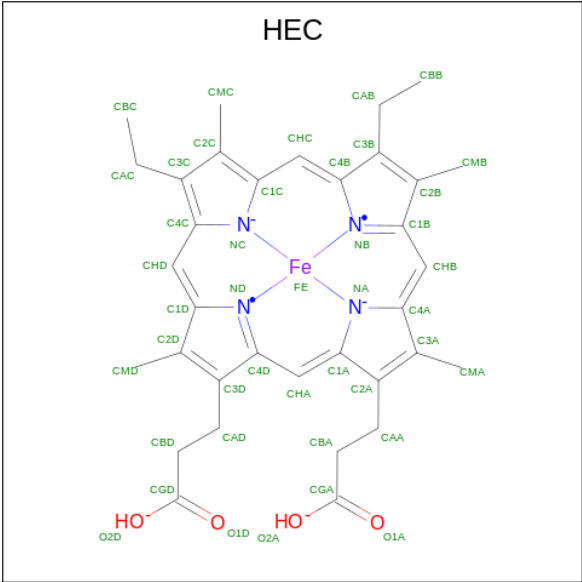
Mol	Chain	Residues	Atoms				AltConf	Trace
6	B	46	Total 374	C 252	N 59	O 63	0	0
6	E	47	Total 382	C 258	N 60	O 64	0	0
6	G	46	Total 374	C 252	N 59	O 63	0	0
6	J	45	Total 367	C 248	N 58	O 61	0	0
6	N	44	Total 363	C 246	N 57	O 60	0	0
6	P	45	Total 368	C 249	N 58	O 61	0	0
6	R	45	Total 367	C 248	N 58	O 61	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	T	45	Total 367	C 248	N 58	O 61	0	0
6	V	44	Total 363	C 246	N 57	O 60	0	0
6	X	46	Total 374	C 252	N 59	O 63	0	0
6	Z	45	Total 368	C 249	N 58	O 61	0	0
6	2	46	Total 374	C 252	N 59	O 63	0	0
6	4	45	Total 367	C 248	N 58	O 61	0	0
6	6	44	Total 363	C 246	N 57	O 60	0	0
6	8	44	Total 363	C 246	N 57	O 60	0	0
6	0	48	Total 386	C 260	N 61	O 65	0	0

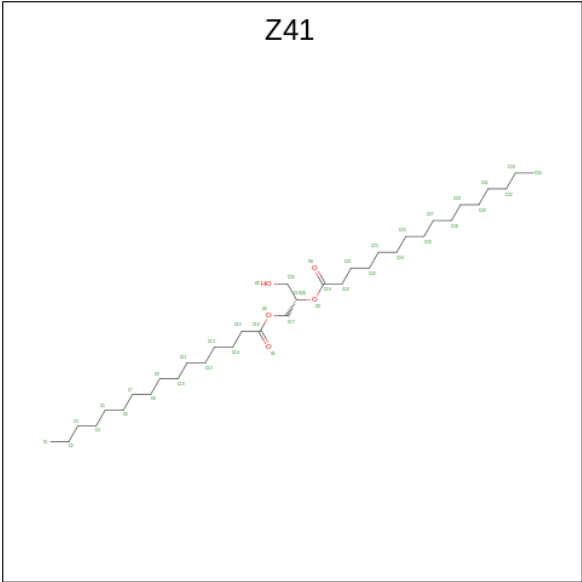
- # HEM

- Molecule 8 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



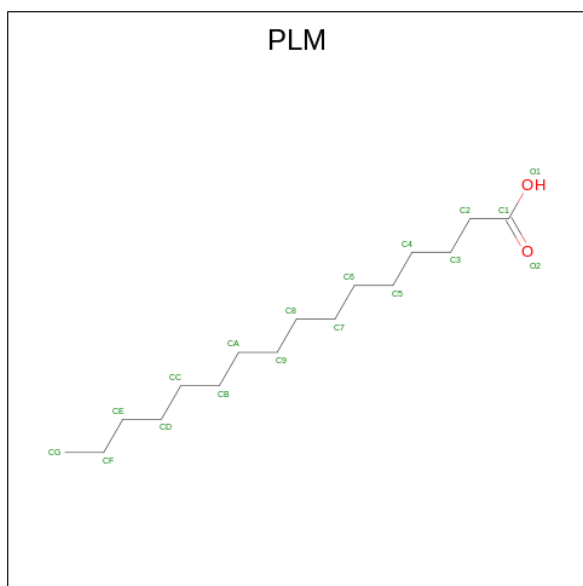
Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 9 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (CCD ID: Z41) (formula: $C_{35}H_{68}O_5$).



Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			26	22	4	

- Molecule 10 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total	C	O	0
			12	11	1	

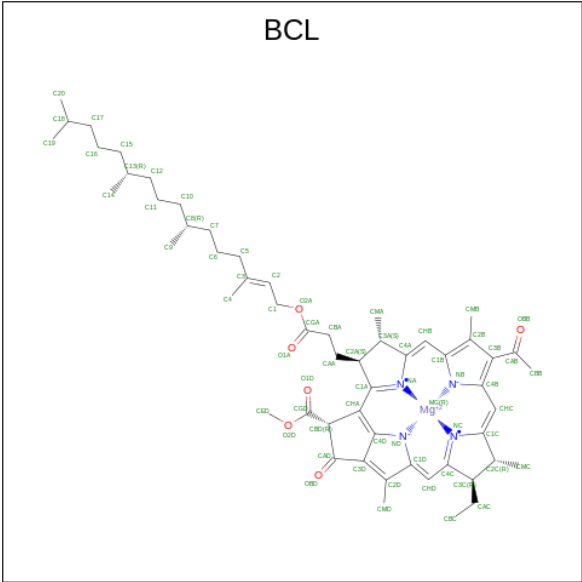
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	C	2	Total	Mg	0
			2	2	

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
12	L	1	Total	Ca	0
			1	1	

- Molecule 13 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

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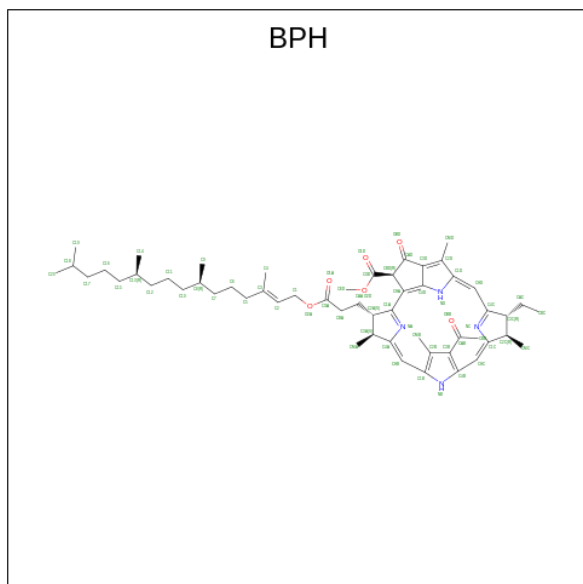
Mol	Chain	Residues	Atoms					AltConf
13	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
13	9	1	Total 66	C 55	Mg 1	N 4	O 6	0

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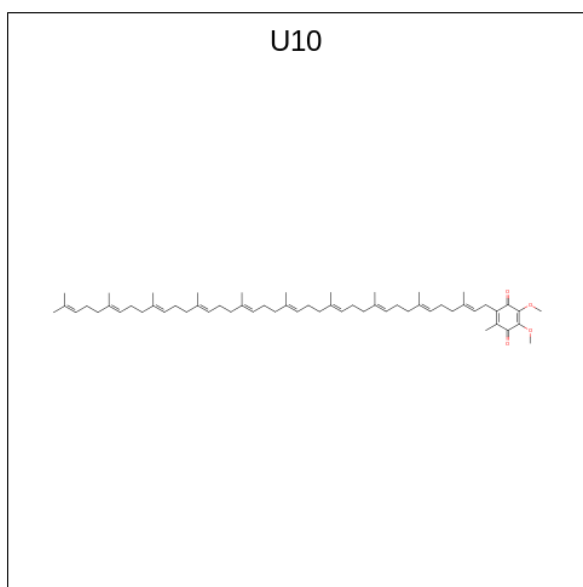
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
13	0	1	66	55	1	4	6	0

- Molecule 14 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



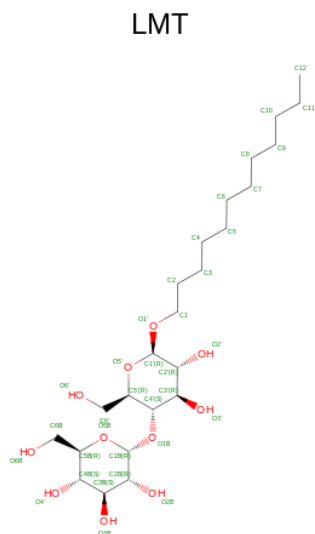
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
14	L	1	65	55	4	6	0
14	M	1	65	55	4	6	0

- Molecule 15 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
15	L	1	Total	C	O	0
			33	29	4	
15	L	1	Total	C	O	0
			18	14	4	
15	L	1	Total	C	O	0
			30	26	4	
15	D	1	Total	C	O	0
			46	42	4	
15	U	1	Total	C	O	0
			18	14	4	
15	Y	1	Total	C	O	0
			20	16	4	
15	1	1	Total	C	O	0
			45	41	4	
15	7	1	Total	C	O	0
			53	49	4	

- Molecule 16 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

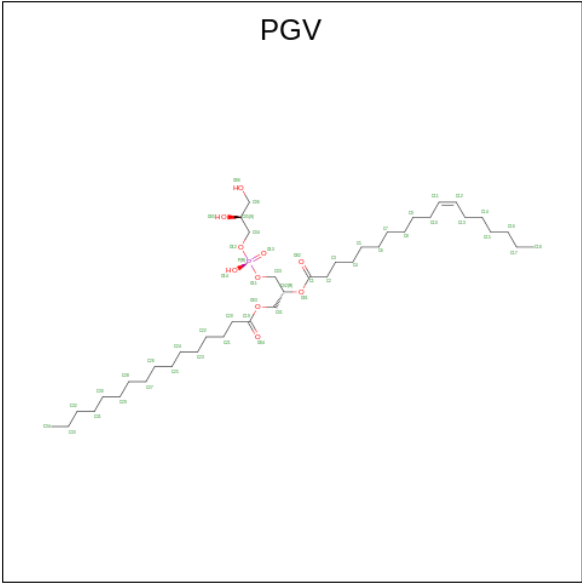


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Mol	Chain	Residues	Atoms			AltConf
16	Z	1	Total	C	O	0
			35	24	11	
16	Z	1	Total	C	O	0
			35	24	11	
16	4	1	Total	C	O	0
			35	24	11	
16	4	1	Total	C	O	0
			32	21	11	
16	5	1	Total	C	O	0
			30	19	11	
16	7	1	Total	C	O	0
			31	20	11	
16	9	1	Total	C	O	0
			25	14	11	

- Molecule 17 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
17	L	1	Total	C	O	P	0
			36	27	8	1	
17	L	1	Total	C	O	P	0
			51	40	10	1	
17	M	1	Total	C	O	P	0
			37	26	10	1	

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Mol	Chain	Residues	Atoms				AltConf
17	M	1	Total 29	C 18	O 10	P 1	0
17	M	1	Total 35	C 26	O 8	P 1	0
17	M	1	Total 20	C 9	O 10	P 1	0
17	H	1	Total 43	C 32	O 10	P 1	0
17	H	1	Total 43	C 32	O 10	P 1	0
17	H	1	Total 51	C 40	O 10	P 1	0
17	A	1	Total 17	C 8	O 8	P 1	0
17	B	1	Total 44	C 33	O 10	P 1	0
17	D	1	Total 40	C 29	O 10	P 1	0
17	E	1	Total 44	C 33	O 10	P 1	0
17	G	1	Total 44	C 33	O 10	P 1	0
17	J	1	Total 44	C 33	O 10	P 1	0
17	K	1	Total 46	C 35	O 10	P 1	0
17	N	1	Total 44	C 33	O 10	P 1	0
17	P	1	Total 44	C 33	O 10	P 1	0
17	R	1	Total 44	C 33	O 10	P 1	0
17	T	1	Total 44	C 33	O 10	P 1	0
17	V	1	Total 44	C 33	O 10	P 1	0
17	X	1	Total 44	C 33	O 10	P 1	0
17	2	1	Total 44	C 33	O 10	P 1	0
17	2	1	Total 44	C 33	O 10	P 1	0

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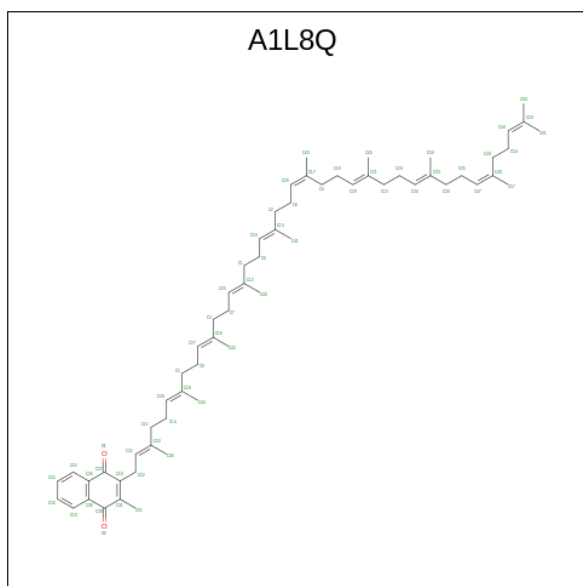
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Mol	Chain	Residues	Atoms				AltConf
17	4	1	Total	C	O	P	0
			44	33	10	1	
17	8	1	Total	C	O	P	0
			44	33	10	1	
17	8	1	Total	C	O	P	0
			44	33	10	1	
17	0	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 18 is FE (III) ION (CCD ID: FE) (formula: Fe).

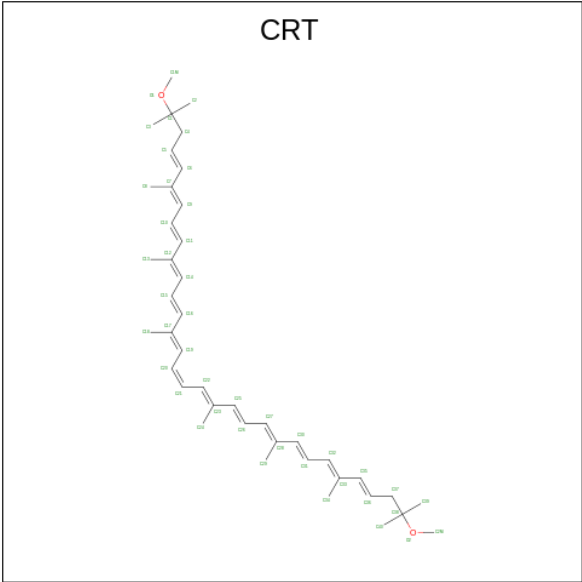
Mol	Chain	Residues	Atoms		AltConf
18	M	1	Total	Fe	0
			1	1	

- Molecule 19 is Menaquinone 10 (CCD ID: A1L8Q) (formula: C₆₁H₈₈O₂).



Mol	Chain	Residues	Atoms			AltConf
19	M	1	Total	C	O	0
			63	61	2	

- Molecule 20 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



Mol	Chain	Residues	Atoms			AltConf
20	M	1	Total	C	O	0
			44	42	2	
20	B	1	Total	C	O	0
			44	42	2	
20	E	1	Total	C	O	0
			44	42	2	
20	G	1	Total	C	O	0
			44	42	2	
20	J	1	Total	C	O	0
			44	42	2	
20	N	1	Total	C	O	0
			44	42	2	
20	P	1	Total	C	O	0
			44	42	2	
20	R	1	Total	C	O	0
			44	42	2	
20	T	1	Total	C	O	0
			44	42	2	
20	V	1	Total	C	O	0
			44	42	2	
20	Y	1	Total	C	O	0
			44	42	2	
20	Z	1	Total	C	O	0
			44	42	2	
20	2	1	Total	C	O	0
			44	42	2	
20	4	1	Total	C	O	0
			44	42	2	

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Mol	Chain	Residues	Atoms			AltConf
20	6	1	Total	C	O	0
			44	42	2	
20	8	1	Total	C	O	0
			44	42	2	
20	0	1	Total	C	O	0
			44	42	2	

- Molecule 21 is water.

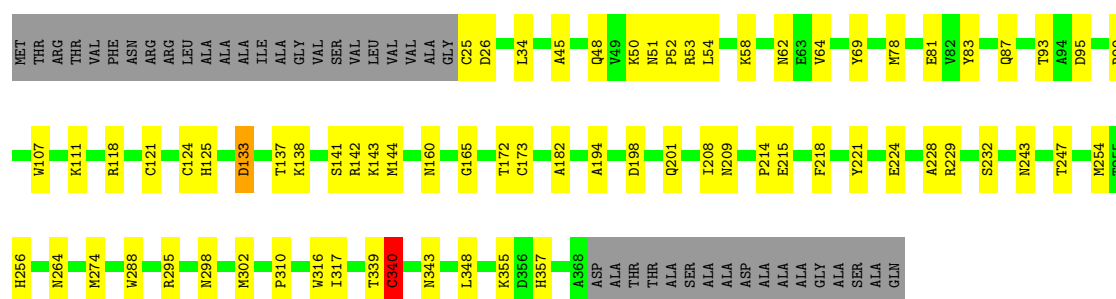
Mol	Chain	Residues	Atoms		AltConf
21	C	47	Total	O	0
			47	47	
21	L	19	Total	O	0
			19	19	
21	M	24	Total	O	0
			24	24	
21	H	5	Total	O	0
			5	5	
21	A	1	Total	O	0
			1	1	
21	D	1	Total	O	0
			1	1	
21	S	1	Total	O	0
			1	1	
21	W	1	Total	O	0
			1	1	

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.

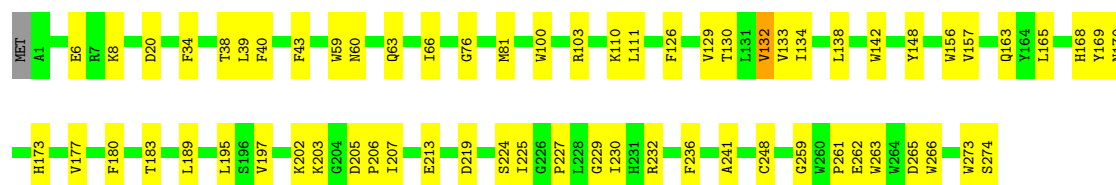
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C: 



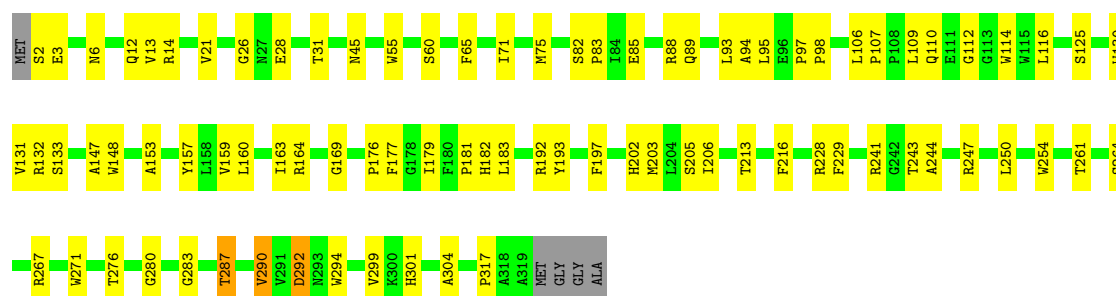
- Molecule 2: Reaction center protein L chain

Chain L: 



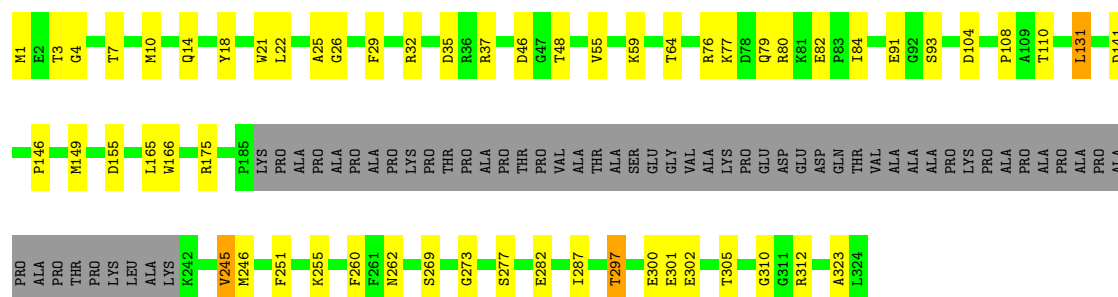
- Molecule 3: Reaction center protein M chain

Chain M: 



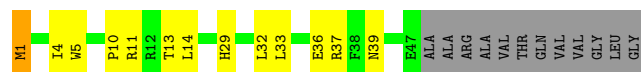
- Molecule 4: Photosynthetic reaction center subunit H

Chain H:  65% 17% 17%



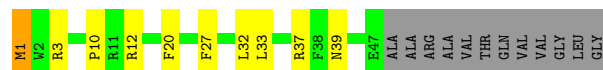
- Molecule 5: Light-harvesting complex 1 alpha chain

Chain A:  58% 20% 20%



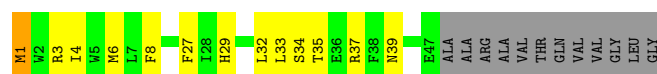
- Molecule 5: Light-harvesting complex 1 alpha chain

Chain D:  63% 15% 20%



- Molecule 5: Light-harvesting complex 1 alpha chain

Chain F:  58% 20% 20%



- Molecule 5: Light-harvesting complex 1 alpha chain

Chain I:  61% 19% 20%



- Molecule 5: Light-harvesting complex 1 alpha chain

Chain K:  56% 22% 20%

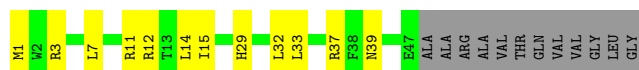


- Molecule 5: Light-harvesting complex 1 alpha chain

Chain O:  54% 24% 20%



- Molecule 5: Light-harvesting complex 1 alpha chain



- Molecule 5: Light-harvesting complex 1 alpha chain



- Molecule 5: Light-harvesting complex 1 alpha chain



- Molecule 5: Light-harvesting complex 1 alpha chain



- Molecule 5: Light-harvesting complex 1 alpha chain



- Molecule 5: Light-harvesting complex 1 alpha chain



- Molecule 5: Light-harvesting complex 1 alpha chain





- Molecule 5: Light-harvesting complex 1 alpha chain



- Molecule 5: Light-harvesting complex 1 alpha chain



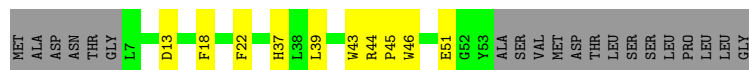
- Molecule 5: Light-harvesting complex 1 alpha chain



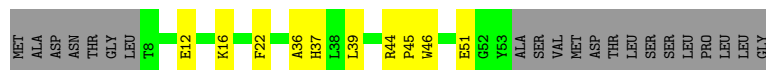
- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain





- Molecule 6: Light-harvesting complex 1 beta chain



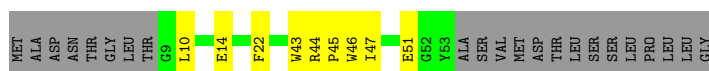
- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



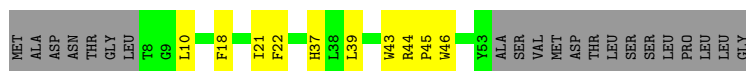
- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain

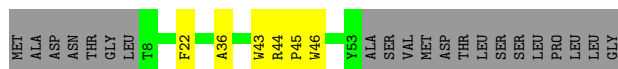


- Molecule 6: Light-harvesting complex 1 beta chain





- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	229234	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.250	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	311.6, 311.6, 311.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: U10, CRT, A1L8Q, HEM, CA, PLM, PGV, BCL, FME, HEC, FE, BPH, MG, LMT, Z41

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	0.15	0/2750	0.37	1/3759 (0.0%)
2	L	0.11	0/2263	0.28	0/3093
3	M	0.11	0/2617	0.26	0/3592
4	H	0.10	0/2165	0.27	0/2940
5	1	0.09	0/418	0.21	0/567
5	3	0.09	0/409	0.23	0/555
5	5	0.11	0/418	0.26	0/567
5	7	0.11	0/418	0.29	0/567
5	9	0.11	0/418	0.25	0/567
5	A	0.09	0/418	0.22	0/567
5	D	0.09	0/418	0.22	0/567
5	F	0.09	0/418	0.22	0/567
5	I	0.09	0/418	0.24	0/567
5	K	0.08	0/418	0.22	0/567
5	O	0.10	0/418	0.25	0/567
5	Q	0.10	0/418	0.23	0/567
5	S	0.10	0/418	0.23	0/567
5	U	0.09	0/418	0.22	0/567
5	W	0.10	0/418	0.23	0/567
5	Y	0.10	0/409	0.24	0/555
6	0	0.11	0/401	0.29	0/547
6	2	0.10	0/389	0.23	0/531
6	4	0.08	0/382	0.22	0/521
6	6	0.10	0/378	0.29	0/516
6	8	0.10	0/378	0.25	0/516
6	B	0.10	0/389	0.25	0/531
6	E	0.09	0/397	0.23	0/542
6	G	0.10	0/389	0.24	0/531
6	J	0.10	0/382	0.22	0/521
6	N	0.11	0/378	0.27	0/516
6	P	0.10	0/383	0.26	0/523
6	R	0.11	0/382	0.32	0/521

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	T	0.11	0/382	0.27	0/521
6	V	0.08	0/378	0.24	0/516
6	X	0.08	0/389	0.21	0/531
6	Z	0.09	0/383	0.21	0/523
All	All	0.11	0/22625	0.27	1/30839 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	CYS	CA-CB-SG	8.35	133.60	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	340	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2675	0	2496	56	0
2	L	2175	0	2131	58	0
3	M	2518	0	2464	69	0
4	H	2109	0	2052	42	0
5	1	414	0	417	11	0
5	3	405	0	411	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	5	414	0	417	12	0
5	7	414	0	417	14	0
5	9	414	0	417	16	0
5	A	414	0	417	9	0
5	D	414	0	417	12	0
5	F	414	0	417	11	0
5	I	414	0	417	9	0
5	K	414	0	417	15	0
5	O	414	0	417	18	0
5	Q	414	0	417	12	0
5	S	414	0	417	13	0
5	U	414	0	417	13	0
5	W	414	0	417	12	0
5	Y	405	0	411	17	0
6	0	386	0	374	16	0
6	2	374	0	360	9	0
6	4	367	0	353	13	0
6	6	363	0	350	12	0
6	8	363	0	350	13	0
6	B	374	0	360	14	0
6	E	382	0	371	13	0
6	G	374	0	360	9	0
6	J	367	0	353	10	0
6	N	363	0	350	17	0
6	P	368	0	355	13	0
6	R	367	0	353	11	0
6	T	367	0	353	9	0
6	V	363	0	350	11	0
6	X	374	0	360	14	0
6	Z	368	0	355	9	0
7	C	43	0	30	8	0
8	C	129	0	90	3	0
9	C	26	0	0	1	0
10	C	12	0	18	0	0
11	C	2	0	0	0	0
12	L	1	0	0	0	0
13	0	66	0	74	7	0
13	1	66	0	74	4	0
13	2	66	0	74	5	0
13	3	66	0	74	4	0
13	4	66	0	74	4	0
13	5	66	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	6	66	0	74	6	0
13	7	66	0	74	3	0
13	8	66	0	74	8	0
13	9	66	0	74	5	0
13	A	66	0	74	3	0
13	B	66	0	74	7	0
13	D	66	0	74	3	0
13	E	66	0	74	6	0
13	F	66	0	74	5	0
13	G	66	0	74	7	0
13	I	66	0	74	6	0
13	J	66	0	74	3	0
13	K	66	0	74	4	0
13	L	198	0	222	10	0
13	M	66	0	74	9	0
13	N	66	0	74	5	0
13	O	66	0	74	3	0
13	P	66	0	74	6	0
13	Q	66	0	74	3	0
13	R	66	0	74	5	0
13	S	66	0	74	3	0
13	T	66	0	74	8	0
13	U	66	0	74	5	0
13	V	66	0	74	7	0
13	W	66	0	74	7	0
13	X	66	0	74	7	0
13	Y	66	0	74	3	0
13	Z	66	0	74	5	0
14	L	65	0	76	1	0
14	M	65	0	76	5	0
15	1	45	0	59	2	0
15	7	53	0	71	7	0
15	D	46	0	60	3	0
15	L	81	0	89	16	0
15	U	18	0	15	0	0
15	Y	20	0	19	3	0
16	4	67	0	83	3	0
16	5	30	0	33	4	0
16	7	31	0	35	7	0
16	9	25	0	23	0	0
16	B	34	0	41	0	0
16	D	31	0	35	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	E	35	0	46	0	0
16	F	32	0	37	0	0
16	H	26	0	25	3	0
16	J	30	0	33	0	0
16	K	35	0	46	1	0
16	L	32	0	37	2	0
16	M	31	0	35	3	0
16	O	35	0	46	2	0
16	P	35	0	46	2	0
16	T	35	0	46	0	0
16	V	35	0	46	0	0
16	X	34	0	41	1	0
16	Z	70	0	92	1	0
17	0	44	0	56	7	0
17	2	88	0	112	8	0
17	4	44	0	56	3	0
17	8	88	0	112	10	0
17	A	17	0	12	2	0
17	B	44	0	56	6	0
17	D	40	0	50	2	0
17	E	44	0	56	4	0
17	G	44	0	56	2	0
17	H	137	0	187	11	0
17	J	44	0	56	5	0
17	K	46	0	63	4	0
17	L	87	0	122	6	0
17	M	121	0	125	6	0
17	N	44	0	56	3	0
17	P	44	0	56	3	0
17	R	44	0	56	2	0
17	T	44	0	56	5	0
17	V	44	0	56	5	0
17	X	44	0	56	5	0
18	M	1	0	0	0	0
19	M	63	0	0	0	0
20	0	44	0	60	3	0
20	2	44	0	60	3	0
20	4	44	0	60	5	0
20	6	44	0	60	12	0
20	8	44	0	60	7	0
20	B	44	0	60	4	0
20	E	44	0	60	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	G	44	0	60	4	0
20	J	44	0	60	5	0
20	M	44	0	60	5	0
20	N	44	0	60	7	0
20	P	44	0	60	4	0
20	R	44	0	60	5	0
20	T	44	0	60	7	0
20	V	44	0	60	11	0
20	Y	44	0	60	5	0
20	Z	44	0	60	4	0
21	A	1	0	0	0	0
21	C	47	0	0	2	0
21	D	1	0	0	0	0
21	H	5	0	0	0	0
21	L	19	0	0	1	0
21	M	24	0	0	0	0
21	S	1	0	0	0	0
21	W	1	0	0	0	0
All	All	27731	0	28078	690	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 12.

All (690) 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:124:CYS:SG	7:C:401:HEM:HAC	1.82	1.20
1:C:124:CYS:SG	7:C:401:HEM:CAC	2.43	1.06
1:C:198:ASP:OD1	21:C:501:HOH:O	1.88	0.89
3:M:287:THR:HB	3:M:294:TRP:HE1	1.46	0.79
4:H:297:THR:HG22	4:H:300:GLU:H	1.50	0.76
1:C:247:THR:HG21	3:M:192:ARG:HB2	1.65	0.76
2:L:81:MET:HE3	5:9:34:SER:HB2	1.68	0.75
6:8:43:TRP:HB2	17:8:101:PGV:H212	1.69	0.75
1:C:142:ARG:NH1	7:C:401:HEM:O1D	2.20	0.75
5:O:6:MET:HE1	6:P:12:GLU:HA	1.67	0.74
5:7:32:LEU:HD11	13:8:103:BCL:HHD	1.69	0.73
5:D:32:LEU:HD11	13:E:102:BCL:HHD	1.70	0.72
16:5:401:LMT:H21	16:7:103:LMT:H42	1.72	0.71
5:K:1:FME:HCN	16:P:104:LMT:H111	1.72	0.71
5:O:7:LEU:HD22	5:Q:11:ARG:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:18:PHE:HB2	20:V:101:CRT:H23	1.71	0.70
5:Q:32:LEU:HD11	13:R:102:BCL:HHD	1.72	0.70
3:M:241:ARG:NH2	4:H:76:ARG:O	2.25	0.69
2:L:168:HIS:HB3	3:M:183:LEU:HD13	1.75	0.69
5:Y:32:LEU:HD11	13:Z:102:BCL:HHD	1.73	0.69
6:2:22:PHE:HA	20:2:102:CRT:H14	1.75	0.68
1:C:133:ASP:OD2	1:C:142:ARG:NH2	2.27	0.68
4:H:108:PRO:HB2	4:H:310:GLY:HA2	1.74	0.67
5:D:1:FME:H	15:D:104:U10:H352	1.59	0.67
6:R:47:ILE:HG21	17:R:103:PGV:H212	1.76	0.67
5:3:32:LEU:HD11	13:4:102:BCL:HHD	1.77	0.67
5:O:32:LEU:HD11	13:P:102:BCL:HHD	1.77	0.66
5:W:37:ARG:NH1	6:X:45:PRO:O	2.29	0.66
1:C:121:CYS:HB2	7:C:401:HEM:HHC	1.77	0.65
5:A:32:LEU:HD11	13:B:102:BCL:HHD	1.77	0.65
6:R:51:GLU:OE2	6:R:51:GLU:N	2.22	0.65
13:7:102:BCL:H3C	17:8:101:PGV:H242	1.79	0.65
2:L:138:LEU:O	16:L:305:LMT:O6'	2.09	0.65
5:K:32:LEU:HD11	13:N:102:BCL:HHD	1.78	0.65
3:M:228:ARG:O	4:H:305:THR:OG1	2.14	0.65
5:9:32:LEU:HD11	13:0:102:BCL:HHD	1.78	0.65
5:F:32:LEU:HD11	13:G:102:BCL:HHD	1.78	0.65
5:5:32:LEU:HD11	13:6:102:BCL:HHD	1.79	0.65
2:L:40:PHE:HZ	15:7:101:U10:H353	1.62	0.64
5:I:32:LEU:HD11	13:J:102:BCL:HHD	1.79	0.64
4:H:91:GLU:HB3	17:A:101:PGV:H062	1.80	0.64
5:1:37:ARG:O	6:2:44:ARG:NH1	2.30	0.64
3:M:3:GLU:N	3:M:3:GLU:OE2	2.29	0.64
5:F:6:MET:HB2	20:J:101:CRT:H1M1	1.81	0.63
17:B:103:PGV:H212	6:E:43:TRP:HB2	1.80	0.63
17:M:406:PGV:H201	16:H:402:LMT:H3B	1.79	0.63
16:M:409:LMT:H31	17:K:102:PGV:H251	1.81	0.63
13:A:102:BCL:HMB2	20:0:101:CRT:H35	1.81	0.62
5:F:1:FME:O1	5:F:3:ARG:NH1	2.32	0.62
2:L:43:PHE:HB2	17:L:307:PGV:H343	1.80	0.62
5:5:37:ARG:NH1	6:6:45:PRO:O	2.33	0.62
1:C:121:CYS:HB2	7:C:401:HEM:CHC	2.30	0.61
6:B:43:TRP:HB2	17:0:103:PGV:H231	1.81	0.61
13:L:302:BCL:H191	17:L:307:PGV:H101	1.83	0.61
4:H:14:GLN:NE2	17:H:401:PGV:O13	2.31	0.61
2:L:183:THR:HG21	3:M:213:THR:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:403:BPH:HBB3	14:M:403:BPH:HHC	1.83	0.61
5:U:32:LEU:HD11	13:V:102:BCL:HHD	1.81	0.61
2:L:197:VAL:HG11	2:L:213:GLU:HG3	1.83	0.61
6:J:18:PHE:HA	20:J:101:CRT:H6	1.83	0.61
5:S:37:ARG:NH1	6:T:45:PRO:O	2.33	0.60
13:B:102:BCL:H172	17:B:103:PGV:H61	1.84	0.60
4:H:59:LYS:H	4:H:59:LYS:HD3	1.66	0.60
5:7:37:ARG:O	6:8:44:ARG:NH1	2.33	0.60
5:Y:37:ARG:O	6:Z:44:ARG:NH1	2.31	0.60
5:F:37:ARG:NH1	6:G:45:PRO:O	2.34	0.60
3:M:159:VAL:HA	3:M:163:ILE:HB	1.83	0.60
5:K:33:LEU:O	5:K:39:ASN:ND2	2.35	0.60
1:C:232:SER:OG	3:M:292:ASP:OD2	2.15	0.59
5:Y:1:FME:HG3	16:Z:104:LMT:H61	1.84	0.59
2:L:213:GLU:HB3	15:L:304:U10:H4M2	1.83	0.59
6:R:46:TRP:CD2	13:R:102:BCL:H2C	2.37	0.59
17:V:103:PGV:H212	6:X:43:TRP:HB2	1.83	0.59
5:3:33:LEU:O	5:3:39:ASN:ND2	2.35	0.59
1:C:160:ASN:HA	1:C:165:GLY:HA3	1.84	0.59
5:7:6:MET:HE1	6:8:15:ALA:HB3	1.84	0.59
5:1:32:LEU:HD11	13:2:103:BCL:HHD	1.83	0.59
6:B:46:TRP:CD2	13:B:102:BCL:H2C	2.38	0.59
2:L:39:LEU:HD22	17:L:307:PGV:H341	1.85	0.58
6:4:18:PHE:HB2	20:4:101:CRT:H21A	1.84	0.58
5:Y:33:LEU:O	5:Y:39:ASN:ND2	2.36	0.58
13:0:102:BCL:H121	17:0:103:PGV:H91	1.84	0.58
17:T:103:PGV:H212	6:V:43:TRP:HB2	1.84	0.58
2:L:60:ASN:HB3	2:L:63:GLN:HB2	1.86	0.58
5:D:33:LEU:O	5:D:39:ASN:ND2	2.36	0.58
5:7:33:LEU:O	5:7:39:ASN:ND2	2.36	0.58
13:R:102:BCL:HBB2	17:R:103:PGV:H301	1.85	0.57
1:C:64:VAL:HG22	1:C:348:LEU:HD13	1.85	0.57
6:N:46:TRP:CD2	13:N:102:BCL:H2C	2.39	0.57
5:O:1:FME:SD	5:O:1:FME:N	2.76	0.57
6:R:20:LYS:HE3	6:R:24:GLN:HE22	1.69	0.57
5:S:32:LEU:HD11	13:T:102:BCL:HHD	1.86	0.57
6:X:46:TRP:HZ2	17:X:102:PGV:H82	1.69	0.57
5:1:37:ARG:NH1	6:2:45:PRO:O	2.38	0.57
5:I:37:ARG:O	6:J:44:ARG:NH1	2.33	0.57
5:K:16:ALA:HB1	16:K:103:LMT:H6D	1.86	0.57
6:V:22:PHE:HA	20:V:101:CRT:H14	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:7:101:U10:H1M2	16:7:103:LMT:H51	1.87	0.57
1:C:144:MET:HE1	1:C:302:MET:HE1	1.87	0.57
6:E:46:TRP:CD2	13:E:102:BCL:H2C	2.39	0.57
6:G:46:TRP:CD2	13:G:102:BCL:H2C	2.39	0.57
6:P:46:TRP:CD2	13:P:102:BCL:H2C	2.40	0.57
5:W:32:LEU:HD11	13:X:101:BCL:HHD	1.85	0.57
4:H:175:ARG:NH2	4:H:301:GLU:OE2	2.38	0.57
4:H:282:GLU:OE1	4:H:282:GLU:N	2.34	0.57
16:D:103:LMT:H6B	16:D:103:LMT:H3O2	1.52	0.57
17:K:102:PGV:H241	17:K:102:PGV:H42	1.86	0.57
5:3:37:ARG:O	6:4:44:ARG:NH1	2.34	0.57
5:W:33:LEU:O	5:W:39:ASN:ND2	2.38	0.57
6:0:46:TRP:CD2	13:0:102:BCL:H2C	2.39	0.57
14:M:403:BPH:HBC3	14:M:403:BPH:HHD	1.87	0.57
1:C:93:THR:HG22	1:C:95:ASP:H	1.70	0.57
5:S:7:LEU:HD21	20:V:101:CRT:H1M1	1.86	0.57
20:G:101:CRT:H35	13:I:101:BCL:HMB1	1.87	0.56
5:K:37:ARG:O	6:N:44:ARG:NH1	2.34	0.56
6:X:46:TRP:CD2	13:X:101:BCL:H2C	2.40	0.56
1:C:45:ALA:HB2	2:L:156:TRP:CD1	2.40	0.56
17:H:401:PGV:H221	17:D:101:PGV:H82	1.87	0.56
17:B:103:PGV:H251	6:E:39:LEU:HB3	1.87	0.56
5:U:29:HIS:CE1	13:V:102:BCL:HMD3	2.40	0.56
5:U:37:ARG:O	6:V:44:ARG:NH1	2.34	0.56
20:V:101:CRT:H392	13:W:101:BCL:HBB2	1.87	0.56
1:C:194:ALA:O	3:M:114:TRP:NE1	2.36	0.56
16:4:105:LMT:H2B	6:6:29:PHE:HD1	1.70	0.56
5:7:37:ARG:NH1	6:8:45:PRO:O	2.38	0.56
1:C:264:ASN:HA	2:L:165:LEU:HD21	1.88	0.56
20:E:101:CRT:H35	13:F:101:BCL:HMB1	1.87	0.56
13:V:102:BCL:H152	17:V:103:PGV:H72	1.87	0.56
20:B:101:CRT:H35	13:D:102:BCL:HMB1	1.88	0.56
3:M:28:GLU:OE1	5:Q:12:ARG:NH1	2.39	0.56
5:9:2:TRP:CE2	6:0:16:LYS:HE3	2.40	0.56
3:M:243:THR:N	4:H:302:GLU:OE2	2.37	0.55
6:V:46:TRP:CD2	13:V:102:BCL:H2C	2.41	0.55
6:Z:46:TRP:CD2	13:Z:102:BCL:H2C	2.41	0.55
6:8:46:TRP:HZ2	17:8:104:PGV:H92	1.71	0.55
20:8:102:CRT:H343	5:9:26:ILE:HG22	1.87	0.55
2:L:59:TRP:HD1	17:D:101:PGV:H061	1.71	0.55
5:9:37:ARG:O	6:0:44:ARG:NH1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:60:SER:O	3:M:125:SER:OG	2.24	0.55
13:N:102:BCL:H143	17:N:103:PGV:H91	1.89	0.55
6:2:46:TRP:CD2	13:2:103:BCL:H2C	2.41	0.55
3:M:98:PRO:HA	3:M:112:GLY:HA3	1.88	0.55
6:T:46:TRP:CD2	13:T:102:BCL:H2C	2.42	0.55
3:M:287:THR:HB	3:M:294:TRP:NE1	2.19	0.55
6:8:46:TRP:CD2	13:8:103:BCL:H2C	2.41	0.55
3:M:12:GLN:OE1	3:M:14:ARG:NH2	2.40	0.55
5:1:46:MET:HE2	6:2:44:ARG:HG2	1.89	0.55
1:C:182:ALA:HB3	1:C:339:THR:HA	1.88	0.54
3:M:26:GLY:O	5:O:12:ARG:NH1	2.40	0.54
15:7:101:U10:H43	15:7:101:U10:H38	1.89	0.54
5:1:1:FME:HCN	16:4:104:LMT:H91	1.88	0.54
2:L:130:THR:HA	2:L:134:ILE:HB	1.89	0.54
6:0:22:PHE:CD2	20:0:101:CRT:H14	2.43	0.54
3:M:94:ALA:HB2	3:M:181:PRO:HG2	1.90	0.54
6:X:43:TRP:CD2	6:X:44:ARG:HG3	2.42	0.54
13:X:101:BCL:H143	17:X:102:PGV:H91	1.90	0.54
5:Y:13:THR:HG23	15:Y:103:U10:H3M2	1.89	0.54
6:B:43:TRP:CD2	6:B:44:ARG:HG3	2.42	0.54
6:J:46:TRP:CD2	13:J:102:BCL:H2C	2.43	0.54
5:W:29:HIS:CE1	13:X:101:BCL:HMD3	2.43	0.54
6:4:18:PHE:HA	20:4:101:CRT:H6	1.90	0.54
1:C:62:ASN:HB3	1:C:348:LEU:HA	1.90	0.54
6:E:43:TRP:CD2	6:E:44:ARG:HG3	2.43	0.54
5:F:33:LEU:O	5:F:39:ASN:ND2	2.41	0.54
6:B:51:GLU:OE1	17:B:103:PGV:O05	2.26	0.53
13:T:102:BCL:H121	17:T:103:PGV:H92	1.90	0.53
4:H:7:THR:HG1	5:F:34:SER:HG	1.43	0.53
5:F:37:ARG:O	6:G:44:ARG:NH1	2.32	0.53
6:Z:22:PHE:HA	20:Z:101:CRT:H14	1.90	0.53
3:M:169:GLY:HA3	16:M:409:LMT:H3B	1.91	0.53
6:G:22:PHE:HA	20:G:101:CRT:H14	1.90	0.53
6:J:18:PHE:HB2	20:J:101:CRT:H21A	1.90	0.53
13:I:101:BCL:H122	13:I:101:BCL:H51	1.91	0.53
20:T:101:CRT:H35	13:U:102:BCL:HMB2	1.91	0.53
5:5:37:ARG:O	6:6:44:ARG:NH1	2.40	0.53
1:C:48:GLN:HG2	1:C:50:LYS:HD3	1.90	0.53
5:3:37:ARG:NH1	6:4:45:PRO:O	2.42	0.53
6:8:43:TRP:CD2	6:8:44:ARG:HG3	2.44	0.53
2:L:236:PHE:HB2	15:L:308:U10:H8	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:43:TRP:CD2	6:R:44:ARG:HG3	2.43	0.53
16:L:305:LMT:H2'	16:5:401:LMT:H2'	1.91	0.53
5:Y:6:MET:HE3	5:Y:6:MET:HA	1.91	0.53
2:L:225:ILE:HG12	2:L:229:GLY:HA3	1.91	0.53
20:P:101:CRT:H35	13:Q:101:BCL:HMB1	1.91	0.52
5:Y:7:LEU:HB3	5:1:11:ARG:HG3	1.90	0.52
17:2:104:PGV:H232	6:4:39:LEU:HB3	1.90	0.52
1:C:118:ARG:HD3	1:C:317:ILE:HD12	1.90	0.52
13:L:302:BCL:HBC2	13:M:402:BCL:HBC2	1.89	0.52
5:5:42:GLU:OE2	16:5:401:LMT:O3B	2.27	0.52
13:G:102:BCL:H18	17:G:103:PGV:H61	1.92	0.52
5:I:37:ARG:NH1	6:J:45:PRO:O	2.43	0.52
6:6:46:TRP:CD2	13:6:102:BCL:H2C	2.45	0.52
3:M:280:GLY:HA2	13:M:402:BCL:HED2	1.91	0.52
6:4:46:TRP:CD2	13:4:102:BCL:H2C	2.44	0.52
1:C:173:CYS:HA	1:C:340:CYS:CB	2.40	0.52
4:H:77:LYS:O	4:H:79:GLN:NE2	2.42	0.52
16:D:103:LMT:O3'	16:D:103:LMT:O6B	2.27	0.52
4:H:80:ARG:NH2	4:H:104:ASP:O	2.43	0.52
5:A:29:HIS:CE1	13:B:102:BCL:HMD3	2.45	0.52
5:S:7:LEU:HD12	20:V:101:CRT:H82	1.92	0.52
5:3:7:LEU:HD21	20:6:101:CRT:H32A	1.92	0.52
4:H:25:ALA:HB1	17:H:403:PGV:H241	1.92	0.51
1:C:137:THR:O	1:C:141:SER:OG	2.26	0.51
2:L:232:ARG:NH2	3:M:6:ASN:OD1	2.43	0.51
5:D:1:FME:O1	5:D:3:ARG:NH1	2.44	0.51
5:5:18:PHE:HZ	20:6:101:CRT:H131	1.75	0.51
15:L:304:U10:H251	15:L:309:U10:H211	1.92	0.51
5:I:33:LEU:O	5:I:39:ASN:ND2	2.44	0.51
2:L:132:VAL:HG13	2:L:133:VAL:HG23	1.91	0.51
3:M:65:PHE:CZ	5:S:23:VAL:HG22	2.46	0.51
6:0:43:TRP:CD2	6:0:44:ARG:HG3	2.46	0.51
2:L:40:PHE:CZ	15:7:101:U10:H353	2.45	0.51
5:9:37:ARG:NH1	6:0:45:PRO:O	2.44	0.51
1:C:121:CYS:CB	7:C:401:HEM:HHC	2.41	0.51
14:L:303:BPH:CBB	14:L:303:BPH:HHC	2.41	0.51
3:M:97:PRO:HD3	3:M:176:PRO:HB3	1.92	0.51
5:D:37:ARG:NH1	6:E:45:PRO:O	2.44	0.51
6:N:22:PHE:CD2	20:N:101:CRT:H14	2.45	0.51
6:2:36:ALA:HB1	17:2:101:PGV:H282	1.92	0.51
1:C:87:GLN:OE1	1:C:142:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:40:PHE:CE2	15:7:101:U10:H311	2.46	0.51
3:M:109:LEU:HD22	3:M:114:TRP:CE2	2.46	0.51
5:3:4:ILE:HD11	5:3:8:PHE:CE2	2.45	0.50
6:4:47:ILE:HG13	17:4:103:PGV:H52	1.93	0.50
6:6:21:ILE:HB	20:6:101:CRT:H6	1.94	0.50
5:D:12:ARG:HB2	15:D:104:U10:H4M2	1.93	0.50
5:Q:3:ARG:HD3	20:T:101:CRT:H41	1.94	0.50
5:U:19:THR:HG23	13:U:102:BCL:H162	1.92	0.50
4:H:7:THR:HB	5:F:35:THR:HG22	1.93	0.50
1:C:173:CYS:HA	1:C:340:CYS:HB3	1.94	0.50
2:L:225:ILE:HG22	15:L:304:U10:H8	1.93	0.50
20:V:101:CRT:H35	13:W:101:BCL:HMB2	1.92	0.50
20:8:102:CRT:H35	13:9:101:BCL:C1B	2.41	0.50
3:M:153:ALA:HB1	13:M:402:BCL:H71	1.92	0.50
17:J:103:PGV:H211	6:N:43:TRP:HB2	1.94	0.50
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.76	0.50
3:M:301:HIS:HB3	17:H:401:PGV:H032	1.94	0.50
4:H:26:GLY:HA3	16:H:402:LMT:H12	1.94	0.50
6:X:18:PHE:HB2	20:Y:101:CRT:H21A	1.94	0.50
17:J:103:PGV:H282	6:N:36:ALA:HB1	1.94	0.49
17:8:104:PGV:H232	6:0:39:LEU:HB3	1.94	0.49
5:D:27:PHE:HD1	16:D:103:LMT:H61	1.76	0.49
6:8:22:PHE:HA	20:8:102:CRT:H14	1.94	0.49
13:0:102:BCL:H152	17:0:103:PGV:H72	1.94	0.49
4:H:277:SER:OG	4:H:312:ARG:NH2	2.40	0.49
6:J:12:GLU:O	6:J:16:LYS:HG2	2.12	0.49
17:P:103:PGV:H282	6:R:36:ALA:HB1	1.95	0.49
3:M:82:SER:HB3	3:M:85:GLU:HB2	1.94	0.49
5:U:18:PHE:HE1	20:V:101:CRT:H182	1.78	0.49
6:X:43:TRP:CE2	6:X:44:ARG:HG3	2.48	0.49
13:0:102:BCL:H192	17:0:103:PGV:H52	1.93	0.49
6:J:22:PHE:CD2	20:J:101:CRT:H14	2.48	0.49
1:C:243:ASN:O	1:C:247:THR:HG23	2.13	0.49
4:H:29:PHE:HZ	4:H:55:VAL:HG22	1.78	0.49
1:C:310:PRO:O	1:C:316:TRP:NE1	2.36	0.49
6:2:43:TRP:CD2	6:2:44:ARG:HG3	2.48	0.49
6:4:43:TRP:CD2	6:4:44:ARG:HG3	2.48	0.49
5:7:40:TRP:CZ2	13:7:102:BCL:HHC	2.48	0.49
5:9:10:PRO:HB3	6:0:18:PHE:CE1	2.48	0.49
6:B:43:TRP:CE2	6:B:44:ARG:HG3	2.48	0.49
5:D:1:FME:HE1	20:G:101:CRT:H133	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:18:PHE:HA	20:N:101:CRT:H6	1.95	0.49
5:5:40:TRP:CZ2	13:5:402:BCL:HHC	2.47	0.49
5:O:47:GLU:HG3	6:P:54:ALA:HB3	1.94	0.49
20:2:102:CRT:H35	13:3:101:BCL:HMB1	1.94	0.49
2:L:202:LYS:O	2:L:205:ASP:HB2	2.13	0.48
2:L:274:SER:N	5:W:34:SER:OG	2.46	0.48
3:M:299:VAL:HG12	3:M:304:ALA:HB3	1.95	0.48
5:K:3:ARG:HD2	20:P:101:CRT:H41	1.95	0.48
2:L:111:LEU:O	3:M:247:ARG:NH1	2.46	0.48
6:J:23:VAL:O	6:J:27:ILE:HG12	2.13	0.48
6:N:46:TRP:HZ2	17:N:103:PGV:H101	1.79	0.48
15:L:304:U10:H101	15:L:304:U10:H13	1.95	0.48
3:M:205:SER:OG	3:M:276:THR:O	2.25	0.48
5:9:22:PHE:O	5:9:26:ILE:HG23	2.12	0.48
15:L:309:U10:H4M3	3:M:179:ILE:HG21	1.94	0.48
5:1:33:LEU:O	5:1:39:ASN:ND2	2.46	0.48
1:C:254:MET:HB3	8:C:403:HEC:C4B	2.44	0.48
6:N:11:SER:OG	6:N:13:ASP:OD1	2.28	0.48
5:O:6:MET:HA	6:P:10:LEU:HD21	1.96	0.48
16:5:401:LMT:O6'	16:7:103:LMT:O2'	2.29	0.48
13:B:102:BCL:H2	13:B:102:BCL:H62	1.58	0.48
6:E:13:ASP:OD1	6:E:13:ASP:N	2.37	0.48
13:V:102:BCL:H172	17:V:103:PGV:H51	1.96	0.48
5:W:21:LEU:HB3	13:W:101:BCL:H12	1.96	0.48
20:Y:101:CRT:H35	13:Y:102:BCL:HMB1	1.96	0.48
3:M:261:THR:H	3:M:264:SER:HG	1.60	0.47
5:Q:37:ARG:O	6:R:44:ARG:NH1	2.46	0.47
5:W:37:ARG:O	6:X:44:ARG:NH1	2.45	0.47
6:2:43:TRP:HB2	17:2:101:PGV:H201	1.95	0.47
5:I:5:TRP:HZ3	5:I:13:THR:HG21	1.79	0.47
5:U:40:TRP:CZ2	13:U:102:BCL:HHC	2.49	0.47
13:X:101:BCL:HBA1	13:X:101:BCL:H3A	1.40	0.47
5:Y:18:PHE:HE1	20:Z:101:CRT:H182	1.79	0.47
5:Y:27:PHE:HZ	5:1:30:PHE:HZ	1.62	0.47
3:M:290:VAL:HG22	4:H:4:GLY:HA2	1.96	0.47
5:7:5:TRP:HB2	6:8:15:ALA:HB1	1.95	0.47
5:9:10:PRO:HG2	6:0:10:LEU:HD11	1.95	0.47
5:A:37:ARG:O	6:B:44:ARG:NH1	2.45	0.47
13:E:102:BCL:H143	13:E:102:BCL:H161	1.78	0.47
5:O:2:TRP:CG	6:P:16:LYS:HD2	2.49	0.47
6:P:47:ILE:HG21	17:P:103:PGV:H212	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:GLN:HB3	1:C:214:PRO:HA	1.96	0.47
20:R:101:CRT:H10	20:R:101:CRT:H81	1.78	0.47
6:V:43:TRP:CD2	6:V:44:ARG:HG3	2.50	0.47
2:L:180:PHE:CD2	2:L:241:ALA:HB1	2.50	0.47
17:L:307:PGV:H302	17:L:307:PGV:H272	1.75	0.47
4:H:21:TRP:NE1	17:H:401:PGV:O04	2.46	0.47
5:W:22:PHE:HB2	13:W:101:BCL:H2	1.96	0.47
4:H:260:PHE:C	4:H:262:ASN:H	2.21	0.47
5:A:5:TRP:HZ3	5:A:13:THR:HG21	1.80	0.47
17:E:103:PGV:H282	6:G:36:ALA:HB1	1.96	0.47
6:P:19:HIS:O	6:P:23:VAL:HG23	2.13	0.47
13:V:102:BCL:HBA1	13:V:102:BCL:H3A	1.45	0.47
6:6:43:TRP:CD2	6:6:44:ARG:HG3	2.50	0.47
3:M:164:ARG:NH2	3:M:193:TYR:OH	2.47	0.47
5:K:44:ASN:O	6:N:44:ARG:NH2	2.47	0.47
3:M:157:TYR:CZ	20:M:405:CRT:H293	2.50	0.47
6:B:51:GLU:OE2	6:B:51:GLU:N	2.31	0.47
6:R:26:PHE:HD2	6:R:27:ILE:HD12	1.80	0.47
20:6:101:CRT:H5	20:6:101:CRT:H23	1.54	0.47
5:7:20:PHE:HE1	5:9:22:PHE:CZ	2.33	0.47
1:C:78:MET:HB2	1:C:81:GLU:HG2	1.97	0.46
1:C:83:TYR:HB3	7:C:401:HEM:CGA	2.45	0.46
2:L:265:ASP:OD1	21:L:401:HOH:O	2.19	0.46
5:U:37:ARG:NH1	6:V:45:PRO:O	2.48	0.46
5:3:3:ARG:HG3	5:3:3:ARG:HH11	1.80	0.46
5:7:34:SER:HA	16:7:103:LMT:O3B	2.15	0.46
1:C:125:HIS:CE1	1:C:138:LYS:HE3	2.51	0.46
2:L:34:PHE:O	2:L:38:THR:OG1	2.24	0.46
17:V:103:PGV:H221	6:X:39:LEU:HB3	1.96	0.46
13:6:102:BCL:H152	17:8:101:PGV:H72	1.96	0.46
13:S:101:BCL:H101	13:S:101:BCL:H62	1.50	0.46
1:C:228:ALA:O	8:C:403:HEC:HAA2	2.15	0.46
4:H:141:ASP:OD1	4:H:141:ASP:N	2.48	0.46
6:E:22:PHE:CD2	20:E:101:CRT:H14	2.50	0.46
13:4:102:BCL:HBA1	13:4:102:BCL:H3A	1.71	0.46
6:0:41:TRP:CH2	17:0:103:PGV:H21	2.50	0.46
3:M:83:PRO:HD3	5:U:30:PHE:HB3	1.97	0.46
3:M:130:TRP:NE1	3:M:147:ALA:O	2.46	0.46
20:J:101:CRT:H35	13:K:101:BCL:HMB1	1.97	0.46
5:K:30:PHE:CZ	17:K:102:PGV:H31	2.50	0.46
5:3:14:LEU:HD23	5:3:14:LEU:HA	1.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:7:103:LMT:O2B	16:7:103:LMT:H6E	2.16	0.46
13:B:102:BCL:H102	13:B:102:BCL:H61	1.44	0.46
13:Z:102:BCL:H3A	13:Z:102:BCL:HBA1	1.46	0.46
13:Z:102:BCL:H93	13:Z:102:BCL:H112	1.74	0.46
13:5:402:BCL:H143	13:5:402:BCL:H111	1.69	0.46
2:L:6:GLU:HA	3:M:250:LEU:HD11	1.98	0.46
6:R:43:TRP:CE2	6:R:44:ARG:HG3	2.50	0.46
5:W:3:ARG:HD3	6:Z:17:GLU:OE2	2.16	0.46
6:X:18:PHE:HA	20:Y:101:CRT:H6	1.96	0.46
17:4:103:PGV:H292	6:6:36:ALA:HB1	1.98	0.46
2:L:8:LYS:HD2	4:H:110:THR:HG23	1.98	0.46
17:M:407:PGV:O12	17:M:407:PGV:O06	2.28	0.46
13:E:102:BCL:H151	17:E:103:PGV:H72	1.97	0.46
13:G:102:BCL:H122	17:G:103:PGV:H92	1.98	0.46
13:X:101:BCL:H18	17:X:102:PGV:H42	1.98	0.46
5:Y:44:ASN:O	6:Z:44:ARG:NH2	2.43	0.46
20:Z:101:CRT:H35	13:1:101:BCL:HMB1	1.97	0.46
13:2:103:BCL:HBA1	13:2:103:BCL:H3A	1.60	0.46
4:H:22:LEU:HD11	5:F:27:PHE:HE1	1.81	0.46
20:N:101:CRT:H35	13:O:101:BCL:HMB1	1.97	0.46
6:T:10:LEU:HD22	6:T:14:GLU:HB2	1.98	0.46
6:4:43:TRP:CE2	6:4:44:ARG:HG3	2.51	0.46
15:7:101:U10:H322	5:9:22:PHE:HE2	1.80	0.46
13:0:102:BCL:H18	13:0:102:BCL:H151	1.61	0.46
1:C:51:ASN:HB3	1:C:54:LEU:HB3	1.96	0.46
3:M:65:PHE:HZ	5:S:23:VAL:HG22	1.80	0.46
6:B:10:LEU:HG	6:B:14:GLU:HB3	1.98	0.46
13:G:102:BCL:HBA1	13:G:102:BCL:H3A	1.49	0.46
6:N:13:ASP:OD1	6:N:13:ASP:N	2.48	0.46
6:4:24:GLN:HB3	16:4:104:LMT:H42	1.97	0.46
6:0:11:SER:OG	6:0:14:GLU:HG3	2.16	0.46
1:C:34:LEU:HA	1:C:52:PRO:HD3	1.97	0.45
2:L:219:ASP:O	3:M:132:ARG:NH2	2.49	0.45
5:3:3:ARG:HB3	20:6:101:CRT:H31A	1.97	0.45
3:M:71:ILE:O	3:M:75:MET:HG3	2.16	0.45
3:M:95:LEU:HB3	3:M:177:PHE:HB2	1.98	0.45
6:G:12:GLU:O	6:G:16:LYS:HG3	2.15	0.45
13:5:402:BCL:H102	13:5:402:BCL:H61	1.47	0.45
13:E:102:BCL:H193	17:E:103:PGV:H21	1.99	0.45
13:6:102:BCL:H162	13:6:102:BCL:H192	1.73	0.45
6:8:43:TRP:CE2	6:8:44:ARG:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ASN:OD1	1:C:165:GLY:N	2.47	0.45
1:C:288:TRP:CE3	3:M:317:PRO:HB2	2.51	0.45
3:M:283:GLY:O	3:M:287:THR:HG22	2.17	0.45
3:M:301:HIS:ND1	17:H:401:PGV:O14	2.43	0.45
4:H:146:PRO:HD2	4:H:165:LEU:HD11	1.98	0.45
5:A:10:PRO:HB3	6:B:18:PHE:CE1	2.52	0.45
6:J:46:TRP:HE1	17:J:103:PGV:H81	1.80	0.45
17:2:104:PGV:H232	17:2:104:PGV:H261	1.80	0.45
1:C:111:LYS:H	1:C:111:LYS:HG2	1.60	0.45
13:L:310:BCL:H18	13:L:310:BCL:H151	1.76	0.45
6:B:46:TRP:HZ2	17:B:103:PGV:H101	1.80	0.45
5:K:37:ARG:NH1	6:N:45:PRO:O	2.49	0.45
5:5:27:PHE:HE1	16:7:103:LMT:H62	1.81	0.45
1:C:274:MET:HE2	1:C:274:MET:HB2	1.88	0.45
17:L:307:PGV:H102	17:L:307:PGV:H131	1.72	0.45
17:L:307:PGV:H11	13:L:310:BCL:H91	1.97	0.45
4:H:166:TRP:CD2	4:H:246:MET:HE1	2.52	0.45
5:K:9:ASP:O	5:K:13:THR:HG22	2.16	0.45
13:N:102:BCL:HBA1	13:N:102:BCL:H3A	1.67	0.45
20:T:101:CRT:H10	20:T:101:CRT:H81	1.86	0.45
5:5:33:LEU:O	5:5:39:ASN:ND2	2.49	0.45
6:8:10:LEU:HD23	6:8:14:GLU:HG3	1.98	0.45
4:H:46:ASP:OD2	4:H:48:THR:OG1	2.30	0.45
20:E:101:CRT:H35	13:F:101:BCL:CMB	2.46	0.45
20:R:101:CRT:H20	20:R:101:CRT:H181	1.84	0.45
6:T:51:GLU:H	6:T:51:GLU:CD	2.21	0.45
13:6:102:BCL:H122	17:8:101:PGV:H72	1.99	0.45
13:8:103:BCL:H121	17:8:104:PGV:H292	1.99	0.45
1:C:298:ASN:HA	1:C:302:MET:HB2	1.99	0.45
6:N:18:PHE:HB2	20:N:101:CRT:H21A	1.98	0.45
5:Q:29:HIS:CE1	13:R:102:BCL:HMD1	2.52	0.45
5:U:5:TRP:HZ3	5:U:13:THR:HG21	1.82	0.45
15:Y:103:U10:H1M1	15:Y:103:U10:H71	1.68	0.45
2:L:103:ARG:NH2	3:M:254:TRP:O	2.50	0.45
2:L:263:TRP:O	2:L:266:TRP:HD1	1.99	0.45
6:E:46:TRP:HZ2	17:E:103:PGV:H82	1.82	0.45
5:U:1:FME:O1	5:U:3:ARG:HG3	2.17	0.45
3:M:28:GLU:CD	5:Q:11:ARG:HH12	2.24	0.45
6:B:51:GLU:H	6:B:51:GLU:CD	2.20	0.45
6:T:43:TRP:CE2	6:T:44:ARG:HG3	2.52	0.45
13:W:101:BCL:HMD3	6:X:37:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2:43:TRP:CE2	6:2:44:ARG:HG3	2.52	0.45
15:L:308:U10:H102	15:L:308:U10:H1M1	1.98	0.44
4:H:149:MET:HB3	4:H:273:GLY:HA2	1.98	0.44
5:D:27:PHE:CD1	16:D:103:LMT:H61	2.51	0.44
5:U:3:ARG:HH11	6:X:21:ILE:HD11	1.82	0.44
5:W:40:TRP:CZ2	13:W:101:BCL:HHC	2.52	0.44
2:L:236:PHE:CE2	15:L:308:U10:H4M3	2.53	0.44
13:M:402:BCL:H202	20:M:405:CRT:H16	1.98	0.44
5:O:37:ARG:NH1	6:P:45:PRO:O	2.49	0.44
20:P:101:CRT:H35	13:Q:101:BCL:CMB	2.48	0.44
5:S:29:HIS:CE1	13:T:102:BCL:HMD1	2.52	0.44
5:1:40:TRP:CZ2	13:1:101:BCL:HHC	2.53	0.44
6:8:13:ASP:HA	6:8:16:LYS:HB2	1.98	0.44
4:H:245:VAL:HG22	4:H:287:ILE:HB	1.99	0.44
17:H:403:PGV:H251	13:F:101:BCL:H191	1.99	0.44
6:E:43:TRP:CE2	6:E:44:ARG:HG3	2.52	0.44
5:I:21:LEU:HB3	13:I:101:BCL:H12	2.00	0.44
5:S:37:ARG:O	6:T:44:ARG:NH1	2.43	0.44
13:U:102:BCL:HMD3	6:V:37:HIS:CE1	2.53	0.44
5:3:27:PHE:CZ	5:5:30:PHE:HZ	2.35	0.44
6:6:18:PHE:HA	20:6:101:CRT:C5	2.47	0.44
20:8:102:CRT:H10	20:8:102:CRT:H81	1.84	0.44
5:9:40:TRP:CZ2	13:9:101:BCL:HHC	2.52	0.44
2:L:205:ASP:OD1	2:L:206:PRO:HD2	2.17	0.44
6:T:43:TRP:CD2	6:T:44:ARG:HG3	2.52	0.44
5:Y:22:PHE:HB2	13:Y:102:BCL:H2	2.00	0.44
1:C:143:LYS:HD3	1:C:143:LYS:HA	1.83	0.44
4:H:255:LYS:O	4:H:269:SER:OG	2.28	0.44
6:P:11:SER:HB3	6:P:14:GLU:HB2	2.00	0.44
6:E:51:GLU:H	6:E:51:GLU:CD	2.25	0.44
20:V:101:CRT:H10	20:V:101:CRT:H81	1.66	0.44
20:6:101:CRT:H20	20:6:101:CRT:H181	1.81	0.44
6:8:36:ALA:HB1	17:8:101:PGV:H282	2.00	0.44
1:C:218:PHE:HE1	1:C:256:HIS:CG	2.35	0.44
1:C:229:ARG:NE	8:C:403:HEC:O2D	2.31	0.44
3:M:179:ILE:O	3:M:182:HIS:ND1	2.44	0.44
5:Y:14:LEU:HD23	5:Y:14:LEU:HA	1.87	0.44
6:6:43:TRP:CE2	6:6:44:ARG:HG3	2.53	0.44
20:8:102:CRT:H35	13:9:101:BCL:C2B	2.47	0.44
13:T:102:BCL:HBB2	17:T:103:PGV:H291	2.00	0.43
16:X:103:LMT:H5'	16:X:103:LMT:O5B	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:403:BPH:H6C1	14:M:403:BPH:H4C1	1.49	0.43
20:M:405:CRT:H2M1	5:O:31:ILE:HG12	2.00	0.43
17:H:404:PGV:H332	5:D:20:PHE:HA	1.99	0.43
6:B:12:GLU:O	6:B:16:LYS:HD3	2.18	0.43
6:B:43:TRP:HB2	17:O:103:PGV:H201	2.00	0.43
2:L:76:GLY:HA3	16:7:103:LMT:H3B	2.00	0.43
20:B:101:CRT:H10	20:B:101:CRT:H81	1.78	0.43
5:F:4:ILE:HD11	5:F:8:PHE:HE2	1.83	0.43
17:J:103:PGV:H22	17:J:103:PGV:H51	1.83	0.43
20:N:101:CRT:H35	13:O:101:BCL:CMB	2.49	0.43
5:S:14:LEU:HD23	5:S:14:LEU:HA	1.89	0.43
5:7:35:THR:HG21	5:9:41:LEU:HB3	1.99	0.43
2:L:142:TRP:CD2	15:7:101:U10:H4M3	2.53	0.43
16:M:409:LMT:O2'	16:O:102:LMT:H12	2.18	0.43
13:B:102:BCL:HBB2	17:B:103:PGV:H302	2.00	0.43
13:G:102:BCL:H161	13:G:102:BCL:H192	1.75	0.43
13:I:101:BCL:HMD3	6:J:37:HIS:CE1	2.53	0.43
13:Q:101:BCL:H202	13:Q:101:BCL:H161	1.73	0.43
5:Y:40:TRP:CZ2	13:Y:102:BCL:HHC	2.53	0.43
13:Z:102:BCL:HBB2	17:2:101:PGV:H291	1.99	0.43
2:L:189:LEU:HB3	15:L:304:U10:H1M2	2.00	0.43
5:Y:1:FME:O	5:Y:4:ILE:HG22	2.18	0.43
20:6:101:CRT:H10	20:6:101:CRT:H81	1.77	0.43
13:8:103:BCL:H172	17:8:104:PGV:H62	2.00	0.43
3:M:160:LEU:HD21	13:M:402:BCL:OBD	2.18	0.43
4:H:32:ARG:NH1	4:H:35:ASP:OD2	2.51	0.43
4:H:155:ASP:OD1	4:H:155:ASP:N	2.52	0.43
5:A:33:LEU:O	5:A:39:ASN:ND2	2.51	0.43
6:B:22:PHE:CD2	20:B:101:CRT:H14	2.54	0.43
20:B:101:CRT:H35	13:D:102:BCL:CMB	2.49	0.43
20:G:101:CRT:H35	13:I:101:BCL:CMB	2.48	0.43
13:P:102:BCL:HBA1	13:P:102:BCL:H3A	1.64	0.43
6:V:43:TRP:CE2	6:V:44:ARG:HG3	2.53	0.43
3:M:130:TRP:O	3:M:133:SER:OG	2.27	0.43
5:Y:26:ILE:HD13	5:Y:26:ILE:HA	1.92	0.43
6:O:43:TRP:CE2	6:O:44:ARG:HG3	2.53	0.43
6:R:22:PHE:HA	20:R:101:CRT:H11	2.01	0.43
20:2:102:CRT:H10	20:2:102:CRT:H81	1.75	0.43
13:2:103:BCL:H13	17:2:104:PGV:H92	2.01	0.43
5:3:1:FME:HE2	5:3:1:FME:HA	2.00	0.43
5:3:31:ILE:O	5:3:35:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:8:103:BCL:H61	13:8:103:BCL:H41	1.86	0.43
6:0:7:LEU:HD23	6:0:7:LEU:HA	1.84	0.43
4:H:131:LEU:HD12	4:H:131:LEU:HA	1.79	0.43
13:T:102:BCL:H171	17:T:103:PGV:H52	2.01	0.43
5:U:6:MET:HE3	5:U:6:MET:HB3	1.84	0.43
3:M:55:TRP:HZ3	17:M:410:PGV:H012	1.84	0.42
13:M:402:BCL:HAA2	13:M:402:BCL:HBD	1.99	0.42
5:O:34:SER:HA	16:O:102:LMT:O3'	2.19	0.42
5:Q:33:LEU:O	5:Q:39:ASN:ND2	2.52	0.42
6:X:22:PHE:HA	20:Y:101:CRT:H14	2.00	0.42
17:X:102:PGV:H282	6:Z:36:ALA:HB1	2.00	0.42
6:Z:37:HIS:ND1	17:2:101:PGV:H132	2.34	0.42
2:L:170:ASN:HB3	2:L:173:HIS:HB3	2.02	0.42
3:M:89:GLN:O	3:M:93:LEU:HG	2.19	0.42
13:O:101:BCL:H202	13:O:101:BCL:H162	1.81	0.42
6:V:21:ILE:HB	20:V:101:CRT:H9	2.02	0.42
6:Z:43:TRP:CD2	6:Z:44:ARG:HG3	2.54	0.42
6:0:48:PRO:HA	6:0:53:TYR:CE2	2.54	0.42
1:C:172:THR:O	1:C:340:CYS:HB2	2.18	0.42
4:H:146:PRO:HB2	4:H:165:LEU:HD21	2.01	0.42
2:L:227:PRO:HA	15:L:304:U10:H3M3	2.02	0.42
13:L:311:BCL:H92	13:L:311:BCL:H43	2.00	0.42
3:M:110:GLN:HE22	5:S:42:GLU:CD	2.27	0.42
5:A:1:FME:O	5:A:4:ILE:HG22	2.20	0.42
5:I:40:TRP:CE3	13:I:101:BCL:HBC2	2.54	0.42
5:K:40:TRP:CD2	13:K:101:BCL:H2C	2.54	0.42
20:6:101:CRT:H35	13:7:102:BCL:HMB1	2.02	0.42
5:7:24:LEU:HD23	13:8:103:BCL:HED3	2.01	0.42
6:P:51:GLU:OE2	6:P:51:GLU:N	2.45	0.42
13:X:101:BCL:H72	17:X:102:PGV:H12	2.01	0.42
13:M:402:BCL:H2	14:M:403:BPH:HHC	2.01	0.42
4:H:82:GLU:HB3	4:H:84:ILE:HG12	2.02	0.42
13:K:101:BCL:H2	13:K:101:BCL:H61	1.84	0.42
13:P:102:BCL:H92	13:P:102:BCL:H61	1.74	0.42
20:6:101:CRT:H11	20:6:101:CRT:H15	1.73	0.42
2:L:273:TRP:CD2	3:M:88:ARG:HB2	2.55	0.42
3:M:148:TRP:CE2	17:M:406:PGV:H21	2.55	0.42
15:D:104:U10:H271	15:D:104:U10:H322	2.01	0.42
5:1:14:LEU:HD23	5:1:14:LEU:HA	1.89	0.42
13:1:101:BCL:H192	13:1:101:BCL:H162	1.73	0.42
1:C:69:TYR:CE2	1:C:99:ARG:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:405:CRT:H181	20:M:405:CRT:H20	1.79	0.42
5:I:3:ARG:HD3	20:N:101:CRT:H41	2.01	0.42
6:T:22:PHE:HA	20:T:101:CRT:H14	2.01	0.42
6:T:47:ILE:HD12	17:T:103:PGV:H231	2.02	0.42
20:T:101:CRT:H26	20:T:101:CRT:H241	1.92	0.42
3:M:55:TRP:CZ3	17:M:410:PGV:H012	2.55	0.42
3:M:106:LEU:HA	3:M:107:PRO:HD3	1.89	0.42
5:O:14:LEU:HD23	5:O:14:LEU:HA	1.90	0.42
6:P:41:TRP:CH2	17:P:103:PGV:H41	2.55	0.42
1:C:26:ASP:OD1	21:C:502:HOH:O	2.21	0.42
13:L:311:BCL:H143	13:M:402:BCL:H193	2.02	0.42
4:H:1:MET:HE3	4:H:1:MET:HB3	1.74	0.42
15:1:102:U10:H172	15:1:102:U10:H151	1.82	0.42
13:3:101:BCL:H2	13:3:101:BCL:H62	1.70	0.42
5:5:27:PHE:CZ	5:7:30:PHE:HZ	2.38	0.42
2:L:230:ILE:HG21	15:L:304:U10:H3M2	2.02	0.41
5:O:7:LEU:HD23	5:O:7:LEU:HA	1.91	0.41
6:6:18:PHE:HA	20:6:101:CRT:H5	2.01	0.41
6:6:22:PHE:HA	20:6:101:CRT:H11	2.01	0.41
20:8:102:CRT:H35	13:9:101:BCL:CHB	2.50	0.41
6:0:46:TRP:HZ2	17:0:103:PGV:H101	1.85	0.41
2:L:40:PHE:CD1	5:9:23:VAL:HG22	2.55	0.41
2:L:157:VAL:HG21	13:L:310:BCL:HHD	2.02	0.41
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.02	0.41
4:H:323:ALA:O	5:5:12:ARG:HD2	2.19	0.41
1:C:51:ASN:OD1	1:C:53:ARG:NH2	2.53	0.41
1:C:208:ILE:HD13	1:C:215:GLU:HA	2.02	0.41
20:M:405:CRT:H5	20:M:405:CRT:H33	1.52	0.41
4:H:21:TRP:CH2	17:H:401:PGV:H251	2.56	0.41
5:W:12:ARG:CZ	5:Y:11:ARG:HH21	2.33	0.41
5:Y:8:PHE:HB3	15:Y:103:U10:H4M1	2.02	0.41
6:Z:51:GLU:HB3	6:Z:54:ALA:HB3	2.02	0.41
5:3:1:FME:O1	5:3:3:ARG:HG3	2.21	0.41
13:3:101:BCL:H143	13:3:101:BCL:H111	1.84	0.41
20:4:101:CRT:H20	20:4:101:CRT:H181	1.85	0.41
6:6:41:TRP:CZ2	17:8:101:PGV:H22	2.56	0.41
4:H:18:TYR:CE1	17:H:401:PGV:H201	2.55	0.41
4:H:37:ARG:NH1	4:H:59:LYS:O	2.54	0.41
20:E:101:CRT:H10	20:E:101:CRT:H81	1.85	0.41
6:N:48:PRO:HA	6:N:53:TYR:CE1	2.55	0.41
6:R:18:PHE:HB2	20:R:101:CRT:H23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:40:TRP:CZ2	13:3:101:BCL:HHC	2.55	0.41
13:4:102:BCL:H122	17:4:103:PGV:H102	2.02	0.41
13:6:102:BCL:CGA	13:6:102:BCL:H3A	2.49	0.41
20:8:102:CRT:H15	20:8:102:CRT:H131	1.75	0.41
1:C:124:CYS:HB2	7:C:401:HEM:C3C	2.55	0.41
2:L:110:LYS:HB2	2:L:110:LYS:HE2	1.93	0.41
2:L:236:PHE:HB2	15:L:308:U10:C8	2.50	0.41
15:L:309:U10:H3M2	15:L:309:U10:O2	2.20	0.41
13:S:101:BCL:H141	13:S:101:BCL:H161	1.73	0.41
2:L:129:VAL:HA	2:L:132:VAL:HG12	2.02	0.41
3:M:116:LEU:HD12	3:M:116:LEU:HA	1.93	0.41
3:M:228:ARG:HB2	4:H:251:PHE:CE2	2.56	0.41
13:A:102:BCL:CMB	20:0:101:CRT:H35	2.48	0.41
13:F:101:BCL:H2	13:F:101:BCL:H61	1.64	0.41
6:N:53:TYR:CE2	5:O:43:GLY:HA3	2.55	0.41
5:O:10:PRO:HB3	6:P:18:PHE:CE1	2.55	0.41
15:1:102:U10:H72	15:1:102:U10:H1M1	1.75	0.41
5:5:40:TRP:CE3	13:5:402:BCL:HBC2	2.56	0.41
1:C:107:TRP:HZ2	1:C:357:HIS:CE1	2.38	0.41
13:L:302:BCL:H141	13:L:302:BCL:H162	1.81	0.41
13:L:310:BCL:HMD2	3:M:206:ILE:HD13	2.01	0.41
3:M:148:TRP:NE1	17:M:406:PGV:H21	2.35	0.41
13:D:102:BCL:HMD3	6:E:37:HIS:CE1	2.56	0.41
5:F:29:HIS:CE1	13:G:102:BCL:HMD1	2.55	0.41
5:K:10:PRO:HB3	6:N:18:PHE:CE1	2.56	0.41
20:N:101:CRT:H81	20:N:101:CRT:H10	1.79	0.41
6:P:43:TRP:CE2	6:P:44:ARG:HD2	2.56	0.41
13:P:102:BCL:H202	13:P:102:BCL:H162	1.76	0.41
5:S:1:FME:O1	5:S:3:ARG:NH1	2.53	0.41
5:7:27:PHE:CZ	5:9:30:PHE:HZ	2.39	0.41
2:L:195:LEU:HD21	3:M:267:ARG:HG3	2.02	0.41
2:L:225:ILE:CG2	15:L:304:U10:H8	2.50	0.41
1:C:173:CYS:HA	1:C:340:CYS:HB2	2.02	0.41
2:L:66:ILE:HB	2:L:148:TYR:HB2	2.03	0.41
2:L:126:PHE:HA	2:L:129:VAL:HG22	2.03	0.41
2:L:177:VAL:HG22	13:L:302:BCL:CHB	2.51	0.41
2:L:259:GLY:O	2:L:262:GLU:HB2	2.21	0.41
15:L:309:U10:H72	15:L:309:U10:H1M1	1.89	0.41
5:A:11:ARG:HH21	17:A:101:PGV:H05	1.86	0.41
5:D:37:ARG:O	6:E:44:ARG:NH1	2.48	0.41
6:G:51:GLU:OE2	6:G:51:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:29:HIS:CE1	13:J:102:BCL:HMD1	2.56	0.41
17:J:103:PGV:H241	6:N:39:LEU:HB3	2.03	0.41
5:K:1:FME:HE1	20:P:101:CRT:H133	2.02	0.41
5:K:3:ARG:HH12	16:P:104:LMT:H122	1.85	0.41
13:K:101:BCL:H101	13:K:101:BCL:H62	1.51	0.41
5:O:7:LEU:HD21	20:R:101:CRT:H1M1	2.02	0.41
5:Q:14:LEU:HD23	5:Q:14:LEU:HA	1.85	0.41
5:S:19:THR:O	5:S:23:VAL:HG23	2.21	0.41
13:U:102:BCL:HBC3	13:U:102:BCL:H2C	1.90	0.41
5:W:40:TRP:CE3	13:W:101:BCL:HBC2	2.56	0.41
20:Z:101:CRT:H10	20:Z:101:CRT:H81	1.72	0.41
13:2:103:BCL:H3A	13:2:103:BCL:H43	2.02	0.41
17:2:104:PGV:H292	6:4:36:ALA:HB1	2.02	0.41
5:7:15:ILE:HD13	5:7:15:ILE:HA	1.94	0.41
5:9:19:THR:O	5:9:23:VAL:HG23	2.20	0.41
1:C:45:ALA:O	2:L:163:GLN:NE2	2.54	0.41
3:M:55:TRP:HB2	5:Q:15:ILE:HG21	2.02	0.41
3:M:271:TRP:HZ2	16:H:402:LMT:H2B	1.86	0.41
4:H:10:MET:HE3	4:H:10:MET:HB3	1.84	0.41
13:A:102:BCL:H62	13:A:102:BCL:H102	1.89	0.41
13:E:102:BCL:H192	6:G:39:LEU:HD22	2.03	0.41
6:N:41:TRP:CZ2	17:N:103:PGV:H22	2.56	0.41
5:O:7:LEU:O	5:Q:11:ARG:HD2	2.21	0.41
13:R:102:BCL:HBA1	13:R:102:BCL:H3A	1.61	0.41
20:T:101:CRT:H20	20:T:101:CRT:H181	1.85	0.41
15:L:304:U10:H171	15:L:304:U10:H151	1.81	0.40
6:V:22:PHE:CD2	20:V:101:CRT:H14	2.55	0.40
5:1:6:MET:HB2	20:4:101:CRT:H1M1	2.03	0.40
13:1:101:BCL:HBC3	13:1:101:BCL:HHD	2.03	0.40
13:8:103:BCL:H141	13:8:103:BCL:H162	1.89	0.40
2:L:224:SER:O	3:M:45:ASN:HB2	2.20	0.40
5:Q:7:LEU:HD12	20:T:101:CRT:H82	2.04	0.40
13:T:102:BCL:H142	13:T:102:BCL:H111	1.74	0.40
13:V:102:BCL:H151	6:X:39:LEU:HD13	2.03	0.40
1:C:221:TYR:O	1:C:295:ARG:NH1	2.54	0.40
2:L:189:LEU:HD11	14:M:403:BPH:HED1	2.03	0.40
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.57	0.40
5:D:10:PRO:HB3	6:E:18:PHE:CZ	2.56	0.40
13:F:101:BCL:HMD3	6:G:37:HIS:CE1	2.57	0.40
5:K:29:HIS:CE1	13:N:102:BCL:HMD1	2.55	0.40
17:K:102:PGV:H131	17:K:102:PGV:H102	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:28:ILE:HD12	13:P:102:BCL:O1D	2.22	0.40
5:S:40:TRP:CE3	13:S:101:BCL:HBC2	2.56	0.40
13:T:102:BCL:H162	13:T:102:BCL:H141	1.88	0.40
17:V:103:PGV:H231	17:V:103:PGV:H262	1.76	0.40
6:4:22:PHE:CD2	20:4:101:CRT:H14	2.57	0.40
6:4:48:PRO:HA	6:4:53:TYR:CE1	2.56	0.40
13:9:101:BCL:HMD3	6:0:37:HIS:CE1	2.56	0.40
1:C:25:CYS:HB3	9:C:405:Z41:C17	2.43	0.40
1:C:58:LYS:NZ	1:C:343:ASN:O	2.45	0.40
1:C:209:ASN:CG	2:L:262:GLU:HG3	2.47	0.40
3:M:197:PHE:CE1	13:M:402:BCL:HMC2	2.57	0.40
3:M:203:MET:SD	17:H:401:PGV:H32	2.61	0.40
5:U:14:LEU:HD23	5:U:14:LEU:HA	1.90	0.40
20:Y:101:CRT:H20	20:Y:101:CRT:H181	1.85	0.40
13:0:102:BCL:HBA1	13:0:102:BCL:H3A	1.65	0.40
2:L:169:TYR:CG	2:L:261:PRO:HG3	2.56	0.40
5:A:14:LEU:HD23	5:A:14:LEU:HA	1.92	0.40
20:V:101:CRT:H15	20:V:101:CRT:H131	1.95	0.40
13:8:103:BCL:HBA1	13:8:103:BCL:H3A	1.59	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	342/385 (89%)	329 (96%)	13 (4%)	0	100	100
2	L	272/275 (99%)	265 (97%)	7 (3%)	0	100	100
3	M	316/323 (98%)	310 (98%)	6 (2%)	0	100	100
4	H	264/324 (82%)	258 (98%)	6 (2%)	0	100	100
5	1	45/59 (76%)	44 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	3	44/59 (75%)	43 (98%)	1 (2%)	0	100	100
5	5	45/59 (76%)	45 (100%)	0	0	100	100
5	7	45/59 (76%)	44 (98%)	1 (2%)	0	100	100
5	9	45/59 (76%)	45 (100%)	0	0	100	100
5	A	45/59 (76%)	45 (100%)	0	0	100	100
5	D	45/59 (76%)	44 (98%)	1 (2%)	0	100	100
5	F	45/59 (76%)	43 (96%)	2 (4%)	0	100	100
5	I	45/59 (76%)	45 (100%)	0	0	100	100
5	K	45/59 (76%)	44 (98%)	1 (2%)	0	100	100
5	O	45/59 (76%)	45 (100%)	0	0	100	100
5	Q	45/59 (76%)	45 (100%)	0	0	100	100
5	S	45/59 (76%)	43 (96%)	2 (4%)	0	100	100
5	U	45/59 (76%)	45 (100%)	0	0	100	100
5	W	45/59 (76%)	45 (100%)	0	0	100	100
5	Y	44/59 (75%)	44 (100%)	0	0	100	100
6	0	46/67 (69%)	44 (96%)	2 (4%)	0	100	100
6	2	44/67 (66%)	42 (96%)	2 (4%)	0	100	100
6	4	43/67 (64%)	42 (98%)	1 (2%)	0	100	100
6	6	42/67 (63%)	39 (93%)	3 (7%)	0	100	100
6	8	42/67 (63%)	39 (93%)	3 (7%)	0	100	100
6	B	44/67 (66%)	41 (93%)	3 (7%)	0	100	100
6	E	45/67 (67%)	42 (93%)	3 (7%)	0	100	100
6	G	44/67 (66%)	41 (93%)	3 (7%)	0	100	100
6	J	43/67 (64%)	41 (95%)	2 (5%)	0	100	100
6	N	42/67 (63%)	39 (93%)	3 (7%)	0	100	100
6	P	43/67 (64%)	41 (95%)	2 (5%)	0	100	100
6	R	43/67 (64%)	40 (93%)	3 (7%)	0	100	100
6	T	43/67 (64%)	40 (93%)	3 (7%)	0	100	100
6	V	42/67 (63%)	39 (93%)	3 (7%)	0	100	100
6	X	44/67 (66%)	41 (93%)	3 (7%)	0	100	100
6	Z	43/67 (64%)	40 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2605/3323 (78%)	2522 (97%)	83 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	289/313 (92%)	286 (99%)	3 (1%)	68	82
2	L	218/219 (100%)	213 (98%)	5 (2%)	44	63
3	M	251/253 (99%)	242 (96%)	9 (4%)	31	47
4	H	219/258 (85%)	213 (97%)	6 (3%)	39	58
5	1	42/49 (86%)	41 (98%)	1 (2%)	43	62
5	3	41/49 (84%)	41 (100%)	0	100	100
5	5	42/49 (86%)	41 (98%)	1 (2%)	43	62
5	7	42/49 (86%)	42 (100%)	0	100	100
5	9	42/49 (86%)	40 (95%)	2 (5%)	23	35
5	A	42/49 (86%)	41 (98%)	1 (2%)	43	62
5	D	42/49 (86%)	42 (100%)	0	100	100
5	F	42/49 (86%)	42 (100%)	0	100	100
5	I	42/49 (86%)	42 (100%)	0	100	100
5	K	42/49 (86%)	42 (100%)	0	100	100
5	O	42/49 (86%)	41 (98%)	1 (2%)	43	62
5	Q	42/49 (86%)	42 (100%)	0	100	100
5	S	42/49 (86%)	42 (100%)	0	100	100
5	U	42/49 (86%)	42 (100%)	0	100	100
5	W	42/49 (86%)	42 (100%)	0	100	100
5	Y	41/49 (84%)	41 (100%)	0	100	100
6	0	39/55 (71%)	38 (97%)	1 (3%)	40	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	2	38/55 (69%)	38 (100%)	0	100	100
6	4	37/55 (67%)	37 (100%)	0	100	100
6	6	37/55 (67%)	35 (95%)	2 (5%)	20	29
6	8	37/55 (67%)	35 (95%)	2 (5%)	20	29
6	B	38/55 (69%)	38 (100%)	0	100	100
6	E	39/55 (71%)	39 (100%)	0	100	100
6	G	38/55 (69%)	38 (100%)	0	100	100
6	J	37/55 (67%)	37 (100%)	0	100	100
6	N	37/55 (67%)	37 (100%)	0	100	100
6	P	37/55 (67%)	37 (100%)	0	100	100
6	R	37/55 (67%)	37 (100%)	0	100	100
6	T	37/55 (67%)	37 (100%)	0	100	100
6	V	37/55 (67%)	37 (100%)	0	100	100
6	X	38/55 (69%)	37 (97%)	1 (3%)	40	59
6	Z	37/55 (67%)	37 (100%)	0	100	100
All	All	2247/2707 (83%)	2212 (98%)	35 (2%)	54	73

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	133	ASP
1	C	224	GLU
1	C	355	LYS
2	L	20	ASP
2	L	132	VAL
2	L	203	LYS
2	L	207	ILE
2	L	248	CYS
3	M	2	SER
3	M	13	VAL
3	M	21	VAL
3	M	31	THR
3	M	131	VAL
3	M	216	PHE
3	M	287	THR
3	M	290	VAL
3	M	292	ASP

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Mol	Chain	Res	Type
4	H	3	THR
4	H	64	THR
4	H	93	SER
4	H	131	LEU
4	H	245	VAL
4	H	297	THR
5	A	36	GLU
5	O	36	GLU
6	X	10	LEU
5	1	46	MET
5	5	14	LEU
6	6	17	GLU
6	6	25	SER
6	8	11	SER
6	8	23	VAL
5	9	26	ILE
5	9	42	GLU
6	0	51	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	122	ASN
1	C	129	ASN
1	C	177	ASN
1	C	209	ASN
1	C	243	ASN
1	C	343	ASN
2	L	60	ASN
3	M	80	ASN
4	H	258	ASN
6	E	24	GLN
5	F	44	ASN
6	P	24	GLN
5	Q	44	ASN
6	R	24	GLN
5	U	44	ASN
6	X	24	GLN
6	2	24	GLN
6	4	24	GLN
6	8	24	GLN
5	9	44	ASN

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Mol	Chain	Res	Type
6	0	24	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FME	Y	1	5	8,9,10	0.47	0	7,9,11	1.16	1 (14%)
5	FME	O	1	5	8,9,10	0.51	0	7,9,11	1.02	1 (14%)
5	FME	S	1	5	8,9,10	0.50	0	7,9,11	1.12	1 (14%)
5	FME	9	1	5	8,9,10	0.52	0	7,9,11	0.89	1 (14%)
5	FME	W	1	5	8,9,10	0.49	0	7,9,11	1.10	1 (14%)
5	FME	F	1	5	8,9,10	0.51	0	7,9,11	0.98	1 (14%)
5	FME	7	1	5	8,9,10	0.52	0	7,9,11	0.98	1 (14%)
5	FME	Q	1	5	8,9,10	0.53	0	7,9,11	0.96	1 (14%)
5	FME	3	1	5	8,9,10	0.51	0	7,9,11	1.01	1 (14%)
5	FME	K	1	5	8,9,10	0.51	0	7,9,11	1.09	1 (14%)
5	FME	1	1	5	8,9,10	0.51	0	7,9,11	0.95	1 (14%)
5	FME	5	1	5	8,9,10	0.50	0	7,9,11	1.02	1 (14%)
5	FME	U	1	5	8,9,10	0.52	0	7,9,11	0.96	1 (14%)
5	FME	A	1	5	8,9,10	0.49	0	7,9,11	1.13	1 (14%)
5	FME	D	1	5	8,9,10	0.48	0	7,9,11	1.12	1 (14%)
5	FME	I	1	5	8,9,10	0.50	0	7,9,11	1.11	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FME	Y	1	5	-	1/7/9/11	-
5	FME	O	1	5	-	3/7/9/11	-
5	FME	S	1	5	-	0/7/9/11	-
5	FME	9	1	5	-	2/7/9/11	-
5	FME	W	1	5	-	1/7/9/11	-
5	FME	F	1	5	-	1/7/9/11	-
5	FME	7	1	5	-	0/7/9/11	-
5	FME	Q	1	5	-	2/7/9/11	-
5	FME	3	1	5	-	0/7/9/11	-
5	FME	K	1	5	-	1/7/9/11	-
5	FME	1	1	5	-	2/7/9/11	-
5	FME	5	1	5	-	0/7/9/11	-
5	FME	U	1	5	-	0/7/9/11	-
5	FME	A	1	5	-	2/7/9/11	-
5	FME	D	1	5	-	2/7/9/11	-
5	FME	I	1	5	-	0/7/9/11	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	1	FME	O-C-CA	-2.77	117.51	124.78
5	A	1	FME	O-C-CA	-2.69	117.73	124.78
5	I	1	FME	O-C-CA	-2.69	117.73	124.78
5	D	1	FME	O-C-CA	-2.69	117.74	124.78
5	S	1	FME	O-C-CA	-2.68	117.74	124.78
5	W	1	FME	O-C-CA	-2.65	117.85	124.78
5	K	1	FME	O-C-CA	-2.63	117.89	124.78
5	O	1	FME	O-C-CA	-2.55	118.08	124.78
5	3	1	FME	O-C-CA	-2.50	118.22	124.78
5	F	1	FME	O-C-CA	-2.49	118.26	124.78
5	7	1	FME	O-C-CA	-2.48	118.27	124.78
5	5	1	FME	O-C-CA	-2.46	118.33	124.78
5	Q	1	FME	O-C-CA	-2.43	118.40	124.78
5	U	1	FME	O-C-CA	-2.43	118.41	124.78
5	1	1	FME	O-C-CA	-2.42	118.44	124.78
5	9	1	FME	O-C-CA	-2.25	118.87	124.78

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1	FME	C-CA-CB-CG
5	F	1	FME	O1-CN-N-CA
5	K	1	FME	CA-CB-CG-SD
5	O	1	FME	O1-CN-N-CA
5	O	1	FME	N-CA-CB-CG
5	O	1	FME	C-CA-CB-CG
5	Q	1	FME	O1-CN-N-CA
5	W	1	FME	O1-CN-N-CA
5	9	1	FME	O1-CN-N-CA
5	D	1	FME	N-CA-CB-CG
5	9	1	FME	N-CA-CB-CG
5	1	1	FME	N-CA-CB-CG
5	Q	1	FME	N-CA-CB-CG
5	A	1	FME	C-CA-CB-CG
5	Y	1	FME	C-CA-CB-CG
5	A	1	FME	CB-CA-N-CN
5	1	1	FME	CB-CA-N-CN

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	1	FME	2	0
5	O	1	FME	1	0
5	S	1	FME	1	0
5	F	1	FME	1	0
5	3	1	FME	2	0
5	K	1	FME	2	0
5	1	1	FME	1	0
5	U	1	FME	1	0
5	A	1	FME	1	0
5	D	1	FME	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 123 ligands modelled in this entry, 4 are monoatomic - leaving 119 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
15	U10	7	101	-	53,53,63	0.60	2 (3%)	64,67,79	0.52	0
20	CRT	E	101	-	41,43,43	0.72	0	50,54,54	1.76	14 (28%)
20	CRT	R	101	-	41,43,43	0.72	0	50,54,54	1.77	13 (26%)
17	PGV	2	101	-	43,43,50	0.98	2 (4%)	45,49,56	1.00	2 (4%)
16	LMT	O	102	-	36,36,36	0.45	0	47,47,47	0.73	1 (2%)
17	PGV	R	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.01	2 (4%)
13	BCL	W	101	5	69,74,74	1.80	18 (26%)	83,115,115	2.53	27 (32%)
20	CRT	N	101	-	41,43,43	0.71	0	50,54,54	1.84	13 (26%)
19	A1L8Q	M	404	-	64,64,64	0.33	1 (1%)	78,81,81	0.61	1 (1%)
17	PGV	H	401	-	42,42,50	0.99	2 (4%)	45,48,56	1.16	3 (6%)
10	PLM	C	406	1	11,11,17	0.39	0	10,10,17	0.46	0
16	LMT	F	102	-	33,33,36	0.44	0	44,44,47	0.72	1 (2%)
13	BCL	A	102	5	69,74,74	1.80	17 (24%)	83,115,115	2.60	26 (31%)
13	BCL	E	102	6	69,74,74	1.78	18 (26%)	83,115,115	2.46	23 (27%)
17	PGV	B	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.12	4 (8%)
13	BCL	Y	102	5	69,74,74	1.80	17 (24%)	83,115,115	2.54	24 (28%)
13	BCL	7	102	5	69,74,74	1.78	17 (24%)	83,115,115	2.51	26 (31%)
17	PGV	M	406	-	36,36,50	1.07	2 (5%)	39,42,56	1.12	3 (7%)
13	BCL	O	101	5	69,74,74	1.79	18 (26%)	83,115,115	2.56	25 (30%)
13	BCL	G	102	6	69,74,74	1.78	18 (26%)	83,115,115	2.45	24 (28%)
13	BCL	0	102	6	69,74,74	1.79	18 (26%)	83,115,115	2.50	24 (28%)
13	BCL	6	102	6	69,74,74	1.77	17 (24%)	83,115,115	2.47	24 (28%)
17	PGV	8	104	-	43,43,50	0.98	2 (4%)	45,49,56	1.08	3 (6%)
16	LMT	4	105	-	33,33,36	0.43	0	44,44,47	0.65	1 (2%)
13	BCL	V	102	6	69,74,74	1.76	18 (26%)	83,115,115	2.44	24 (28%)
13	BCL	5	402	5	69,74,74	1.81	17 (24%)	83,115,115	2.50	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PGV	4	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.07	3 (6%)
17	PGV	D	101	-	39,39,50	1.03	2 (5%)	42,45,56	1.06	2 (4%)
16	LMT	H	402	-	27,27,36	0.46	0	37,38,47	0.81	1 (2%)
13	BCL	Q	101	5	69,74,74	1.80	18 (26%)	83,115,115	2.57	23 (27%)
16	LMT	9	102	-	26,26,36	0.48	0	37,37,47	0.77	1 (2%)
15	U10	L	309	-	30,30,63	0.79	1 (3%)	36,39,79	0.71	0
13	BCL	N	102	6	69,74,74	1.78	18 (26%)	83,115,115	2.47	23 (27%)
17	PGV	E	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.06	3 (6%)
13	BCL	8	103	6	69,74,74	1.78	17 (24%)	83,115,115	2.47	25 (30%)
16	LMT	J	104	-	31,31,36	0.45	0	42,42,47	0.75	1 (2%)
16	LMT	D	103	-	32,32,36	0.42	0	43,43,47	0.78	1 (2%)
17	PGV	H	404	-	50,50,50	0.93	2 (4%)	53,56,56	1.02	3 (5%)
13	BCL	K	101	5	69,74,74	1.80	18 (26%)	83,115,115	2.54	24 (28%)
20	CRT	T	101	-	41,43,43	0.72	0	50,54,54	1.83	13 (26%)
20	CRT	6	101	-	41,43,43	0.71	0	50,54,54	2.09	16 (32%)
20	CRT	J	101	-	41,43,43	0.72	0	50,54,54	1.81	16 (32%)
17	PGV	T	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.12	3 (6%)
20	CRT	2	102	-	41,43,43	0.72	0	50,54,54	1.87	14 (28%)
15	U10	1	102	-	45,45,63	0.67	2 (4%)	54,57,79	0.53	0
13	BCL	Z	102	6	69,74,74	1.78	18 (26%)	83,115,115	2.45	25 (30%)
9	Z41	C	405	1	25,25,39	0.32	0	27,27,41	0.29	0
13	BCL	D	102	5	69,74,74	1.80	18 (26%)	83,115,115	2.53	25 (30%)
15	U10	D	104	-	46,46,63	0.70	2 (4%)	55,58,79	0.69	0
17	PGV	M	410	-	19,19,50	1.70	3 (15%)	20,24,56	1.36	1 (5%)
16	LMT	7	103	-	32,32,36	0.42	0	43,43,47	1.14	4 (9%)
17	PGV	K	102	-	45,45,50	0.97	2 (4%)	48,51,56	0.99	2 (4%)
17	PGV	L	306	-	35,35,50	1.13	2 (5%)	39,40,56	1.16	3 (7%)
20	CRT	G	101	-	41,43,43	0.71	0	50,54,54	1.77	14 (28%)
17	PGV	0	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.02	3 (6%)
16	LMT	P	104	-	36,36,36	0.41	0	47,47,47	0.73	1 (2%)
16	LMT	K	103	-	36,36,36	0.44	0	47,47,47	0.80	0
13	BCL	I	101	5	69,74,74	1.80	17 (24%)	83,115,115	2.52	25 (30%)
15	U10	U	101	-	18,18,63	1.04	2 (11%)	22,25,79	0.85	0
17	PGV	H	403	-	42,42,50	1.00	2 (4%)	45,48,56	1.13	3 (6%)
20	CRT	P	101	-	41,43,43	0.71	0	50,54,54	1.79	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCL	1	101	5	69,74,74	1.79	17 (24%)	83,115,115	2.50	24 (28%)
13	BCL	L	310	2	69,74,74	1.78	18 (26%)	83,115,115	2.49	25 (30%)
16	LMT	L	305	-	33,33,36	0.48	0	44,44,47	0.84	2 (4%)
13	BCL	T	102	6	69,74,74	1.77	17 (24%)	83,115,115	2.48	25 (30%)
13	BCL	U	102	5	69,74,74	1.80	17 (24%)	83,115,115	2.46	25 (30%)
16	LMT	5	401	-	31,31,36	0.42	0	42,42,47	0.69	1 (2%)
16	LMT	Z	103	-	36,36,36	0.46	0	47,47,47	1.14	3 (6%)
14	BPH	L	303	-	59,70,70	0.77	2 (3%)	61,101,101	0.90	2 (3%)
17	PGV	2	104	-	43,43,50	0.99	2 (4%)	45,49,56	1.11	3 (6%)
20	CRT	8	102	-	41,43,43	0.73	0	50,54,54	2.38	16 (32%)
17	PGV	P	103	-	43,43,50	1.00	2 (4%)	45,49,56	1.12	4 (8%)
13	BCL	J	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.44	24 (28%)
13	BCL	M	402	3	69,74,74	1.81	17 (24%)	83,115,115	2.56	26 (31%)
16	LMT	Z	104	-	36,36,36	0.40	0	47,47,47	0.79	1 (2%)
13	BCL	4	102	6	69,74,74	1.78	18 (26%)	83,115,115	2.45	23 (27%)
13	BCL	B	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.46	24 (28%)
15	U10	Y	103	-	20,20,63	0.98	2 (10%)	24,27,79	0.91	0
17	PGV	J	103	-	43,43,50	0.98	2 (4%)	45,49,56	0.98	2 (4%)
20	CRT	0	101	-	41,43,43	0.70	0	50,54,54	1.75	12 (24%)
13	BCL	9	101	5	69,74,74	1.80	18 (26%)	83,115,115	2.51	24 (28%)
17	PGV	A	101	-	16,16,50	0.54	0	17,20,56	0.74	0
17	PGV	N	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.03	3 (6%)
8	HEC	C	404	1	50,50,50	1.75	11 (22%)	68,82,82	1.88	18 (26%)
16	LMT	E	104	-	36,36,36	0.42	0	47,47,47	0.72	1 (2%)
7	HEM	C	401	1	50,50,50	1.59	7 (14%)	66,82,82	1.66	16 (24%)
13	BCL	L	302	2	69,74,74	1.78	18 (26%)	83,115,115	2.59	28 (33%)
8	HEC	C	402	1	50,50,50	1.78	10 (20%)	68,82,82	1.79	18 (26%)
13	BCL	S	101	5	69,74,74	1.80	18 (26%)	83,115,115	2.59	26 (31%)
15	U10	L	308	-	18,18,63	1.07	2 (11%)	22,25,79	0.73	0
17	PGV	X	102	-	43,43,50	0.99	2 (4%)	45,49,56	0.97	2 (4%)
20	CRT	4	101	-	41,43,43	0.72	0	50,54,54	1.79	14 (28%)
13	BCL	R	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.43	24 (28%)
17	PGV	L	307	-	50,50,50	0.91	2 (4%)	53,56,56	0.99	3 (5%)
15	U10	L	304	-	33,33,63	0.78	2 (6%)	40,43,79	0.81	0
20	CRT	M	405	-	41,43,43	0.71	0	50,54,54	3.42	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PGV	G	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.02	2 (4%)
16	LMT	4	104	-	36,36,36	0.41	0	47,47,47	0.82	1 (2%)
16	LMT	B	104	-	35,35,36	0.43	0	46,46,47	0.79	0
13	BCL	P	102	6	69,74,74	1.77	17 (24%)	83,115,115	2.50	25 (30%)
17	PGV	M	408	-	34,34,50	1.15	2 (5%)	37,39,56	1.28	4 (10%)
13	BCL	X	101	6	69,74,74	1.76	18 (26%)	83,115,115	2.46	24 (28%)
16	LMT	T	104	-	36,36,36	0.38	0	47,47,47	0.69	1 (2%)
13	BCL	2	103	6	69,74,74	1.78	18 (26%)	83,115,115	2.48	23 (27%)
8	HEC	C	403	1	50,50,50	1.76	10 (20%)	68,82,82	1.82	18 (26%)
16	LMT	M	409	-	32,32,36	0.43	0	43,43,47	0.80	1 (2%)
20	CRT	Z	101	-	41,43,43	0.72	0	50,54,54	1.88	13 (26%)
20	CRT	B	101	-	41,43,43	0.71	0	50,54,54	1.89	15 (30%)
14	BPH	M	403	-	59,70,70	0.73	3 (5%)	61,101,101	0.89	2 (3%)
16	LMT	X	103	-	35,35,36	0.50	0	46,46,47	1.07	3 (6%)
20	CRT	Y	101	-	41,43,43	0.72	0	50,54,54	1.77	14 (28%)
16	LMT	V	104	-	36,36,36	0.43	0	47,47,47	0.95	3 (6%)
17	PGV	M	407	-	28,28,50	1.21	2 (7%)	31,34,56	1.24	3 (9%)
13	BCL	L	311	3	69,74,74	1.79	17 (24%)	83,115,115	2.49	24 (28%)
20	CRT	V	101	-	41,43,43	0.72	0	50,54,54	1.96	14 (28%)
13	BCL	F	101	5	69,74,74	1.79	18 (26%)	83,115,115	2.54	24 (28%)
13	BCL	3	101	5	69,74,74	1.81	17 (24%)	83,115,115	2.44	23 (27%)
17	PGV	V	103	-	43,43,50	0.99	2 (4%)	45,49,56	1.11	3 (6%)
17	PGV	8	101	-	43,43,50	0.98	2 (4%)	45,49,56	1.02	2 (4%)

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
15	U10	7	101	-	-	18/51/75/87	0/1/1/1
20	CRT	E	101	-	-	2/51/51/51	-
20	CRT	R	101	-	-	4/51/51/51	-
17	PGV	2	101	-	-	8/48/48/55	-
16	LMT	O	102	-	-	4/21/61/61	0/2/2/2
17	PGV	R	103	-	-	12/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCL	W	101	5	-	8/41/137/137	-
20	CRT	N	101	-	-	2/51/51/51	-
19	A1L8Q	M	404	-	-	16/59/79/79	0/2/2/2
17	PGV	H	401	-	-	16/47/47/55	-
10	PLM	C	406	1	-	2/8/9/15	-
16	LMT	F	102	-	-	4/18/58/61	0/2/2/2
13	BCL	A	102	5	-	7/41/137/137	-
13	BCL	E	102	6	-	15/41/137/137	-
17	PGV	B	103	-	-	17/48/48/55	-
13	BCL	Y	102	5	-	17/41/137/137	-
13	BCL	7	102	5	-	14/41/137/137	-
17	PGV	M	406	-	-	13/41/41/55	-
13	BCL	O	101	5	-	14/41/137/137	-
13	BCL	G	102	6	-	21/41/137/137	-
13	BCL	0	102	6	-	14/41/137/137	-
13	BCL	6	102	6	-	10/41/137/137	-
17	PGV	8	104	-	-	13/48/48/55	-
16	LMT	4	105	-	-	5/18/58/61	0/2/2/2
13	BCL	V	102	6	-	18/41/137/137	-
13	BCL	5	402	5	-	13/41/137/137	-
17	PGV	4	103	-	-	12/48/48/55	-
17	PGV	D	101	-	-	11/44/44/55	-
16	LMT	H	402	-	-	3/12/52/61	0/2/2/2
13	BCL	Q	101	5	-	13/41/137/137	-
16	LMT	9	102	-	-	1/11/51/61	0/2/2/2
15	U10	L	309	-	-	8/24/48/87	0/1/1/1
13	BCL	N	102	6	-	16/41/137/137	-
17	PGV	E	103	-	-	15/48/48/55	-
13	BCL	8	103	6	-	19/41/137/137	-
16	LMT	J	104	-	-	2/16/56/61	0/2/2/2
16	LMT	D	103	-	-	7/17/57/61	0/2/2/2
17	PGV	H	404	-	-	14/55/55/55	-
13	BCL	K	101	5	-	16/41/137/137	-
20	CRT	T	101	-	-	3/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CRT	6	101	-	-	11/51/51/51	-
20	CRT	J	101	-	-	7/51/51/51	-
17	PGV	T	103	-	-	13/48/48/55	-
20	CRT	2	102	-	-	7/51/51/51	-
15	U10	1	102	-	-	7/42/66/87	0/1/1/1
13	BCL	Z	102	6	-	19/41/137/137	-
9	Z41	C	405	1	-	11/26/26/41	-
13	BCL	D	102	5	-	10/41/137/137	-
15	U10	D	104	-	-	17/43/67/87	0/1/1/1
17	PGV	M	410	-	-	8/22/22/55	-
16	LMT	7	103	-	-	5/17/57/61	0/2/2/2
17	PGV	K	102	-	-	18/50/50/55	-
17	PGV	L	306	-	-	5/37/37/55	-
20	CRT	G	101	-	-	6/51/51/51	-
17	PGV	0	103	-	-	8/48/48/55	-
16	LMT	P	104	-	-	6/21/61/61	0/2/2/2
16	LMT	K	103	-	-	10/21/61/61	0/2/2/2
13	BCL	I	101	5	-	11/41/137/137	-
15	U10	U	101	-	-	1/9/33/87	0/1/1/1
17	PGV	H	403	-	-	22/47/47/55	-
20	CRT	P	101	-	-	0/51/51/51	-
13	BCL	1	101	5	-	14/41/137/137	-
13	BCL	L	310	2	-	12/41/137/137	-
16	LMT	L	305	-	-	6/18/58/61	0/2/2/2
13	BCL	T	102	6	-	16/41/137/137	-
13	BCL	U	102	5	-	13/41/137/137	-
16	LMT	5	401	-	-	2/16/56/61	0/2/2/2
16	LMT	Z	103	-	-	7/21/61/61	0/2/2/2
14	BPH	L	303	-	-	6/37/105/105	0/5/6/6
17	PGV	2	104	-	-	9/48/48/55	-
20	CRT	8	102	-	-	7/51/51/51	-
17	PGV	P	103	-	-	10/48/48/55	-
13	BCL	J	102	6	-	21/41/137/137	-
13	BCL	M	402	3	-	15/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMT	Z	104	-	-	6/21/61/61	0/2/2/2
13	BCL	4	102	6	-	13/41/137/137	-
13	BCL	B	102	6	-	17/41/137/137	-
15	U10	Y	103	-	-	2/12/36/87	0/1/1/1
17	PGV	J	103	-	-	6/48/48/55	-
20	CRT	0	101	-	-	3/51/51/51	-
13	BCL	9	101	5	-	15/41/137/137	-
17	PGV	A	101	-	-	8/19/19/55	-
17	PGV	N	103	-	-	11/48/48/55	-
8	HEC	C	404	1	1/1/3/7	4/14/54/54	-
16	LMT	E	104	-	-	5/21/61/61	0/2/2/2
7	HEM	C	401	1	-	6/14/54/54	-
13	BCL	L	302	2	-	10/41/137/137	-
8	HEC	C	402	1	1/1/3/7	4/14/54/54	-
13	BCL	S	101	5	-	13/41/137/137	-
15	U10	L	308	-	-	2/9/33/87	0/1/1/1
17	PGV	X	102	-	-	12/48/48/55	-
20	CRT	4	101	-	-	5/51/51/51	-
13	BCL	R	102	6	-	16/41/137/137	-
17	PGV	L	307	-	-	19/55/55/55	-
15	U10	L	304	-	-	6/27/51/87	0/1/1/1
20	CRT	M	405	-	-	7/51/51/51	-
17	PGV	G	103	-	-	9/48/48/55	-
16	LMT	4	104	-	-	5/21/61/61	0/2/2/2
16	LMT	B	104	-	-	8/20/60/61	0/2/2/2
13	BCL	P	102	6	-	17/41/137/137	-
17	PGV	M	408	-	-	9/36/36/55	-
13	BCL	X	101	6	-	17/41/137/137	-
16	LMT	T	104	-	-	3/21/61/61	0/2/2/2
13	BCL	2	103	6	-	18/41/137/137	-
8	HEC	C	403	1	1/1/3/7	4/14/54/54	-
16	LMT	M	409	-	-	2/17/57/61	0/2/2/2
20	CRT	Z	101	-	-	4/51/51/51	-
20	CRT	B	101	-	-	6/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BPH	M	403	-	-	8/37/105/105	0/5/6/6
16	LMT	X	103	-	-	10/20/60/61	0/2/2/2
20	CRT	Y	101	-	-	1/51/51/51	-
16	LMT	V	104	-	-	4/21/61/61	0/2/2/2
17	PGV	M	407	-	-	9/33/33/55	-
13	BCL	L	311	3	-	12/41/137/137	-
20	CRT	V	101	-	-	7/51/51/51	-
13	BCL	F	101	5	-	13/41/137/137	-
13	BCL	3	101	5	-	13/41/137/137	-
17	PGV	V	103	-	-	17/48/48/55	-
17	PGV	8	101	-	-	14/48/48/55	-

All (748) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	M	410	PGV	O01-C1	5.62	1.45	1.33
7	C	401	HEM	FE-NB	5.45	2.11	1.94
8	C	402	HEC	FE-NB	5.36	2.11	1.94
8	C	404	HEC	FE-NB	5.34	2.11	1.94
13	M	402	BCL	O2D-CGD	5.23	1.46	1.33
8	C	403	HEC	FE-NB	5.21	2.11	1.94
13	L	302	BCL	O2D-CGD	5.15	1.45	1.33
13	W	101	BCL	O2D-CGD	5.14	1.45	1.33
13	K	101	BCL	O2D-CGD	5.14	1.45	1.33
13	Z	102	BCL	O2D-CGD	5.14	1.45	1.33
13	5	402	BCL	O2D-CGD	5.13	1.45	1.33
13	3	101	BCL	O2D-CGD	5.13	1.45	1.33
13	I	101	BCL	O2D-CGD	5.13	1.45	1.33
13	8	103	BCL	O2D-CGD	5.13	1.45	1.33
13	Y	102	BCL	O2D-CGD	5.13	1.45	1.33
13	0	102	BCL	O2D-CGD	5.13	1.45	1.33
13	D	102	BCL	O2D-CGD	5.12	1.45	1.33
13	G	102	BCL	O2D-CGD	5.12	1.45	1.33
13	Q	101	BCL	O2D-CGD	5.11	1.45	1.33
13	V	102	BCL	O2D-CGD	5.11	1.45	1.33
13	4	102	BCL	O2D-CGD	5.11	1.45	1.33
13	O	101	BCL	O2D-CGD	5.10	1.45	1.33
13	9	101	BCL	O2D-CGD	5.10	1.45	1.33
13	N	102	BCL	O2D-CGD	5.10	1.45	1.33
13	U	102	BCL	O2D-CGD	5.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	103	BCL	O2D-CGD	5.09	1.45	1.33
13	F	101	BCL	O2D-CGD	5.09	1.45	1.33
13	S	101	BCL	O2D-CGD	5.09	1.45	1.33
13	7	102	BCL	O2D-CGD	5.09	1.45	1.33
13	J	102	BCL	O2D-CGD	5.08	1.45	1.33
13	R	102	BCL	O2D-CGD	5.08	1.45	1.33
13	E	102	BCL	O2D-CGD	5.08	1.45	1.33
13	A	102	BCL	O2D-CGD	5.08	1.45	1.33
13	6	102	BCL	O2D-CGD	5.08	1.45	1.33
13	X	101	BCL	O2D-CGD	5.07	1.45	1.33
13	1	101	BCL	O2D-CGD	5.07	1.45	1.33
13	T	102	BCL	O2D-CGD	5.06	1.45	1.33
13	L	310	BCL	O2D-CGD	5.06	1.45	1.33
13	P	102	BCL	O2D-CGD	5.03	1.45	1.33
13	B	102	BCL	O2D-CGD	5.03	1.45	1.33
13	L	311	BCL	O2D-CGD	4.92	1.45	1.33
13	L	302	BCL	C3D-C4D	-4.67	1.33	1.44
13	M	402	BCL	C3D-C4D	-4.65	1.33	1.44
13	L	311	BCL	C3D-C4D	-4.64	1.33	1.44
13	8	103	BCL	C3D-C4D	-4.61	1.33	1.44
13	L	310	BCL	C3D-C4D	-4.60	1.33	1.44
13	E	102	BCL	C3D-C4D	-4.58	1.33	1.44
13	Y	102	BCL	C3D-C4D	-4.58	1.33	1.44
13	Z	102	BCL	C3D-C4D	-4.58	1.33	1.44
13	3	101	BCL	C3D-C4D	-4.58	1.33	1.44
13	U	102	BCL	C3D-C4D	-4.57	1.33	1.44
13	0	102	BCL	C3D-C4D	-4.57	1.33	1.44
13	Q	101	BCL	C3D-C4D	-4.57	1.33	1.44
13	9	101	BCL	C3D-C4D	-4.57	1.33	1.44
13	I	101	BCL	C3D-C4D	-4.55	1.33	1.44
13	5	402	BCL	C3D-C4D	-4.55	1.33	1.44
13	P	102	BCL	C3D-C4D	-4.55	1.33	1.44
13	S	101	BCL	C3D-C4D	-4.55	1.33	1.44
13	4	102	BCL	C3D-C4D	-4.55	1.33	1.44
13	W	101	BCL	C3D-C4D	-4.54	1.33	1.44
13	D	102	BCL	C3D-C4D	-4.54	1.33	1.44
13	K	101	BCL	C3D-C4D	-4.54	1.33	1.44
13	F	101	BCL	C3D-C4D	-4.54	1.33	1.44
13	N	102	BCL	C3D-C4D	-4.54	1.33	1.44
13	7	102	BCL	C3D-C4D	-4.53	1.33	1.44
13	6	102	BCL	C3D-C4D	-4.53	1.33	1.44
13	A	102	BCL	C3D-C4D	-4.53	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	102	BCL	C3D-C4D	-4.53	1.34	1.44
13	2	103	BCL	C3D-C4D	-4.53	1.34	1.44
13	J	102	BCL	C3D-C4D	-4.53	1.34	1.44
13	T	102	BCL	C3D-C4D	-4.53	1.34	1.44
13	X	101	BCL	C3D-C4D	-4.52	1.34	1.44
13	O	101	BCL	C3D-C4D	-4.52	1.34	1.44
13	1	101	BCL	C3D-C4D	-4.52	1.34	1.44
13	R	102	BCL	C3D-C4D	-4.51	1.34	1.44
13	G	102	BCL	C3D-C4D	-4.50	1.34	1.44
13	V	102	BCL	C3D-C4D	-4.47	1.34	1.44
13	Q	101	BCL	C3B-C4B	4.42	1.49	1.41
13	A	102	BCL	C3B-C4B	4.41	1.49	1.41
13	D	102	BCL	C3B-C4B	4.40	1.49	1.41
13	Y	102	BCL	C3B-C4B	4.39	1.49	1.41
13	M	402	BCL	C3B-C4B	4.36	1.49	1.41
13	I	101	BCL	C3B-C4B	4.36	1.49	1.41
13	3	101	BCL	C3B-C4B	4.36	1.49	1.41
13	L	310	BCL	O2A-CGA	4.35	1.46	1.33
13	F	101	BCL	C3B-C4B	4.35	1.49	1.41
13	K	101	BCL	C3B-C4B	4.35	1.49	1.41
8	C	402	HEC	CBC-CAC	-4.35	1.32	1.51
13	5	402	BCL	C3B-C4B	4.31	1.49	1.41
13	S	101	BCL	C3B-C4B	4.31	1.49	1.41
13	A	102	BCL	O2A-CGA	4.31	1.45	1.33
13	P	102	BCL	O2A-CGA	4.30	1.45	1.33
17	H	404	PGV	O03-C19	4.30	1.45	1.33
13	N	102	BCL	O2A-CGA	4.29	1.45	1.33
13	9	101	BCL	C3B-C4B	4.29	1.49	1.41
13	6	102	BCL	O2A-CGA	4.29	1.45	1.33
17	X	102	PGV	O03-C19	4.28	1.45	1.33
13	1	101	BCL	O2A-CGA	4.28	1.45	1.33
13	3	101	BCL	O2A-CGA	4.28	1.45	1.33
13	U	102	BCL	O2A-CGA	4.27	1.45	1.33
13	0	102	BCL	O2A-CGA	4.27	1.45	1.33
13	U	102	BCL	C3B-C4B	4.27	1.49	1.41
13	M	402	BCL	O2A-CGA	4.26	1.45	1.33
13	K	101	BCL	O2A-CGA	4.26	1.45	1.33
17	G	103	PGV	O03-C19	4.26	1.45	1.33
17	M	408	PGV	O03-C19	4.26	1.45	1.33
17	L	306	PGV	O03-C19	4.26	1.45	1.33
13	L	302	BCL	C3B-C4B	4.26	1.49	1.41
13	4	102	BCL	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	M	407	PGV	O03-C19	4.25	1.45	1.33
13	E	102	BCL	O2A-CGA	4.25	1.45	1.33
13	T	102	BCL	O2A-CGA	4.25	1.45	1.33
17	T	103	PGV	O03-C19	4.25	1.45	1.33
13	N	102	BCL	C3B-C4B	4.24	1.49	1.41
17	K	102	PGV	O03-C19	4.24	1.45	1.33
13	W	101	BCL	C3B-C4B	4.24	1.49	1.41
13	J	102	BCL	O2A-CGA	4.24	1.45	1.33
13	O	101	BCL	C3B-C4B	4.24	1.49	1.41
13	9	101	BCL	O2A-CGA	4.24	1.45	1.33
13	5	402	BCL	O2A-CGA	4.24	1.45	1.33
17	P	103	PGV	O03-C19	4.23	1.45	1.33
17	N	103	PGV	O03-C19	4.23	1.45	1.33
13	R	102	BCL	O2A-CGA	4.23	1.45	1.33
17	D	101	PGV	O03-C19	4.23	1.45	1.33
17	R	103	PGV	O03-C19	4.23	1.45	1.33
13	Y	102	BCL	O2A-CGA	4.23	1.45	1.33
13	7	102	BCL	O2A-CGA	4.23	1.45	1.33
17	0	103	PGV	O03-C19	4.23	1.45	1.33
17	M	408	PGV	O01-C1	4.22	1.46	1.34
17	2	101	PGV	O03-C19	4.22	1.45	1.33
13	1	101	BCL	C3B-C4B	4.22	1.48	1.41
13	8	103	BCL	O2A-CGA	4.22	1.45	1.33
17	8	104	PGV	O03-C19	4.22	1.45	1.33
13	O	101	BCL	O2A-CGA	4.21	1.45	1.33
13	Q	101	BCL	O2A-CGA	4.21	1.45	1.33
13	L	311	BCL	O2A-CGA	4.21	1.45	1.33
17	J	103	PGV	O03-C19	4.21	1.45	1.33
17	V	103	PGV	O03-C19	4.21	1.45	1.33
17	H	403	PGV	O03-C19	4.21	1.45	1.33
17	E	103	PGV	O03-C19	4.21	1.45	1.33
17	L	307	PGV	O03-C19	4.21	1.45	1.33
13	I	101	BCL	O2A-CGA	4.21	1.45	1.33
13	S	101	BCL	O2A-CGA	4.21	1.45	1.33
13	P	102	BCL	C3B-C4B	4.21	1.48	1.41
13	2	103	BCL	O2A-CGA	4.21	1.45	1.33
17	4	103	PGV	O03-C19	4.21	1.45	1.33
17	8	101	PGV	O03-C19	4.21	1.45	1.33
17	2	104	PGV	O03-C19	4.20	1.45	1.33
13	Z	102	BCL	O2A-CGA	4.19	1.45	1.33
13	0	102	BCL	C3B-C4B	4.19	1.48	1.41
13	F	101	BCL	O2A-CGA	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	402	HEC	FE-NC	4.19	2.09	1.95
17	B	103	PGV	O03-C19	4.19	1.45	1.33
17	P	103	PGV	O01-C1	4.19	1.46	1.34
13	8	103	BCL	C3B-C4B	4.19	1.48	1.41
13	W	101	BCL	O2A-CGA	4.18	1.45	1.33
8	C	402	HEC	CBB-CAB	-4.17	1.32	1.51
13	G	102	BCL	C3B-C4B	4.17	1.48	1.41
13	V	102	BCL	O2A-CGA	4.17	1.45	1.33
17	L	306	PGV	O01-C1	4.17	1.46	1.34
8	C	404	HEC	FE-NC	4.17	2.09	1.95
13	2	103	BCL	C3B-C4B	4.16	1.48	1.41
13	T	102	BCL	C3B-C4B	4.16	1.48	1.41
13	D	102	BCL	O2A-CGA	4.16	1.45	1.33
13	X	101	BCL	O2A-CGA	4.15	1.45	1.33
13	G	102	BCL	O2A-CGA	4.15	1.45	1.33
17	M	406	PGV	O03-C19	4.15	1.45	1.33
13	B	102	BCL	C3B-C4B	4.15	1.48	1.41
17	H	404	PGV	O01-C1	4.15	1.46	1.34
13	6	102	BCL	C3B-C4B	4.15	1.48	1.41
13	B	102	BCL	O2A-CGA	4.14	1.45	1.33
17	H	403	PGV	O01-C1	4.14	1.46	1.34
17	2	104	PGV	O01-C1	4.14	1.46	1.34
17	K	102	PGV	O01-C1	4.13	1.46	1.34
17	E	103	PGV	O01-C1	4.13	1.46	1.34
13	X	101	BCL	C3B-C4B	4.13	1.48	1.41
13	J	102	BCL	C3B-C4B	4.13	1.48	1.41
13	L	302	BCL	O2A-CGA	4.12	1.45	1.33
17	H	401	PGV	O01-C1	4.11	1.45	1.34
17	V	103	PGV	O01-C1	4.11	1.45	1.34
17	B	103	PGV	O01-C1	4.11	1.45	1.34
17	4	103	PGV	O01-C1	4.11	1.45	1.34
8	C	403	HEC	FE-NC	4.11	2.09	1.95
13	R	102	BCL	C3B-C4B	4.10	1.48	1.41
13	7	102	BCL	C3B-C4B	4.10	1.48	1.41
17	M	407	PGV	O01-C1	4.10	1.45	1.34
17	H	401	PGV	O03-C19	4.09	1.45	1.33
17	T	103	PGV	O01-C1	4.09	1.45	1.34
17	N	103	PGV	O01-C1	4.09	1.45	1.34
13	L	311	BCL	C3B-C4B	4.09	1.48	1.41
17	R	103	PGV	O01-C1	4.09	1.45	1.34
17	8	104	PGV	O01-C1	4.09	1.45	1.34
7	C	401	HEM	FE-NC	4.09	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	101	PGV	O01-C1	4.09	1.45	1.34
13	E	102	BCL	C3B-C4B	4.08	1.48	1.41
17	2	101	PGV	O01-C1	4.08	1.45	1.34
17	X	102	PGV	O01-C1	4.07	1.45	1.34
17	0	103	PGV	O01-C1	4.07	1.45	1.34
8	C	403	HEC	CBB-CAB	-4.07	1.33	1.51
13	Z	102	BCL	C3B-C4B	4.07	1.48	1.41
8	C	403	HEC	CBC-CAC	-4.07	1.33	1.51
13	4	102	BCL	C3B-C4B	4.06	1.48	1.41
17	L	307	PGV	O01-C1	4.06	1.45	1.34
17	G	103	PGV	O01-C1	4.06	1.45	1.34
17	8	101	PGV	O01-C1	4.06	1.45	1.34
13	V	102	BCL	C3B-C4B	4.05	1.48	1.41
13	L	310	BCL	C3B-C4B	4.04	1.48	1.41
17	M	406	PGV	O01-C1	4.04	1.45	1.34
17	J	103	PGV	O01-C1	4.03	1.45	1.34
8	C	404	HEC	CBC-CAC	-4.03	1.33	1.51
8	C	404	HEC	CBB-CAB	-3.92	1.34	1.51
13	3	101	BCL	CHD-C1D	3.85	1.45	1.38
13	5	402	BCL	CHD-C1D	3.82	1.45	1.38
13	U	102	BCL	CHD-C1D	3.81	1.45	1.38
13	Y	102	BCL	CHD-C1D	3.81	1.45	1.38
13	9	101	BCL	CHD-C1D	3.76	1.45	1.38
13	F	101	BCL	CHD-C1D	3.76	1.45	1.38
13	7	102	BCL	CHD-C1D	3.75	1.45	1.38
13	L	311	BCL	CHD-C1D	3.74	1.45	1.38
13	1	101	BCL	CHD-C1D	3.71	1.45	1.38
13	D	102	BCL	CHD-C1D	3.70	1.45	1.38
13	Q	101	BCL	CHD-C1D	3.70	1.45	1.38
13	I	101	BCL	CHD-C1D	3.68	1.45	1.38
13	K	101	BCL	CHD-C1D	3.68	1.45	1.38
13	2	103	BCL	OBD-CAD	3.67	1.28	1.22
13	A	102	BCL	OBD-CAD	3.67	1.28	1.22
13	W	101	BCL	OBD-CAD	3.66	1.28	1.22
13	J	102	BCL	OBD-CAD	3.66	1.28	1.22
13	O	101	BCL	OBD-CAD	3.66	1.28	1.22
13	K	101	BCL	OBD-CAD	3.66	1.28	1.22
13	1	101	BCL	OBD-CAD	3.65	1.28	1.22
13	L	310	BCL	CHD-C1D	3.65	1.45	1.38
13	G	102	BCL	OBD-CAD	3.65	1.28	1.22
13	T	102	BCL	OBD-CAD	3.65	1.28	1.22
13	7	102	BCL	OBD-CAD	3.65	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q	101	BCL	OBD-CAD	3.65	1.28	1.22
13	Z	102	BCL	OBD-CAD	3.65	1.28	1.22
13	8	103	BCL	OBD-CAD	3.64	1.28	1.22
13	5	402	BCL	OBD-CAD	3.64	1.28	1.22
13	9	101	BCL	OBD-CAD	3.64	1.28	1.22
13	V	102	BCL	OBD-CAD	3.64	1.28	1.22
13	D	102	BCL	OBD-CAD	3.64	1.28	1.22
13	6	102	BCL	CHD-C1D	3.64	1.45	1.38
13	4	102	BCL	OBD-CAD	3.63	1.28	1.22
13	Y	102	BCL	OBD-CAD	3.63	1.28	1.22
13	N	102	BCL	OBD-CAD	3.63	1.28	1.22
13	3	101	BCL	OBD-CAD	3.63	1.28	1.22
13	X	101	BCL	OBD-CAD	3.62	1.28	1.22
13	0	102	BCL	OBD-CAD	3.62	1.28	1.22
13	S	101	BCL	CHD-C1D	3.62	1.45	1.38
13	R	102	BCL	OBD-CAD	3.62	1.28	1.22
13	F	101	BCL	OBD-CAD	3.62	1.28	1.22
13	O	101	BCL	CHD-C1D	3.62	1.45	1.38
13	L	302	BCL	CHD-C1D	3.61	1.45	1.38
13	W	101	BCL	CHD-C1D	3.61	1.45	1.38
13	P	102	BCL	OBD-CAD	3.61	1.28	1.22
13	U	102	BCL	OBD-CAD	3.61	1.28	1.22
13	I	101	BCL	OBD-CAD	3.61	1.28	1.22
13	B	102	BCL	OBD-CAD	3.60	1.28	1.22
8	C	402	HEC	C4B-NB	-3.60	1.34	1.40
13	E	102	BCL	OBD-CAD	3.60	1.28	1.22
13	4	102	BCL	CHD-C1D	3.60	1.45	1.38
13	L	310	BCL	OBD-CAD	3.59	1.28	1.22
13	M	402	BCL	CHD-C1D	3.59	1.45	1.38
13	E	102	BCL	CHD-C1D	3.59	1.45	1.38
13	N	102	BCL	CHD-C1D	3.57	1.45	1.38
13	6	102	BCL	OBD-CAD	3.57	1.28	1.22
13	L	302	BCL	OBD-CAD	3.56	1.28	1.22
13	I	101	BCL	CHB-C1B	3.56	1.47	1.39
13	X	101	BCL	CHD-C1D	3.55	1.45	1.38
13	5	402	BCL	CHB-C1B	3.55	1.47	1.39
13	2	103	BCL	CHD-C1D	3.54	1.45	1.38
13	8	103	BCL	CHD-C1D	3.54	1.45	1.38
13	T	102	BCL	CHD-C1D	3.54	1.45	1.38
13	J	102	BCL	CHD-C1D	3.53	1.45	1.38
13	Z	102	BCL	CHD-C1D	3.53	1.45	1.38
13	A	102	BCL	CHD-C1D	3.53	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	101	BCL	CHB-C1B	3.52	1.47	1.39
13	0	102	BCL	CHD-C1D	3.52	1.45	1.38
13	W	101	BCL	CHB-C1B	3.51	1.47	1.39
13	S	101	BCL	OBD-CAD	3.51	1.28	1.22
13	G	102	BCL	CHD-C1D	3.51	1.45	1.38
13	7	102	BCL	CHB-C1B	3.51	1.47	1.39
13	L	311	BCL	OBD-CAD	3.51	1.28	1.22
13	U	102	BCL	CHB-C1B	3.50	1.47	1.39
17	M	410	PGV	O01-C02	-3.49	1.42	1.46
13	L	311	BCL	CHB-C1B	3.49	1.47	1.39
13	B	102	BCL	CHD-C1D	3.49	1.45	1.38
13	P	102	BCL	CHD-C1D	3.48	1.45	1.38
13	O	101	BCL	CHB-C1B	3.47	1.47	1.39
13	R	102	BCL	CHB-C1B	3.47	1.47	1.39
13	K	101	BCL	CHB-C1B	3.46	1.47	1.39
13	9	101	BCL	CHB-C1B	3.45	1.47	1.39
13	A	102	BCL	CHB-C1B	3.45	1.47	1.39
13	Y	102	BCL	CHB-C1B	3.45	1.47	1.39
13	3	101	BCL	CHC-C4B	3.44	1.47	1.39
13	1	101	BCL	CHB-C1B	3.44	1.47	1.39
13	F	101	BCL	CHB-C1B	3.43	1.47	1.39
13	M	402	BCL	CHB-C1B	3.43	1.47	1.39
13	Q	101	BCL	CHB-C1B	3.43	1.47	1.39
13	L	310	BCL	CHB-C1B	3.42	1.47	1.39
13	M	402	BCL	OBD-CAD	3.42	1.28	1.22
13	4	102	BCL	CHB-C1B	3.41	1.47	1.39
13	D	102	BCL	CHB-C1B	3.41	1.47	1.39
13	B	102	BCL	CHB-C1B	3.40	1.47	1.39
13	R	102	BCL	CHD-C1D	3.40	1.45	1.38
13	S	101	BCL	CHB-C1B	3.40	1.47	1.39
13	V	102	BCL	CHB-C1B	3.39	1.47	1.39
13	0	102	BCL	CHB-C1B	3.38	1.47	1.39
13	G	102	BCL	CHB-C1B	3.37	1.47	1.39
13	2	103	BCL	CHB-C1B	3.37	1.47	1.39
13	8	103	BCL	CHB-C1B	3.37	1.47	1.39
13	V	102	BCL	CHD-C1D	3.37	1.44	1.38
7	C	401	HEM	C1B-NB	-3.35	1.34	1.40
13	6	102	BCL	CHB-C1B	3.35	1.46	1.39
13	E	102	BCL	CHB-C1B	3.35	1.46	1.39
13	P	102	BCL	CHB-C1B	3.35	1.46	1.39
13	T	102	BCL	CHB-C1B	3.34	1.46	1.39
13	M	402	BCL	CHC-C4B	3.34	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	102	BCL	CHB-C1B	3.34	1.46	1.39
13	I	101	BCL	CHC-C4B	3.32	1.46	1.39
13	L	302	BCL	CHC-C4B	3.32	1.46	1.39
13	X	101	BCL	CHB-C1B	3.30	1.46	1.39
13	N	102	BCL	CHB-C1B	3.30	1.46	1.39
13	U	102	BCL	CHC-C4B	3.29	1.46	1.39
13	5	402	BCL	CHC-C4B	3.29	1.46	1.39
13	J	102	BCL	CHB-C1B	3.28	1.46	1.39
13	8	103	BCL	CHC-C4B	3.26	1.46	1.39
8	C	403	HEC	C4B-NB	-3.26	1.34	1.40
13	S	101	BCL	CHC-C4B	3.25	1.46	1.39
8	C	404	HEC	C4B-NB	-3.25	1.34	1.40
8	C	402	HEC	C1D-ND	-3.24	1.34	1.40
13	7	102	BCL	CHC-C4B	3.23	1.46	1.39
13	T	102	BCL	CHC-C4B	3.23	1.46	1.39
13	N	102	BCL	CHC-C4B	3.23	1.46	1.39
13	A	102	BCL	CHC-C4B	3.22	1.46	1.39
13	W	101	BCL	CHC-C4B	3.22	1.46	1.39
13	L	302	BCL	CHB-C1B	3.22	1.46	1.39
13	D	102	BCL	CHC-C4B	3.21	1.46	1.39
13	1	101	BCL	CHC-C4B	3.21	1.46	1.39
13	B	102	BCL	CHC-C4B	3.21	1.46	1.39
13	O	101	BCL	CHC-C4B	3.21	1.46	1.39
13	0	102	BCL	CHC-C4B	3.21	1.46	1.39
13	R	102	BCL	CHC-C4B	3.21	1.46	1.39
13	P	102	BCL	CHC-C4B	3.20	1.46	1.39
13	L	311	BCL	CHC-C4B	3.20	1.46	1.39
13	F	101	BCL	CHC-C4B	3.20	1.46	1.39
13	Q	101	BCL	CHC-C4B	3.20	1.46	1.39
13	9	101	BCL	CHC-C4B	3.20	1.46	1.39
13	E	102	BCL	CHC-C4B	3.20	1.46	1.39
13	4	102	BCL	CHC-C4B	3.19	1.46	1.39
13	X	101	BCL	CHC-C4B	3.19	1.46	1.39
13	K	101	BCL	CHC-C4B	3.19	1.46	1.39
13	J	102	BCL	CHC-C4B	3.18	1.46	1.39
13	Z	102	BCL	CHC-C4B	3.17	1.46	1.39
13	6	102	BCL	CHC-C4B	3.17	1.46	1.39
13	G	102	BCL	CHC-C4B	3.16	1.46	1.39
8	C	404	HEC	C1D-ND	-3.16	1.34	1.40
13	L	310	BCL	CHC-C4B	3.16	1.46	1.39
13	Y	102	BCL	CHC-C4B	3.14	1.46	1.39
13	V	102	BCL	CHC-C4B	3.14	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	403	HEC	C1D-ND	-3.13	1.34	1.40
13	2	103	BCL	CHC-C4B	3.13	1.46	1.39
7	C	401	HEM	C4D-ND	-3.12	1.34	1.40
13	L	311	BCL	C4B-NB	-3.07	1.34	1.37
13	L	311	BCL	C3D-C2D	3.02	1.47	1.39
13	R	102	BCL	C3D-C2D	3.01	1.47	1.39
13	Z	102	BCL	C3D-C2D	3.01	1.47	1.39
14	M	403	BPH	C4D-CHA	3.00	1.44	1.39
13	E	102	BCL	C3D-C2D	2.99	1.47	1.39
13	7	102	BCL	C3D-C2D	2.99	1.47	1.39
14	L	303	BPH	C4D-CHA	2.99	1.44	1.39
13	3	101	BCL	C3D-C2D	2.98	1.47	1.39
13	5	402	BCL	C3D-C2D	2.98	1.47	1.39
13	0	102	BCL	C3D-C2D	2.98	1.47	1.39
13	L	310	BCL	C3D-C2D	2.98	1.47	1.39
13	9	101	BCL	C3D-C2D	2.98	1.47	1.39
13	4	102	BCL	C3D-C2D	2.98	1.47	1.39
13	V	102	BCL	C3D-C2D	2.97	1.47	1.39
13	W	101	BCL	C3D-C2D	2.97	1.47	1.39
13	U	102	BCL	C3D-C2D	2.96	1.47	1.39
13	X	101	BCL	C3D-C2D	2.96	1.47	1.39
13	2	103	BCL	C3D-C2D	2.96	1.47	1.39
13	G	102	BCL	C3D-C2D	2.95	1.47	1.39
13	8	103	BCL	C3D-C2D	2.95	1.47	1.39
13	Y	102	BCL	C3D-C2D	2.94	1.47	1.39
13	I	101	BCL	C3D-C2D	2.94	1.47	1.39
13	N	102	BCL	C3D-C2D	2.94	1.47	1.39
13	D	102	BCL	C3D-C2D	2.94	1.47	1.39
13	J	102	BCL	C3D-C2D	2.94	1.47	1.39
13	P	102	BCL	C3D-C2D	2.94	1.47	1.39
13	B	102	BCL	C3D-C2D	2.93	1.47	1.39
13	T	102	BCL	C3D-C2D	2.93	1.47	1.39
13	6	102	BCL	C3D-C2D	2.93	1.47	1.39
13	F	101	BCL	C3D-C2D	2.93	1.47	1.39
13	K	101	BCL	C3D-C2D	2.92	1.47	1.39
13	1	101	BCL	C3D-C2D	2.91	1.47	1.39
13	A	102	BCL	C3D-C2D	2.91	1.47	1.39
13	Q	101	BCL	C3D-C2D	2.91	1.47	1.39
13	S	101	BCL	C3D-C2D	2.90	1.47	1.39
13	O	101	BCL	C3D-C2D	2.89	1.47	1.39
13	3	101	BCL	CHD-C4C	2.87	1.47	1.39
13	L	311	BCL	C1D-C2D	2.87	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	102	BCL	C1D-ND	-2.87	1.34	1.37
13	L	311	BCL	CHD-C4C	2.87	1.47	1.39
13	V	102	BCL	C1D-ND	-2.86	1.34	1.37
13	U	102	BCL	CHD-C4C	2.85	1.47	1.39
13	M	402	BCL	C3D-C2D	2.85	1.46	1.39
13	1	101	BCL	C4B-NB	-2.85	1.34	1.37
13	W	101	BCL	C4B-NB	-2.83	1.34	1.37
13	Z	102	BCL	C1D-ND	-2.83	1.34	1.37
13	Q	101	BCL	C1D-C2D	2.83	1.50	1.45
13	L	310	BCL	C4B-NB	-2.83	1.34	1.37
13	9	101	BCL	CHD-C4C	2.83	1.47	1.39
13	U	102	BCL	C4B-NB	-2.82	1.34	1.37
13	Y	102	BCL	CHD-C4C	2.82	1.47	1.39
13	D	102	BCL	C1D-C2D	2.82	1.50	1.45
13	0	102	BCL	C1D-ND	-2.81	1.34	1.37
13	D	102	BCL	CHD-C4C	2.81	1.47	1.39
13	5	402	BCL	C1D-C2D	2.81	1.50	1.45
13	1	101	BCL	CHD-C4C	2.81	1.47	1.39
13	3	101	BCL	C1D-C2D	2.81	1.50	1.45
13	K	101	BCL	C1D-C2D	2.80	1.50	1.45
13	L	310	BCL	C1D-ND	-2.80	1.34	1.37
13	Q	101	BCL	CHD-C4C	2.80	1.47	1.39
13	N	102	BCL	C1D-ND	-2.80	1.34	1.37
13	P	102	BCL	C1D-ND	-2.80	1.34	1.37
13	Y	102	BCL	C1D-C2D	2.80	1.50	1.45
13	S	101	BCL	C4B-NB	-2.80	1.34	1.37
13	G	102	BCL	C4B-NB	-2.79	1.34	1.37
13	J	102	BCL	C1D-ND	-2.79	1.34	1.37
13	O	101	BCL	C1D-C2D	2.79	1.50	1.45
13	2	103	BCL	C4B-NB	-2.79	1.34	1.37
13	M	402	BCL	C1D-C2D	2.79	1.50	1.45
13	S	101	BCL	C1D-C2D	2.78	1.50	1.45
13	K	101	BCL	C4B-NB	-2.77	1.34	1.37
13	Z	102	BCL	C4B-NB	-2.77	1.34	1.37
13	5	402	BCL	CHD-C4C	2.77	1.47	1.39
13	F	101	BCL	CHD-C4C	2.77	1.47	1.39
13	U	102	BCL	C1D-C2D	2.77	1.50	1.45
13	E	102	BCL	C1D-ND	-2.77	1.34	1.37
13	O	101	BCL	CHD-C4C	2.77	1.47	1.39
13	4	102	BCL	C4B-NB	-2.76	1.34	1.37
13	7	102	BCL	CHD-C4C	2.76	1.47	1.39
13	F	101	BCL	C1D-C2D	2.76	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	102	BCL	C4B-NB	-2.76	1.34	1.37
13	B	102	BCL	C1D-ND	-2.76	1.34	1.37
13	9	101	BCL	C4B-NB	-2.76	1.34	1.37
13	0	102	BCL	C4B-NB	-2.76	1.34	1.37
13	N	102	BCL	C4B-NB	-2.75	1.34	1.37
13	L	302	BCL	C3D-C2D	2.75	1.46	1.39
13	9	101	BCL	C1D-C2D	2.75	1.50	1.45
13	O	101	BCL	C4B-NB	-2.74	1.34	1.37
13	J	102	BCL	C4B-NB	-2.74	1.34	1.37
13	K	101	BCL	CHD-C4C	2.74	1.47	1.39
13	5	402	BCL	C4B-NB	-2.74	1.34	1.37
13	W	101	BCL	CHD-C4C	2.73	1.46	1.39
13	A	102	BCL	C1D-C2D	2.73	1.50	1.45
13	1	101	BCL	C1D-C2D	2.73	1.50	1.45
13	T	102	BCL	C1D-ND	-2.72	1.34	1.37
13	I	101	BCL	CHD-C4C	2.72	1.46	1.39
13	4	102	BCL	C1D-ND	-2.72	1.34	1.37
13	L	302	BCL	C4B-NB	-2.71	1.34	1.37
13	R	102	BCL	C4B-NB	-2.71	1.34	1.37
13	A	102	BCL	C4B-NB	-2.71	1.34	1.37
13	G	102	BCL	C1D-ND	-2.71	1.34	1.37
13	F	101	BCL	C4B-NB	-2.71	1.34	1.37
13	7	102	BCL	C4B-NB	-2.71	1.34	1.37
13	M	402	BCL	C4B-NB	-2.71	1.34	1.37
13	I	101	BCL	C1D-C2D	2.71	1.50	1.45
13	S	101	BCL	CHD-C4C	2.71	1.46	1.39
13	8	103	BCL	C1D-ND	-2.70	1.34	1.37
13	W	101	BCL	C1D-C2D	2.70	1.50	1.45
13	T	102	BCL	C4B-NB	-2.69	1.34	1.37
13	L	310	BCL	CHD-C4C	2.69	1.46	1.39
13	7	102	BCL	C1D-C2D	2.69	1.50	1.45
13	8	103	BCL	C4B-NB	-2.69	1.34	1.37
13	A	102	BCL	CHD-C4C	2.68	1.46	1.39
13	X	101	BCL	C1D-ND	-2.67	1.34	1.37
15	L	308	U10	C3-C2	-2.67	1.41	1.48
13	2	103	BCL	C1D-ND	-2.67	1.34	1.37
13	L	302	BCL	CHD-C4C	2.67	1.46	1.39
13	E	102	BCL	C4B-NB	-2.65	1.34	1.37
13	X	101	BCL	C4B-NB	-2.65	1.34	1.37
13	L	302	BCL	C1D-C2D	2.65	1.50	1.45
13	P	102	BCL	C4B-NB	-2.65	1.34	1.37
13	M	402	BCL	CHD-C4C	2.65	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	102	U10	C3-C2	-2.65	1.41	1.48
13	B	102	BCL	C4B-NB	-2.64	1.34	1.37
13	D	102	BCL	C4B-NB	-2.64	1.34	1.37
13	L	311	BCL	C1D-ND	-2.64	1.34	1.37
13	6	102	BCL	CHD-C4C	2.63	1.46	1.39
15	D	104	U10	C3-C2	-2.63	1.41	1.48
13	V	102	BCL	C4B-NB	-2.63	1.34	1.37
13	2	103	BCL	CHD-C4C	2.62	1.46	1.39
13	4	102	BCL	CHD-C4C	2.62	1.46	1.39
13	6	102	BCL	C4B-NB	-2.61	1.34	1.37
7	C	401	HEM	C1C-C2C	-2.61	1.40	1.45
15	Y	103	U10	C3-C2	-2.61	1.41	1.48
13	X	101	BCL	CHD-C4C	2.61	1.46	1.39
13	Q	101	BCL	C4B-NB	-2.61	1.34	1.37
13	7	102	BCL	C1B-C2B	2.61	1.49	1.43
13	E	102	BCL	CHD-C4C	2.61	1.46	1.39
13	3	101	BCL	C4B-NB	-2.60	1.34	1.37
13	8	103	BCL	CHD-C4C	2.60	1.46	1.39
13	0	102	BCL	CHD-C4C	2.59	1.46	1.39
13	T	102	BCL	CHD-C4C	2.59	1.46	1.39
13	P	102	BCL	CHD-C4C	2.59	1.46	1.39
13	S	101	BCL	C1B-C2B	2.58	1.49	1.43
13	2	103	BCL	C1B-C2B	2.58	1.49	1.43
13	J	102	BCL	CHD-C4C	2.58	1.46	1.39
13	N	102	BCL	CHD-C4C	2.57	1.46	1.39
13	O	101	BCL	C1D-ND	-2.57	1.34	1.37
13	I	101	BCL	C1D-ND	-2.57	1.34	1.37
13	L	302	BCL	C1D-ND	-2.57	1.34	1.37
15	L	309	U10	C4-C5	-2.56	1.41	1.48
13	I	101	BCL	C4B-NB	-2.56	1.34	1.37
13	Z	102	BCL	CHD-C4C	2.56	1.46	1.39
13	6	102	BCL	C1D-ND	-2.56	1.34	1.37
15	U	101	U10	C3-C2	-2.56	1.41	1.48
13	A	102	BCL	C1D-ND	-2.55	1.34	1.37
13	4	102	BCL	C1B-C2B	2.55	1.49	1.43
13	G	102	BCL	CHD-C4C	2.55	1.46	1.39
13	9	101	BCL	C1D-ND	-2.55	1.34	1.37
17	M	410	PGV	O03-C19	2.55	1.45	1.33
13	Q	101	BCL	C1D-ND	-2.55	1.34	1.37
13	1	101	BCL	C1D-ND	-2.54	1.34	1.37
13	R	102	BCL	CHD-C4C	2.54	1.46	1.39
13	B	102	BCL	CHD-C4C	2.54	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	102	BCL	C1B-C2B	2.54	1.49	1.43
13	9	101	BCL	C1B-C2B	2.54	1.49	1.43
13	W	101	BCL	C1D-ND	-2.53	1.34	1.37
13	V	102	BCL	CHD-C4C	2.53	1.46	1.39
13	B	102	BCL	C1B-C2B	2.53	1.49	1.43
13	5	402	BCL	C1B-C2B	2.53	1.49	1.43
13	I	101	BCL	C1B-C2B	2.52	1.49	1.43
13	2	103	BCL	C1D-C2D	2.52	1.50	1.45
13	0	102	BCL	C1B-C2B	2.52	1.49	1.43
13	6	102	BCL	C1B-C2B	2.51	1.49	1.43
15	D	104	U10	C4-C5	-2.51	1.41	1.48
13	S	101	BCL	C1D-ND	-2.51	1.34	1.37
13	R	102	BCL	C1B-C2B	2.51	1.49	1.43
13	6	102	BCL	C1D-C2D	2.51	1.50	1.45
13	0	102	BCL	C1D-C2D	2.51	1.50	1.45
7	C	401	HEM	C3B-C4B	2.51	1.49	1.44
13	M	402	BCL	C1B-C2B	2.50	1.49	1.43
13	K	101	BCL	C1D-ND	-2.50	1.34	1.37
13	F	101	BCL	C1D-ND	-2.50	1.34	1.37
13	M	402	BCL	C1D-ND	-2.50	1.34	1.37
8	C	404	HEC	FE-ND	-2.50	1.87	1.94
13	O	101	BCL	C1B-C2B	2.50	1.49	1.43
13	Y	102	BCL	C1D-ND	-2.49	1.34	1.37
15	L	304	U10	C3-C2	-2.49	1.41	1.48
13	E	102	BCL	C1B-C2B	2.49	1.49	1.43
13	L	310	BCL	C1D-C2D	2.49	1.50	1.45
13	Z	102	BCL	C1B-C2B	2.49	1.49	1.43
13	Y	102	BCL	C1B-C2B	2.49	1.49	1.43
13	1	101	BCL	C1B-C2B	2.48	1.49	1.43
13	J	102	BCL	C1B-C2B	2.48	1.49	1.43
13	M	402	BCL	C1B-NB	-2.48	1.34	1.37
13	D	102	BCL	C1B-C2B	2.48	1.49	1.43
13	T	102	BCL	C1D-C2D	2.48	1.50	1.45
13	D	102	BCL	C1D-ND	-2.47	1.34	1.37
13	N	102	BCL	C1B-C2B	2.47	1.49	1.43
13	V	102	BCL	C1B-C2B	2.47	1.49	1.43
13	P	102	BCL	C1D-C2D	2.46	1.50	1.45
13	T	102	BCL	C1B-C2B	2.46	1.49	1.43
13	8	103	BCL	C1D-C2D	2.46	1.50	1.45
13	U	102	BCL	C1D-ND	-2.46	1.34	1.37
13	L	311	BCL	C1B-C2B	2.46	1.49	1.43
13	A	102	BCL	C1B-C2B	2.46	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	101	BCL	C1B-C2B	2.46	1.49	1.43
13	Q	101	BCL	C1B-C2B	2.46	1.49	1.43
13	8	103	BCL	C1B-C2B	2.46	1.49	1.43
13	X	101	BCL	C1B-C2B	2.46	1.49	1.43
13	5	402	BCL	C1D-ND	-2.45	1.34	1.37
13	W	101	BCL	C1B-C2B	2.45	1.49	1.43
13	U	102	BCL	C1B-C2B	2.45	1.49	1.43
13	F	101	BCL	C1B-C2B	2.45	1.49	1.43
13	E	102	BCL	C1D-C2D	2.44	1.50	1.45
13	P	102	BCL	C1B-C2B	2.44	1.49	1.43
13	N	102	BCL	C1B-NB	-2.44	1.34	1.37
15	L	308	U10	C4-C5	-2.43	1.41	1.48
13	7	102	BCL	C1D-ND	-2.43	1.34	1.37
13	G	102	BCL	C1D-C2D	2.43	1.50	1.45
13	3	101	BCL	C1B-C2B	2.42	1.49	1.43
13	N	102	BCL	C1D-C2D	2.42	1.50	1.45
13	4	102	BCL	C1D-C2D	2.42	1.50	1.45
8	C	403	HEC	C4A-C3A	-2.41	1.40	1.45
13	3	101	BCL	MG-NC	-2.40	2.00	2.06
13	L	311	BCL	MG-NA	-2.40	2.00	2.06
8	C	403	HEC	FE-ND	-2.40	1.87	1.94
15	L	304	U10	C4-C5	-2.39	1.42	1.48
13	X	101	BCL	C1D-C2D	2.38	1.50	1.45
13	B	102	BCL	C1D-C2D	2.38	1.50	1.45
13	3	101	BCL	C1D-ND	-2.38	1.34	1.37
13	V	102	BCL	C1B-NB	-2.37	1.34	1.37
13	J	102	BCL	C1D-C2D	2.35	1.50	1.45
13	L	302	BCL	C1B-C2B	2.34	1.48	1.43
8	C	402	HEC	FE-ND	-2.34	1.87	1.94
13	W	101	BCL	MG-NA	-2.34	2.00	2.06
13	J	102	BCL	C1B-NB	-2.34	1.34	1.37
13	R	102	BCL	C1D-C2D	2.33	1.49	1.45
15	7	101	U10	C3-C2	-2.33	1.42	1.48
13	L	310	BCL	C1B-NB	-2.33	1.34	1.37
13	Q	101	BCL	C1B-NB	-2.31	1.34	1.37
13	Z	102	BCL	C1B-NB	-2.31	1.34	1.37
13	5	402	BCL	MG-NC	-2.31	2.00	2.06
13	3	101	BCL	C1B-NB	-2.31	1.34	1.37
13	L	310	BCL	C1B-C2B	2.31	1.48	1.43
13	U	102	BCL	MG-NA	-2.29	2.00	2.06
13	S	101	BCL	MG-NA	-2.29	2.00	2.06
13	A	102	BCL	C1B-NB	-2.29	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	101	BCL	C1B-NB	-2.29	1.35	1.37
13	P	102	BCL	C1B-NB	-2.28	1.35	1.37
13	K	101	BCL	C1B-NB	-2.28	1.35	1.37
8	C	404	HEC	C1A-C2A	-2.28	1.41	1.45
13	D	102	BCL	C1B-NB	-2.28	1.35	1.37
13	B	102	BCL	C1B-NB	-2.27	1.35	1.37
8	C	404	HEC	C4B-C3B	2.27	1.49	1.45
13	5	402	BCL	MG-NA	-2.27	2.00	2.06
13	X	101	BCL	C1B-NB	-2.27	1.35	1.37
13	E	102	BCL	C1B-NB	-2.27	1.35	1.37
13	3	101	BCL	MG-NA	-2.27	2.00	2.06
13	Y	102	BCL	C1B-NB	-2.26	1.35	1.37
13	Z	102	BCL	C1D-C2D	2.26	1.49	1.45
13	U	102	BCL	C1B-NB	-2.26	1.35	1.37
13	G	102	BCL	C1B-NB	-2.25	1.35	1.37
13	6	102	BCL	C1B-NB	-2.25	1.35	1.37
15	Y	103	U10	C4-C5	-2.25	1.42	1.48
13	A	102	BCL	MG-NA	-2.25	2.00	2.06
7	C	401	HEM	FE-ND	-2.25	1.87	1.94
13	6	102	BCL	MG-NC	-2.25	2.00	2.06
13	0	102	BCL	C1B-NB	-2.24	1.35	1.37
8	C	404	HEC	C4A-C3A	-2.24	1.40	1.45
13	7	102	BCL	MG-NC	-2.24	2.00	2.06
15	U	101	U10	C4-C5	-2.24	1.42	1.48
13	I	101	BCL	C1B-NB	-2.24	1.35	1.37
13	I	101	BCL	MG-NC	-2.24	2.00	2.06
13	9	101	BCL	C1B-NB	-2.24	1.35	1.37
13	4	102	BCL	C1B-NB	-2.24	1.35	1.37
13	V	102	BCL	C1D-C2D	2.23	1.49	1.45
13	M	402	BCL	MG-NC	-2.23	2.01	2.06
13	D	102	BCL	MG-NC	-2.23	2.01	2.06
13	8	103	BCL	C1B-NB	-2.23	1.35	1.37
13	2	103	BCL	C1B-NB	-2.23	1.35	1.37
13	1	101	BCL	C1B-NB	-2.23	1.35	1.37
13	U	102	BCL	MG-NC	-2.23	2.01	2.06
8	C	402	HEC	C4A-C3A	-2.23	1.40	1.45
13	L	310	BCL	MG-NC	-2.23	2.01	2.06
13	L	310	BCL	MG-NA	-2.23	2.01	2.06
13	O	101	BCL	C1B-NB	-2.22	1.35	1.37
13	K	101	BCL	MG-NA	-2.22	2.01	2.06
13	L	302	BCL	C1B-NB	-2.22	1.35	1.37
13	I	101	BCL	MG-NA	-2.22	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Y	102	BCL	MG-NA	-2.21	2.01	2.06
13	7	102	BCL	MG-NA	-2.20	2.01	2.06
13	8	103	BCL	MG-NC	-2.20	2.01	2.06
13	E	102	BCL	MG-NA	-2.20	2.01	2.06
8	C	403	HEC	C1A-C2A	-2.20	1.41	1.45
13	Q	101	BCL	MG-NA	-2.19	2.01	2.06
13	L	302	BCL	MG-NC	-2.19	2.01	2.06
8	C	402	HEC	C1A-C2A	-2.19	1.41	1.45
13	E	102	BCL	MG-NC	-2.19	2.01	2.06
13	4	102	BCL	MG-NA	-2.19	2.01	2.06
13	T	102	BCL	C1B-NB	-2.19	1.35	1.37
13	F	101	BCL	C1B-NB	-2.18	1.35	1.37
13	4	102	BCL	MG-NC	-2.18	2.01	2.06
13	L	311	BCL	MG-NC	-2.18	2.01	2.06
13	G	102	BCL	CHC-C1C	-2.18	1.32	1.37
13	D	102	BCL	MG-NA	-2.17	2.01	2.06
8	C	404	HEC	C1B-NB	-2.17	1.34	1.38
13	W	101	BCL	MG-NC	-2.16	2.01	2.06
14	M	403	BPH	C3A-C2A	-2.16	1.52	1.54
13	R	102	BCL	C1B-NB	-2.16	1.35	1.37
15	7	101	U10	C4-C5	-2.16	1.42	1.48
13	5	402	BCL	C1B-NB	-2.16	1.35	1.37
13	W	101	BCL	C1B-NB	-2.16	1.35	1.37
13	1	101	BCL	MG-NA	-2.16	2.01	2.06
13	9	101	BCL	MG-NC	-2.15	2.01	2.06
13	A	102	BCL	MG-NC	-2.15	2.01	2.06
8	C	403	HEC	C1B-NB	-2.15	1.34	1.38
13	Z	102	BCL	MG-NC	-2.14	2.01	2.06
13	N	102	BCL	MG-NC	-2.14	2.01	2.06
13	2	103	BCL	MG-NC	-2.14	2.01	2.06
13	L	302	BCL	CHB-C4A	-2.14	1.32	1.37
13	Q	101	BCL	MG-NC	-2.14	2.01	2.06
13	6	102	BCL	MG-NA	-2.14	2.01	2.06
13	T	102	BCL	MG-NC	-2.14	2.01	2.06
13	8	103	BCL	MG-NA	-2.13	2.01	2.06
13	9	101	BCL	MG-NA	-2.13	2.01	2.06
13	O	101	BCL	MG-NA	-2.13	2.01	2.06
13	M	402	BCL	MG-NA	-2.13	2.01	2.06
13	O	101	BCL	MG-NC	-2.13	2.01	2.06
13	2	103	BCL	CHC-C1C	-2.12	1.32	1.37
13	F	101	BCL	MG-NA	-2.12	2.01	2.06
13	V	102	BCL	CHC-C1C	-2.12	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	101	BCL	MG-NC	-2.12	2.01	2.06
13	2	103	BCL	MG-NA	-2.12	2.01	2.06
13	L	311	BCL	C1B-NB	-2.11	1.35	1.37
13	L	310	BCL	CHC-C1C	-2.11	1.32	1.37
13	B	102	BCL	MG-NC	-2.11	2.01	2.06
13	N	102	BCL	MG-NA	-2.11	2.01	2.06
13	Y	102	BCL	MG-NC	-2.11	2.01	2.06
13	R	102	BCL	MG-NA	-2.11	2.01	2.06
13	0	102	BCL	MG-NA	-2.11	2.01	2.06
13	S	101	BCL	MG-NC	-2.10	2.01	2.06
8	C	402	HEC	C1B-NB	-2.10	1.34	1.38
13	0	102	BCL	MG-NC	-2.09	2.01	2.06
13	J	102	BCL	CHC-C1C	-2.09	1.32	1.37
13	P	102	BCL	MG-NC	-2.09	2.01	2.06
13	V	102	BCL	MG-NC	-2.09	2.01	2.06
13	0	102	BCL	CHC-C1C	-2.09	1.32	1.37
13	F	101	BCL	MG-NC	-2.09	2.01	2.06
13	G	102	BCL	MG-NC	-2.09	2.01	2.06
13	Z	102	BCL	CHC-C1C	-2.08	1.32	1.37
13	R	102	BCL	MG-NC	-2.08	2.01	2.06
13	S	101	BCL	CHC-C1C	-2.08	1.32	1.37
13	7	102	BCL	C1B-NB	-2.08	1.35	1.37
15	1	102	U10	C4-C5	-2.08	1.42	1.48
13	B	102	BCL	MG-NA	-2.07	2.01	2.06
13	P	102	BCL	MG-NA	-2.07	2.01	2.06
13	V	102	BCL	MG-NA	-2.07	2.01	2.06
13	G	102	BCL	MG-NA	-2.06	2.01	2.06
13	X	101	BCL	MG-NC	-2.06	2.01	2.06
14	L	303	BPH	C1B-C2B	2.05	1.41	1.39
13	R	102	BCL	CHC-C1C	-2.05	1.32	1.37
13	J	102	BCL	MG-NA	-2.05	2.01	2.06
13	T	102	BCL	MG-NA	-2.05	2.01	2.06
13	L	302	BCL	MG-NA	-2.04	2.01	2.06
13	J	102	BCL	MG-NC	-2.04	2.01	2.06
13	O	101	BCL	CHC-C1C	-2.04	1.32	1.37
13	X	101	BCL	MG-NA	-2.04	2.01	2.06
13	N	102	BCL	CHC-C1C	-2.04	1.32	1.37
13	Z	102	BCL	MG-NA	-2.03	2.01	2.06
13	F	101	BCL	CHC-C1C	-2.03	1.32	1.37
13	K	101	BCL	MG-NC	-2.03	2.01	2.06
13	9	101	BCL	CHC-C1C	-2.03	1.32	1.37
13	B	102	BCL	CHC-C1C	-2.02	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	102	BCL	CHC-C1C	-2.02	1.32	1.37
13	X	101	BCL	CHC-C1C	-2.02	1.32	1.37
13	K	101	BCL	CHC-C1C	-2.02	1.32	1.37
13	D	102	BCL	CHC-C1C	-2.02	1.32	1.37
19	M	404	A1L8Q	C19-C31	2.01	1.38	1.35
13	Q	101	BCL	CHC-C1C	-2.01	1.32	1.37
13	4	102	BCL	CHC-C1C	-2.01	1.32	1.37
14	M	403	BPH	C1B-C2B	2.01	1.41	1.39
13	W	101	BCL	CHC-C1C	-2.01	1.32	1.37

All (1301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	M	405	CRT	C2-C1-C4	-16.98	84.78	110.86
20	M	405	CRT	C3-C1-C4	-11.13	93.77	110.86
13	L	302	BCL	C2B-C1B-NB	10.60	117.34	110.23
13	P	102	BCL	C2B-C1B-NB	10.46	117.25	110.23
13	Q	101	BCL	C2B-C1B-NB	10.37	117.18	110.23
13	6	102	BCL	C2B-C1B-NB	10.35	117.17	110.23
13	X	101	BCL	C2B-C1B-NB	10.33	117.16	110.23
13	D	102	BCL	C2B-C1B-NB	10.28	117.12	110.23
13	0	102	BCL	C2B-C1B-NB	10.26	117.11	110.23
13	N	102	BCL	C2B-C1B-NB	10.24	117.10	110.23
13	F	101	BCL	C2B-C1B-NB	10.19	117.06	110.23
13	K	101	BCL	C2B-C1B-NB	10.19	117.06	110.23
13	8	103	BCL	C2B-C1B-NB	10.17	117.05	110.23
13	V	102	BCL	C2B-C1B-NB	10.17	117.05	110.23
13	J	102	BCL	C2B-C1B-NB	10.16	117.05	110.23
13	A	102	BCL	C2B-C1B-NB	10.15	117.04	110.23
13	T	102	BCL	C2B-C1B-NB	10.15	117.03	110.23
13	Z	102	BCL	C2B-C1B-NB	10.13	117.02	110.23
13	Y	102	BCL	C2B-C1B-NB	10.12	117.01	110.23
13	2	103	BCL	C2B-C1B-NB	10.09	117.00	110.23
13	B	102	BCL	C2B-C1B-NB	10.07	116.98	110.23
13	O	101	BCL	C2B-C1B-NB	10.03	116.95	110.23
13	L	310	BCL	C2B-C1B-NB	10.02	116.95	110.23
13	4	102	BCL	C2B-C1B-NB	9.98	116.92	110.23
13	9	101	BCL	C2B-C1B-NB	9.98	116.92	110.23
13	U	102	BCL	C2B-C1B-NB	9.98	116.92	110.23
13	G	102	BCL	C2B-C1B-NB	9.97	116.92	110.23
13	R	102	BCL	C2B-C1B-NB	9.96	116.91	110.23
13	S	101	BCL	C2B-C1B-NB	9.96	116.91	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	402	BCL	C2B-C1B-NB	9.92	116.89	110.23
13	E	102	BCL	C2B-C1B-NB	9.92	116.89	110.23
13	1	101	BCL	C2B-C1B-NB	9.90	116.87	110.23
13	W	101	BCL	C2B-C1B-NB	9.86	116.84	110.23
13	7	102	BCL	C2B-C1B-NB	9.80	116.80	110.23
13	I	101	BCL	C2B-C1B-NB	9.79	116.80	110.23
13	L	311	BCL	C2B-C1B-NB	9.73	116.76	110.23
13	3	101	BCL	C2B-C1B-NB	9.63	116.69	110.23
13	5	402	BCL	C2B-C1B-NB	9.61	116.67	110.23
13	L	311	BCL	CHD-C1D-ND	-8.55	116.59	124.45
13	S	101	BCL	CHD-C1D-ND	-8.55	116.60	124.45
13	Q	101	BCL	CHD-C1D-ND	-8.53	116.62	124.45
13	W	101	BCL	CHD-C1D-ND	-8.49	116.65	124.45
13	M	402	BCL	CHD-C1D-ND	-8.49	116.65	124.45
13	F	101	BCL	CHD-C1D-ND	-8.49	116.66	124.45
13	A	102	BCL	CHD-C1D-ND	-8.48	116.66	124.45
13	K	101	BCL	CHD-C1D-ND	-8.46	116.68	124.45
13	Y	102	BCL	CHD-C1D-ND	-8.44	116.70	124.45
13	5	402	BCL	CHD-C1D-ND	-8.42	116.71	124.45
13	O	101	BCL	CHD-C1D-ND	-8.42	116.72	124.45
13	3	101	BCL	CHD-C1D-ND	-8.41	116.72	124.45
13	L	310	BCL	CHD-C1D-ND	-8.38	116.75	124.45
13	1	101	BCL	CHD-C1D-ND	-8.38	116.76	124.45
13	M	402	BCL	CMD-C2D-C1D	8.35	139.44	124.71
13	L	302	BCL	CHD-C1D-ND	-8.34	116.79	124.45
13	I	101	BCL	CHD-C1D-ND	-8.33	116.80	124.45
13	L	302	BCL	CMD-C2D-C1D	8.31	139.37	124.71
13	D	102	BCL	CHD-C1D-ND	-8.30	116.82	124.45
13	U	102	BCL	CHD-C1D-ND	-8.30	116.83	124.45
13	7	102	BCL	CHD-C1D-ND	-8.28	116.84	124.45
13	9	101	BCL	CHD-C1D-ND	-8.25	116.87	124.45
13	Q	101	BCL	CMD-C2D-C1D	8.24	139.24	124.71
13	O	101	BCL	CMD-C2D-C1D	8.20	139.17	124.71
13	S	101	BCL	CMD-C2D-C1D	8.13	139.05	124.71
13	3	101	BCL	CMD-C2D-C1D	8.13	139.03	124.71
13	Y	102	BCL	CMD-C2D-C1D	8.09	138.98	124.71
13	K	101	BCL	CMD-C2D-C1D	8.06	138.93	124.71
13	1	101	BCL	CMD-C2D-C1D	8.06	138.92	124.71
13	F	101	BCL	CMD-C2D-C1D	8.06	138.91	124.71
13	L	311	BCL	CMD-C2D-C1D	8.05	138.89	124.71
13	A	102	BCL	CMD-C2D-C1D	8.04	138.89	124.71
13	D	102	BCL	CMD-C2D-C1D	8.03	138.87	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	402	BCL	CMD-C2D-C1D	8.02	138.84	124.71
13	U	102	BCL	CMD-C2D-C1D	8.00	138.81	124.71
13	9	101	BCL	CMD-C2D-C1D	7.99	138.80	124.71
13	W	101	BCL	CMD-C2D-C1D	7.96	138.74	124.71
13	7	102	BCL	CMD-C2D-C1D	7.95	138.73	124.71
13	I	101	BCL	CMD-C2D-C1D	7.93	138.69	124.71
13	6	102	BCL	CHD-C1D-ND	-7.76	117.33	124.45
13	8	103	BCL	CHD-C1D-ND	-7.73	117.35	124.45
13	2	103	BCL	CHD-C1D-ND	-7.72	117.36	124.45
13	E	102	BCL	CHD-C1D-ND	-7.71	117.37	124.45
13	0	102	BCL	CHD-C1D-ND	-7.71	117.37	124.45
13	4	102	BCL	CHD-C1D-ND	-7.70	117.38	124.45
13	N	102	BCL	CHD-C1D-ND	-7.70	117.38	124.45
13	B	102	BCL	CHD-C1D-ND	-7.66	117.42	124.45
13	T	102	BCL	CHD-C1D-ND	-7.65	117.43	124.45
13	P	102	BCL	CHD-C1D-ND	-7.64	117.43	124.45
13	X	101	BCL	CHD-C1D-ND	-7.61	117.47	124.45
13	L	310	BCL	CMD-C2D-C1D	7.54	138.00	124.71
13	G	102	BCL	CHD-C1D-ND	-7.53	117.53	124.45
13	R	102	BCL	CHD-C1D-ND	-7.51	117.56	124.45
13	J	102	BCL	CHD-C1D-ND	-7.49	117.57	124.45
13	6	102	BCL	CMD-C2D-C1D	7.46	137.85	124.71
13	P	102	BCL	CMD-C2D-C1D	7.39	137.74	124.71
13	T	102	BCL	CMD-C2D-C1D	7.39	137.74	124.71
13	V	102	BCL	CHD-C1D-ND	-7.38	117.67	124.45
13	2	103	BCL	CMD-C2D-C1D	7.37	137.70	124.71
13	Z	102	BCL	CHD-C1D-ND	-7.35	117.70	124.45
13	8	103	BCL	CMD-C2D-C1D	7.32	137.62	124.71
13	4	102	BCL	CMD-C2D-C1D	7.30	137.59	124.71
13	N	102	BCL	CMD-C2D-C1D	7.30	137.57	124.71
13	E	102	BCL	CMD-C2D-C1D	7.26	137.52	124.71
13	G	102	BCL	CMD-C2D-C1D	7.25	137.49	124.71
13	0	102	BCL	CMD-C2D-C1D	7.24	137.47	124.71
13	B	102	BCL	CMD-C2D-C1D	7.21	137.42	124.71
13	X	101	BCL	CMD-C2D-C1D	7.16	137.34	124.71
13	J	102	BCL	CMD-C2D-C1D	7.02	137.09	124.71
20	6	101	CRT	C15-C14-C12	-6.96	117.38	127.31
13	V	102	BCL	CMD-C2D-C1D	6.93	136.93	124.71
13	Z	102	BCL	CMD-C2D-C1D	6.92	136.91	124.71
13	R	102	BCL	CMD-C2D-C1D	6.88	136.84	124.71
20	8	102	CRT	C40-C38-C39	5.89	121.44	110.37
20	V	101	CRT	C10-C9-C7	-5.75	119.11	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	8	102	CRT	C39-C38-C37	5.59	119.45	110.86
20	M	405	CRT	C3-C1-C2	5.54	120.79	110.37
13	V	102	BCL	C2D-C1D-ND	5.33	114.03	110.10
13	B	102	BCL	C2D-C1D-ND	5.33	114.03	110.10
13	A	102	BCL	C2D-C1D-ND	5.31	114.02	110.10
13	R	102	BCL	C2D-C1D-ND	5.28	113.99	110.10
13	O	101	BCL	C2D-C1D-ND	5.27	113.98	110.10
13	T	102	BCL	C2D-C1D-ND	5.25	113.97	110.10
13	0	102	BCL	C2D-C1D-ND	5.25	113.97	110.10
13	P	102	BCL	C2D-C1D-ND	5.23	113.96	110.10
13	2	103	BCL	C2D-C1D-ND	5.23	113.96	110.10
13	N	102	BCL	C2D-C1D-ND	5.21	113.94	110.10
13	S	101	BCL	C2D-C1D-ND	5.21	113.94	110.10
13	L	310	BCL	O2D-CGD-CBD	5.20	120.51	111.27
13	X	101	BCL	C2D-C1D-ND	5.16	113.90	110.10
13	I	101	BCL	C2D-C1D-ND	5.15	113.90	110.10
13	G	102	BCL	C2D-C1D-ND	5.14	113.89	110.10
13	J	102	BCL	C2D-C1D-ND	5.14	113.89	110.10
13	Z	102	BCL	C2D-C1D-ND	5.13	113.88	110.10
20	V	101	CRT	C5-C6-C7	-5.13	118.14	125.89
13	F	101	BCL	C2D-C1D-ND	5.12	113.88	110.10
13	1	101	BCL	C2D-C1D-ND	5.11	113.87	110.10
13	4	102	BCL	C2D-C1D-ND	5.09	113.86	110.10
13	Q	101	BCL	C2D-C1D-ND	5.09	113.85	110.10
17	M	410	PGV	O01-C1-O02	-5.08	119.10	125.57
13	K	101	BCL	C2D-C1D-ND	5.08	113.85	110.10
13	M	402	BCL	C3D-C2D-C1D	-5.08	98.90	105.83
13	8	103	BCL	C2D-C1D-ND	5.06	113.84	110.10
13	O	101	BCL	C3D-C2D-C1D	-5.04	98.95	105.83
13	A	102	BCL	C3D-C2D-C1D	-5.03	98.97	105.83
13	M	402	BCL	C2D-C1D-ND	5.02	113.80	110.10
13	S	101	BCL	C3D-C2D-C1D	-5.00	99.00	105.83
13	E	102	BCL	C2D-C1D-ND	5.00	113.79	110.10
13	D	102	BCL	C2D-C1D-ND	4.98	113.78	110.10
13	7	102	BCL	C2D-C1D-ND	4.97	113.77	110.10
13	A	102	BCL	O2D-CGD-CBD	4.97	120.10	111.27
13	L	302	BCL	C2D-C1D-ND	4.96	113.76	110.10
13	1	101	BCL	C3D-C2D-C1D	-4.96	99.06	105.83
13	Q	101	BCL	C3D-C2D-C1D	-4.96	99.07	105.83
13	Y	102	BCL	C2D-C1D-ND	4.94	113.75	110.10
13	6	102	BCL	C2D-C1D-ND	4.93	113.73	110.10
13	F	101	BCL	C3D-C2D-C1D	-4.92	99.12	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K	101	BCL	C3D-C2D-C1D	-4.92	99.12	105.83
13	I	101	BCL	C3D-C2D-C1D	-4.91	99.12	105.83
13	D	102	BCL	C3D-C2D-C1D	-4.91	99.13	105.83
13	L	311	BCL	C3D-C2D-C1D	-4.91	99.13	105.83
8	C	403	HEC	CHC-C4B-NB	4.91	130.42	124.37
13	7	102	BCL	C3D-C2D-C1D	-4.89	99.15	105.83
20	T	101	CRT	C21-C22-C23	-4.89	120.33	127.31
13	9	101	BCL	C3D-C2D-C1D	-4.89	99.16	105.83
13	W	101	BCL	C2D-C1D-ND	4.89	113.71	110.10
13	9	101	BCL	C2D-C1D-ND	4.89	113.71	110.10
13	U	102	BCL	C3D-C2D-C1D	-4.88	99.17	105.83
13	O	101	BCL	O2D-CGD-CBD	4.88	119.94	111.27
13	Y	102	BCL	C3D-C2D-C1D	-4.88	99.18	105.83
13	5	402	BCL	C3D-C2D-C1D	-4.87	99.18	105.83
20	8	102	CRT	C40-C38-C37	4.87	118.34	110.86
13	S	101	BCL	CHD-C4C-NC	4.86	130.48	125.08
13	3	101	BCL	C3D-C2D-C1D	-4.86	99.20	105.83
13	L	302	BCL	C3D-C2D-C1D	-4.86	99.20	105.83
20	Z	101	CRT	C10-C9-C7	-4.85	120.39	127.31
20	N	101	CRT	C21-C22-C23	-4.84	120.40	127.31
13	W	101	BCL	C3D-C2D-C1D	-4.84	99.22	105.83
13	L	310	BCL	C2D-C1D-ND	4.84	113.67	110.10
13	5	402	BCL	C2D-C1D-ND	4.83	113.67	110.10
13	9	101	BCL	O2D-CGD-CBD	4.82	119.84	111.27
20	Z	101	CRT	C21-C22-C23	-4.81	120.44	127.31
20	Z	101	CRT	C5-C6-C7	-4.81	118.62	125.89
13	2	103	BCL	C3D-C2D-C1D	-4.81	99.27	105.83
13	5	402	BCL	O2D-CGD-CBD	4.81	119.81	111.27
13	T	102	BCL	C3D-C2D-C1D	-4.80	99.29	105.83
13	0	102	BCL	C3D-C2D-C1D	-4.79	99.29	105.83
13	N	102	BCL	C3D-C2D-C1D	-4.79	99.29	105.83
13	P	102	BCL	C3D-C2D-C1D	-4.79	99.30	105.83
13	M	402	BCL	CHD-C4C-NC	4.79	130.39	125.08
13	B	102	BCL	C3D-C2D-C1D	-4.78	99.30	105.83
20	B	101	CRT	C21-C22-C23	-4.77	120.50	127.31
13	U	102	BCL	C2D-C1D-ND	4.77	113.62	110.10
13	4	102	BCL	C3D-C2D-C1D	-4.76	99.33	105.83
20	J	101	CRT	C21-C22-C23	-4.76	120.51	127.31
13	Q	101	BCL	O2D-CGD-CBD	4.76	119.73	111.27
13	3	101	BCL	O2D-CGD-CBD	4.76	119.73	111.27
13	L	311	BCL	C2D-C1D-ND	4.75	113.61	110.10
7	C	401	HEM	CHD-C1D-ND	4.74	129.57	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	101	CRT	C21-C22-C23	-4.74	120.54	127.31
13	G	102	BCL	C3D-C2D-C1D	-4.74	99.36	105.83
20	V	101	CRT	C21-C22-C23	-4.74	120.55	127.31
13	I	101	BCL	O2D-CGD-CBD	4.74	119.69	111.27
20	4	101	CRT	C21-C22-C23	-4.73	120.55	127.31
13	E	102	BCL	C3D-C2D-C1D	-4.73	99.38	105.83
13	L	311	BCL	O2D-CGD-CBD	4.72	119.66	111.27
13	A	102	BCL	CHD-C4C-NC	4.72	130.31	125.08
13	8	103	BCL	C3D-C2D-C1D	-4.72	99.40	105.83
20	P	101	CRT	C21-C22-C23	-4.71	120.59	127.31
13	D	102	BCL	O2D-CGD-CBD	4.71	119.63	111.27
20	8	102	CRT	C15-C14-C12	-4.70	120.60	127.31
13	6	102	BCL	C3D-C2D-C1D	-4.70	99.41	105.83
13	V	102	BCL	C3D-C2D-C1D	-4.70	99.42	105.83
13	K	101	BCL	O2D-CGD-CBD	4.69	119.61	111.27
13	Y	102	BCL	O2D-CGD-CBD	4.68	119.59	111.27
13	L	310	BCL	C3D-C2D-C1D	-4.68	99.45	105.83
13	X	101	BCL	C3D-C2D-C1D	-4.67	99.45	105.83
13	Z	102	BCL	C3D-C2D-C1D	-4.66	99.46	105.83
13	J	102	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
20	Y	101	CRT	C21-C22-C23	-4.66	120.66	127.31
13	R	102	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
20	2	102	CRT	C21-C22-C23	-4.66	120.66	127.31
13	U	102	BCL	O2D-CGD-CBD	4.65	119.53	111.27
20	E	101	CRT	C21-C22-C23	-4.62	120.72	127.31
8	C	404	HEC	CHD-C1D-ND	4.61	130.06	124.37
13	W	101	BCL	O2D-CGD-CBD	4.59	119.43	111.27
13	7	102	BCL	O2D-CGD-CBD	4.59	119.42	111.27
13	0	102	BCL	O2D-CGD-CBD	4.58	119.41	111.27
13	F	101	BCL	O2D-CGD-CBD	4.57	119.39	111.27
20	G	101	CRT	C21-C22-C23	-4.55	120.81	127.31
13	0	102	BCL	CHD-C4C-NC	4.55	130.13	125.08
13	N	102	BCL	CHD-C4C-NC	4.54	130.12	125.08
13	P	102	BCL	O2D-CGD-CBD	4.54	119.33	111.27
13	E	102	BCL	O2D-CGD-CBD	4.52	119.30	111.27
13	Z	102	BCL	O2D-CGD-CBD	4.51	119.29	111.27
20	2	102	CRT	C10-C9-C7	-4.51	120.87	127.31
13	P	102	BCL	CHD-C4C-NC	4.51	130.09	125.08
13	1	101	BCL	O2D-CGD-CBD	4.51	119.28	111.27
20	6	101	CRT	C10-C9-C7	-4.51	120.88	127.31
13	3	101	BCL	C2D-C1D-ND	4.51	113.42	110.10
13	4	102	BCL	O2D-CGD-CBD	4.49	119.25	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	103	BCL	CHD-C4C-NC	4.49	130.06	125.08
13	S	101	BCL	C3C-C4C-CHD	-4.48	113.82	123.39
8	C	404	HEC	CHA-C4D-ND	4.48	129.28	124.42
13	N	102	BCL	O2D-CGD-CBD	4.47	119.22	111.27
13	A	102	BCL	C3C-C4C-CHD	-4.45	113.87	123.39
17	P	103	PGV	O01-C1-C2	4.45	121.10	111.50
13	P	102	BCL	C3C-C4C-CHD	-4.45	113.89	123.39
13	X	101	BCL	CHD-C4C-NC	4.44	130.00	125.08
13	B	102	BCL	O2D-CGD-CBD	4.43	119.14	111.27
13	G	102	BCL	O2D-CGD-CBD	4.43	119.14	111.27
13	0	102	BCL	C3C-C4C-CHD	-4.42	113.96	123.39
13	R	102	BCL	C3C-C4C-CHD	-4.41	113.97	123.39
13	I	101	BCL	CHD-C4C-NC	4.41	129.97	125.08
20	B	101	CRT	C5-C6-C7	-4.40	119.24	125.89
13	E	102	BCL	CHD-C4C-NC	4.40	129.96	125.08
13	J	102	BCL	O2D-CGD-CBD	4.40	119.08	111.27
13	X	101	BCL	C3C-C4C-CHD	-4.39	114.00	123.39
13	B	102	BCL	CHD-C4C-NC	4.39	129.96	125.08
13	2	103	BCL	C3C-C4C-CHD	-4.38	114.03	123.39
13	T	102	BCL	CHD-C4C-NC	4.38	129.94	125.08
13	B	102	BCL	C1D-ND-C4D	-4.38	103.22	106.33
17	H	401	PGV	O01-C1-C2	4.38	120.94	111.50
13	B	102	BCL	C3C-C4C-CHD	-4.38	114.04	123.39
20	0	101	CRT	C21-C22-C23	-4.37	121.07	127.31
13	L	302	BCL	CHD-C4C-NC	4.37	129.93	125.08
13	J	102	BCL	CHD-C4C-NC	4.37	129.93	125.08
13	R	102	BCL	O2D-CGD-CBD	4.37	119.03	111.27
13	A	102	BCL	C1D-ND-C4D	-4.36	103.23	106.33
13	T	102	BCL	C1D-ND-C4D	-4.36	103.24	106.33
13	0	102	BCL	C1D-ND-C4D	-4.36	103.24	106.33
13	R	102	BCL	C1D-ND-C4D	-4.36	103.24	106.33
13	N	102	BCL	C3C-C4C-CHD	-4.36	114.08	123.39
13	6	102	BCL	O2D-CGD-CBD	4.36	119.02	111.27
13	X	101	BCL	C1D-ND-C4D	-4.36	103.24	106.33
17	B	103	PGV	O01-C1-C2	4.34	120.85	111.50
13	S	101	BCL	C1D-ND-C4D	-4.34	103.25	106.33
13	R	102	BCL	CHD-C4C-NC	4.34	129.89	125.08
13	T	102	BCL	C3C-C4C-CHD	-4.33	114.14	123.39
13	J	102	BCL	C3C-C4C-CHD	-4.33	114.15	123.39
13	V	102	BCL	C3C-C4C-CHD	-4.33	114.15	123.39
13	O	101	BCL	C1D-ND-C4D	-4.32	103.26	106.33
17	V	103	PGV	O01-C1-C2	4.32	120.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	103	BCL	C1D-ND-C4D	-4.32	103.27	106.33
13	T	102	BCL	O2D-CGD-CBD	4.32	118.94	111.27
13	G	102	BCL	CHD-C4C-NC	4.32	129.87	125.08
13	L	302	BCL	C1D-ND-C4D	-4.31	103.27	106.33
17	H	403	PGV	O01-C1-C2	4.31	120.79	111.50
13	L	302	BCL	C3C-C4C-CHD	-4.31	114.19	123.39
13	F	101	BCL	C1D-ND-C4D	-4.31	103.28	106.33
13	8	103	BCL	O2D-CGD-CBD	4.30	118.91	111.27
13	Q	101	BCL	C1D-ND-C4D	-4.30	103.28	106.33
13	8	103	BCL	C1D-ND-C4D	-4.29	103.28	106.33
13	M	402	BCL	C3C-C4C-CHD	-4.29	114.22	123.39
13	X	101	BCL	O2D-CGD-CBD	4.29	118.90	111.27
13	8	103	BCL	CHD-C4C-NC	4.29	129.84	125.08
13	I	101	BCL	C1D-ND-C4D	-4.29	103.29	106.33
13	K	101	BCL	C1D-ND-C4D	-4.29	103.29	106.33
13	2	103	BCL	O2D-CGD-CBD	4.29	118.88	111.27
13	P	102	BCL	C1D-ND-C4D	-4.28	103.29	106.33
17	2	104	PGV	O01-C1-C2	4.28	120.72	111.50
20	T	101	CRT	C5-C6-C7	-4.28	119.43	125.89
13	G	102	BCL	C3C-C4C-CHD	-4.28	114.25	123.39
20	8	102	CRT	C20-C19-C17	-4.27	121.21	127.31
13	W	101	BCL	CHD-C4C-NC	4.27	129.82	125.08
8	C	403	HEC	CHA-C4D-ND	4.27	129.06	124.42
20	M	405	CRT	C21-C22-C23	-4.27	121.22	127.31
8	C	402	HEC	CHC-C4B-NB	4.26	129.63	124.37
14	L	303	BPH	C4D-CHA-CBD	-4.26	106.59	108.52
20	2	102	CRT	C5-C6-C7	-4.26	119.46	125.89
20	R	101	CRT	C21-C22-C23	-4.24	121.26	127.31
17	T	103	PGV	O01-C1-C2	4.24	120.64	111.50
13	V	102	BCL	CHD-C4C-NC	4.24	129.78	125.08
13	E	102	BCL	C3C-C4C-CHD	-4.23	114.35	123.39
13	8	103	BCL	C3C-C4C-CHD	-4.23	114.36	123.39
13	V	102	BCL	C1D-ND-C4D	-4.23	103.33	106.33
13	Z	102	BCL	C3C-C4C-CHD	-4.22	114.37	123.39
13	J	102	BCL	C1D-ND-C4D	-4.22	103.34	106.33
13	3	101	BCL	CHC-C4B-NB	-4.20	119.81	124.26
20	M	405	CRT	C20-C19-C17	-4.20	121.31	127.31
20	8	102	CRT	C21-C22-C23	-4.20	121.32	127.31
13	G	102	BCL	C1D-ND-C4D	-4.20	103.35	106.33
13	Z	102	BCL	CHD-C4C-NC	4.19	129.73	125.08
13	S	101	BCL	CHC-C4B-NB	-4.19	119.82	124.26
13	Y	102	BCL	C1D-ND-C4D	-4.19	103.36	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	102	BCL	CHD-C4C-NC	4.18	129.72	125.08
13	M	402	BCL	C1D-ND-C4D	-4.18	103.37	106.33
13	D	102	BCL	C1D-ND-C4D	-4.18	103.37	106.33
13	V	102	BCL	O2D-CGD-CBD	4.17	118.68	111.27
13	1	101	BCL	C1D-ND-C4D	-4.17	103.37	106.33
13	S	101	BCL	O2D-CGD-CBD	4.17	118.68	111.27
13	O	101	BCL	CHD-C4C-NC	4.16	129.70	125.08
13	N	102	BCL	C1D-ND-C4D	-4.16	103.38	106.33
17	M	407	PGV	O01-C1-C2	4.16	120.46	111.50
13	Z	102	BCL	C1D-ND-C4D	-4.15	103.39	106.33
13	K	101	BCL	CHD-C4C-NC	4.15	129.68	125.08
13	5	402	BCL	CHC-C4B-NB	-4.15	119.87	124.26
13	4	102	BCL	CHD-C4C-NC	4.15	129.68	125.08
13	9	101	BCL	CHC-C4B-NB	-4.15	119.87	124.26
20	R	101	CRT	C10-C9-C7	-4.14	121.39	127.31
20	B	101	CRT	C10-C9-C7	-4.14	121.40	127.31
13	L	311	BCL	CHD-C4C-NC	4.14	129.67	125.08
13	Y	102	BCL	CHC-C4B-NB	-4.13	119.88	124.26
13	L	310	BCL	CHD-C4C-NC	4.13	129.67	125.08
8	C	402	HEC	CHA-C4D-ND	4.13	128.91	124.42
17	E	103	PGV	O01-C1-C2	4.12	120.38	111.50
13	Q	101	BCL	CHC-C4B-NB	-4.11	119.91	124.26
13	6	102	BCL	CHD-C4C-NC	4.11	129.64	125.08
17	M	408	PGV	O01-C1-C2	4.10	120.35	111.50
13	I	101	BCL	C3C-C4C-CHD	-4.10	114.63	123.39
13	6	102	BCL	C1D-ND-C4D	-4.10	103.42	106.33
17	L	306	PGV	O01-C1-C2	4.10	120.33	111.50
13	5	402	BCL	CHD-C4C-NC	4.09	129.62	125.08
13	4	102	BCL	C1D-ND-C4D	-4.08	103.44	106.33
13	Q	101	BCL	CHD-C4C-NC	4.08	129.60	125.08
13	4	102	BCL	C3C-C4C-CHD	-4.06	114.72	123.39
13	Y	102	BCL	CHD-C4C-NC	4.06	129.58	125.08
13	M	402	BCL	O2D-CGD-CBD	4.06	118.47	111.27
13	E	102	BCL	C1D-ND-C4D	-4.05	103.46	106.33
13	F	101	BCL	CHD-C4C-NC	4.05	129.58	125.08
13	L	302	BCL	O2D-CGD-CBD	4.05	118.46	111.27
20	N	101	CRT	C10-C9-C7	-4.04	121.55	127.31
13	7	102	BCL	C1D-ND-C4D	-4.03	103.47	106.33
13	D	102	BCL	CHC-C4B-NB	-4.03	119.99	124.26
20	0	101	CRT	C5-C6-C7	-4.02	119.81	125.89
13	L	310	BCL	C1D-ND-C4D	-4.02	103.48	106.33
13	O	101	BCL	C3C-C4C-CHD	-3.99	114.86	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	402	HEC	CHD-C1D-ND	3.99	129.29	124.37
13	W	101	BCL	C1D-ND-C4D	-3.99	103.50	106.33
13	5	402	BCL	C1D-ND-C4D	-3.98	103.51	106.33
13	6	102	BCL	C3C-C4C-CHD	-3.98	114.89	123.39
13	9	101	BCL	C1D-ND-C4D	-3.98	103.51	106.33
20	J	101	CRT	C20-C19-C17	-3.97	121.64	127.31
13	W	101	BCL	C3C-C4C-CHD	-3.97	114.91	123.39
17	D	101	PGV	O01-C1-C2	3.97	120.05	111.50
8	C	404	HEC	CHB-C1B-NB	3.96	128.72	124.42
13	E	102	BCL	C1-C2-C3	-3.95	119.21	126.04
13	K	101	BCL	CHC-C4B-NB	-3.95	120.08	124.26
17	M	406	PGV	O01-C1-C2	3.95	120.01	111.50
17	G	103	PGV	O01-C1-C2	3.94	119.98	111.50
13	W	101	BCL	CHC-C4B-NB	-3.92	120.11	124.26
13	K	101	BCL	C3C-C4C-CHD	-3.92	115.01	123.39
13	L	311	BCL	C1D-ND-C4D	-3.90	103.56	106.33
17	R	103	PGV	O01-C1-C2	3.90	119.92	111.50
17	4	103	PGV	O01-C1-C2	3.90	119.91	111.50
13	S	101	BCL	C1-C2-C3	-3.90	119.30	126.04
17	8	104	PGV	O01-C1-C2	3.90	119.90	111.50
20	E	101	CRT	C20-C19-C17	-3.88	121.77	127.31
13	L	310	BCL	C3C-C4C-CHD	-3.88	115.10	123.39
13	F	101	BCL	CHC-C4B-NB	-3.88	120.15	124.26
13	F	101	BCL	C3C-C4C-CHD	-3.88	115.11	123.39
13	U	102	BCL	C1D-ND-C4D	-3.88	103.58	106.33
13	A	102	BCL	CHC-C4B-NB	-3.87	120.16	124.26
20	2	102	CRT	C20-C19-C17	-3.87	121.78	127.31
13	1	101	BCL	CHD-C4C-NC	3.87	129.37	125.08
13	U	102	BCL	CHC-C4B-NB	-3.87	120.16	124.26
13	D	102	BCL	CHD-C4C-NC	3.87	129.37	125.08
8	C	403	HEC	C4B-NB-C1B	3.86	109.06	105.07
13	1	101	BCL	CHC-C4B-NB	-3.85	120.18	124.26
13	7	102	BCL	C3C-C4C-CHD	-3.84	115.20	123.39
13	Q	101	BCL	C3C-C4C-CHD	-3.83	115.21	123.39
17	L	307	PGV	O01-C1-C2	3.83	119.75	111.50
17	H	404	PGV	O01-C1-C2	3.83	119.75	111.50
13	Y	102	BCL	C3C-C4C-CHD	-3.83	115.22	123.39
20	P	101	CRT	C20-C19-C17	-3.83	121.85	127.31
20	R	101	CRT	C5-C6-C7	-3.82	120.12	125.89
20	6	101	CRT	C18-C17-C16	3.81	124.08	118.08
13	L	311	BCL	CHC-C4B-NB	-3.81	120.22	124.26
13	O	101	BCL	CHC-C4B-NB	-3.81	120.22	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	103	PGV	O01-C1-C2	3.81	119.71	111.50
8	C	403	HEC	CHD-C1D-ND	3.80	129.06	124.37
20	R	101	CRT	C20-C19-C17	-3.80	121.89	127.31
14	M	403	BPH	C4D-CHA-CBD	-3.80	106.80	108.52
20	G	101	CRT	C10-C9-C7	-3.78	121.91	127.31
20	N	101	CRT	C20-C19-C17	-3.78	121.91	127.31
13	9	101	BCL	CHD-C4C-NC	3.78	129.28	125.08
20	B	101	CRT	C20-C19-C17	-3.76	121.94	127.31
13	N	102	BCL	CHC-C4B-NB	-3.75	120.29	124.26
8	C	404	HEC	C4B-NB-C1B	3.73	108.93	105.07
13	L	311	BCL	C3C-C4C-CHD	-3.73	115.43	123.39
13	1	101	BCL	C3C-C4C-CHD	-3.73	115.43	123.39
13	4	102	BCL	C1-C2-C3	-3.72	119.60	126.04
20	0	101	CRT	C20-C19-C17	-3.72	122.00	127.31
17	8	101	PGV	O01-C1-C2	3.72	119.52	111.50
17	0	103	PGV	O01-C1-C2	3.72	119.51	111.50
8	C	402	HEC	C4C-NC-C1C	3.71	108.98	105.35
13	I	101	BCL	CHC-C4B-NB	-3.70	120.34	124.26
13	5	402	BCL	C3C-C4C-CHD	-3.70	115.49	123.39
17	K	102	PGV	O01-C1-C2	3.70	119.47	111.50
16	X	103	LMT	C1B-O1B-C4'	3.69	127.09	117.96
20	G	101	CRT	C5-C6-C7	-3.69	120.32	125.89
20	0	101	CRT	C10-C9-C7	-3.68	122.05	127.31
20	4	101	CRT	C20-C19-C17	-3.67	122.07	127.31
13	8	103	BCL	C1-C2-C3	-3.67	119.70	126.04
13	D	102	BCL	C3C-C4C-CHD	-3.66	115.57	123.39
8	C	404	HEC	C4C-NC-C1C	3.66	108.93	105.35
20	Y	101	CRT	C20-C19-C17	-3.65	122.09	127.31
13	L	311	BCL	C1-C2-C3	-3.65	119.73	126.04
20	T	101	CRT	C20-C19-C17	-3.65	122.10	127.31
17	2	101	PGV	O01-C1-C2	3.64	119.35	111.50
13	9	101	BCL	C3C-C4C-CHD	-3.64	115.62	123.39
20	N	101	CRT	C5-C6-C7	-3.62	120.43	125.89
13	M	402	BCL	CHC-C4B-NB	-3.61	120.43	124.26
13	U	102	BCL	CHD-C4C-NC	3.61	129.09	125.08
8	C	403	HEC	CHB-C1B-NB	3.60	128.32	124.42
20	8	102	CRT	C10-C9-C7	-3.59	122.18	127.31
13	3	101	BCL	C1D-ND-C4D	-3.59	103.78	106.33
20	G	101	CRT	C20-C19-C17	-3.58	122.20	127.31
13	L	302	BCL	CHC-C4B-NB	-3.58	120.47	124.26
20	Z	101	CRT	C20-C19-C17	-3.56	122.23	127.31
13	7	102	BCL	CHC-C4B-NB	-3.55	120.50	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	102	BCL	CHC-C4B-NB	-3.54	120.51	124.26
7	C	401	HEM	CHA-C4D-ND	3.53	128.73	124.37
8	C	402	HEC	C4B-NB-C1B	3.52	108.71	105.07
13	L	310	BCL	C3D-C4D-ND	3.52	115.93	110.24
13	M	402	BCL	CHB-C1B-NB	-3.51	120.55	124.26
13	7	102	BCL	CHB-C1B-NB	-3.51	120.55	124.26
13	R	102	BCL	C3D-C4D-ND	3.50	115.90	110.24
13	S	101	BCL	CHB-C1B-NB	-3.50	120.55	124.26
13	6	102	BCL	CHB-C1B-NB	-3.50	120.55	124.26
13	X	101	BCL	C3D-C4D-ND	3.50	115.89	110.24
13	0	102	BCL	C3D-C4D-ND	3.49	115.88	110.24
17	J	103	PGV	O01-C1-C2	3.49	119.02	111.50
8	C	404	HEC	CHC-C4B-NB	3.48	128.67	124.37
8	C	403	HEC	C4C-NC-C1C	3.48	108.75	105.35
13	8	103	BCL	C3D-C4D-ND	3.47	115.84	110.24
13	P	102	BCL	CHC-C4B-NB	-3.46	120.59	124.26
13	7	102	BCL	C1-C2-C3	-3.46	120.06	126.04
13	T	102	BCL	C3D-C4D-ND	3.45	115.82	110.24
13	L	311	BCL	C3D-C4D-ND	3.45	115.82	110.24
13	4	102	BCL	CHC-C4B-NB	-3.45	120.61	124.26
13	2	103	BCL	CHC-C4B-NB	-3.45	120.61	124.26
13	E	102	BCL	CHC-C4B-NB	-3.44	120.61	124.26
7	C	401	HEM	CHC-C4B-NB	3.43	128.15	124.42
13	6	102	BCL	C1-C2-C3	-3.43	120.11	126.04
13	B	102	BCL	C3D-C4D-ND	3.42	115.77	110.24
13	G	102	BCL	CHC-C4B-NB	-3.42	120.64	124.26
13	Z	102	BCL	C3D-C4D-ND	3.42	115.77	110.24
13	Q	101	BCL	C3D-C4D-ND	3.42	115.76	110.24
13	Y	102	BCL	C3D-C4D-ND	3.41	115.76	110.24
13	P	102	BCL	C3D-C4D-ND	3.41	115.76	110.24
13	L	302	BCL	C3D-C4D-ND	3.41	115.75	110.24
13	I	101	BCL	C3D-C4D-ND	3.41	115.75	110.24
13	2	103	BCL	C3D-C4D-ND	3.40	115.75	110.24
13	F	101	BCL	C3D-C4D-ND	3.40	115.74	110.24
13	K	101	BCL	C3D-C4D-ND	3.40	115.74	110.24
13	8	103	BCL	CHC-C4B-NB	-3.40	120.66	124.26
13	G	102	BCL	C3D-C4D-ND	3.40	115.73	110.24
13	J	102	BCL	C3D-C4D-ND	3.39	115.72	110.24
13	D	102	BCL	C3D-C4D-ND	3.39	115.72	110.24
13	0	102	BCL	CHC-C4B-NB	-3.39	120.67	124.26
13	E	102	BCL	C3D-C4D-ND	3.38	115.71	110.24
13	Y	102	BCL	C1-C2-C3	-3.38	120.20	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	402	BCL	C3D-C4D-ND	3.38	115.70	110.24
8	C	404	HEC	CBB-CAB-C3B	3.38	121.74	112.43
13	4	102	BCL	CHB-C1B-NB	-3.37	120.69	124.26
13	S	101	BCL	C3D-C4D-ND	3.37	115.69	110.24
13	6	102	BCL	C3D-C4D-ND	3.37	115.68	110.24
13	J	102	BCL	CHC-C4B-NB	-3.36	120.69	124.26
13	O	101	BCL	C3D-C4D-ND	3.36	115.68	110.24
16	Z	103	LMT	C3B-C4B-C5B	3.36	116.23	110.24
13	A	102	BCL	C3D-C4D-ND	3.36	115.67	110.24
13	1	101	BCL	C3D-C4D-ND	3.35	115.66	110.24
20	V	101	CRT	C20-C19-C17	-3.35	122.52	127.31
13	9	101	BCL	C3D-C4D-ND	3.35	115.66	110.24
20	P	101	CRT	C5-C6-C7	-3.35	120.83	125.89
13	V	102	BCL	C3D-C4D-ND	3.35	115.65	110.24
8	C	404	HEC	CAD-CBD-CGD	-3.34	106.41	113.60
13	2	103	BCL	CHB-C1B-NB	-3.34	120.72	124.26
7	C	401	HEM	C1B-NB-C4B	3.34	108.52	105.07
13	4	102	BCL	C3D-C4D-ND	3.34	115.64	110.24
13	5	402	BCL	C3D-C4D-ND	3.34	115.64	110.24
13	B	102	BCL	CHC-C4B-NB	-3.33	120.73	124.26
20	8	102	CRT	O2-C38-C39	-3.33	86.09	108.97
13	E	102	BCL	CHB-C1B-NB	-3.32	120.74	124.26
13	N	102	BCL	C3D-C4D-ND	3.32	115.60	110.24
20	T	101	CRT	C10-C9-C7	-3.32	122.58	127.31
13	L	310	BCL	CHC-C4B-NB	-3.31	120.75	124.26
13	7	102	BCL	C3D-C4D-ND	3.31	115.59	110.24
13	W	101	BCL	C3D-C4D-ND	3.31	115.59	110.24
13	T	102	BCL	C1-C2-C3	-3.30	120.34	126.04
13	U	102	BCL	C3D-C4D-ND	3.30	115.57	110.24
13	R	102	BCL	CHB-C1B-NB	-3.28	120.78	124.26
13	V	102	BCL	CHC-C4B-NB	-3.28	120.78	124.26
13	X	101	BCL	CHC-C4B-NB	-3.28	120.79	124.26
13	N	102	BCL	CHB-C1B-NB	-3.28	120.79	124.26
13	G	102	BCL	CHB-C1B-NB	-3.27	120.80	124.26
13	V	102	BCL	CHB-C1B-NB	-3.26	120.80	124.26
20	4	101	CRT	C10-C9-C7	-3.26	122.66	127.31
8	C	402	HEC	CHB-C1B-NB	3.25	127.95	124.42
20	E	101	CRT	C10-C9-C7	-3.25	122.67	127.31
16	X	103	LMT	O1B-C4'-C5'	3.25	118.36	109.45
13	Z	102	BCL	CHC-C4B-NB	-3.25	120.82	124.26
20	Y	101	CRT	C10-C9-C7	-3.25	122.67	127.31
13	3	101	BCL	C3D-C4D-ND	3.24	115.48	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	9	101	BCL	CHB-C1B-NB	-3.24	120.83	124.26
13	V	102	BCL	C1-C2-C3	-3.22	120.47	126.04
13	0	102	BCL	CHB-C1B-NB	-3.21	120.85	124.26
13	3	101	BCL	CHD-C4C-NC	3.21	128.65	125.08
13	5	402	BCL	CHB-C1B-NB	-3.20	120.86	124.26
7	C	401	HEM	CHB-C1B-NB	3.20	128.32	124.37
13	U	102	BCL	C3C-C4C-CHD	-3.20	116.55	123.39
13	R	102	BCL	CHC-C4B-NB	-3.20	120.87	124.26
13	J	102	BCL	C1-C2-C3	-3.18	120.54	126.04
13	T	102	BCL	CHC-C4B-NB	-3.18	120.89	124.26
13	P	102	BCL	CHB-C1B-NB	-3.17	120.90	124.26
13	Z	102	BCL	CHB-C1B-NB	-3.14	120.93	124.26
13	B	102	BCL	CHB-C1B-NB	-3.14	120.93	124.26
13	J	102	BCL	CHB-C1B-NB	-3.13	120.94	124.26
13	Q	101	BCL	CHB-C1B-NB	-3.13	120.94	124.26
20	6	101	CRT	C20-C19-C17	-3.13	122.85	127.31
17	X	102	PGV	O01-C1-C2	3.13	118.24	111.50
13	T	102	BCL	CHB-C1B-NB	-3.12	120.95	124.26
13	L	302	BCL	C1-C2-C3	-3.12	120.65	126.04
13	L	310	BCL	C1-C2-C3	-3.11	120.66	126.04
13	O	101	BCL	C1-C2-C3	-3.11	120.67	126.04
13	D	102	BCL	CHB-C1B-NB	-3.11	120.97	124.26
13	X	101	BCL	CHB-C1B-NB	-3.10	120.97	124.26
13	B	102	BCL	C1-C2-C3	-3.10	120.69	126.04
13	8	103	BCL	CHB-C1B-NB	-3.10	120.98	124.26
13	U	102	BCL	CHB-C1B-NB	-3.09	120.98	124.26
13	G	102	BCL	C1-C2-C3	-3.09	120.70	126.04
13	2	103	BCL	C1-C2-C3	-3.09	120.70	126.04
13	1	101	BCL	CHB-C1B-NB	-3.09	120.99	124.26
8	C	403	HEC	CBC-CAC-C3C	3.07	120.91	112.43
16	Z	103	LMT	O5B-C5B-C4B	3.07	115.28	109.69
20	V	101	CRT	C32-C31-C30	-3.07	113.63	123.22
20	8	102	CRT	C34-C33-C35	3.07	122.92	118.08
20	8	102	CRT	O2-C38-C40	-3.07	87.86	108.97
13	A	102	BCL	C1-C2-C3	-3.07	120.74	126.04
17	H	401	PGV	C02-O01-C1	-3.06	110.25	117.79
20	8	102	CRT	C5-C6-C7	-3.06	121.26	125.89
20	P	101	CRT	C10-C9-C7	-3.06	122.94	127.31
7	C	401	HEM	C4B-C3B-C2B	-3.05	104.69	107.11
13	L	311	BCL	CHB-C1B-NB	-3.05	121.03	124.26
13	Y	102	BCL	CHB-C1B-NB	-3.02	121.06	124.26
13	3	101	BCL	C1-C2-C3	-3.01	120.83	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	7	103	LMT	C4B-C3B-C2B	-3.01	105.56	110.82
20	J	101	CRT	C32-C31-C30	-3.01	113.83	123.22
20	B	101	CRT	C32-C31-C30	-3.00	113.85	123.22
13	M	402	BCL	C1-C2-C3	-3.00	120.86	126.04
20	6	101	CRT	C8-C7-C6	2.99	122.78	118.08
13	L	302	BCL	CHB-C1B-NB	-2.99	121.10	124.26
20	4	101	CRT	C32-C31-C30	-2.98	113.92	123.22
13	I	101	BCL	CHB-C1B-NB	-2.98	121.10	124.26
13	W	101	BCL	CHB-C1B-NB	-2.97	121.11	124.26
7	C	401	HEM	CHD-C1D-C2D	-2.97	120.34	124.98
8	C	403	HEC	CBD-CAD-C3D	-2.97	104.39	112.63
13	0	102	BCL	C4-C3-C5	2.97	120.26	115.27
20	Y	101	CRT	C5-C6-C7	-2.97	121.41	125.89
20	4	101	CRT	C5-C6-C7	-2.97	121.41	125.89
13	Q	101	BCL	C4B-C3B-C2B	-2.97	103.59	108.36
13	D	102	BCL	C4-C3-C5	2.96	120.26	115.27
13	O	101	BCL	CHB-C1B-NB	-2.96	121.12	124.26
13	K	101	BCL	C4-C3-C5	2.96	120.25	115.27
16	7	103	LMT	C1B-O5B-C5B	2.96	119.50	113.69
13	K	101	BCL	CHB-C1B-NB	-2.96	121.12	124.26
13	2	103	BCL	CHB-C4A-NA	2.96	128.61	124.51
16	4	104	LMT	C1B-O1B-C4'	-2.96	110.64	117.96
17	M	408	PGV	O03-C19-C20	2.96	121.19	111.91
13	I	101	BCL	C4-C3-C5	2.96	120.24	115.27
20	T	101	CRT	C32-C31-C30	-2.95	114.02	123.22
13	S	101	BCL	C4B-C3B-C2B	-2.95	103.62	108.36
13	F	101	BCL	CHB-C1B-NB	-2.94	121.14	124.26
7	C	401	HEM	C4C-NC-C1C	2.94	108.23	105.35
20	Y	101	CRT	C32-C31-C30	-2.94	114.05	123.22
14	M	403	BPH	C2B-C1B-NB	-2.94	107.50	109.53
13	W	101	BCL	C4-C3-C5	2.93	120.20	115.27
13	A	102	BCL	C4B-C3B-C2B	-2.93	103.65	108.36
13	J	102	BCL	CHB-C4A-NA	2.93	128.56	124.51
13	F	101	BCL	C4B-C3B-C2B	-2.92	103.67	108.36
20	B	101	CRT	C21-C20-C19	-2.91	117.52	123.47
13	0	102	BCL	CHB-C4A-NA	2.91	128.53	124.51
13	N	102	BCL	CHB-C4A-NA	2.90	128.53	124.51
13	F	101	BCL	C4-C3-C5	2.90	120.16	115.27
13	A	102	BCL	CHB-C1B-NB	-2.90	121.19	124.26
13	Z	102	BCL	C1-C2-C3	-2.90	121.03	126.04
13	G	102	BCL	C4B-C3B-C2B	-2.90	103.70	108.36
13	K	101	BCL	C4B-C3B-C2B	-2.89	103.70	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	102	BCL	C4B-C3B-C2B	-2.89	103.71	108.36
13	Z	102	BCL	C4-C3-C5	2.89	120.13	115.27
13	I	101	BCL	C4B-C3B-C2B	-2.89	103.72	108.36
13	S	101	BCL	O2A-CGA-CBA	2.89	120.96	111.91
13	Y	102	BCL	C4B-C3B-C2B	-2.89	103.72	108.36
8	C	404	HEC	CAC-C3C-C4C	2.88	128.92	124.92
13	O	101	BCL	C4B-C3B-C2B	-2.88	103.73	108.36
13	9	101	BCL	C4B-C3B-C2B	-2.87	103.74	108.36
17	B	103	PGV	C02-O01-C1	-2.87	110.72	117.79
17	H	403	PGV	C02-O01-C1	-2.87	110.73	117.79
13	L	302	BCL	C4-C3-C5	2.86	120.09	115.27
13	N	102	BCL	C4B-C3B-C2B	-2.86	103.76	108.36
13	5	402	BCL	C4B-C3B-C2B	-2.86	103.76	108.36
13	P	102	BCL	C4-C3-C5	2.86	120.08	115.27
13	E	102	BCL	CHB-C4A-NA	2.85	128.46	124.51
20	J	101	CRT	C5-C6-C7	-2.85	121.58	125.89
20	P	101	CRT	C32-C31-C30	-2.85	114.32	123.22
16	E	104	LMT	C1B-O1B-C4'	-2.85	110.91	117.96
20	Z	101	CRT	C32-C31-C30	-2.85	114.32	123.22
20	E	101	CRT	C32-C31-C30	-2.85	114.32	123.22
14	L	303	BPH	C2B-C1B-NB	-2.85	107.56	109.53
13	G	102	BCL	CHB-C4A-NA	2.85	128.45	124.51
17	T	103	PGV	C02-O01-C1	-2.84	110.79	117.79
16	Z	104	LMT	C1B-O1B-C4'	-2.84	110.93	117.96
20	N	101	CRT	C21-C20-C19	-2.84	117.66	123.47
13	R	102	BCL	C1-C2-C3	-2.84	121.14	126.04
13	9	101	BCL	C1-C2-C3	-2.83	121.14	126.04
20	2	102	CRT	C32-C31-C30	-2.83	114.38	123.22
13	X	101	BCL	C4-C3-C5	2.83	120.03	115.27
17	P	103	PGV	C02-O01-C1	-2.83	110.82	117.79
20	V	101	CRT	C8-C7-C9	-2.83	118.96	122.92
16	L	305	LMT	C1B-O1B-C4'	-2.83	110.96	117.96
13	O	101	BCL	O2A-CGA-CBA	2.83	120.78	111.91
13	M	402	BCL	C4B-C3B-C2B	-2.83	103.81	108.36
13	R	102	BCL	C4-C3-C5	2.83	120.03	115.27
13	5	402	BCL	C4-C3-C5	2.82	120.02	115.27
13	T	102	BCL	C4-C3-C5	2.82	120.02	115.27
13	Z	102	BCL	CHB-C4A-NA	2.82	128.41	124.51
13	0	102	BCL	C1-C2-C3	-2.82	121.16	126.04
13	L	302	BCL	O2A-CGA-CBA	2.82	120.76	111.91
13	2	103	BCL	C4B-C3B-C2B	-2.81	103.83	108.36
20	8	102	CRT	C32-C31-C30	-2.81	114.44	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	9	101	BCL	C4-C3-C5	2.81	120.00	115.27
13	V	102	BCL	C1C-NC-C4C	-2.81	105.44	106.71
13	P	102	BCL	CHB-C4A-NA	2.81	128.40	124.51
13	T	102	BCL	CHC-C1C-NC	2.81	128.39	124.51
13	3	101	BCL	CHB-C1B-NB	-2.80	121.29	124.26
13	R	102	BCL	CHC-C1C-NC	2.80	128.38	124.51
13	2	103	BCL	CHC-C1C-NC	2.80	128.38	124.51
13	J	102	BCL	C4B-C3B-C2B	-2.79	103.86	108.36
13	X	101	BCL	CHC-C1C-NC	2.79	128.37	124.51
13	J	102	BCL	CHC-C1C-NC	2.79	128.37	124.51
13	B	102	BCL	C4B-C3B-C2B	-2.79	103.87	108.36
20	J	101	CRT	C10-C9-C7	-2.79	123.33	127.31
13	5	402	BCL	C1-C2-C3	-2.79	121.22	126.04
13	6	102	BCL	CHB-C4A-NA	2.78	128.36	124.51
20	0	101	CRT	C32-C31-C30	-2.78	114.54	123.22
13	3	101	BCL	C4B-C3B-C2B	-2.78	103.89	108.36
20	E	101	CRT	C5-C6-C7	-2.78	121.69	125.89
13	M	402	BCL	O2A-CGA-CBA	2.78	120.62	111.91
13	L	302	BCL	CHC-C1C-NC	2.77	128.34	124.51
13	8	103	BCL	CHB-C4A-NA	2.77	128.34	124.51
13	T	102	BCL	CHB-C4A-NA	2.77	128.34	124.51
13	X	101	BCL	CHB-C4A-NA	2.77	128.34	124.51
20	P	101	CRT	C21-C20-C19	-2.77	117.81	123.47
13	B	102	BCL	CHC-C1C-NC	2.76	128.34	124.51
13	P	102	BCL	CHC-C1C-NC	2.76	128.33	124.51
13	W	101	BCL	C1-C2-C3	-2.76	121.28	126.04
13	J	102	BCL	C4-C3-C5	2.76	119.91	115.27
13	B	102	BCL	CHB-C4A-NA	2.75	128.32	124.51
20	G	101	CRT	C32-C31-C30	-2.75	114.62	123.22
20	N	101	CRT	C32-C31-C30	-2.75	114.63	123.22
13	2	103	BCL	C4-C3-C5	2.75	119.89	115.27
20	6	101	CRT	C32-C31-C30	-2.74	114.66	123.22
13	0	102	BCL	CHC-C1C-NC	2.74	128.31	124.51
13	8	103	BCL	CHC-C1C-NC	2.74	128.30	124.51
13	0	102	BCL	C4B-C3B-C2B	-2.74	103.96	108.36
13	Q	101	BCL	C4-C3-C5	2.74	119.87	115.27
13	P	102	BCL	C4B-C3B-C2B	-2.73	103.96	108.36
16	5	401	LMT	C1B-O1B-C4'	-2.73	111.21	117.96
13	1	101	BCL	C4B-C3B-C2B	-2.73	103.97	108.36
16	J	104	LMT	C1B-O1B-C4'	-2.73	111.21	117.96
16	F	102	LMT	C1B-O1B-C4'	-2.73	111.21	117.96
13	L	310	BCL	CHB-C1B-NB	-2.72	121.37	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	V	102	BCL	CHC-C1C-NC	2.72	128.28	124.51
13	P	102	BCL	C1-C2-C3	-2.72	121.34	126.04
13	5	402	BCL	O2A-CGA-CBA	2.72	120.44	111.91
20	R	101	CRT	C32-C31-C30	-2.72	114.73	123.22
13	V	102	BCL	C4B-C3B-C2B	-2.72	103.99	108.36
13	A	102	BCL	CHC-C1C-NC	2.71	128.26	124.51
8	C	404	HEC	C1D-ND-C4D	2.71	107.87	105.07
17	H	404	PGV	O03-C19-C20	2.71	120.41	111.91
8	C	404	HEC	CBC-CAC-C3C	2.71	119.90	112.43
13	E	102	BCL	C4B-C3B-C2B	-2.71	104.00	108.36
13	R	102	BCL	CHB-C4A-NA	2.71	128.25	124.51
13	G	102	BCL	CHC-C1C-NC	2.71	128.25	124.51
13	V	102	BCL	CHB-C4A-NA	2.70	128.25	124.51
17	M	406	PGV	C02-O01-C1	-2.70	111.14	117.79
13	L	310	BCL	CHC-C1C-NC	2.70	128.25	124.51
13	E	102	BCL	C4-C3-C5	2.70	119.82	115.27
13	X	101	BCL	C4B-C3B-C2B	-2.70	104.01	108.36
20	6	101	CRT	C8-C7-C9	-2.70	119.14	122.92
13	N	102	BCL	CHC-C1C-NC	2.70	128.24	124.51
13	Z	102	BCL	C4B-C3B-C2B	-2.70	104.02	108.36
13	4	102	BCL	CHB-C4A-NA	2.70	128.24	124.51
13	W	101	BCL	C4B-C3B-C2B	-2.70	104.02	108.36
13	F	101	BCL	O2A-CGA-CBA	2.70	120.37	111.91
13	1	101	BCL	C4-C3-C5	2.69	119.80	115.27
13	8	103	BCL	C4B-C3B-C2B	-2.69	104.03	108.36
13	1	101	BCL	O2A-CGA-CBA	2.69	120.36	111.91
20	V	101	CRT	C21-C20-C19	-2.69	117.96	123.47
13	L	302	BCL	CMD-C2D-C3D	-2.69	121.43	127.61
8	C	402	HEC	CAD-CBD-CGD	-2.69	107.82	113.60
13	L	310	BCL	C4-C3-C5	2.69	119.79	115.27
13	L	310	BCL	C1D-CHD-C4C	-2.68	120.15	126.62
8	C	403	HEC	CHA-C1A-NA	2.68	127.34	124.44
13	Z	102	BCL	CHC-C1C-NC	2.68	128.22	124.51
13	X	101	BCL	C1-C2-C3	-2.68	121.41	126.04
13	G	102	BCL	C4-C3-C5	2.68	119.78	115.27
13	L	302	BCL	C4B-C3B-C2B	-2.68	104.05	108.36
17	V	103	PGV	C02-O01-C1	-2.68	111.20	117.79
13	F	101	BCL	CHC-C1C-NC	2.68	128.21	124.51
17	J	103	PGV	O03-C19-C20	2.68	120.31	111.91
13	9	101	BCL	O2A-CGA-CBA	2.68	120.30	111.91
13	U	102	BCL	C4B-C3B-C2B	-2.67	104.06	108.36
13	1	101	BCL	C1-C2-C3	-2.67	121.42	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	402	HEC	CHA-C1A-NA	2.67	127.33	124.44
20	J	101	CRT	C9-C10-C11	-2.67	114.88	123.22
13	E	102	BCL	O2A-CGA-CBA	2.67	120.29	111.91
20	4	101	CRT	C21-C20-C19	-2.67	118.01	123.47
13	R	102	BCL	C4B-C3B-C2B	-2.67	104.07	108.36
13	N	102	BCL	C4-C3-C5	2.67	119.75	115.27
13	U	102	BCL	C1-C2-C3	-2.66	121.44	126.04
13	D	102	BCL	C1-C2-C3	-2.66	121.44	126.04
13	3	101	BCL	C3C-C4C-CHD	-2.66	117.71	123.39
13	L	302	BCL	CMB-C2B-C3B	2.66	133.12	125.93
16	9	102	LMT	C1B-O1B-C4'	-2.66	111.38	117.96
13	Y	102	BCL	C4-C3-C5	2.66	119.74	115.27
8	C	402	HEC	CBC-CAC-C3C	2.66	119.75	112.43
20	8	102	CRT	C36-C35-C33	2.65	129.90	125.89
13	7	102	BCL	CHB-C4A-NA	2.65	128.18	124.51
13	L	310	BCL	C4B-C3B-C2B	-2.65	104.09	108.36
13	O	101	BCL	CHC-C1C-NC	2.65	128.18	124.51
17	8	104	PGV	C02-O01-C1	-2.65	111.27	117.79
13	3	101	BCL	CMB-C2B-C3B	2.65	133.08	125.93
13	U	102	BCL	C4-C3-C5	2.65	119.72	115.27
17	H	403	PGV	O03-C19-C20	2.64	120.20	111.91
13	T	102	BCL	C4B-C3B-C2B	-2.64	104.11	108.36
17	M	407	PGV	O03-C19-C20	2.64	120.20	111.91
13	6	102	BCL	CHC-C1C-NC	2.64	128.16	124.51
13	D	102	BCL	CMB-C2B-C3B	2.64	133.06	125.93
13	K	101	BCL	CHC-C1C-NC	2.64	128.16	124.51
13	T	102	BCL	C2A-C1A-CHA	-2.64	119.25	123.86
13	4	102	BCL	CHC-C1C-NC	2.64	128.16	124.51
20	T	101	CRT	C21-C20-C19	-2.64	118.07	123.47
13	O	101	BCL	C4-C3-C5	2.64	119.70	115.27
13	F	101	BCL	CHB-C4A-NA	2.63	128.15	124.51
13	Q	101	BCL	CHB-C4A-NA	2.63	128.15	124.51
13	S	101	BCL	CHB-C4A-NA	2.62	128.13	124.51
13	I	101	BCL	CHC-C1C-NC	2.62	128.13	124.51
13	U	102	BCL	O2A-CGA-CBA	2.62	120.12	111.91
13	E	102	BCL	CHC-C1C-NC	2.62	128.13	124.51
17	D	101	PGV	O03-C19-C20	2.61	120.11	111.91
20	J	101	CRT	C26-C27-C28	-2.61	123.58	127.31
17	0	103	PGV	O03-C19-C20	2.61	120.11	111.91
13	6	102	BCL	C4B-C3B-C2B	-2.61	104.16	108.36
13	L	311	BCL	O2A-CGA-CBA	2.61	120.10	111.91
13	M	402	BCL	CAA-C2A-C3A	-2.61	105.63	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q	101	BCL	C1-C2-C3	-2.61	121.53	126.04
13	4	102	BCL	C4B-C3B-C2B	-2.61	104.17	108.36
20	Y	101	CRT	C21-C20-C19	-2.60	118.15	123.47
13	Q	101	BCL	CHC-C1C-NC	2.60	128.10	124.51
13	A	102	BCL	CMB-C2B-C3B	2.60	132.94	125.93
17	2	104	PGV	C02-O01-C1	-2.59	111.40	117.79
20	J	101	CRT	C34-C33-C35	2.59	122.16	118.08
16	P	104	LMT	C1B-O1B-C4'	-2.59	111.55	117.96
20	E	101	CRT	C21-C20-C19	-2.59	118.17	123.47
13	X	101	BCL	C2A-C1A-CHA	-2.59	119.33	123.86
8	C	402	HEC	CHA-C4D-C3D	-2.59	121.03	124.84
13	I	101	BCL	O2A-CGA-CBA	2.59	120.03	111.91
13	K	101	BCL	O2A-CGA-CBA	2.59	120.03	111.91
13	M	402	BCL	CMD-C2D-C3D	-2.59	121.66	127.61
20	M	405	CRT	C31-C32-C33	-2.59	123.62	127.31
13	R	102	BCL	C2A-C1A-CHA	-2.59	119.34	123.86
13	7	102	BCL	C4-C3-C5	2.59	119.62	115.27
8	C	403	HEC	CHA-C4D-C3D	-2.58	121.04	124.84
13	Y	102	BCL	CMB-C2B-C3B	2.58	132.91	125.93
13	D	102	BCL	CHB-C4A-NA	2.58	128.09	124.51
20	Z	101	CRT	C21-C20-C19	-2.58	118.18	123.47
13	U	102	BCL	CHB-C4A-NA	2.58	128.08	124.51
13	F	101	BCL	CMB-C2B-C3B	2.58	132.90	125.93
13	L	310	BCL	CMB-C2B-C3B	2.58	132.89	125.93
13	3	101	BCL	O2A-CGA-CBA	2.57	119.99	111.91
13	Q	101	BCL	CMD-C2D-C3D	-2.57	121.69	127.61
13	L	311	BCL	C4-C3-C5	2.57	119.60	115.27
20	Y	101	CRT	C26-C27-C28	-2.57	123.64	127.31
13	M	402	BCL	CED-O2D-CGD	2.57	121.75	115.94
17	K	102	PGV	O03-C19-C20	2.57	119.98	111.91
13	Q	101	BCL	CMB-C2B-C3B	2.57	132.87	125.93
17	8	104	PGV	O03-C19-C20	2.57	119.97	111.91
13	O	101	BCL	CHB-C4A-NA	2.57	128.07	124.51
20	J	101	CRT	C13-C12-C11	2.57	122.12	118.08
13	Z	102	BCL	O2A-CGA-CBA	2.57	119.96	111.91
8	C	403	HEC	CBB-CAB-C3B	2.56	119.50	112.43
13	X	101	BCL	CMB-C2B-C3B	2.56	132.85	125.93
13	K	101	BCL	CMB-C2B-C3B	2.56	132.85	125.93
13	N	102	BCL	CMB-C2B-C3B	2.56	132.85	125.93
13	6	102	BCL	C4-C3-C5	2.56	119.58	115.27
20	M	405	CRT	C5-C6-C7	-2.56	122.02	125.89
20	N	101	CRT	C14-C15-C16	-2.56	115.23	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	402	LMT	C1B-O1B-C4'	-2.56	111.64	117.96
13	L	310	BCL	O2A-CGA-CBA	2.56	119.93	111.91
13	9	101	BCL	CMB-C2B-C3B	2.56	132.83	125.93
13	A	102	BCL	O2A-CGA-CBA	2.55	119.92	111.91
13	I	101	BCL	C1-C2-C3	-2.55	121.63	126.04
20	Y	101	CRT	C34-C33-C35	2.55	122.09	118.08
17	L	306	PGV	O03-C19-C20	2.55	119.90	111.91
20	6	101	CRT	C21-C20-C19	-2.55	118.26	123.47
13	3	101	BCL	CMD-C2D-C3D	-2.54	121.76	127.61
13	8	103	BCL	C2A-C1A-CHA	-2.54	119.42	123.86
13	D	102	BCL	O2A-CGA-CBA	2.54	119.88	111.91
13	M	402	BCL	CMB-C2B-C3B	2.54	132.78	125.93
13	W	101	BCL	O2A-CGA-CBA	2.54	119.87	111.91
13	P	102	BCL	C2A-C1A-CHA	-2.54	119.42	123.86
17	8	101	PGV	O03-C19-C20	2.54	119.86	111.91
13	Z	102	BCL	CMB-C2B-C3B	2.53	132.78	125.93
20	Z	101	CRT	C14-C15-C16	-2.53	115.31	123.22
20	4	101	CRT	C14-C15-C16	-2.53	115.32	123.22
20	Y	101	CRT	C14-C15-C16	-2.53	115.32	123.22
13	8	103	BCL	C4-C3-C5	2.53	119.53	115.27
13	Q	101	BCL	O2A-CGA-CBA	2.53	119.84	111.91
17	G	103	PGV	O03-C19-C20	2.53	119.84	111.91
17	H	401	PGV	O03-C19-C20	2.52	119.83	111.91
13	0	102	BCL	CMB-C2B-C3B	2.52	132.74	125.93
13	Z	102	BCL	C1C-NC-C4C	-2.52	105.57	106.71
20	N	101	CRT	C34-C33-C35	2.51	122.04	118.08
13	1	101	BCL	CHB-C4A-NA	2.51	127.99	124.51
13	O	101	BCL	CMB-C2B-C3B	2.51	132.71	125.93
20	0	101	CRT	C21-C20-C19	-2.51	118.33	123.47
13	7	102	BCL	C4B-C3B-C2B	-2.51	104.32	108.36
13	A	102	BCL	CHB-C4A-NA	2.51	127.98	124.51
20	4	101	CRT	C34-C33-C35	2.51	122.03	118.08
13	W	101	BCL	CHB-C4A-NA	2.51	127.98	124.51
13	N	102	BCL	C1-C2-C3	-2.51	121.71	126.04
20	4	101	CRT	C26-C27-C28	-2.51	123.73	127.31
17	T	103	PGV	O03-C19-C20	2.51	119.77	111.91
13	Y	102	BCL	CMD-C2D-C3D	-2.51	121.85	127.61
20	6	101	CRT	C5-C6-C7	2.50	129.68	125.89
13	A	102	BCL	C4-C3-C5	2.50	119.48	115.27
13	P	102	BCL	CMB-C2B-C3B	2.50	132.69	125.93
13	B	102	BCL	C2A-C1A-CHA	-2.50	119.49	123.86
20	G	101	CRT	C14-C15-C16	-2.50	115.42	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	102	CRT	C14-C15-C16	-2.50	115.43	123.22
13	V	102	BCL	C4-C3-C5	2.49	119.47	115.27
13	Y	102	BCL	CHB-C4A-NA	2.49	127.96	124.51
8	C	404	HEC	C1A-CHA-C4D	-2.49	120.68	126.06
20	T	101	CRT	C14-C15-C16	-2.49	115.44	123.22
13	J	102	BCL	CMB-C2B-C3B	2.49	132.66	125.93
13	O	101	BCL	CMD-C2D-C3D	-2.49	121.88	127.61
16	V	104	LMT	C1B-O1B-C4'	-2.49	111.80	117.96
20	J	101	CRT	C21-C20-C19	-2.49	118.37	123.47
8	C	404	HEC	CHA-C4D-C3D	-2.49	121.18	124.84
13	U	102	BCL	CMB-C2B-C3B	2.49	132.65	125.93
17	4	103	PGV	C02-O01-C1	-2.49	111.67	117.79
8	C	404	HEC	CHB-C1B-C2B	-2.49	121.09	124.98
17	4	103	PGV	O03-C19-C20	2.49	119.71	111.91
13	I	101	BCL	CMB-C2B-C3B	2.48	132.64	125.93
13	A	102	BCL	C1C-NC-C4C	-2.48	105.59	106.71
13	G	102	BCL	CMB-C2B-C3B	2.48	132.63	125.93
20	M	405	CRT	C26-C27-C28	-2.48	123.77	127.31
13	V	102	BCL	C2A-C1A-CHA	-2.48	119.52	123.86
13	D	102	BCL	CHC-C1C-NC	2.48	127.94	124.51
7	C	401	HEM	CBA-CAA-C2A	-2.48	105.74	112.63
13	K	101	BCL	CHB-C4A-NA	2.48	127.94	124.51
13	0	102	BCL	C2A-C1A-CHA	-2.48	119.53	123.86
13	Y	102	BCL	CHC-C1C-NC	2.48	127.94	124.51
13	K	101	BCL	C1-C2-C3	-2.48	121.76	126.04
8	C	403	HEC	C1D-ND-C4D	2.47	107.63	105.07
16	M	409	LMT	C1B-O1B-C4'	-2.47	111.84	117.96
13	W	101	BCL	CMB-C2B-C3B	2.47	132.61	125.93
13	5	402	BCL	CMB-C2B-C3B	2.47	132.61	125.93
13	Y	102	BCL	O2A-CGA-CBA	2.47	119.67	111.91
13	6	102	BCL	CMB-C2B-C3B	2.47	132.60	125.93
13	S	101	BCL	CHC-C1C-NC	2.47	127.92	124.51
13	W	101	BCL	C4A-NA-C1A	2.46	107.81	106.71
13	S	101	BCL	CMD-C2D-C3D	-2.46	121.95	127.61
17	L	307	PGV	O03-C19-C20	2.46	119.63	111.91
13	L	310	BCL	O2D-CGD-O1D	-2.46	119.03	123.84
13	X	101	BCL	O2A-CGA-CBA	2.46	119.63	111.91
13	K	101	BCL	CMD-C2D-C3D	-2.46	121.96	127.61
17	0	103	PGV	C02-O01-C1	-2.46	111.74	117.79
20	E	101	CRT	C34-C33-C35	2.46	121.95	118.08
13	1	101	BCL	CMB-C2B-C3B	2.46	132.57	125.93
13	9	101	BCL	CHB-C4A-NA	2.46	127.91	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	101	CRT	C14-C15-C16	-2.46	115.55	123.22
13	S	101	BCL	CMB-C2B-C3B	2.46	132.56	125.93
20	B	101	CRT	C34-C33-C35	2.45	121.94	118.08
13	V	102	BCL	CMB-C2B-C3B	2.45	132.56	125.93
13	F	101	BCL	CMD-C2D-C3D	-2.45	121.97	127.61
13	L	311	BCL	CMD-C2D-C3D	-2.45	121.97	127.61
13	5	402	BCL	CMD-C2D-C3D	-2.45	121.97	127.61
13	J	102	BCL	C2A-C1A-CHA	-2.45	119.57	123.86
20	M	405	CRT	C9-C10-C11	-2.45	115.57	123.22
13	M	402	BCL	CHB-C4A-NA	2.45	127.90	124.51
20	G	101	CRT	C34-C33-C35	2.45	121.94	118.08
13	G	102	BCL	O2A-CGA-CBA	2.45	119.59	111.91
13	G	102	BCL	C2A-C1A-CHA	-2.45	119.58	123.86
13	0	102	BCL	O2A-CGA-CBA	2.45	119.58	111.91
20	B	101	CRT	C29-C28-C30	2.44	121.93	118.08
13	2	103	BCL	C2A-C1A-CHA	-2.44	119.59	123.86
20	2	102	CRT	C21-C20-C19	-2.44	118.47	123.47
20	N	101	CRT	C13-C12-C11	2.44	121.92	118.08
13	D	102	BCL	CMD-C2D-C3D	-2.44	122.00	127.61
13	3	101	BCL	C1D-CHD-C4C	-2.44	120.74	126.62
20	J	101	CRT	C29-C28-C30	2.44	121.92	118.08
17	R	103	PGV	O03-C19-C20	2.44	119.55	111.91
20	M	405	CRT	C10-C9-C7	-2.44	123.83	127.31
20	0	101	CRT	C34-C33-C35	2.44	121.91	118.08
13	2	103	BCL	CMB-C2B-C3B	2.43	132.50	125.93
13	U	102	BCL	CMD-C2D-C3D	-2.43	122.02	127.61
20	P	101	CRT	C9-C10-C11	-2.43	115.63	123.22
13	1	101	BCL	CMD-C2D-C3D	-2.43	122.02	127.61
13	P	102	BCL	C1C-NC-C4C	-2.43	105.61	106.71
8	C	402	HEC	CHB-C1B-C2B	-2.43	121.19	124.98
20	E	101	CRT	C14-C15-C16	-2.43	115.64	123.22
20	B	101	CRT	C27-C26-C25	-2.43	115.64	123.22
13	7	102	BCL	O2A-CGA-CBA	2.43	119.53	111.91
13	G	102	BCL	C1C-NC-C4C	-2.43	105.61	106.71
13	4	102	BCL	C1D-CHD-C4C	-2.43	120.77	126.62
13	8	103	BCL	CMB-C2B-C3B	2.43	132.48	125.93
13	W	101	BCL	CMD-C2D-C3D	-2.42	122.04	127.61
8	C	402	HEC	C1A-CHA-C4D	-2.42	120.83	126.06
13	L	302	BCL	CHB-C4A-NA	2.42	127.86	124.51
20	6	101	CRT	C26-C27-C28	-2.42	123.85	127.31
20	P	101	CRT	C14-C15-C16	-2.42	115.66	123.22
16	V	104	LMT	O5B-C5B-C4B	-2.42	105.30	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	9	101	BCL	CMD-C2D-C3D	-2.42	122.05	127.61
20	0	101	CRT	C14-C15-C16	-2.42	115.67	123.22
20	E	101	CRT	C26-C27-C28	-2.42	123.86	127.31
13	L	310	BCL	C2A-C1A-CHA	-2.42	119.63	123.86
13	W	101	BCL	C1D-CHD-C4C	-2.42	120.79	126.62
20	2	102	CRT	C27-C26-C25	-2.42	115.68	123.22
16	4	105	LMT	C1B-O1B-C4'	-2.41	111.99	117.96
17	L	306	PGV	O14-P-O13	2.41	120.13	110.68
17	E	103	PGV	C02-O01-C1	-2.41	111.85	117.79
13	4	102	BCL	C1C-NC-C4C	-2.41	105.62	106.71
13	4	102	BCL	CMB-C2B-C3B	2.41	132.44	125.93
13	W	101	BCL	C1C-NC-C4C	-2.41	105.62	106.71
20	B	101	CRT	C14-C15-C16	-2.41	115.71	123.22
20	4	101	CRT	C13-C12-C11	2.41	121.87	118.08
13	B	102	BCL	C1C-NC-C4C	-2.40	105.62	106.71
20	V	101	CRT	C34-C33-C35	2.40	121.86	118.08
17	N	103	PGV	O03-C19-C20	2.40	119.45	111.91
13	B	102	BCL	CMB-C2B-C3B	2.40	132.42	125.93
13	L	302	BCL	C2A-C1A-CHA	-2.40	119.66	123.86
20	Z	101	CRT	C8-C7-C9	-2.40	119.56	122.92
8	C	403	HEC	C1A-CHA-C4D	-2.40	120.89	126.06
13	R	102	BCL	C1C-NC-C4C	-2.40	105.63	106.71
13	P	102	BCL	O2D-CGD-O1D	-2.39	119.16	123.84
13	3	101	BCL	C4-C3-C5	2.39	119.30	115.27
20	P	101	CRT	C34-C33-C35	2.39	121.84	118.08
20	0	101	CRT	C27-C26-C25	-2.39	115.76	123.22
13	7	102	BCL	CMD-C2D-C3D	-2.39	122.12	127.61
13	M	402	BCL	CHC-C1C-NC	2.39	127.81	124.51
20	2	102	CRT	C29-C28-C30	2.38	121.83	118.08
16	O	102	LMT	C1B-O1B-C4'	-2.38	112.07	117.96
13	Z	102	BCL	C2A-C1A-CHA	-2.38	119.69	123.86
13	A	102	BCL	CAC-C3C-C4C	-2.38	107.30	112.58
20	Y	101	CRT	C13-C12-C11	2.38	121.83	118.08
20	4	101	CRT	C29-C28-C30	2.38	121.83	118.08
13	A	102	BCL	CMD-C2D-C3D	-2.38	122.15	127.61
20	6	101	CRT	C34-C33-C35	2.38	121.82	118.08
20	E	101	CRT	C9-C10-C11	-2.38	115.80	123.22
20	4	101	CRT	C9-C10-C11	-2.38	115.81	123.22
20	T	101	CRT	C34-C33-C35	2.37	121.82	118.08
20	Y	101	CRT	C27-C26-C25	-2.37	115.81	123.22
13	E	102	BCL	CMB-C2B-C3B	2.37	132.34	125.93
20	M	405	CRT	C14-C15-C16	-2.37	115.81	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	102	BCL	C1D-CHD-C4C	-2.37	120.90	126.62
20	6	101	CRT	C18-C17-C19	-2.37	119.60	122.92
17	2	101	PGV	O03-C19-C20	2.37	119.35	111.91
20	Z	101	CRT	C34-C33-C35	2.37	121.81	118.08
13	A	102	BCL	O2D-CGD-O1D	-2.37	119.20	123.84
8	C	404	HEC	CHA-C1A-NA	2.37	127.00	124.44
16	V	104	LMT	C1B-C2B-C3B	2.37	114.93	110.00
13	L	302	BCL	O2A-CGA-O1A	-2.37	117.61	123.59
13	T	102	BCL	O2D-CGD-O1D	-2.37	119.21	123.84
13	5	402	BCL	CHB-C4A-NA	2.37	127.79	124.51
20	4	101	CRT	C27-C26-C25	-2.37	115.83	123.22
13	O	101	BCL	O2D-CGD-O1D	-2.37	119.21	123.84
20	2	102	CRT	C34-C33-C35	2.37	121.81	118.08
17	M	407	PGV	C02-O01-C1	-2.37	111.97	117.79
13	M	402	BCL	C1D-CHD-C4C	-2.36	120.92	126.62
20	G	101	CRT	C21-C20-C19	-2.36	118.63	123.47
13	B	102	BCL	O2A-CGA-CBA	2.36	119.33	111.91
13	T	102	BCL	CMB-C2B-C3B	2.36	132.31	125.93
17	M	406	PGV	O03-C19-C20	2.36	119.32	111.91
13	L	311	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
20	T	101	CRT	C13-C12-C11	2.36	121.80	118.08
13	I	101	BCL	CMD-C2D-C3D	-2.36	122.18	127.61
20	Y	101	CRT	C29-C28-C30	2.36	121.79	118.08
8	C	402	HEC	C1D-ND-C4D	2.36	107.51	105.07
13	6	102	BCL	C2A-C1A-CHA	-2.36	119.74	123.86
13	L	311	BCL	CHB-C4A-NA	2.36	127.77	124.51
13	6	102	BCL	C1D-CHD-C4C	-2.35	120.94	126.62
16	T	104	LMT	C1B-O1B-C4'	-2.35	112.14	117.96
13	Y	102	BCL	C2A-C1A-CHA	-2.35	119.75	123.86
13	4	102	BCL	C2A-C1A-CHA	-2.35	119.75	123.86
20	N	101	CRT	C27-C26-C25	-2.35	115.88	123.22
20	2	102	CRT	C8-C7-C9	-2.35	119.63	122.92
13	B	102	BCL	O2D-CGD-O1D	-2.35	119.25	123.84
13	R	102	BCL	CMB-C2B-C3B	2.35	132.26	125.93
13	L	311	BCL	C4B-C3B-C2B	-2.34	104.59	108.36
13	3	101	BCL	O2D-CGD-O1D	-2.34	119.25	123.84
13	F	101	BCL	C2A-C1A-CHA	-2.34	119.76	123.86
13	V	102	BCL	O2A-CGA-CBA	2.34	119.26	111.91
17	N	103	PGV	C02-O01-C1	-2.34	112.02	117.79
13	G	102	BCL	O2D-CGD-O1D	-2.34	119.26	123.84
13	9	101	BCL	O2D-CGD-O1D	-2.34	119.27	123.84
17	V	103	PGV	O03-C19-C20	2.34	119.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R	101	CRT	C15-C14-C12	-2.34	123.97	127.31
17	X	102	PGV	O03-C19-C20	2.34	119.24	111.91
20	P	101	CRT	C26-C27-C28	-2.34	123.97	127.31
13	N	102	BCL	O2D-CGD-O1D	-2.34	119.27	123.84
13	I	101	BCL	CHB-C4A-NA	2.33	127.74	124.51
13	K	101	BCL	O2D-CGD-O1D	-2.33	119.28	123.84
8	C	402	HEC	O2D-CGD-CBD	2.33	121.52	114.03
20	G	101	CRT	C26-C27-C28	-2.33	123.98	127.31
13	E	102	BCL	O2D-CGD-O1D	-2.33	119.28	123.84
13	O	101	BCL	C2A-C1A-CHA	-2.33	119.79	123.86
13	M	402	BCL	C4-C3-C5	2.33	119.19	115.27
20	M	405	CRT	C32-C31-C30	-2.33	115.96	123.22
13	L	310	BCL	CHB-C4A-NA	2.33	127.73	124.51
20	N	101	CRT	C26-C27-C28	-2.32	124.00	127.31
20	8	102	CRT	C27-C26-C25	-2.32	115.97	123.22
13	5	402	BCL	O2D-CGD-O1D	-2.32	119.30	123.84
13	Q	101	BCL	O2D-CGD-O1D	-2.32	119.30	123.84
13	J	102	BCL	O2D-CGD-O1D	-2.32	119.31	123.84
7	C	401	HEM	CBD-CAD-C3D	-2.32	106.19	112.63
16	D	103	LMT	O1B-C4'-C3'	2.32	113.45	107.28
20	P	101	CRT	C27-C26-C25	-2.32	115.98	123.22
13	G	102	BCL	CHC-C4B-C3B	-2.32	124.11	132.35
13	0	102	BCL	O2D-CGD-O1D	-2.32	119.31	123.84
20	V	101	CRT	C29-C28-C30	2.32	121.72	118.08
20	E	101	CRT	C13-C12-C11	2.31	121.72	118.08
16	X	103	LMT	O1B-C1B-O5B	2.31	117.14	110.67
20	E	101	CRT	C27-C26-C25	-2.31	116.00	123.22
20	V	101	CRT	C6-C7-C9	2.31	122.49	118.94
20	R	101	CRT	C26-C27-C28	-2.31	124.01	127.31
20	T	101	CRT	C27-C26-C25	-2.31	116.01	123.22
13	L	311	BCL	C2A-C1A-CHA	-2.31	119.82	123.86
20	J	101	CRT	C27-C26-C25	-2.31	116.02	123.22
13	W	101	BCL	CHC-C1C-NC	2.31	127.70	124.51
13	F	101	BCL	O2D-CGD-O1D	-2.30	119.33	123.84
20	8	102	CRT	C29-C28-C30	2.30	121.71	118.08
13	2	103	BCL	CHC-C4B-C3B	-2.30	124.16	132.35
13	5	402	BCL	C1D-CHD-C4C	-2.30	121.07	126.62
13	W	101	BCL	O2D-CGD-O1D	-2.30	119.34	123.84
20	G	101	CRT	C13-C12-C11	2.30	121.70	118.08
13	U	102	BCL	C1D-CHD-C4C	-2.30	121.07	126.62
20	6	101	CRT	C10-C11-C12	-2.30	119.96	126.42
13	B	102	BCL	CHC-C4B-C3B	-2.30	124.17	132.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	402	HEC	CBB-CAB-C3B	2.30	118.77	112.43
13	Z	102	BCL	CHC-C4B-C3B	-2.30	124.17	132.35
13	I	101	BCL	O2D-CGD-O1D	-2.30	119.35	123.84
13	E	102	BCL	C1D-CHD-C4C	-2.30	121.08	126.62
20	Y	101	CRT	C9-C10-C11	-2.30	116.05	123.22
13	R	102	BCL	O2D-CGD-O1D	-2.30	119.35	123.84
13	D	102	BCL	O2D-CGD-O1D	-2.29	119.35	123.84
13	S	101	BCL	C4-C3-C5	2.29	119.13	115.27
20	R	101	CRT	C27-C26-C25	-2.29	116.06	123.22
13	R	102	BCL	CHC-C4B-C3B	-2.29	124.19	132.35
13	J	102	BCL	CHC-C4B-C3B	-2.29	124.19	132.35
13	B	102	BCL	C1D-CHD-C4C	-2.29	121.09	126.62
13	2	103	BCL	C1D-CHD-C4C	-2.29	121.09	126.62
13	L	302	BCL	CED-O2D-CGD	2.29	121.12	115.94
13	X	101	BCL	CHC-C4B-C3B	-2.29	124.21	132.35
20	P	101	CRT	C29-C28-C30	2.29	121.68	118.08
13	4	102	BCL	C4-C3-C5	2.29	119.12	115.27
13	3	101	BCL	CHB-C4A-NA	2.29	127.67	124.51
13	T	102	BCL	CHC-C4B-C3B	-2.28	124.22	132.35
20	M	405	CRT	C15-C14-C12	-2.28	124.05	127.31
13	N	102	BCL	C1D-CHD-C4C	-2.28	121.11	126.62
8	C	403	HEC	CHB-C4A-NA	2.28	126.91	124.44
13	V	102	BCL	CHC-C4B-C3B	-2.28	124.23	132.35
13	U	102	BCL	O2D-CGD-O1D	-2.28	119.38	123.84
20	P	101	CRT	C13-C12-C11	2.28	121.67	118.08
13	I	101	BCL	CAC-C3C-C4C	-2.28	107.52	112.58
13	G	102	BCL	C1D-CHD-C4C	-2.28	121.12	126.62
13	V	102	BCL	C1D-CHD-C4C	-2.28	121.12	126.62
13	N	102	BCL	O2A-CGA-CBA	2.28	119.05	111.91
13	S	101	BCL	C1D-CHD-C4C	-2.28	121.13	126.62
13	E	102	BCL	C2A-C1A-CHA	-2.28	119.88	123.86
20	R	101	CRT	C21-C20-C19	-2.28	118.81	123.47
13	0	102	BCL	CHC-C4B-C3B	-2.28	124.25	132.35
13	2	103	BCL	O2D-CGD-O1D	-2.28	119.39	123.84
20	Z	101	CRT	C27-C26-C25	-2.28	116.12	123.22
13	N	102	BCL	C2A-C1A-CHA	-2.27	119.88	123.86
13	S	101	BCL	C2A-C1A-CHA	-2.27	119.88	123.86
13	J	102	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
13	1	101	BCL	CHC-C1C-NC	2.27	127.66	124.51
13	B	102	BCL	C4-C3-C5	2.27	119.09	115.27
13	J	102	BCL	C1C-NC-C4C	-2.27	105.69	106.71
13	P	102	BCL	C1D-CHD-C4C	-2.27	121.14	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	311	BCL	CMB-C2B-C3B	2.27	132.06	125.93
20	Z	101	CRT	C13-C12-C11	2.27	121.65	118.08
13	L	302	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
20	T	101	CRT	C29-C28-C30	2.26	121.64	118.08
13	X	101	BCL	C1D-CHD-C4C	-2.26	121.16	126.62
13	Z	102	BCL	O2D-CGD-O1D	-2.26	119.41	123.84
13	K	101	BCL	C2A-C1A-CHA	-2.26	119.90	123.86
13	Y	102	BCL	O2D-CGD-O1D	-2.26	119.42	123.84
13	0	102	BCL	C1D-CHD-C4C	-2.26	121.17	126.62
13	L	302	BCL	C4D-CHA-C1A	-2.26	118.50	121.25
13	8	103	BCL	C1D-CHD-C4C	-2.26	121.17	126.62
13	X	101	BCL	O2D-CGD-O1D	-2.26	119.42	123.84
13	1	101	BCL	C2A-C1A-CHA	-2.26	119.91	123.86
13	A	102	BCL	C1D-CHD-C4C	-2.26	121.17	126.62
7	C	401	HEM	CHD-C4C-NC	2.26	126.88	124.44
13	4	102	BCL	O2D-CGD-O1D	-2.26	119.42	123.84
13	X	101	BCL	C1C-NC-C4C	-2.26	105.69	106.71
13	T	102	BCL	C1D-CHD-C4C	-2.25	121.18	126.62
20	V	101	CRT	C14-C15-C16	-2.25	116.18	123.22
13	7	102	BCL	C1D-CHD-C4C	-2.25	121.19	126.62
13	6	102	BCL	O2D-CGD-O1D	-2.25	119.43	123.84
13	V	102	BCL	O2D-CGD-O1D	-2.25	119.43	123.84
13	I	101	BCL	C1D-CHD-C4C	-2.25	121.19	126.62
20	G	101	CRT	C27-C26-C25	-2.25	116.20	123.22
20	N	101	CRT	C29-C28-C30	2.25	121.62	118.08
20	V	101	CRT	C27-C26-C25	-2.24	116.21	123.22
13	7	102	BCL	O2D-CGD-O1D	-2.24	119.46	123.84
13	P	102	BCL	CHC-C4B-C3B	-2.24	124.38	132.35
13	M	402	BCL	O2D-CGD-O1D	-2.24	119.46	123.84
13	1	101	BCL	O2D-CGD-O1D	-2.24	119.46	123.84
8	C	402	HEC	CHB-C4A-NA	2.24	126.86	124.44
13	P	102	BCL	O2A-CGA-CBA	2.23	118.92	111.91
20	B	101	CRT	C26-C27-C28	-2.23	124.13	127.31
13	8	103	BCL	CHC-C4B-C3B	-2.23	124.42	132.35
16	Z	103	LMT	O1B-C4'-C5'	2.23	115.55	109.45
20	E	101	CRT	C29-C28-C30	2.23	121.59	118.08
20	G	101	CRT	C29-C28-C30	2.22	121.58	118.08
13	E	102	BCL	CHC-C4B-C3B	-2.22	124.44	132.35
20	2	102	CRT	C15-C14-C12	-2.22	124.14	127.31
17	2	104	PGV	O03-C19-C20	2.22	118.88	111.91
13	F	101	BCL	C1-C2-C3	-2.22	122.20	126.04
13	L	311	BCL	C1D-CHD-C4C	-2.22	121.26	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	311	BCL	CHC-C1C-NC	2.22	127.58	124.51
17	M	408	PGV	O14-P-O13	2.22	119.37	110.68
20	R	101	CRT	C34-C33-C35	2.22	121.57	118.08
20	T	101	CRT	C9-C10-C11	-2.22	116.30	123.22
8	C	404	HEC	CHD-C1D-C2D	-2.22	120.57	126.73
13	T	102	BCL	C1C-NC-C4C	-2.22	105.71	106.71
13	U	102	BCL	CHC-C1C-NC	2.21	127.57	124.51
13	2	103	BCL	C1C-NC-C4C	-2.21	105.71	106.71
13	R	102	BCL	C1D-CHD-C4C	-2.21	121.28	126.62
16	7	103	LMT	C1-O1'-C1'	-2.21	110.17	113.84
20	B	101	CRT	C13-C12-C11	2.21	121.56	118.08
13	4	102	BCL	CHC-C4B-C3B	-2.21	124.49	132.35
20	V	101	CRT	C26-C27-C28	-2.21	124.16	127.31
13	5	402	BCL	CAC-C3C-C4C	-2.21	107.69	112.58
13	7	102	BCL	C2A-C1A-CHA	-2.21	120.00	123.86
13	L	310	BCL	CHC-C4B-C3B	-2.21	124.50	132.35
20	R	101	CRT	C14-C15-C16	-2.20	116.34	123.22
13	9	101	BCL	C2A-C1A-CHA	-2.20	120.01	123.86
13	L	310	BCL	CMD-C2D-C3D	-2.20	122.55	127.61
13	W	101	BCL	CAC-C3C-C4C	-2.20	107.69	112.58
20	M	405	CRT	C36-C35-C33	-2.20	122.56	125.89
17	P	103	PGV	O03-C19-C20	2.20	118.82	111.91
13	5	402	BCL	C2A-C1A-CHA	-2.20	120.01	123.86
20	B	101	CRT	C18-C17-C16	2.20	121.54	118.08
13	D	102	BCL	C2A-C1A-CHA	-2.20	120.02	123.86
20	6	101	CRT	C29-C28-C30	2.20	121.54	118.08
8	C	403	HEC	CHB-C1B-C2B	-2.19	121.55	124.98
7	C	401	HEM	CHA-C4D-C3D	-2.19	121.21	125.33
13	I	101	BCL	C2A-C1A-CHA	-2.19	120.03	123.86
20	Z	101	CRT	C29-C28-C30	2.19	121.53	118.08
13	J	102	BCL	O2A-CGA-CBA	2.19	118.78	111.91
13	7	102	BCL	CHC-C1C-NC	2.19	127.54	124.51
16	L	305	LMT	O5B-C1B-C2B	2.19	114.98	110.35
20	B	101	CRT	C8-C7-C9	-2.18	119.86	122.92
13	L	302	BCL	O2D-CGD-O1D	-2.18	119.57	123.84
8	C	403	HEC	C3B-C4B-NB	-2.18	107.74	110.17
13	6	102	BCL	CHC-C4B-C3B	-2.18	124.59	132.35
17	E	103	PGV	O03-C19-C20	2.18	118.75	111.91
13	8	103	BCL	O2D-CGD-O1D	-2.18	119.58	123.84
20	P	101	CRT	C15-C14-C12	-2.18	124.20	127.31
20	N	101	CRT	C9-C10-C11	-2.18	116.43	123.22
20	T	101	CRT	C26-C27-C28	-2.17	124.21	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	101	BCL	CHC-C4B-C3B	-2.17	124.62	132.35
13	L	302	BCL	CHC-C4B-C3B	-2.17	124.62	132.35
13	N	102	BCL	CHC-C4B-C3B	-2.17	124.62	132.35
13	9	101	BCL	CHC-C1C-NC	2.17	127.51	124.51
13	Q	101	BCL	C2A-C1A-CHA	-2.17	120.07	123.86
20	0	101	CRT	C9-C10-C11	-2.17	116.45	123.22
8	C	403	HEC	C3C-C4C-NC	-2.16	107.73	110.15
19	M	404	A1L8Q	C4-C10-C29	2.16	118.97	111.88
13	T	102	BCL	O2A-CGA-CBA	2.16	118.67	111.91
20	R	101	CRT	C8-C7-C9	-2.16	119.90	122.92
13	F	101	BCL	CHC-C4B-C3B	-2.15	124.68	132.35
20	E	101	CRT	C15-C14-C12	-2.15	124.24	127.31
20	0	101	CRT	C13-C12-C11	2.15	121.47	118.08
17	L	307	PGV	C02-O01-C1	-2.15	112.51	117.79
13	R	102	BCL	O2A-CGA-CBA	2.14	118.64	111.91
13	7	102	BCL	CHC-C4B-C3B	-2.14	124.72	132.35
13	I	101	BCL	CHC-C4B-C3B	-2.14	124.73	132.35
7	C	401	HEM	C1A-CHA-C4D	-2.14	121.27	126.34
13	A	102	BCL	CHC-C4B-C3B	-2.13	124.76	132.35
13	Z	102	BCL	C6-C5-C3	-2.13	107.87	113.45
20	V	101	CRT	C15-C14-C12	-2.13	124.27	127.31
13	5	402	BCL	CHC-C1C-NC	2.13	127.45	124.51
8	C	402	HEC	C3C-C4C-NC	-2.13	107.77	110.15
13	M	402	BCL	CHC-C4B-C3B	-2.12	124.80	132.35
13	6	102	BCL	CMD-C2D-C3D	-2.12	122.73	127.61
13	3	101	BCL	C2A-C1A-CHA	-2.12	120.15	123.86
20	2	102	CRT	C13-C12-C11	2.12	121.42	118.08
13	6	102	BCL	C1C-NC-C4C	-2.12	105.75	106.71
13	K	101	BCL	CHC-C4B-C3B	-2.12	124.81	132.35
13	Y	102	BCL	C1D-CHD-C4C	-2.12	121.51	126.62
13	U	102	BCL	C2A-C1A-CHA	-2.12	120.16	123.86
17	H	404	PGV	C02-O01-C1	-2.12	112.58	117.79
13	O	101	BCL	C1C-NC-C4C	-2.12	105.75	106.71
17	M	408	PGV	C03-C02-C01	-2.11	106.80	111.79
17	B	103	PGV	O03-C19-C20	2.11	118.53	111.91
7	C	401	HEM	C4C-CHD-C1D	-2.11	121.51	126.06
16	7	103	LMT	O1'-C1'-C2'	2.10	111.58	108.30
13	Q	101	BCL	CHC-C4B-C3B	-2.09	124.90	132.35
7	C	401	HEM	CHA-C1A-NA	2.09	127.69	123.85
13	D	102	BCL	CHC-C4B-C3B	-2.09	124.92	132.35
13	1	101	BCL	CHC-C4B-C3B	-2.09	124.92	132.35
13	7	102	BCL	CAC-C3C-C4C	-2.09	107.95	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	101	BCL	CHC-C4B-C3B	-2.08	124.94	132.35
20	2	102	CRT	C26-C27-C28	-2.08	124.34	127.31
13	3	101	BCL	CHD-C1D-C2D	2.08	129.84	125.48
20	G	101	CRT	C9-C10-C11	-2.08	116.74	123.22
13	S	101	BCL	O2D-CGD-O1D	-2.07	119.79	123.84
13	A	102	BCL	C2A-C1A-CHA	-2.07	120.24	123.86
13	F	101	BCL	CED-O2D-CGD	2.07	120.61	115.94
13	7	102	BCL	CMB-C2B-C3B	2.06	131.51	125.93
20	6	101	CRT	C27-C26-C25	-2.06	116.78	123.22
20	Z	101	CRT	C26-C27-C28	-2.06	124.37	127.31
13	9	101	BCL	CHC-C4B-C3B	-2.06	125.02	132.35
13	M	402	BCL	C1C-NC-C4C	-2.06	105.78	106.71
20	0	101	CRT	C29-C28-C30	2.06	121.32	118.08
20	J	101	CRT	C20-C21-C22	-2.06	119.26	123.47
13	L	311	BCL	CHD-C1D-C2D	2.05	129.79	125.48
13	O	101	BCL	C1D-CHD-C4C	-2.05	121.67	126.62
8	C	402	HEC	CHD-C1D-C2D	-2.05	121.03	126.73
20	4	101	CRT	C18-C17-C16	2.05	121.31	118.08
13	D	102	BCL	C1D-CHD-C4C	-2.05	121.68	126.62
17	B	103	PGV	O01-C1-O02	-2.05	118.75	123.70
13	W	101	BCL	C2A-C1A-CHA	-2.05	120.28	123.86
20	B	101	CRT	C15-C14-C12	-2.05	124.39	127.31
13	8	103	BCL	O2A-CGA-CBA	2.05	118.33	111.91
20	R	101	CRT	C29-C28-C30	2.04	121.30	118.08
13	Y	102	BCL	CHC-C4B-C3B	-2.04	125.08	132.35
20	J	101	CRT	C11-C12-C14	-2.04	115.80	118.94
13	0	102	BCL	C1C-NC-C4C	-2.04	105.79	106.71
13	W	101	BCL	CHC-C4B-C3B	-2.04	125.10	132.35
13	K	101	BCL	C1D-CHD-C4C	-2.04	121.71	126.62
13	9	101	BCL	C1D-CHD-C4C	-2.04	121.71	126.62
8	C	404	HEC	CAD-C3D-C4D	2.04	128.22	124.66
13	U	102	BCL	CHC-C4B-C3B	-2.04	125.11	132.35
13	8	103	BCL	C1C-NC-C4C	-2.03	105.79	106.71
20	8	102	CRT	C10-C11-C12	-2.03	120.71	126.42
13	7	102	BCL	C1C-NC-C4C	-2.03	105.79	106.71
13	L	310	BCL	C1C-NC-C4C	-2.03	105.80	106.71
17	P	103	PGV	O01-C1-O02	-2.02	118.81	123.70
20	Y	101	CRT	C18-C17-C16	2.02	121.27	118.08
13	P	102	BCL	CMD-C2D-C3D	-2.02	122.96	127.61
8	C	403	HEC	C4A-CHB-C1B	-2.02	121.69	126.06
20	J	101	CRT	C18-C17-C16	2.02	121.26	118.08
13	T	102	BCL	CMD-C2D-C3D	-2.02	122.97	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	101	BCL	C1D-CHD-C4C	-2.02	121.76	126.62
13	5	402	BCL	CHC-C4B-C3B	-2.01	125.19	132.35
13	8	103	BCL	CMD-C2D-C3D	-2.01	122.98	127.61
20	P	101	CRT	C18-C17-C16	2.01	121.25	118.08
7	C	401	HEM	C4D-ND-C1D	2.01	107.15	105.07
13	S	101	BCL	C6-C5-C3	-2.01	108.18	113.45
8	C	404	HEC	C4C-CHD-C1D	-2.01	121.57	126.34
13	S	101	BCL	CED-O2D-CGD	2.01	120.49	115.94
13	L	302	BCL	CHB-C1B-C2B	-2.01	121.56	127.24
13	D	102	BCL	CED-O2D-CGD	2.01	120.48	115.94
13	U	102	BCL	CED-O2D-CGD	2.00	120.47	115.94
20	G	101	CRT	C8-C7-C9	-2.00	120.12	122.92

All (3) chirality outliers are listed below:

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

All (1167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	405	Z41	C15-C16-O2-C17
9	C	405	Z41	O1-C16-O2-C17
9	C	405	Z41	O2-C17-C18-O3
9	C	405	Z41	O2-C17-C18-C35
13	L	302	BCL	CBD-CGD-O2D-CED
13	A	102	BCL	C1A-C2A-CAA-CBA
13	B	102	BCL	C1A-C2A-CAA-CBA
13	B	102	BCL	C3A-C2A-CAA-CBA
13	B	102	BCL	C2C-C3C-CAC-CBC
13	B	102	BCL	C4C-C3C-CAC-CBC
13	D	102	BCL	C2C-C3C-CAC-CBC
13	D	102	BCL	C4C-C3C-CAC-CBC
13	E	102	BCL	C1A-C2A-CAA-CBA
13	E	102	BCL	C2C-C3C-CAC-CBC
13	E	102	BCL	C4C-C3C-CAC-CBC
13	F	101	BCL	C2C-C3C-CAC-CBC
13	F	101	BCL	C4C-C3C-CAC-CBC
13	G	102	BCL	C3A-C2A-CAA-CBA
13	G	102	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
13	G	102	BCL	C4C-C3C-CAC-CBC
13	J	102	BCL	C3A-C2A-CAA-CBA
13	J	102	BCL	C2C-C3C-CAC-CBC
13	J	102	BCL	C4C-C3C-CAC-CBC
13	K	101	BCL	C2C-C3C-CAC-CBC
13	K	101	BCL	C4C-C3C-CAC-CBC
13	N	102	BCL	C3A-C2A-CAA-CBA
13	N	102	BCL	C2C-C3C-CAC-CBC
13	N	102	BCL	C4C-C3C-CAC-CBC
13	O	101	BCL	C2C-C3C-CAC-CBC
13	O	101	BCL	C4C-C3C-CAC-CBC
13	P	102	BCL	C3A-C2A-CAA-CBA
13	P	102	BCL	C2C-C3C-CAC-CBC
13	P	102	BCL	C4C-C3C-CAC-CBC
13	Q	101	BCL	C2C-C3C-CAC-CBC
13	Q	101	BCL	C4C-C3C-CAC-CBC
13	R	102	BCL	C3A-C2A-CAA-CBA
13	R	102	BCL	C2C-C3C-CAC-CBC
13	R	102	BCL	C4C-C3C-CAC-CBC
13	S	101	BCL	C1A-C2A-CAA-CBA
13	S	101	BCL	C3A-C2A-CAA-CBA
13	T	102	BCL	C3A-C2A-CAA-CBA
13	T	102	BCL	C2C-C3C-CAC-CBC
13	T	102	BCL	C4C-C3C-CAC-CBC
13	V	102	BCL	C1A-C2A-CAA-CBA
13	V	102	BCL	C3A-C2A-CAA-CBA
13	V	102	BCL	C2C-C3C-CAC-CBC
13	V	102	BCL	C4C-C3C-CAC-CBC
13	W	101	BCL	C1A-C2A-CAA-CBA
13	X	101	BCL	C3A-C2A-CAA-CBA
13	X	101	BCL	C4C-C3C-CAC-CBC
13	X	101	BCL	C2-C3-C5-C6
13	X	101	BCL	C4-C3-C5-C6
13	Y	102	BCL	C2C-C3C-CAC-CBC
13	Y	102	BCL	C4C-C3C-CAC-CBC
13	Z	102	BCL	C3A-C2A-CAA-CBA
13	Z	102	BCL	C2C-C3C-CAC-CBC
13	Z	102	BCL	C4C-C3C-CAC-CBC
13	1	101	BCL	C2C-C3C-CAC-CBC
13	1	101	BCL	C4C-C3C-CAC-CBC
13	2	103	BCL	C1A-C2A-CAA-CBA
13	2	103	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	2	103	BCL	C2C-C3C-CAC-CBC
13	2	103	BCL	C4C-C3C-CAC-CBC
13	3	101	BCL	C1A-C2A-CAA-CBA
13	4	102	BCL	C3A-C2A-CAA-CBA
13	4	102	BCL	C2C-C3C-CAC-CBC
13	4	102	BCL	C4C-C3C-CAC-CBC
13	6	102	BCL	C3A-C2A-CAA-CBA
13	6	102	BCL	C2C-C3C-CAC-CBC
13	6	102	BCL	C4C-C3C-CAC-CBC
13	6	102	BCL	C11-C10-C8-C9
13	8	103	BCL	C1A-C2A-CAA-CBA
13	8	103	BCL	C3A-C2A-CAA-CBA
13	8	103	BCL	C2C-C3C-CAC-CBC
13	8	103	BCL	C4C-C3C-CAC-CBC
13	9	101	BCL	C1A-C2A-CAA-CBA
13	9	101	BCL	C3A-C2A-CAA-CBA
13	9	101	BCL	C2C-C3C-CAC-CBC
13	9	101	BCL	C4C-C3C-CAC-CBC
13	0	102	BCL	C1A-C2A-CAA-CBA
13	0	102	BCL	C3A-C2A-CAA-CBA
13	0	102	BCL	C2C-C3C-CAC-CBC
13	0	102	BCL	C4C-C3C-CAC-CBC
15	D	104	U10	C1-C6-C7-C8
15	D	104	U10	C5-C6-C7-C8
15	7	101	U10	C32-C33-C34-C35
15	7	101	U10	C32-C33-C34-C36
16	H	402	LMT	O5'-C1'-O1'-C1
16	B	104	LMT	C2-C1-O1'-C1'
16	D	103	LMT	C2'-C1'-O1'-C1
16	D	103	LMT	O5'-C1'-O1'-C1
16	O	102	LMT	C2'-C1'-O1'-C1
16	O	102	LMT	O5'-C1'-O1'-C1
16	V	104	LMT	O5'-C1'-O1'-C1
16	X	103	LMT	O5'-C1'-O1'-C1
16	Z	103	LMT	O5B-C1B-O1B-C4'
16	4	104	LMT	O5'-C1'-O1'-C1
17	L	307	PGV	C03-O11-P-O12
17	L	307	PGV	C03-O11-P-O13
17	L	307	PGV	C03-O11-P-O14
17	M	406	PGV	C03-O11-P-O12
17	M	406	PGV	C03-O11-P-O13
17	M	406	PGV	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
17	M	406	PGV	C04-O12-P-O13
17	M	406	PGV	C04-O12-P-O14
17	M	407	PGV	C03-O11-P-O13
17	M	407	PGV	C03-O11-P-O14
17	M	407	PGV	C04-O12-P-O13
17	M	408	PGV	C2-C1-O01-C02
17	M	410	PGV	C01-C02-O01-C1
17	M	410	PGV	C03-C02-O01-C1
17	M	410	PGV	O02-C1-O01-C02
17	H	401	PGV	C04-O12-P-O11
17	H	401	PGV	C04-O12-P-O13
17	H	401	PGV	C04-O12-P-O14
17	H	403	PGV	C03-O11-P-O14
17	H	403	PGV	O12-C04-C05-C06
17	H	403	PGV	O12-C04-C05-O05
17	H	404	PGV	C03-O11-P-O12
17	H	404	PGV	C03-O11-P-O13
17	H	404	PGV	C04-O12-P-O13
17	H	404	PGV	O03-C01-C02-O01
17	A	101	PGV	C04-O12-P-O13
17	A	101	PGV	C04-O12-P-O14
17	B	103	PGV	C03-O11-P-O14
17	D	101	PGV	C04-O12-P-O11
17	E	103	PGV	C03-O11-P-O12
17	G	103	PGV	C04-O12-P-O11
17	G	103	PGV	C04-O12-P-O13
17	K	102	PGV	C03-O11-P-O13
17	K	102	PGV	C03-O11-P-O14
17	K	102	PGV	C04-O12-P-O11
17	K	102	PGV	O12-C04-C05-O05
17	N	103	PGV	C11-C12-C13-C14
17	P	103	PGV	C03-O11-P-O14
17	P	103	PGV	C04-O12-P-O13
17	R	103	PGV	C03-O11-P-O12
17	V	103	PGV	C03-O11-P-O12
17	V	103	PGV	C03-O11-P-O13
17	V	103	PGV	C11-C12-C13-C14
17	2	101	PGV	C04-O12-P-O13
17	2	104	PGV	C03-O11-P-O12
17	2	104	PGV	C03-O11-P-O13
17	2	104	PGV	C03-O11-P-O14
17	2	104	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
17	8	101	PGV	C03-O11-P-O13
17	8	101	PGV	C04-O12-P-O14
17	8	101	PGV	O03-C01-C02-O01
17	8	104	PGV	C04-O12-P-O13
20	M	405	CRT	C3-C1-O1-C1M
20	M	405	CRT	C3-C1-C4-C5
20	B	101	CRT	C5-C6-C7-C8
20	B	101	CRT	C5-C6-C7-C9
20	E	101	CRT	C15-C16-C17-C18
20	G	101	CRT	O1-C1-C4-C5
20	G	101	CRT	C2-C1-C4-C5
20	G	101	CRT	C3-C1-C4-C5
20	R	101	CRT	C2-C1-C4-C5
20	R	101	CRT	C3-C1-C4-C5
20	T	101	CRT	C15-C16-C17-C18
20	V	101	CRT	O1-C1-C4-C5
20	V	101	CRT	C2-C1-C4-C5
20	V	101	CRT	C3-C1-C4-C5
20	Z	101	CRT	O1-C1-C4-C5
20	Z	101	CRT	C2-C1-C4-C5
20	Z	101	CRT	C3-C1-C4-C5
20	2	102	CRT	C2-C1-C4-C5
20	2	102	CRT	C3-C1-C4-C5
20	6	101	CRT	C1-C4-C5-C6
20	6	101	CRT	C5-C6-C7-C8
20	6	101	CRT	C5-C6-C7-C9
20	6	101	CRT	C15-C16-C17-C18
20	8	102	CRT	C10-C11-C12-C13
20	8	102	CRT	C10-C11-C12-C14
20	8	102	CRT	C36-C37-C38-C39
20	0	101	CRT	C5-C6-C7-C8
16	K	103	LMT	O5B-C1B-O1B-C4'
16	K	103	LMT	C2B-C1B-O1B-C4'
16	B	104	LMT	O5B-C1B-O1B-C4'
16	D	103	LMT	O5B-C1B-O1B-C4'
16	X	103	LMT	O5B-C1B-O1B-C4'
16	7	103	LMT	O5B-C1B-O1B-C4'
13	M	402	BCL	CBD-CGD-O2D-CED
13	0	102	BCL	O1A-CGA-O2A-C1
17	H	401	PGV	O04-C19-O03-C01
16	X	103	LMT	C5'-C4'-O1B-C1B
13	L	302	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	L	306	PGV	O02-C1-O01-C02
13	B	102	BCL	C3-C5-C6-C7
13	6	102	BCL	C3-C5-C6-C7
13	0	102	BCL	CBA-CGA-O2A-C1
13	8	103	BCL	C4-C3-C5-C6
13	L	302	BCL	C3-C5-C6-C7
13	2	103	BCL	CBA-CGA-O2A-C1
17	H	401	PGV	C20-C19-O03-C01
17	M	408	PGV	O02-C1-O01-C02
17	B	103	PGV	O12-C04-C05-O05
17	G	103	PGV	O12-C04-C05-O05
13	J	102	BCL	C3-C5-C6-C7
13	J	102	BCL	CBA-CGA-O2A-C1
13	P	102	BCL	CBA-CGA-O2A-C1
13	R	102	BCL	CBA-CGA-O2A-C1
13	V	102	BCL	CBA-CGA-O2A-C1
13	J	102	BCL	O1A-CGA-O2A-C1
17	L	306	PGV	C2-C1-O01-C02
13	F	101	BCL	C8-C10-C11-C12
13	M	402	BCL	C5-C6-C7-C8
13	P	102	BCL	O1A-CGA-O2A-C1
13	V	102	BCL	O1A-CGA-O2A-C1
13	2	103	BCL	O1A-CGA-O2A-C1
14	M	403	BPH	C4-C3-C5-C6
15	L	304	U10	C15-C14-C16-C17
15	D	104	U10	C35-C34-C36-C37
15	1	102	U10	C12-C11-C9-C10
15	7	101	U10	C25-C24-C26-C27
19	M	404	A1L8Q	C41-C13-C2-C8
19	M	404	A1L8Q	C57-C48-C49-C54
14	M	403	BPH	C2-C3-C5-C6
15	L	304	U10	C13-C14-C16-C17
15	D	104	U10	C33-C34-C36-C37
15	1	102	U10	C12-C11-C9-C8
15	7	101	U10	C23-C24-C26-C27
19	M	404	A1L8Q	C24-C13-C2-C8
19	M	404	A1L8Q	C47-C48-C49-C54
13	V	102	BCL	C2A-CAA-CBA-CGA
16	L	305	LMT	O5'-C5'-C6'-O6'
13	R	102	BCL	O1A-CGA-O2A-C1
15	L	304	U10	C19-C21-C22-C23
15	L	309	U10	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	1	102	U10	C24-C26-C27-C28
15	7	101	U10	C29-C31-C32-C33
13	B	102	BCL	CBA-CGA-O2A-C1
17	H	403	PGV	C20-C19-O03-C01
15	L	304	U10	C7-C8-C9-C10
13	W	101	BCL	C5-C6-C7-C8
17	G	103	PGV	O12-C04-C05-C06
15	L	304	U10	C7-C8-C9-C11
13	I	101	BCL	C3-C5-C6-C7
13	M	402	BCL	O1D-CGD-O2D-CED
13	G	102	BCL	CBA-CGA-O2A-C1
13	N	102	BCL	CBA-CGA-O2A-C1
13	X	101	BCL	CBA-CGA-O2A-C1
13	Z	102	BCL	CBA-CGA-O2A-C1
13	E	102	BCL	C13-C15-C16-C17
17	B	103	PGV	O01-C02-C03-O11
13	7	102	BCL	C5-C6-C7-C8
17	A	101	PGV	O12-C04-C05-O05
13	X	101	BCL	O1A-CGA-O2A-C1
17	H	403	PGV	O04-C19-O03-C01
13	8	103	BCL	C2-C3-C5-C6
13	L	310	BCL	C11-C10-C8-C9
13	L	311	BCL	C11-C10-C8-C9
13	M	402	BCL	C11-C10-C8-C9
13	E	102	BCL	C14-C13-C15-C16
13	J	102	BCL	C11-C10-C8-C9
13	N	102	BCL	C6-C7-C8-C9
13	O	101	BCL	C6-C7-C8-C9
13	P	102	BCL	C6-C7-C8-C9
13	R	102	BCL	C11-C10-C8-C9
13	S	101	BCL	C11-C10-C8-C9
13	V	102	BCL	C11-C10-C8-C9
13	Z	102	BCL	C11-C10-C8-C9
13	2	103	BCL	C6-C7-C8-C9
13	4	102	BCL	C11-C10-C8-C9
13	9	101	BCL	C11-C12-C13-C14
14	M	403	BPH	C11-C10-C8-C9
13	B	102	BCL	C8-C10-C11-C12
13	J	102	BCL	C13-C15-C16-C17
13	B	102	BCL	C2A-CAA-CBA-CGA
20	G	101	CRT	C15-C16-C17-C18
20	2	102	CRT	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	8	102	CRT	C34-C33-C35-C36
20	8	102	CRT	C32-C33-C35-C36
17	R	103	PGV	C2-C1-O01-C02
16	L	305	LMT	C4'-C5'-C6'-O6'
13	G	102	BCL	O1A-CGA-O2A-C1
13	N	102	BCL	O1A-CGA-O2A-C1
13	A	102	BCL	C13-C15-C16-C17
13	2	103	BCL	C10-C11-C12-C13
13	O	101	BCL	C3-C5-C6-C7
13	4	102	BCL	CBA-CGA-O2A-C1
13	K	101	BCL	C5-C6-C7-C8
13	3	101	BCL	C15-C16-C17-C18
13	9	101	BCL	C13-C15-C16-C17
17	L	307	PGV	C19-C20-C21-C22
13	X	101	BCL	C8-C10-C11-C12
13	5	402	BCL	C15-C16-C17-C18
13	Y	102	BCL	C15-C16-C17-C18
13	2	103	BCL	C13-C15-C16-C17
13	8	103	BCL	CBA-CGA-O2A-C1
15	D	104	U10	C22-C23-C24-C26
13	D	102	BCL	C8-C10-C11-C12
13	1	101	BCL	C5-C6-C7-C8
15	D	104	U10	C36-C37-C38-C39
13	G	102	BCL	C11-C10-C8-C7
13	N	102	BCL	C6-C7-C8-C10
13	S	101	BCL	C6-C7-C8-C10
13	5	402	BCL	C6-C7-C8-C10
13	7	102	BCL	C11-C10-C8-C7
17	R	103	PGV	C19-C20-C21-C22
13	6	102	BCL	CBA-CGA-O2A-C1
13	O	101	BCL	C2A-CAA-CBA-CGA
16	L	305	LMT	C2B-C1B-O1B-C4'
13	Z	102	BCL	O1A-CGA-O2A-C1
19	M	404	A1L8Q	C21-C15-C20-C34
16	7	103	LMT	O1'-C1-C2-C3
17	R	103	PGV	O02-C1-O01-C02
13	W	101	BCL	C3-C5-C6-C7
13	Z	102	BCL	C8-C10-C11-C12
13	1	101	BCL	C13-C15-C16-C17
13	B	102	BCL	O1A-CGA-O2A-C1
13	L	302	BCL	C15-C16-C17-C18
13	K	101	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	S	101	BCL	C5-C6-C7-C8
13	T	102	BCL	C10-C11-C12-C13
13	Y	102	BCL	C13-C15-C16-C17
13	7	102	BCL	C10-C11-C12-C13
13	8	103	BCL	C5-C6-C7-C8
16	X	103	LMT	O1'-C1-C2-C3
13	L	311	BCL	CBD-CGD-O2D-CED
13	4	102	BCL	O1A-CGA-O2A-C1
13	Q	101	BCL	C10-C11-C12-C13
13	S	101	BCL	C13-C15-C16-C17
13	U	102	BCL	C8-C10-C11-C12
13	3	101	BCL	C8-C10-C11-C12
13	0	102	BCL	C10-C11-C12-C13
17	M	406	PGV	C04-O12-P-O11
17	M	407	PGV	C03-O11-P-O12
17	H	403	PGV	C03-O11-P-O12
17	H	403	PGV	C04-O12-P-O11
17	A	101	PGV	C04-O12-P-O11
17	K	102	PGV	C03-O11-P-O12
17	P	103	PGV	C03-O11-P-O12
17	T	103	PGV	C03-O11-P-O12
17	4	103	PGV	C03-O11-P-O12
17	4	103	PGV	C04-O12-P-O11
17	8	101	PGV	C04-O12-P-O11
17	M	406	PGV	C20-C19-O03-C01
15	D	104	U10	C22-C23-C24-C25
17	K	102	PGV	O12-C04-C05-C06
13	D	102	BCL	C4-C3-C5-C6
13	T	102	BCL	C8-C10-C11-C12
16	9	102	LMT	O5B-C5B-C6B-O6B
13	M	402	BCL	C3-C5-C6-C7
13	1	101	BCL	C3-C5-C6-C7
17	L	306	PGV	C4-C5-C6-C7
17	M	407	PGV	C19-C20-C21-C22
16	Z	104	LMT	C3-C4-C5-C6
16	T	104	LMT	C2-C3-C4-C5
16	X	103	LMT	C4-C5-C6-C7
17	M	407	PGV	C2-C3-C4-C5
17	H	401	PGV	C25-C26-C27-C28
17	B	103	PGV	C5-C6-C7-C8
17	R	103	PGV	C25-C26-C27-C28
13	O	101	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	Z	103	LMT	C5'-C4'-O1B-C1B
17	M	408	PGV	C01-C02-O01-C1
9	C	405	Z41	C10-C11-C12-C13
16	K	103	LMT	C2-C3-C4-C5
13	8	103	BCL	O1A-CGA-O2A-C1
16	4	105	LMT	C4'-C5'-C6'-O6'
17	E	103	PGV	O12-C04-C05-O05
13	Y	102	BCL	C3-C5-C6-C7
16	L	305	LMT	C4-C5-C6-C7
17	E	103	PGV	C6-C7-C8-C9
13	J	102	BCL	C16-C17-C18-C19
13	S	101	BCL	C16-C17-C18-C19
13	5	402	BCL	C16-C17-C18-C19
13	M	402	BCL	C4-C3-C5-C6
13	L	302	BCL	C11-C10-C8-C9
13	L	310	BCL	C6-C7-C8-C9
13	L	311	BCL	C11-C12-C13-C14
13	3	101	BCL	C11-C12-C13-C14
17	8	104	PGV	C22-C23-C24-C25
13	L	311	BCL	C5-C6-C7-C8
13	S	101	BCL	C2A-CAA-CBA-CGA
13	X	101	BCL	C2A-CAA-CBA-CGA
13	7	102	BCL	C2A-CAA-CBA-CGA
13	6	102	BCL	O1A-CGA-O2A-C1
17	H	403	PGV	C04-C05-C06-O06
20	T	101	CRT	C15-C16-C17-C19
20	6	101	CRT	C15-C16-C17-C19
17	X	102	PGV	C11-C10-C9-C8
17	H	401	PGV	C5-C6-C7-C8
16	5	401	LMT	C1-C2-C3-C4
16	Z	103	LMT	O5'-C5'-C6'-O6'
13	I	101	BCL	C16-C17-C18-C19
13	2	103	BCL	C16-C17-C18-C20
16	Z	103	LMT	O5'-C1'-O1'-C1
17	E	103	PGV	C7-C8-C9-C10
13	D	102	BCL	C5-C6-C7-C8
13	U	102	BCL	C3-C5-C6-C7
14	M	403	BPH	C3-C5-C6-C7
13	T	102	BCL	CBA-CGA-O2A-C1
17	T	103	PGV	C26-C27-C28-C29
13	A	102	BCL	C3A-C2A-CAA-CBA
13	E	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	K	101	BCL	C3A-C2A-CAA-CBA
13	O	101	BCL	C3A-C2A-CAA-CBA
13	W	101	BCL	C3A-C2A-CAA-CBA
13	1	101	BCL	C3A-C2A-CAA-CBA
13	3	101	BCL	C3A-C2A-CAA-CBA
13	5	402	BCL	C3A-C2A-CAA-CBA
13	J	102	BCL	C10-C11-C12-C13
13	Q	101	BCL	C15-C16-C17-C18
17	8	101	PGV	C23-C24-C25-C26
13	I	101	BCL	C16-C17-C18-C20
13	5	402	BCL	C16-C17-C18-C20
13	X	101	BCL	C5-C6-C7-C8
13	M	402	BCL	C2-C3-C5-C6
13	G	102	BCL	C2-C3-C5-C6
13	V	102	BCL	C2-C3-C5-C6
13	3	101	BCL	C2-C3-C5-C6
17	D	101	PGV	C2-C1-O01-C02
17	8	104	PGV	C2-C1-O01-C02
16	P	104	LMT	C7-C8-C9-C10
17	X	102	PGV	C2-C3-C4-C5
13	S	101	BCL	C16-C17-C18-C20
17	H	401	PGV	O12-C04-C05-O05
13	Q	101	BCL	C3-C5-C6-C7
17	M	406	PGV	O04-C19-O03-C01
13	G	102	BCL	C15-C16-C17-C18
17	B	103	PGV	O12-C04-C05-C06
17	8	104	PGV	O02-C1-O01-C02
17	D	101	PGV	C5-C6-C7-C8
13	L	310	BCL	C5-C6-C7-C8
13	1	101	BCL	C15-C16-C17-C18
13	O	101	BCL	O1A-CGA-O2A-C1
17	L	307	PGV	C14-C15-C16-C17
17	R	103	PGV	C6-C7-C8-C9
13	K	101	BCL	C8-C10-C11-C12
13	8	103	BCL	C15-C16-C17-C18
17	X	102	PGV	C6-C7-C8-C9
17	2	104	PGV	C19-C20-C21-C22
17	0	103	PGV	C19-C20-C21-C22
17	H	404	PGV	C23-C24-C25-C26
17	T	103	PGV	C25-C26-C27-C28
13	J	102	BCL	C8-C10-C11-C12
13	1	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	G	102	BCL	C4-C3-C5-C6
13	V	102	BCL	C4-C3-C5-C6
13	3	101	BCL	C4-C3-C5-C6
13	L	302	BCL	C11-C10-C8-C7
13	L	310	BCL	C6-C7-C8-C10
13	L	311	BCL	C11-C12-C13-C15
13	B	102	BCL	C6-C7-C8-C10
13	B	102	BCL	C11-C10-C8-C7
13	F	101	BCL	C2-C3-C5-C6
13	N	102	BCL	C11-C10-C8-C7
13	2	103	BCL	C6-C7-C8-C10
13	3	101	BCL	C11-C10-C8-C7
13	9	101	BCL	C6-C7-C8-C10
13	T	102	BCL	O1A-CGA-O2A-C1
16	7	103	LMT	C2B-C1B-O1B-C4'
17	D	101	PGV	O02-C1-O01-C02
17	H	401	PGV	C1-C2-C3-C4
17	P	103	PGV	C1-C2-C3-C4
17	2	104	PGV	C20-C21-C22-C23
13	P	102	BCL	C5-C6-C7-C8
13	2	103	BCL	C8-C10-C11-C12
17	L	307	PGV	C26-C27-C28-C29
16	K	103	LMT	C5-C6-C7-C8
7	C	401	HEM	C2B-C3B-CAB-CBB
7	C	401	HEM	C2C-C3C-CAC-CBC
13	D	102	BCL	C15-C16-C17-C18
9	C	405	Z41	C20-C19-O3-C18
17	M	406	PGV	C2-C1-O01-C02
17	H	401	PGV	C2-C1-O01-C02
17	B	103	PGV	C2-C1-O01-C02
16	B	104	LMT	C4'-C5'-C6'-O6'
7	C	401	HEM	C4C-C3C-CAC-CBC
9	C	405	Z41	O4-C19-O3-C18
17	H	401	PGV	O02-C1-O01-C02
16	7	103	LMT	C4'-C5'-C6'-O6'
16	Z	104	LMT	C7-C8-C9-C10
17	4	103	PGV	C20-C21-C22-C23
17	G	103	PGV	O03-C01-C02-O01
17	K	102	PGV	O03-C01-C02-O01
17	V	103	PGV	O03-C01-C02-O01
17	4	103	PGV	O03-C01-C02-O01
17	8	104	PGV	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
17	K	102	PGV	C20-C19-O03-C01
17	N	103	PGV	C22-C23-C24-C25
16	H	402	LMT	O5'-C5'-C6'-O6'
16	4	104	LMT	O5'-C5'-C6'-O6'
17	M	408	PGV	C11-C10-C9-C8
13	F	101	BCL	C4-C3-C5-C6
13	D	102	BCL	C2-C3-C5-C6
13	K	101	BCL	C2-C3-C5-C6
16	T	104	LMT	C4-C5-C6-C7
13	S	101	BCL	C6-C7-C8-C9
13	3	101	BCL	C11-C10-C8-C9
17	T	103	PGV	C24-C25-C26-C27
20	E	101	CRT	C15-C16-C17-C19
13	G	102	BCL	C1A-C2A-CAA-CBA
13	J	102	BCL	C1A-C2A-CAA-CBA
13	K	101	BCL	C1A-C2A-CAA-CBA
13	N	102	BCL	C1A-C2A-CAA-CBA
13	O	101	BCL	C1A-C2A-CAA-CBA
13	P	102	BCL	C1A-C2A-CAA-CBA
13	R	102	BCL	C1A-C2A-CAA-CBA
13	T	102	BCL	C1A-C2A-CAA-CBA
13	X	101	BCL	C1A-C2A-CAA-CBA
13	Z	102	BCL	C1A-C2A-CAA-CBA
13	1	101	BCL	C1A-C2A-CAA-CBA
13	4	102	BCL	C1A-C2A-CAA-CBA
13	5	402	BCL	C1A-C2A-CAA-CBA
13	6	102	BCL	C1A-C2A-CAA-CBA
13	J	102	BCL	C16-C17-C18-C20
13	2	103	BCL	C16-C17-C18-C19
17	V	103	PGV	C2-C1-O01-C02
17	X	102	PGV	C2-C1-O01-C02
15	7	101	U10	C31-C32-C33-C34
17	B	103	PGV	C03-O11-P-O12
17	N	103	PGV	C03-O11-P-O12
17	8	101	PGV	C03-O11-P-O12
17	8	104	PGV	C04-O12-P-O11
17	4	103	PGV	C19-C20-C21-C22
15	L	309	U10	C6-C7-C8-C9
13	F	101	BCL	C5-C6-C7-C8
13	U	102	BCL	C10-C11-C12-C13
16	E	104	LMT	O5'-C5'-C6'-O6'
17	B	103	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
17	E	103	PGV	C01-C02-C03-O11
17	8	101	PGV	C01-C02-C03-O11
17	J	103	PGV	C3-C4-C5-C6
16	F	102	LMT	O5'-C5'-C6'-O6'
13	K	101	BCL	C13-C15-C16-C17
16	K	103	LMT	O5B-C5B-C6B-O6B
17	J	103	PGV	C11-C10-C9-C8
20	8	102	CRT	C35-C36-C37-C38
16	M	409	LMT	O5B-C5B-C6B-O6B
17	A	101	PGV	O12-C04-C05-C06
13	K	101	BCL	C4-C3-C5-C6
13	X	101	BCL	C2C-C3C-CAC-CBC
13	0	102	BCL	C15-C16-C17-C18
16	L	305	LMT	O1'-C1-C2-C3
17	H	403	PGV	C5-C6-C7-C8
17	B	103	PGV	C22-C23-C24-C25
17	2	104	PGV	C4-C5-C6-C7
17	M	408	PGV	C4-C5-C6-C7
17	H	403	PGV	C21-C22-C23-C24
16	7	103	LMT	O5B-C5B-C6B-O6B
17	8	101	PGV	O03-C01-C02-C03
16	J	104	LMT	O5'-C5'-C6'-O6'
17	H	401	PGV	C20-C21-C22-C23
13	J	102	BCL	C5-C6-C7-C8
17	H	403	PGV	C15-C16-C17-C18
16	P	104	LMT	O5'-C5'-C6'-O6'
16	F	102	LMT	C6-C7-C8-C9
16	4	104	LMT	C2-C3-C4-C5
16	X	103	LMT	C6-C7-C8-C9
16	5	401	LMT	O5B-C5B-C6B-O6B
17	H	404	PGV	C11-C10-C9-C8
13	R	102	BCL	C5-C6-C7-C8
16	P	104	LMT	O1'-C1-C2-C3
13	B	102	BCL	C5-C6-C7-C8
13	Z	102	BCL	C5-C6-C7-C8
13	2	103	BCL	C5-C6-C7-C8
13	E	102	BCL	C4-C3-C5-C6
13	Y	102	BCL	C4-C3-C5-C6
16	Z	103	LMT	C3'-C4'-O1B-C1B
13	M	402	BCL	CBA-CGA-O2A-C1
13	R	102	BCL	CBD-CGD-O2D-CED
13	N	102	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	X	103	LMT	C5-C6-C7-C8
17	H	401	PGV	O01-C02-C03-O11
17	V	103	PGV	O01-C02-C03-O11
8	C	403	HEC	C2C-C3C-CAC-CBC
13	7	102	BCL	C16-C17-C18-C20
16	L	305	LMT	O5B-C1B-O1B-C4'
20	M	405	CRT	C2-C1-O1-C1M
17	R	103	PGV	O03-C01-C02-O01
17	M	406	PGV	O02-C1-O01-C02
17	X	102	PGV	O02-C1-O01-C02
17	K	102	PGV	O04-C19-O03-C01
16	J	104	LMT	C1-C2-C3-C4
20	M	405	CRT	C2-C1-C4-C5
20	B	101	CRT	C2-C1-C4-C5
20	G	101	CRT	C36-C37-C38-C39
20	J	101	CRT	C36-C37-C38-C39
20	Y	101	CRT	C36-C37-C38-C39
20	2	102	CRT	C36-C37-C38-C39
20	4	101	CRT	C36-C37-C38-C39
20	6	101	CRT	C2-C1-C4-C5
20	6	101	CRT	C3-C1-C4-C5
20	8	102	CRT	C3-C1-C4-C5
13	E	102	BCL	C2-C3-C5-C6
13	E	102	BCL	C11-C10-C8-C7
13	E	102	BCL	C12-C13-C15-C16
13	O	101	BCL	C6-C7-C8-C10
13	P	102	BCL	C6-C7-C8-C10
13	P	102	BCL	C11-C10-C8-C7
13	Y	102	BCL	C2-C3-C5-C6
13	Y	102	BCL	C11-C10-C8-C7
13	Z	102	BCL	C11-C10-C8-C7
13	4	102	BCL	C6-C7-C8-C10
13	4	102	BCL	C11-C10-C8-C7
13	6	102	BCL	C11-C10-C8-C7
13	8	103	BCL	C11-C12-C13-C15
13	9	101	BCL	C11-C12-C13-C15
16	P	104	LMT	C1-C2-C3-C4
17	T	103	PGV	C6-C7-C8-C9
13	B	102	BCL	C11-C10-C8-C9
13	E	102	BCL	C11-C10-C8-C9
13	E	102	BCL	C11-C12-C13-C14
13	F	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	G	102	BCL	C11-C10-C8-C9
13	N	102	BCL	C11-C10-C8-C9
13	P	102	BCL	C11-C10-C8-C9
13	Q	101	BCL	C11-C10-C8-C9
13	X	101	BCL	C11-C12-C13-C14
13	Y	102	BCL	C11-C10-C8-C9
13	1	101	BCL	C6-C7-C8-C9
13	2	103	BCL	C11-C10-C8-C9
13	5	402	BCL	C6-C7-C8-C9
13	8	103	BCL	C11-C12-C13-C14
13	9	101	BCL	C11-C10-C8-C9
17	M	408	PGV	C20-C19-O03-C01
17	D	101	PGV	C20-C19-O03-C01
10	C	406	PLM	C8-C9-CA-CB
20	M	405	CRT	O1-C1-C4-C5
13	M	402	BCL	O1A-CGA-O2A-C1
20	4	101	CRT	C5-C6-C7-C8
16	B	104	LMT	O5'-C5'-C6'-O6'
17	E	103	PGV	O12-C04-C05-C06
17	B	103	PGV	O02-C1-O01-C02
13	2	103	BCL	C15-C16-C17-C18
17	L	307	PGV	C20-C19-O03-C01
16	D	103	LMT	C3-C4-C5-C6
17	4	103	PGV	C01-C02-C03-O11
17	L	307	PGV	C1-C2-C3-C4
13	Z	102	BCL	C4-C3-C5-C6
15	1	102	U10	C15-C14-C16-C17
15	7	101	U10	C12-C11-C9-C10
13	Z	102	BCL	C2-C3-C5-C6
17	L	306	PGV	C6-C7-C8-C9
17	P	103	PGV	C2-C3-C4-C5
17	D	101	PGV	C24-C25-C26-C27
13	L	311	BCL	O1D-CGD-O2D-CED
17	H	404	PGV	C20-C19-O03-C01
17	T	103	PGV	C3-C4-C5-C6
17	G	103	PGV	O03-C01-C02-C03
17	V	103	PGV	O03-C01-C02-C03
17	4	103	PGV	O03-C01-C02-C03
17	8	104	PGV	O03-C01-C02-C03
17	X	102	PGV	C1-C2-C3-C4
16	D	103	LMT	C5'-C4'-O1B-C1B
13	I	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	S	101	BCL	C3-C5-C6-C7
19	M	404	A1L8Q	C4-C10-C29-C21
19	M	404	A1L8Q	C15-C20-C34-C33
17	M	410	PGV	O05-C05-C06-O06
17	E	103	PGV	O01-C02-C03-O11
17	4	103	PGV	O01-C02-C03-O11
17	V	103	PGV	O02-C1-O01-C02
17	G	103	PGV	C7-C8-C9-C10
17	N	103	PGV	O03-C01-C02-O01
17	X	102	PGV	O03-C01-C02-O01
17	L	307	PGV	C22-C23-C24-C25
17	P	103	PGV	C24-C25-C26-C27
16	4	105	LMT	O5'-C5'-C6'-O6'
13	E	102	BCL	C10-C11-C12-C13
15	7	101	U10	C14-C16-C17-C18
15	7	101	U10	C34-C36-C37-C38
13	A	102	BCL	C2-C1-O2A-CGA
15	7	101	U10	C12-C11-C9-C8
13	M	402	BCL	C6-C7-C8-C9
13	O	101	BCL	C11-C10-C8-C9
13	T	102	BCL	C11-C10-C8-C9
13	U	102	BCL	C14-C13-C15-C16
13	W	101	BCL	C6-C7-C8-C9
13	1	101	BCL	C11-C10-C8-C9
13	4	102	BCL	C6-C7-C8-C9
13	4	102	BCL	C11-C12-C13-C14
13	8	103	BCL	C11-C10-C8-C9
13	R	102	BCL	C15-C16-C17-C18
17	E	103	PGV	C05-C04-O12-P
16	K	103	LMT	C1-C2-C3-C4
13	Y	102	BCL	C2A-CAA-CBA-CGA
13	5	402	BCL	C8-C10-C11-C12
20	J	101	CRT	C5-C6-C7-C8
20	J	101	CRT	C15-C16-C17-C18
13	L	310	BCL	C4C-C3C-CAC-CBC
20	G	101	CRT	C15-C16-C17-C19
20	2	102	CRT	C10-C11-C12-C14
20	0	101	CRT	C5-C6-C7-C9
13	D	102	BCL	C10-C11-C12-C13
17	B	103	PGV	C2-C3-C4-C5
17	E	103	PGV	C2-C1-O01-C02
13	Y	102	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
17	T	103	PGV	C11-C12-C13-C14
13	4	102	BCL	C8-C10-C11-C12
17	D	101	PGV	O04-C19-O03-C01
13	M	402	BCL	C6-C7-C8-C10
13	E	102	BCL	C11-C12-C13-C15
13	F	101	BCL	C6-C7-C8-C10
13	F	101	BCL	C11-C10-C8-C7
13	G	102	BCL	C6-C7-C8-C10
13	G	102	BCL	C12-C13-C15-C16
13	I	101	BCL	C11-C10-C8-C7
13	Q	101	BCL	C11-C10-C8-C7
13	T	102	BCL	C11-C10-C8-C7
13	U	102	BCL	C12-C13-C15-C16
13	V	102	BCL	C11-C10-C8-C7
13	W	101	BCL	C6-C7-C8-C10
13	1	101	BCL	C6-C7-C8-C10
13	2	103	BCL	C11-C10-C8-C7
13	3	101	BCL	C11-C12-C13-C15
13	5	402	BCL	C11-C10-C8-C7
13	7	102	BCL	C11-C12-C13-C15
13	8	103	BCL	C11-C10-C8-C7
13	9	101	BCL	C11-C10-C8-C7
17	M	408	PGV	O04-C19-O03-C01
13	7	102	BCL	C16-C17-C18-C19
16	D	103	LMT	C3'-C4'-O1B-C1B
17	N	103	PGV	C19-C20-C21-C22
16	K	103	LMT	C4-C5-C6-C7
16	V	104	LMT	C3-C4-C5-C6
13	A	102	BCL	C5-C6-C7-C8
13	L	302	BCL	C16-C17-C18-C19
16	K	103	LMT	O5'-C1'-O1'-C1
17	H	404	PGV	O03-C01-C02-C03
17	N	103	PGV	O03-C01-C02-C03
16	E	104	LMT	C4B-C5B-C6B-O6B
17	T	103	PGV	O01-C02-C03-O11
7	C	401	HEM	C4B-C3B-CAB-CBB
17	K	102	PGV	C2-C3-C4-C5
13	R	102	BCL	O1D-CGD-O2D-CED
17	E	103	PGV	O02-C1-O01-C02
17	L	307	PGV	O04-C19-O03-C01
17	H	404	PGV	O04-C19-O03-C01
16	Z	104	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	L	310	BCL	C4-C3-C5-C6
13	T	102	BCL	C4-C3-C5-C6
15	L	309	U10	C12-C11-C9-C10
13	L	310	BCL	C2-C3-C5-C6
13	T	102	BCL	C2-C3-C5-C6
13	F	101	BCL	C6-C7-C8-C9
13	G	102	BCL	C6-C7-C8-C9
13	5	402	BCL	C11-C10-C8-C9
13	7	102	BCL	C11-C12-C13-C14
13	0	102	BCL	C6-C7-C8-C9
17	0	103	PGV	C3-C4-C5-C6
13	V	102	BCL	C5-C6-C7-C8
13	Y	102	BCL	CBD-CGD-O2D-CED
17	J	103	PGV	C25-C26-C27-C28
16	M	409	LMT	C2-C3-C4-C5
17	G	103	PGV	C1-C2-C3-C4
17	K	102	PGV	C19-C20-C21-C22
17	8	104	PGV	C19-C20-C21-C22
13	Q	101	BCL	C16-C17-C18-C20
13	N	102	BCL	C2-C1-O2A-CGA
13	P	102	BCL	C2-C1-O2A-CGA
13	X	101	BCL	C2-C1-O2A-CGA
13	1	101	BCL	CBD-CGD-O2D-CED
17	M	407	PGV	C04-O12-P-O11
17	P	103	PGV	C04-O12-P-O11
17	2	101	PGV	C04-O12-P-O11
17	2	104	PGV	C04-O12-P-O11
17	L	307	PGV	C13-C14-C15-C16
17	L	307	PGV	O12-C04-C05-O05
13	P	102	BCL	C4-C3-C5-C6
13	T	102	BCL	C3-C5-C6-C7
17	8	101	PGV	C02-C03-O11-P
17	H	403	PGV	C03-O11-P-O13
17	H	403	PGV	C04-O12-P-O13
17	B	103	PGV	C03-O11-P-O13
17	D	101	PGV	C04-O12-P-O14
17	K	102	PGV	C04-O12-P-O14
17	R	103	PGV	C03-O11-P-O14
17	T	103	PGV	C03-O11-P-O13
17	4	103	PGV	C03-O11-P-O13
17	4	103	PGV	C04-O12-P-O13
17	8	101	PGV	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
13	T	102	BCL	C16-C17-C18-C19
13	3	101	BCL	C16-C17-C18-C19
17	L	306	PGV	C1-C2-C3-C4
17	N	103	PGV	C1-C2-C3-C4
17	8	104	PGV	C1-C2-C3-C4
16	T	104	LMT	O5'-C1'-O1'-C1
17	L	307	PGV	C01-C02-C03-O11
17	H	401	PGV	C01-C02-C03-O11
17	K	102	PGV	C01-C02-C03-O11
17	T	103	PGV	C01-C02-C03-O11
8	C	403	HEC	C4C-C3C-CAC-CBC
13	W	101	BCL	C16-C17-C18-C19
9	C	405	Z41	C13-C14-C15-C16
13	1	101	BCL	O1D-CGD-O2D-CED
13	L	311	BCL	C6-C7-C8-C10
13	L	311	BCL	C11-C10-C8-C7
13	I	101	BCL	C6-C7-C8-C10
13	I	101	BCL	C12-C13-C15-C16
13	J	102	BCL	C6-C7-C8-C10
13	J	102	BCL	C11-C10-C8-C7
13	K	101	BCL	C6-C7-C8-C10
13	Q	101	BCL	C6-C7-C8-C10
13	U	102	BCL	C6-C7-C8-C10
13	V	102	BCL	C6-C7-C8-C10
13	Z	102	BCL	C6-C7-C8-C10
13	Z	102	BCL	C12-C13-C15-C16
13	7	102	BCL	C6-C7-C8-C10
13	0	102	BCL	C6-C7-C8-C10
15	1	102	U10	C13-C14-C16-C17
17	K	102	PGV	O01-C02-C03-O11
16	4	104	LMT	C2-C1-O1'-C1'
13	O	101	BCL	C5-C6-C7-C8
13	Y	102	BCL	O1D-CGD-O2D-CED
16	B	104	LMT	C2B-C1B-O1B-C4'
17	K	102	PGV	O03-C01-C02-C03
17	R	103	PGV	O03-C01-C02-C03
17	B	103	PGV	O03-C01-C02-O01
16	B	104	LMT	C6-C7-C8-C9
17	V	103	PGV	C22-C23-C24-C25
14	L	303	BPH	O2A-C1-C2-C3
16	O	102	LMT	C2B-C1B-O1B-C4'
17	B	103	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	L	302	BCL	C4-C3-C5-C6
13	7	102	BCL	C4-C3-C5-C6
16	Z	104	LMT	C4B-C5B-C6B-O6B
13	S	101	BCL	C15-C16-C17-C18
13	9	101	BCL	C10-C11-C12-C13
13	D	102	BCL	C6-C7-C8-C9
13	I	101	BCL	C11-C10-C8-C9
13	K	101	BCL	C11-C10-C8-C9
13	Z	102	BCL	C6-C7-C8-C9
16	B	104	LMT	O5'-C1'-O1'-C1
8	C	404	HEC	C2B-C3B-CAB-CBB
20	6	101	CRT	C14-C15-C16-C17
20	J	101	CRT	C15-C16-C17-C19
13	0	102	BCL	CBD-CGD-O2D-CED
13	7	102	BCL	C15-C16-C17-C18
13	Q	101	BCL	C16-C17-C18-C19
13	Y	102	BCL	C16-C17-C18-C20
16	Z	104	LMT	O1'-C1-C2-C3
13	0	102	BCL	O1D-CGD-O2D-CED
17	X	102	PGV	C01-C02-O01-C1
17	V	103	PGV	C01-C02-C03-O11
13	V	102	BCL	O1D-CGD-O2D-CED
13	T	102	BCL	C2A-CAA-CBA-CGA
13	L	311	BCL	C2-C1-O2A-CGA
13	M	402	BCL	C2-C1-O2A-CGA
13	L	302	BCL	C16-C17-C18-C20
17	L	307	PGV	C02-C03-O11-P
17	A	101	PGV	C05-C04-O12-P
17	8	101	PGV	O01-C02-C03-O11
17	8	101	PGV	C6-C7-C8-C9
13	R	102	BCL	C16-C17-C18-C20
16	P	104	LMT	C2'-C1'-O1'-C1
17	L	307	PGV	C04-O12-P-O11
17	M	410	PGV	C03-O11-P-O12
17	M	410	PGV	C04-O12-P-O11
17	H	404	PGV	C04-O12-P-O11
17	A	101	PGV	C03-O11-P-O12
17	B	103	PGV	C04-O12-P-O11
17	D	101	PGV	C03-O11-P-O12
17	G	103	PGV	C03-O11-P-O12
17	J	103	PGV	C04-O12-P-O11
17	N	103	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
17	R	103	PGV	C04-O12-P-O11
17	T	103	PGV	C04-O12-P-O11
17	V	103	PGV	C04-O12-P-O11
17	X	102	PGV	C03-O11-P-O12
17	X	102	PGV	C04-O12-P-O11
17	2	101	PGV	C03-O11-P-O12
17	8	104	PGV	C03-O11-P-O12
17	0	103	PGV	C03-O11-P-O12
17	0	103	PGV	C04-O12-P-O11
16	E	104	LMT	C11-C10-C9-C8
20	B	101	CRT	C3-C1-C4-C5
20	B	101	CRT	C36-C37-C38-C39
20	N	101	CRT	C36-C37-C38-C39
20	T	101	CRT	C36-C37-C38-C39
20	6	101	CRT	C36-C37-C38-C39
17	L	307	PGV	C25-C26-C27-C28
17	8	101	PGV	C22-C23-C24-C25
13	J	102	BCL	O1D-CGD-O2D-CED
13	L	310	BCL	C11-C10-C8-C7
13	O	101	BCL	C11-C10-C8-C7
13	X	101	BCL	C11-C12-C13-C15
15	L	309	U10	C12-C11-C9-C8
13	I	101	BCL	C6-C7-C8-C9
13	Q	101	BCL	C6-C7-C8-C9
13	7	102	BCL	C11-C10-C8-C9
17	M	408	PGV	C5-C6-C7-C8
13	Y	102	BCL	O1A-CGA-O2A-C1
20	B	101	CRT	O1-C1-C4-C5
20	4	101	CRT	C36-C37-C38-O2
20	V	101	CRT	C5-C6-C7-C8
20	V	101	CRT	C15-C16-C17-C18
13	6	102	BCL	C15-C16-C17-C18
13	W	101	BCL	C16-C17-C18-C20
13	3	101	BCL	C16-C17-C18-C20
16	F	102	LMT	O1'-C1-C2-C3
16	V	104	LMT	O1'-C1-C2-C3
17	E	103	PGV	C4-C5-C6-C7
16	H	402	LMT	O1'-C1-C2-C3
13	N	102	BCL	C10-C11-C12-C13
14	L	303	BPH	C16-C17-C18-C20
13	Y	102	BCL	CBA-CGA-O2A-C1
17	E	103	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
13	V	102	BCL	CBD-CGD-O2D-CED
16	E	104	LMT	C5-C6-C7-C8
15	D	104	U10	C9-C11-C12-C13
17	K	102	PGV	C6-C7-C8-C9
17	V	103	PGV	C19-C20-C21-C22
8	C	402	HEC	C2B-C3B-CAB-CBB
13	L	310	BCL	C16-C17-C18-C19
15	D	104	U10	C12-C11-C9-C10
13	L	310	BCL	C13-C15-C16-C17
13	G	102	BCL	C13-C15-C16-C17
17	R	103	PGV	C7-C8-C9-C10
13	T	102	BCL	C16-C17-C18-C20
10	C	406	PLM	C7-C8-C9-CA
13	Z	102	BCL	C2A-CAA-CBA-CGA
8	C	404	HEC	C4B-C3B-CAB-CBB
7	C	401	HEM	CAA-CBA-CGA-O1A
17	H	403	PGV	C19-C20-C21-C22
16	V	104	LMT	O5B-C5B-C6B-O6B
13	P	102	BCL	C2-C3-C5-C6
13	7	102	BCL	C2-C3-C5-C6
13	V	102	BCL	C6-C7-C8-C9
13	Z	102	BCL	C14-C13-C15-C16
17	V	103	PGV	C2-C3-C4-C5
17	8	104	PGV	C25-C26-C27-C28
13	P	102	BCL	C13-C15-C16-C17
17	H	404	PGV	C24-C25-C26-C27
17	M	408	PGV	O03-C01-C02-C03
20	6	101	CRT	C13-C12-C14-C15
14	M	403	BPH	O2A-C1-C2-C3
16	P	104	LMT	O5'-C1'-O1'-C1
20	R	101	CRT	C5-C6-C7-C8
17	H	401	PGV	C11-C10-C9-C8
16	Z	103	LMT	O5B-C5B-C6B-O6B
13	M	402	BCL	C11-C10-C8-C7
13	K	101	BCL	C12-C13-C15-C16
13	R	102	BCL	C11-C10-C8-C7
13	8	103	BCL	C6-C7-C8-C10
17	H	403	PGV	C6-C7-C8-C9
7	C	401	HEM	CAA-CBA-CGA-O2A
8	C	402	HEC	CAA-CBA-CGA-O1A
8	C	404	HEC	CAD-CBD-CGD-O1D
8	C	404	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	J	103	PGV	C7-C8-C9-C10
13	U	102	BCL	C16-C17-C18-C19
13	R	102	BCL	C4-C3-C5-C6
15	L	309	U10	C15-C14-C16-C17
16	Z	103	LMT	C4'-C5'-C6'-O6'
17	K	102	PGV	C24-C25-C26-C27
17	N	103	PGV	C24-C25-C26-C27
17	2	101	PGV	O02-C1-O01-C02
20	6	101	CRT	C11-C12-C14-C15
17	0	103	PGV	O03-C01-C02-O01
15	7	101	U10	C19-C21-C22-C23
17	V	103	PGV	C1-C2-C3-C4
13	A	102	BCL	C4-C3-C5-C6
13	J	102	BCL	C4-C3-C5-C6
13	2	103	BCL	C2-C1-O2A-CGA
13	3	101	BCL	C2-C1-O2A-CGA
13	8	103	BCL	C2-C1-O2A-CGA
15	D	104	U10	C12-C11-C9-C8
13	G	102	BCL	O1D-CGD-O2D-CED
16	X	103	LMT	C2B-C1B-O1B-C4'
19	M	404	A1L8Q	C17-C26-C8-C2
17	E	103	PGV	C24-C25-C26-C27
17	D	101	PGV	C26-C27-C28-C29
17	2	101	PGV	O03-C19-C20-C21
16	X	103	LMT	C7-C8-C9-C10
17	H	404	PGV	C2-C3-C4-C5
13	5	402	BCL	C4-C3-C5-C6
14	L	303	BPH	C4-C3-C5-C6
15	D	104	U10	C25-C24-C26-C27
19	M	404	A1L8Q	C42-C16-C3-C7
15	L	309	U10	C1-C6-C7-C8
13	P	102	BCL	C16-C17-C18-C20
13	B	102	BCL	O1D-CGD-O2D-CED
17	B	103	PGV	C11-C12-C13-C14
17	E	103	PGV	C11-C12-C13-C14
13	Y	102	BCL	C5-C6-C7-C8
13	9	101	BCL	C8-C10-C11-C12
13	J	102	BCL	CBD-CGD-O2D-CED
15	L	308	U10	C2-C3-O3-C3M
15	L	308	U10	C5-C4-O4-C4M
15	D	104	U10	C5-C4-O4-C4M
15	1	102	U10	C2-C3-O3-C3M

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Mol	Chain	Res	Type	Atoms
13	0	102	BCL	C4-C3-C5-C6
15	7	101	U10	C40-C39-C41-C42
13	4	102	BCL	C11-C12-C13-C15
14	L	303	BPH	C2-C3-C5-C6
14	L	303	BPH	C11-C12-C13-C15
19	M	404	A1L8Q	C27-C16-C3-C7
17	H	403	PGV	O05-C05-C06-O06
17	4	103	PGV	C6-C7-C8-C9
17	8	101	PGV	C26-C27-C28-C29
14	M	403	BPH	C1-C2-C3-C4
13	O	101	BCL	C16-C17-C18-C20
17	P	103	PGV	O01-C1-C2-C3
13	9	101	BCL	C4-C3-C5-C6
15	D	104	U10	C30-C29-C31-C32
19	M	404	A1L8Q	C20-C15-C21-C45
19	M	404	A1L8Q	C35-C30-C33-C50
13	J	102	BCL	C2-C3-C5-C6
13	L	311	BCL	C6-C7-C8-C9
13	B	102	BCL	C6-C7-C8-C9
13	F	101	BCL	C11-C12-C13-C14
13	G	102	BCL	C14-C13-C15-C16
13	I	101	BCL	C14-C13-C15-C16
13	J	102	BCL	C6-C7-C8-C9
13	K	101	BCL	C14-C13-C15-C16
13	U	102	BCL	C6-C7-C8-C9
13	7	102	BCL	C6-C7-C8-C9
13	8	103	BCL	C6-C7-C8-C9
13	9	101	BCL	C6-C7-C8-C9
14	M	403	BPH	C14-C13-C15-C16
15	L	309	U10	C5-C6-C7-C8
15	Y	103	U10	C5-C6-C7-C8
13	B	102	BCL	CAA-CBA-CGA-O2A
17	V	103	PGV	C9-C10-C11-C12
8	C	402	HEC	CAA-CBA-CGA-O2A
13	L	310	BCL	CAD-CBD-CGD-O2D
14	L	303	BPH	CAD-CBD-CGD-O2D
14	M	403	BPH	CAD-CBD-CGD-O2D
13	R	102	BCL	C16-C17-C18-C19
17	0	103	PGV	C2-C3-C4-C5
13	N	102	BCL	C3-C5-C6-C7
17	K	102	PGV	O02-C1-O01-C02
13	V	102	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	X	101	BCL	CAA-CBA-CGA-O2A
15	7	101	U10	C20-C19-C21-C22
13	R	102	BCL	C2-C3-C5-C6
13	5	402	BCL	C2-C3-C5-C6
15	L	309	U10	C13-C14-C16-C17
15	D	104	U10	C23-C24-C26-C27
15	D	104	U10	C28-C29-C31-C32
15	7	101	U10	C18-C19-C21-C22
13	Z	102	BCL	CAA-CBA-CGA-O2A
17	M	407	PGV	O01-C1-C2-C3
17	V	103	PGV	C23-C24-C25-C26
20	J	101	CRT	C5-C6-C7-C9
20	V	101	CRT	C5-C6-C7-C9
20	V	101	CRT	C15-C16-C17-C19
20	2	102	CRT	C15-C16-C17-C19
20	4	101	CRT	C5-C6-C7-C9
15	D	104	U10	C2-C3-O3-C3M
15	U	101	U10	C2-C3-O3-C3M
19	M	404	A1L8Q	C13-C2-C8-C26
17	2	101	PGV	O01-C02-C03-O11
15	1	102	U10	C31-C32-C33-C34
13	G	102	BCL	CAA-CBA-CGA-O2A
13	X	101	BCL	O2A-C1-C2-C3
8	C	402	HEC	C4B-C3B-CAB-CBB
17	H	404	PGV	C29-C30-C31-C32
17	H	403	PGV	C11-C12-C13-C14
13	L	310	BCL	C16-C17-C18-C20
17	P	103	PGV	C25-C26-C27-C28
16	4	105	LMT	C3-C4-C5-C6
13	L	311	BCL	CHA-CBD-CGD-O1D
13	L	311	BCL	CHA-CBD-CGD-O2D
13	M	402	BCL	CHA-CBD-CGD-O1D
13	M	402	BCL	CHA-CBD-CGD-O2D
13	Q	101	BCL	C4-C3-C5-C6
19	M	404	A1L8Q	C20-C15-C21-C29
19	M	404	A1L8Q	C35-C30-C33-C34
16	B	104	LMT	C4-C5-C6-C7
13	N	102	BCL	CAA-CBA-CGA-O2A
17	M	406	PGV	O03-C19-C20-C21
17	4	103	PGV	O03-C19-C20-C21
17	L	307	PGV	O03-C01-C02-O01
13	I	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
17	H	404	PGV	C4-C5-C6-C7
20	J	101	CRT	C36-C37-C38-C40
20	4	101	CRT	C36-C37-C38-C40
16	K	103	LMT	C3'-C4'-O1B-C1B
17	L	307	PGV	C27-C28-C29-C30
15	7	101	U10	C16-C17-C18-C19
13	L	302	BCL	C2-C3-C5-C6
15	7	101	U10	C24-C26-C27-C28
20	M	405	CRT	C20-C21-C22-C23
16	Z	104	LMT	C6-C7-C8-C9
16	O	102	LMT	O5B-C1B-O1B-C4'
16	4	104	LMT	C9-C10-C11-C12
17	H	403	PGV	O01-C1-C2-C3
15	Y	103	U10	C2-C3-O3-C3M
17	2	101	PGV	C2-C1-O01-C02
13	G	102	BCL	C2A-CAA-CBA-CGA
15	L	304	U10	C11-C12-C13-C14
13	G	102	BCL	CAA-CBA-CGA-O1A
20	J	101	CRT	C36-C37-C38-O2
17	8	104	PGV	O03-C19-C20-C21
13	X	101	BCL	CAA-CBA-CGA-O1A
17	P	103	PGV	O02-C1-C2-C3
13	P	102	BCL	C16-C17-C18-C19
17	2	101	PGV	C2-C3-C4-C5
17	M	410	PGV	C04-C05-C06-O06
13	9	101	BCL	C2-C3-C5-C6
13	0	102	BCL	C2-C3-C5-C6
13	5	402	BCL	C5-C6-C7-C8
16	4	105	LMT	C3'-C4'-O1B-C1B
13	B	102	BCL	CAA-CBA-CGA-O1A
13	Z	102	BCL	CAA-CBA-CGA-O1A
20	N	101	CRT	C15-C16-C17-C19
17	M	406	PGV	C25-C26-C27-C28
13	Q	101	BCL	C1A-C2A-CAA-CBA
13	U	102	BCL	C1A-C2A-CAA-CBA
17	2	104	PGV	O12-C04-C05-C06
13	G	102	BCL	C16-C17-C18-C19
19	M	404	A1L8Q	C12-C25-C7-C3
17	M	407	PGV	O02-C1-C2-C3
17	8	104	PGV	O04-C19-C20-C21
16	K	103	LMT	C5'-C4'-O1B-C1B
16	X	103	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
17	H	401	PGV	C21-C22-C23-C24
17	N	103	PGV	O02-C1-O01-C02
17	O	103	PGV	C25-C26-C27-C28
8	C	403	HEC	CAD-CBD-CGD-O2D
17	L	307	PGV	C04-O12-P-O13
17	M	410	PGV	C03-O11-P-O13
17	A	101	PGV	C03-O11-P-O13
17	E	103	PGV	C03-O11-P-O14
17	N	103	PGV	C03-O11-P-O14
17	T	103	PGV	C04-O12-P-O13
17	V	103	PGV	C04-O12-P-O13
17	X	102	PGV	C04-O12-P-O13
17	O	103	PGV	C04-O12-P-O13
13	E	102	BCL	C16-C17-C18-C19
17	H	403	PGV	C22-C23-C24-C25
13	V	102	BCL	CAA-CBA-CGA-O1A
13	8	103	BCL	C10-C11-C12-C13
9	C	405	Z41	C21-C22-C23-C24
15	7	101	U10	C11-C12-C13-C14
15	7	101	U10	C41-C42-C43-C44
13	S	101	BCL	CAD-CBD-CGD-O1D
13	U	102	BCL	CAD-CBD-CGD-O1D
13	8	103	BCL	CAD-CBD-CGD-O1D
17	X	102	PGV	C03-C02-O01-C1
13	N	102	BCL	CAA-CBA-CGA-O1A
16	4	105	LMT	C5'-C4'-O1B-C1B
17	H	403	PGV	C20-C21-C22-C23
17	D	101	PGV	C25-C26-C27-C28
17	R	103	PGV	C9-C10-C11-C12
9	C	405	Z41	O3-C19-C20-C21
13	A	102	BCL	C15-C16-C17-C18
15	D	104	U10	C16-C17-C18-C19
13	K	101	BCL	C15-C16-C17-C18
16	E	104	LMT	C3-C4-C5-C6
13	U	102	BCL	C16-C17-C18-C20
13	U	102	BCL	C4-C3-C5-C6
20	2	102	CRT	C15-C16-C17-C18
13	D	102	BCL	C6-C7-C8-C10
13	K	101	BCL	C11-C10-C8-C7
13	U	102	BCL	C3A-C2A-CAA-CBA
13	F	101	BCL	CAA-CBA-CGA-O2A
17	T	103	PGV	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	M	405	CRT	C5-C6-C7-C9
20	R	101	CRT	C5-C6-C7-C9
20	Z	101	CRT	C15-C16-C17-C19
20	0	101	CRT	C15-C16-C17-C19
16	D	103	LMT	C2-C1-O1'-C1'
16	F	102	LMT	C2-C3-C4-C5
13	F	101	BCL	CAA-CBA-CGA-O1A
17	H	403	PGV	O02-C1-C2-C3
17	B	103	PGV	O03-C19-C20-C21
8	C	403	HEC	CAD-CBD-CGD-O1D
17	M	406	PGV	O04-C19-C20-C21
17	H	403	PGV	C3-C4-C5-C6
17	J	103	PGV	C24-C25-C26-C27
9	C	405	Z41	C14-C15-C16-O2

There are no ring outliers.

104 monomers are involved in 391 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	7	101	U10	7	0
20	E	101	CRT	4	0
20	R	101	CRT	5	0
17	2	101	PGV	4	0
16	O	102	LMT	2	0
17	R	103	PGV	2	0
13	W	101	BCL	7	0
20	N	101	CRT	7	0
17	H	401	PGV	8	0
13	A	102	BCL	3	0
13	E	102	BCL	6	0
17	B	103	PGV	6	0
13	Y	102	BCL	3	0
13	7	102	BCL	3	0
17	M	406	PGV	3	0
13	O	101	BCL	3	0
13	G	102	BCL	7	0
13	0	102	BCL	7	0
13	6	102	BCL	6	0
17	8	104	PGV	4	0
16	4	105	LMT	1	0
13	V	102	BCL	7	0
13	5	402	BCL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	4	103	PGV	3	0
17	D	101	PGV	2	0
16	H	402	LMT	3	0
13	Q	101	BCL	3	0
15	L	309	U10	4	0
13	N	102	BCL	5	0
17	E	103	PGV	4	0
13	8	103	BCL	8	0
16	D	103	LMT	4	0
17	H	404	PGV	1	0
13	K	101	BCL	4	0
20	T	101	CRT	7	0
20	6	101	CRT	12	0
20	J	101	CRT	5	0
17	T	103	PGV	5	0
20	2	102	CRT	3	0
15	1	102	U10	2	0
13	Z	102	BCL	5	0
9	C	405	Z41	1	0
13	D	102	BCL	3	0
15	D	104	U10	3	0
17	M	410	PGV	2	0
16	7	103	LMT	7	0
17	K	102	PGV	4	0
20	G	101	CRT	4	0
17	0	103	PGV	7	0
16	P	104	LMT	2	0
16	K	103	LMT	1	0
13	I	101	BCL	6	0
17	H	403	PGV	2	0
20	P	101	CRT	4	0
13	1	101	BCL	4	0
13	L	310	BCL	4	0
16	L	305	LMT	2	0
13	T	102	BCL	8	0
13	U	102	BCL	5	0
16	5	401	LMT	4	0
14	L	303	BPH	1	0
17	2	104	PGV	4	0
20	8	102	CRT	7	0
17	P	103	PGV	3	0
13	J	102	BCL	3	0

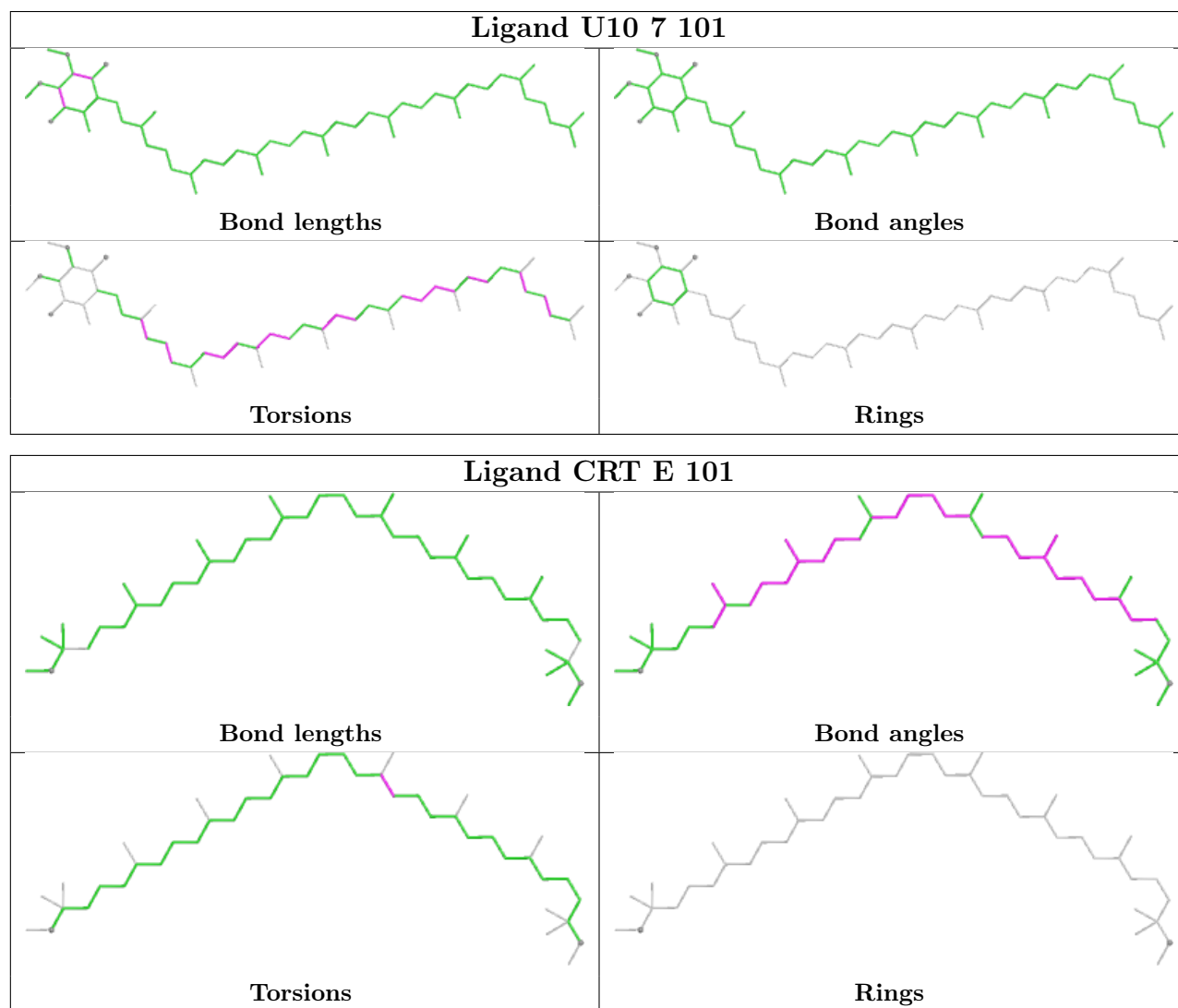
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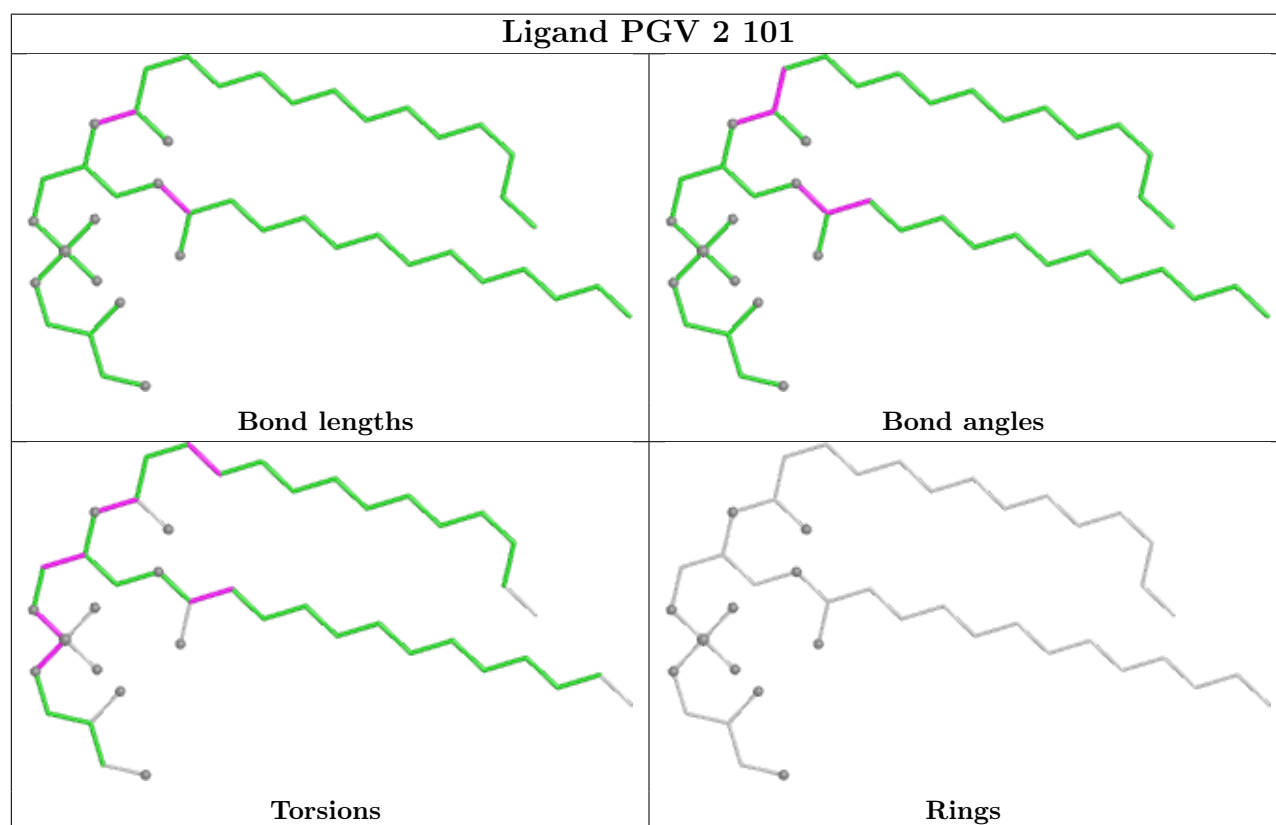
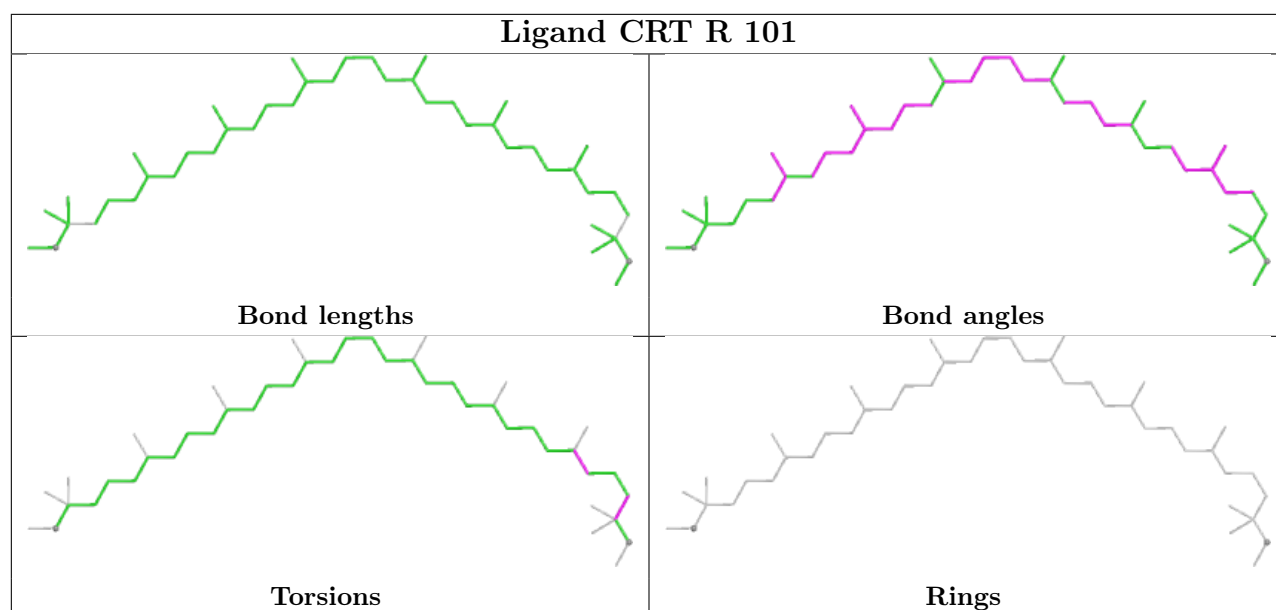
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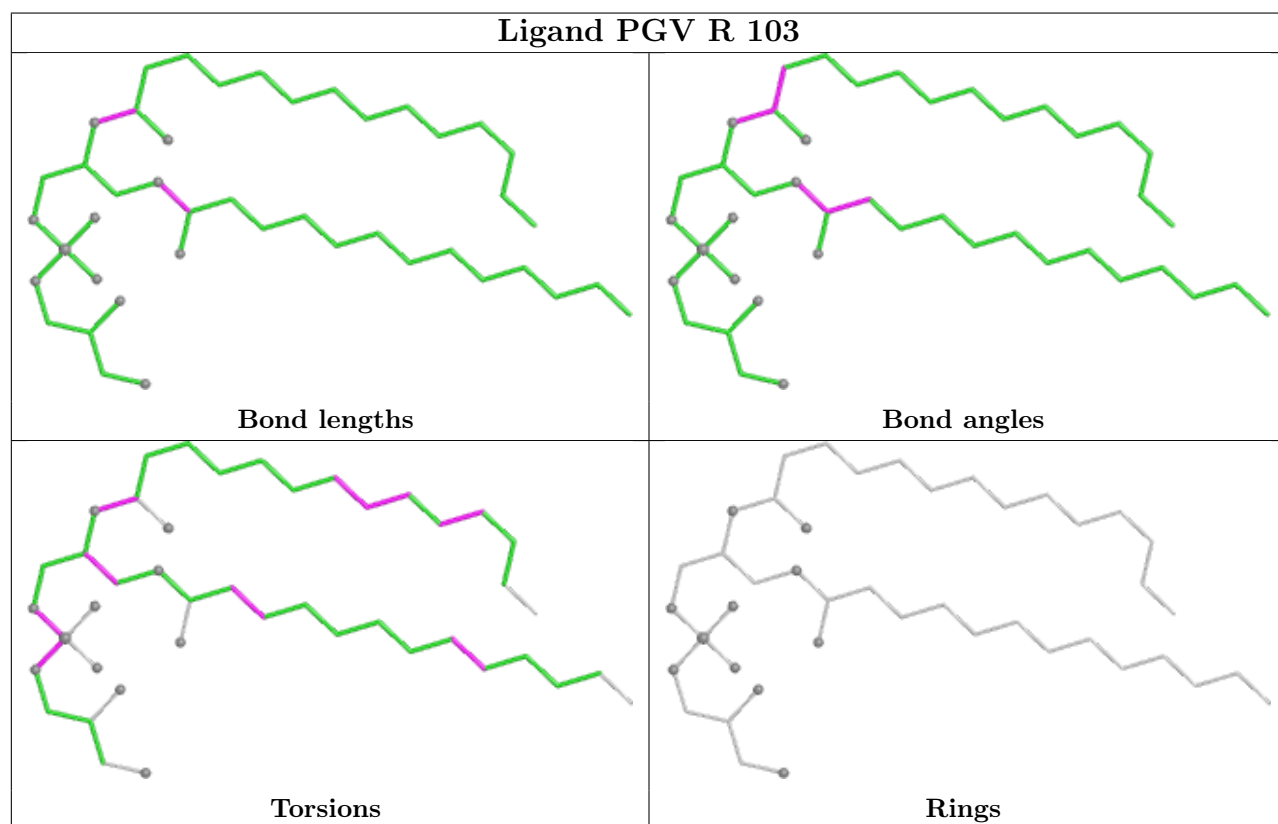
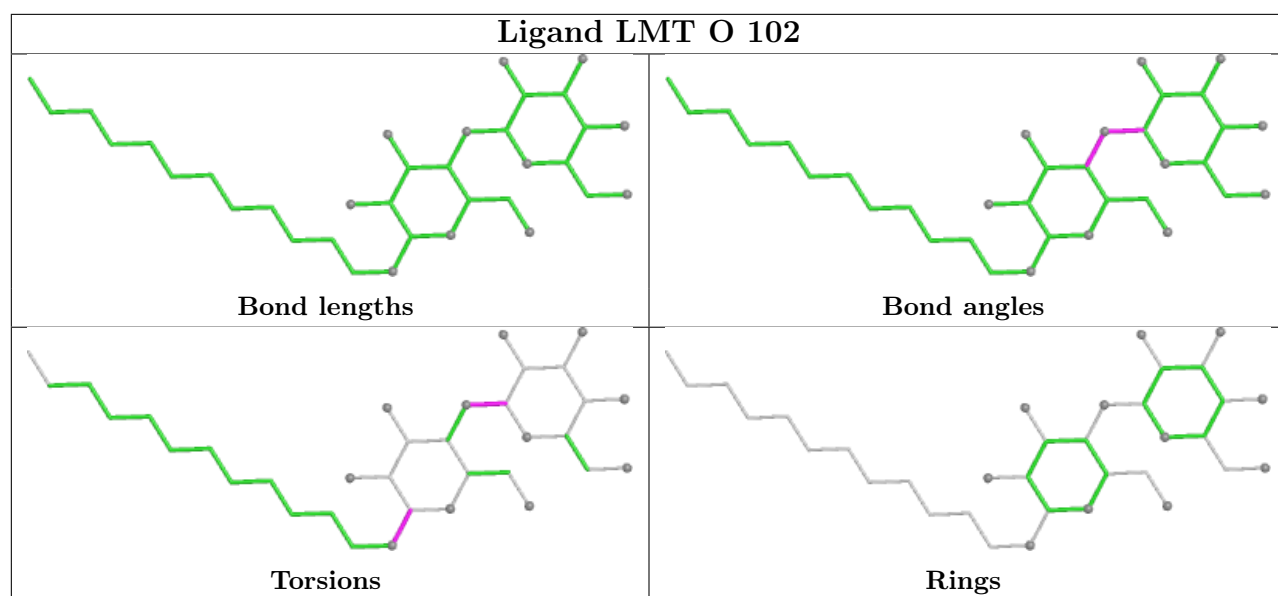
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	402	BCL	9	0
16	Z	104	LMT	1	0
13	4	102	BCL	4	0
13	B	102	BCL	7	0
15	Y	103	U10	3	0
17	J	103	PGV	5	0
20	0	101	CRT	3	0
13	9	101	BCL	5	0
17	A	101	PGV	2	0
17	N	103	PGV	3	0
7	C	401	HEM	8	0
13	L	302	BCL	4	0
13	S	101	BCL	3	0
15	L	308	U10	4	0
17	X	102	PGV	5	0
20	4	101	CRT	5	0
13	R	102	BCL	5	0
17	L	307	PGV	6	0
15	L	304	U10	9	0
20	M	405	CRT	5	0
17	G	103	PGV	2	0
16	4	104	LMT	2	0
13	P	102	BCL	6	0
13	X	101	BCL	7	0
13	2	103	BCL	5	0
8	C	403	HEC	3	0
16	M	409	LMT	3	0
20	Z	101	CRT	4	0
20	B	101	CRT	4	0
14	M	403	BPH	5	0
16	X	103	LMT	1	0
20	Y	101	CRT	5	0
17	M	407	PGV	1	0
13	L	311	BCL	2	0
20	V	101	CRT	11	0
13	F	101	BCL	5	0
13	3	101	BCL	4	0
17	V	103	PGV	5	0
17	8	101	PGV	6	0

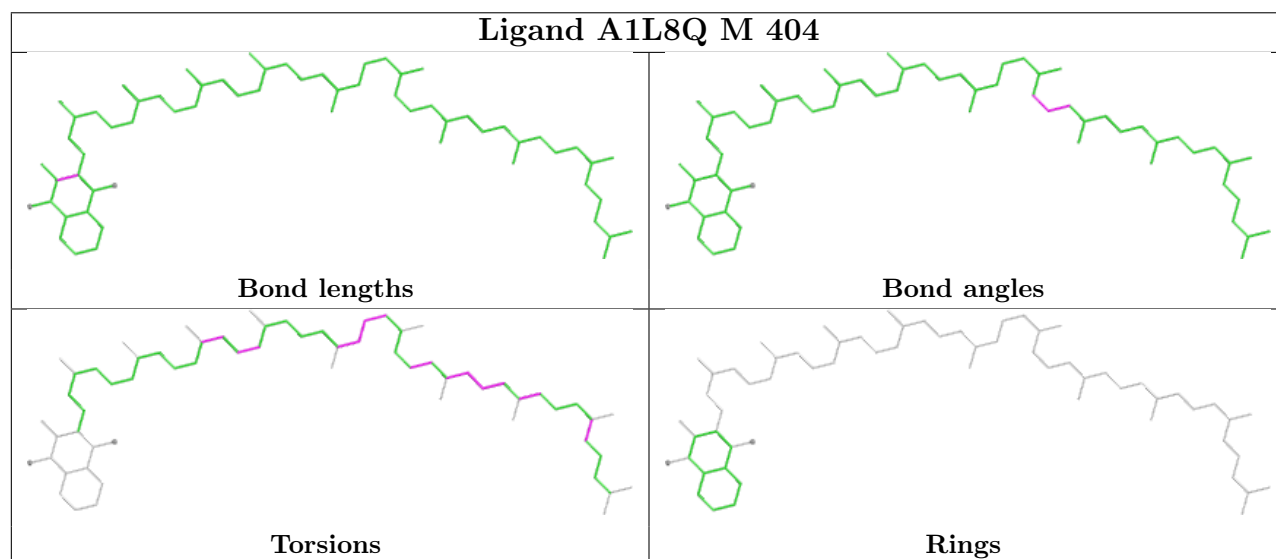
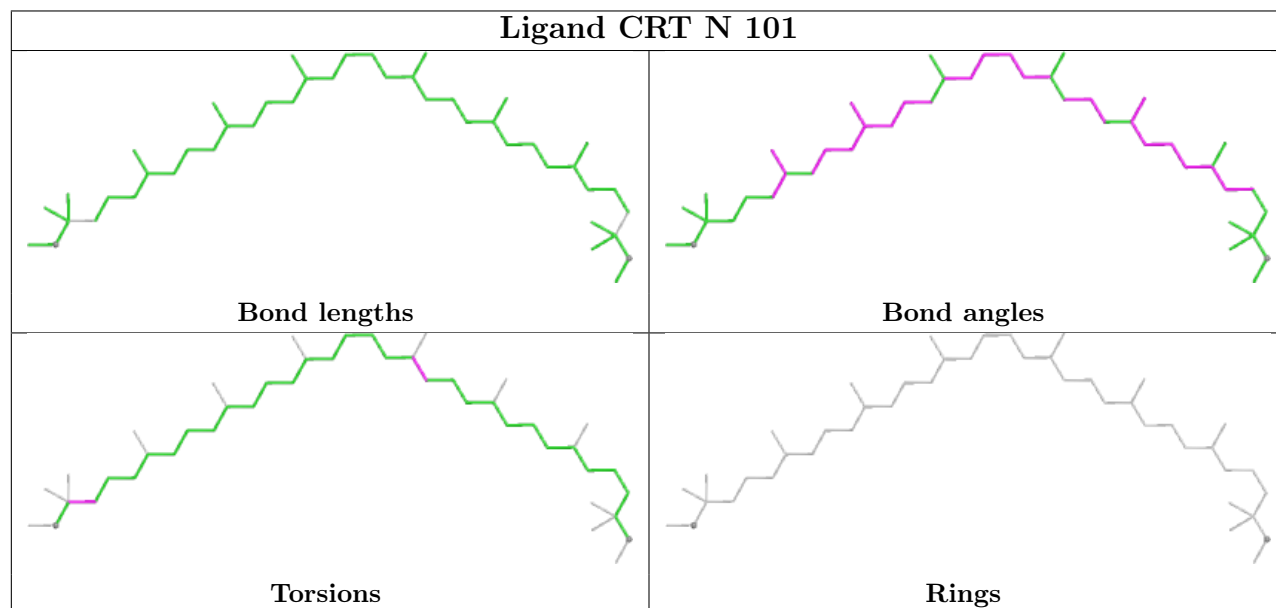
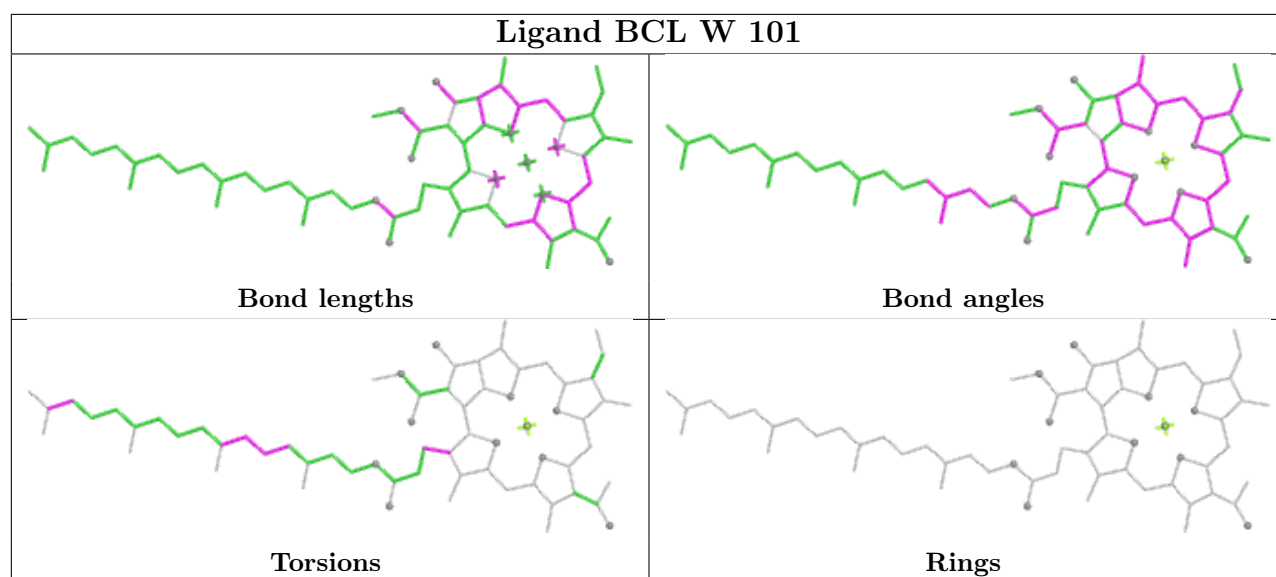
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

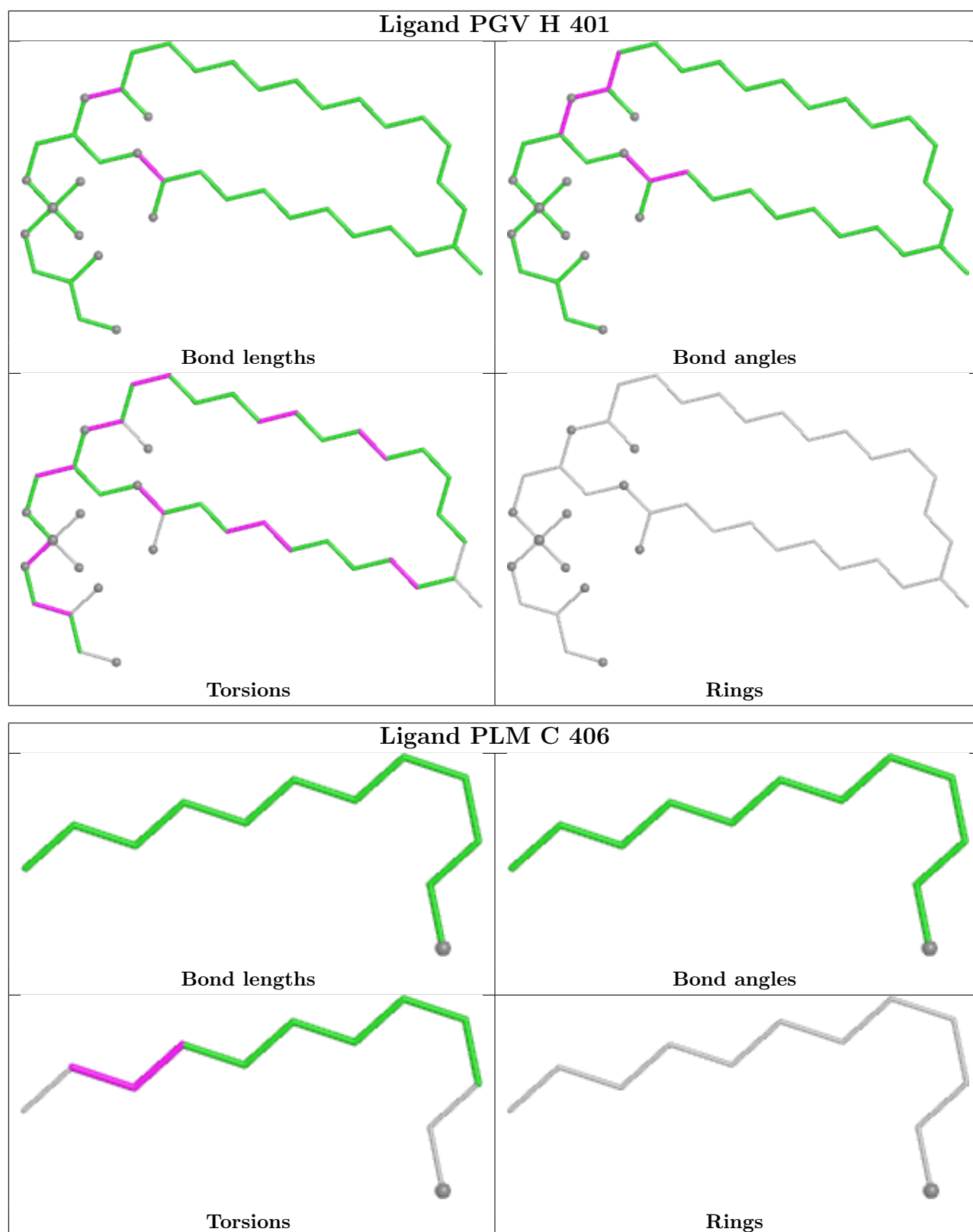
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

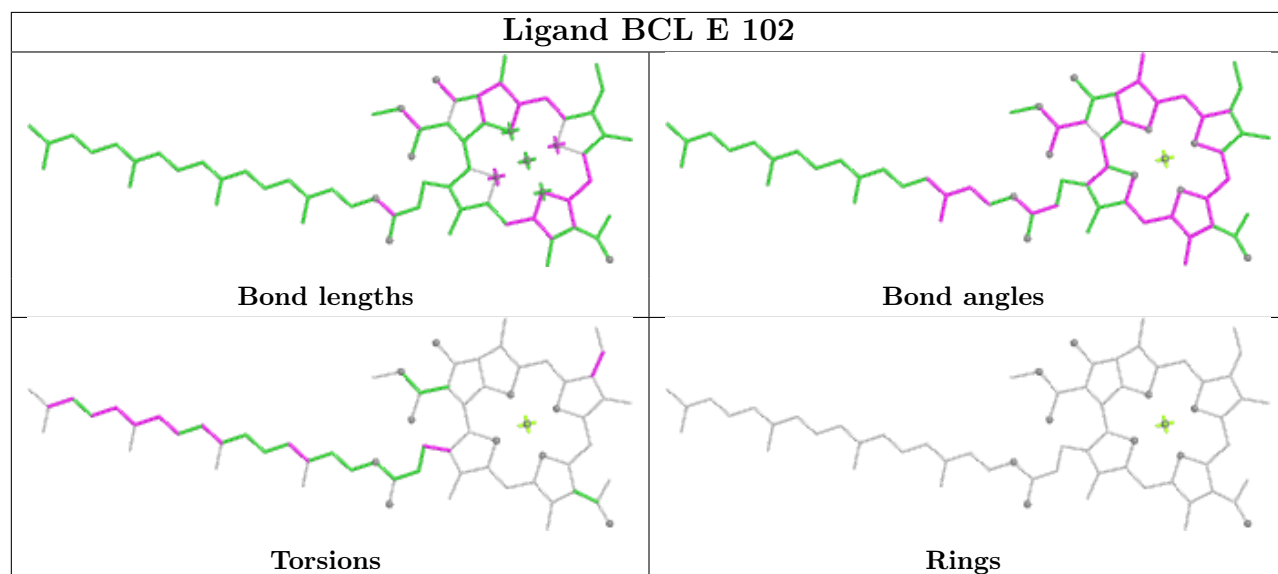
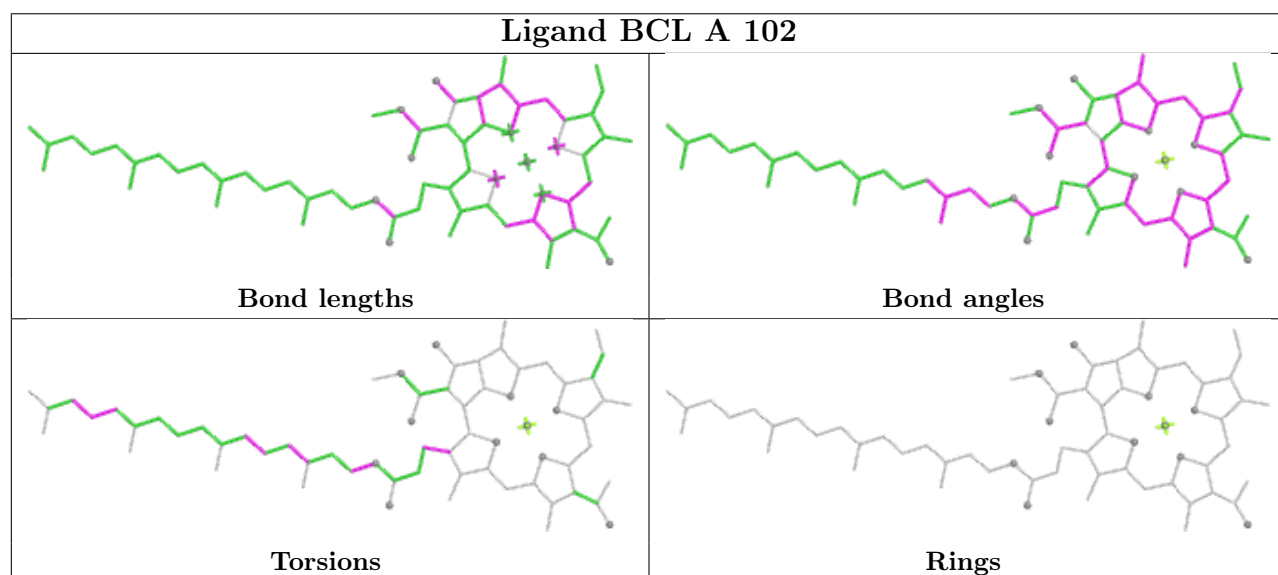
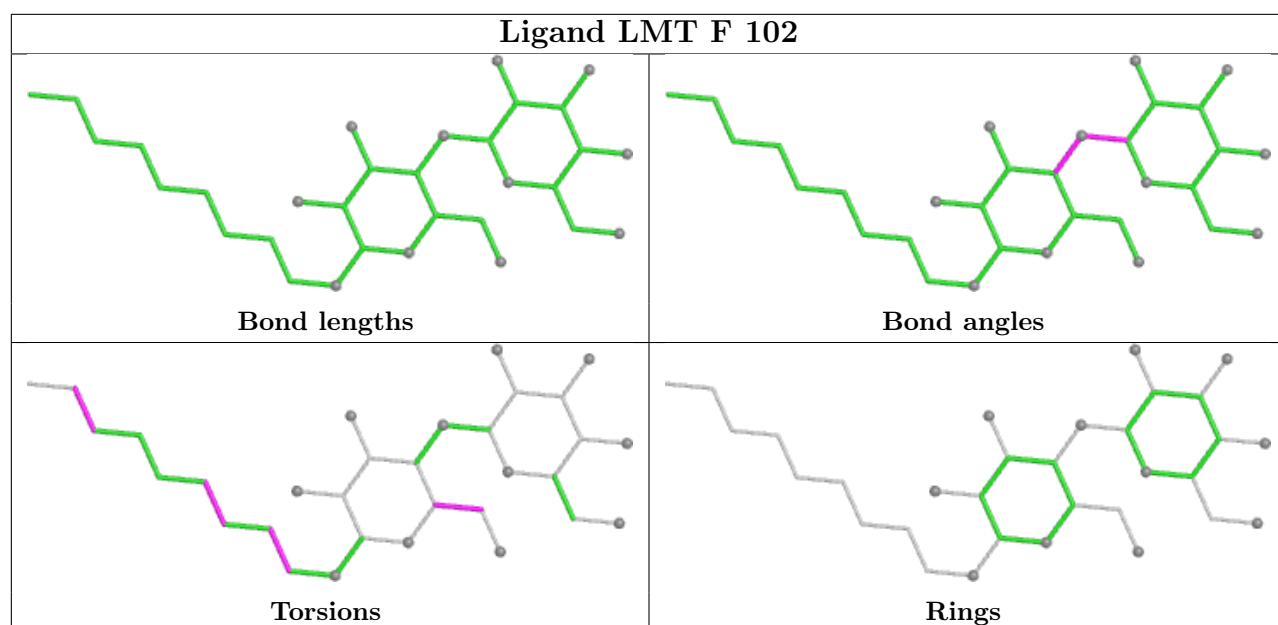


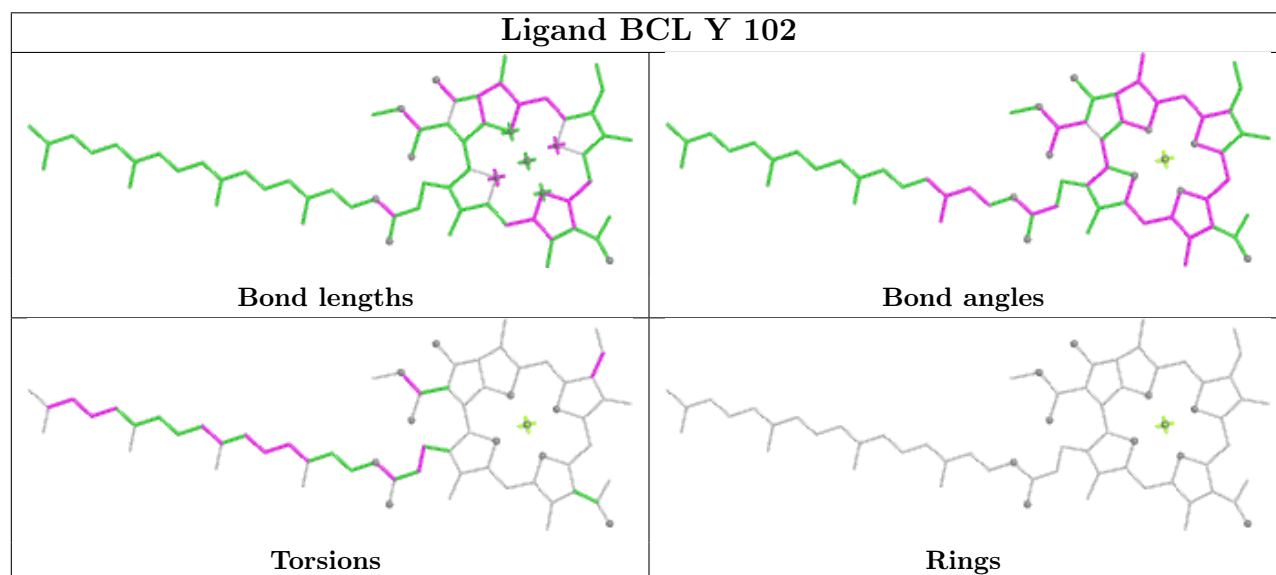
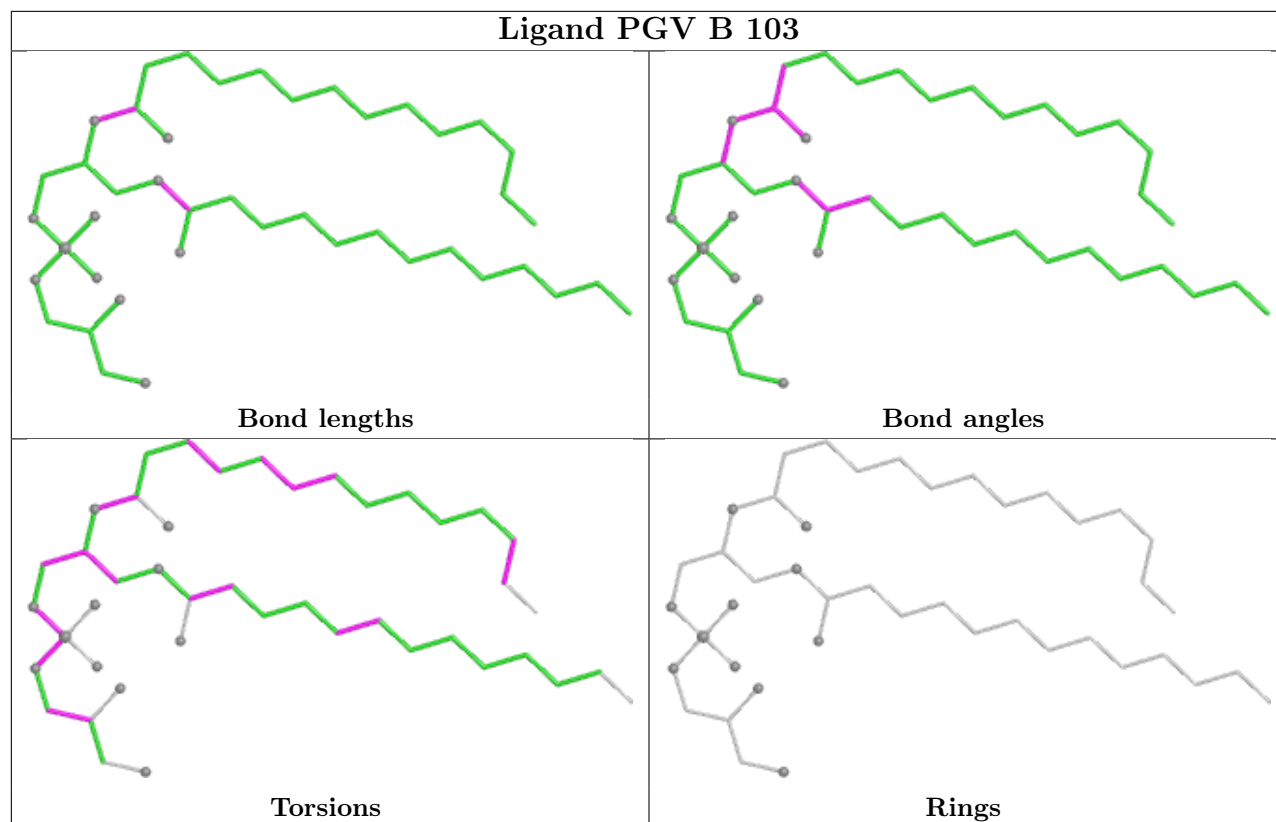


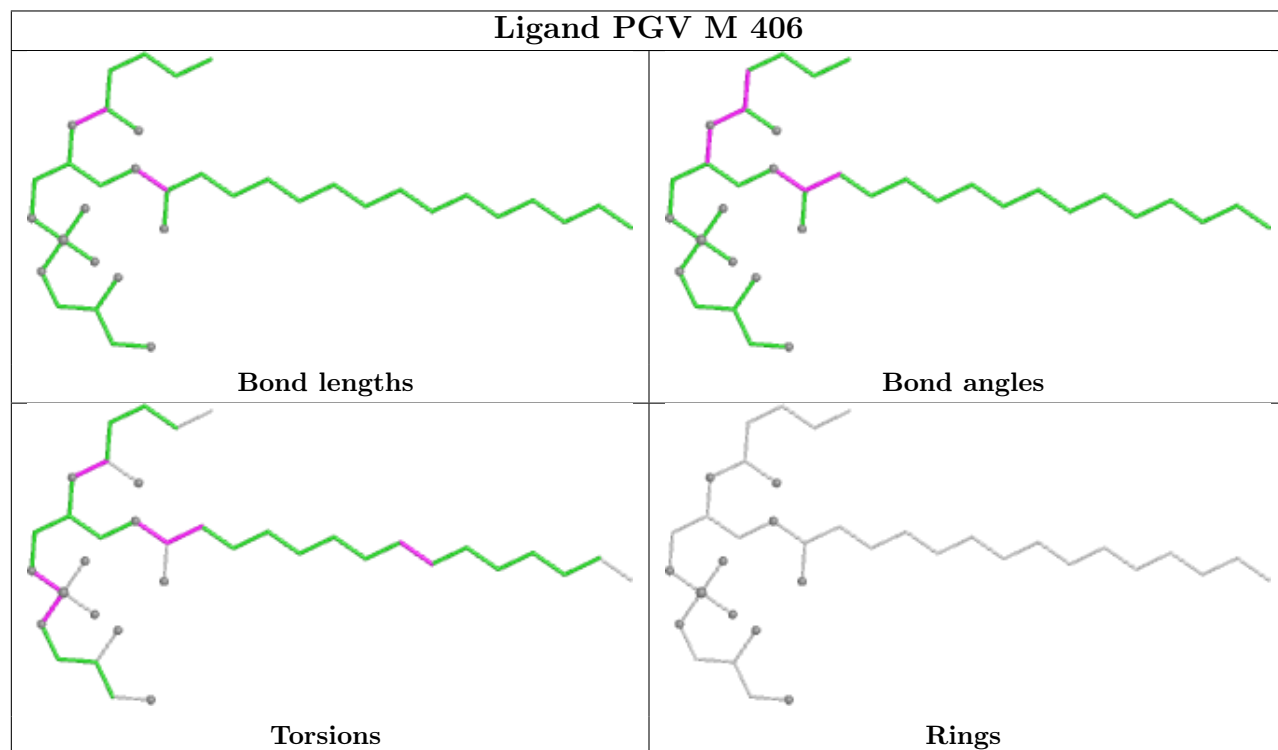
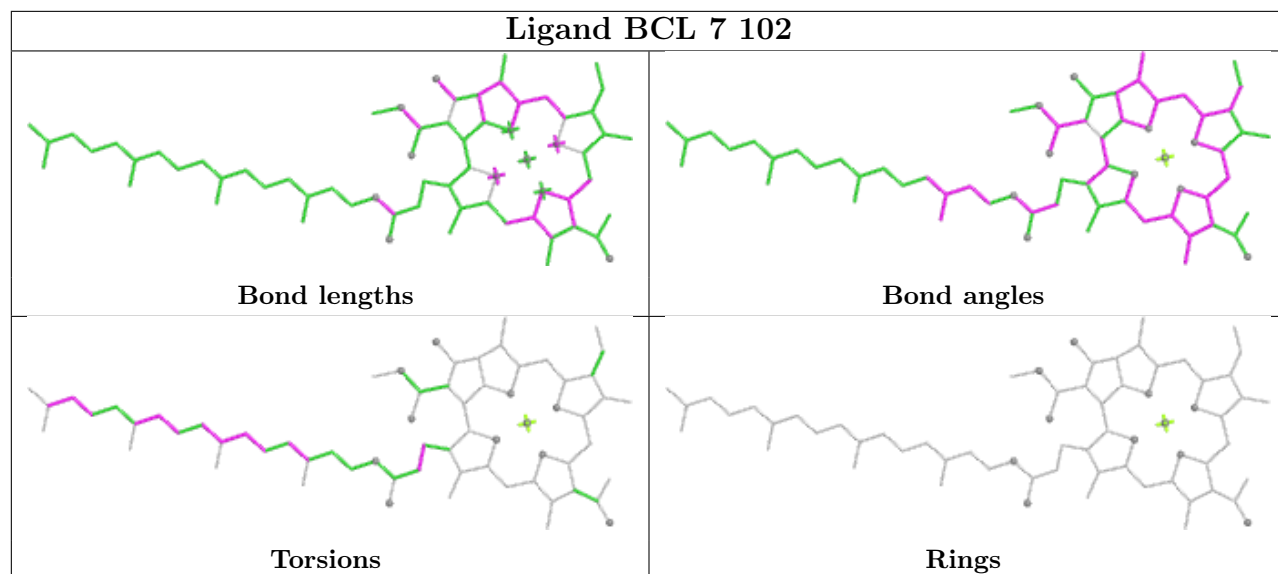


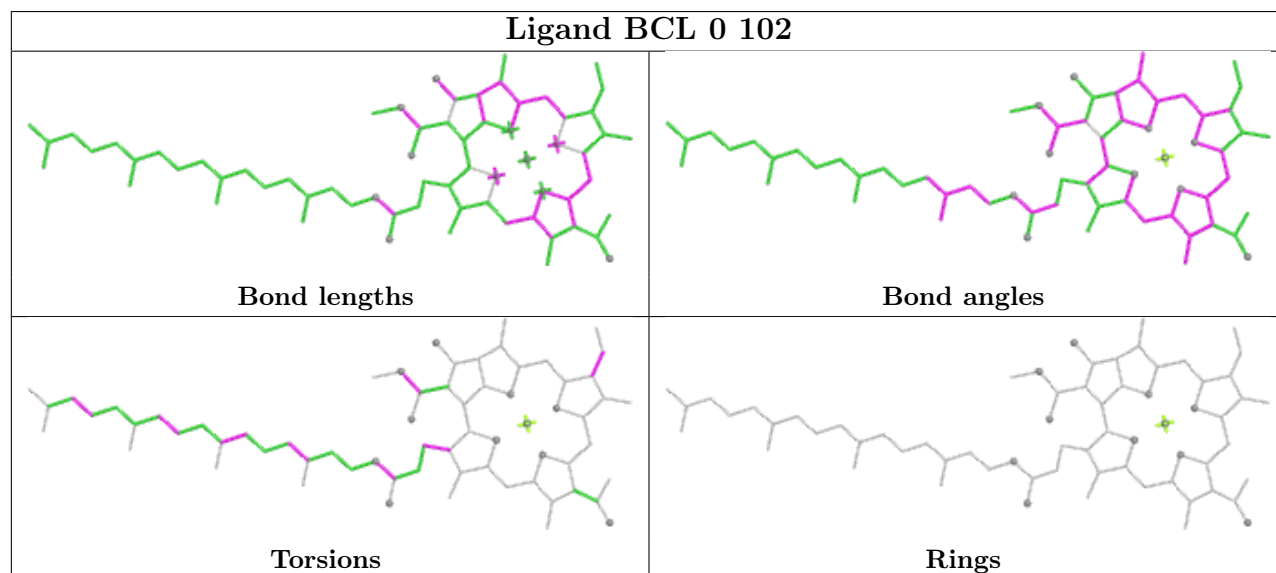
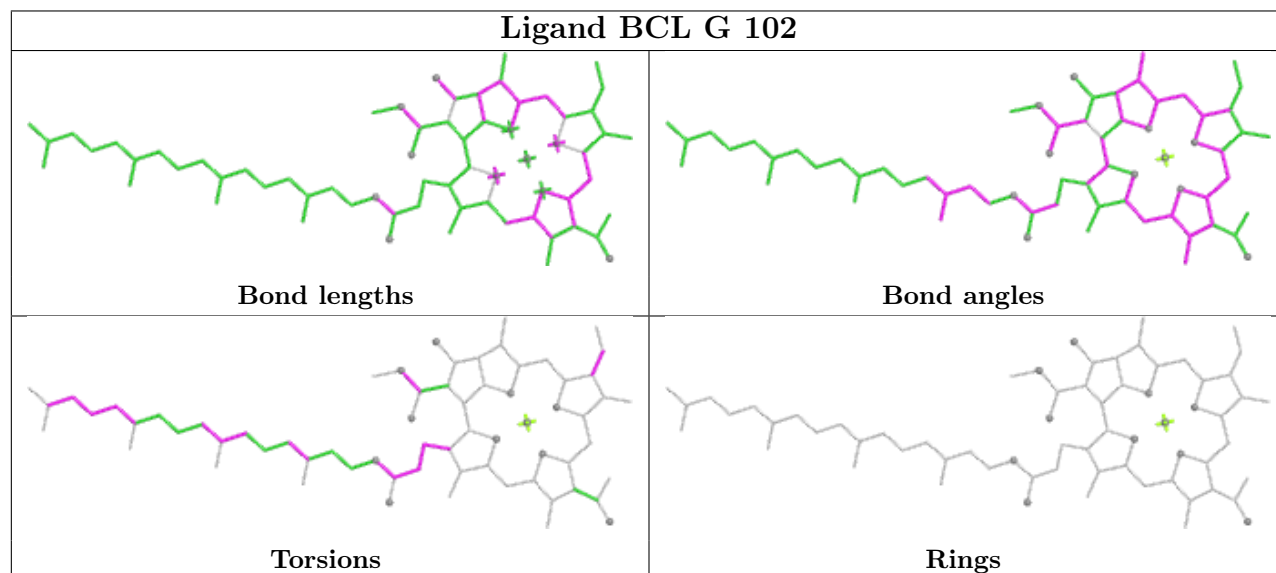
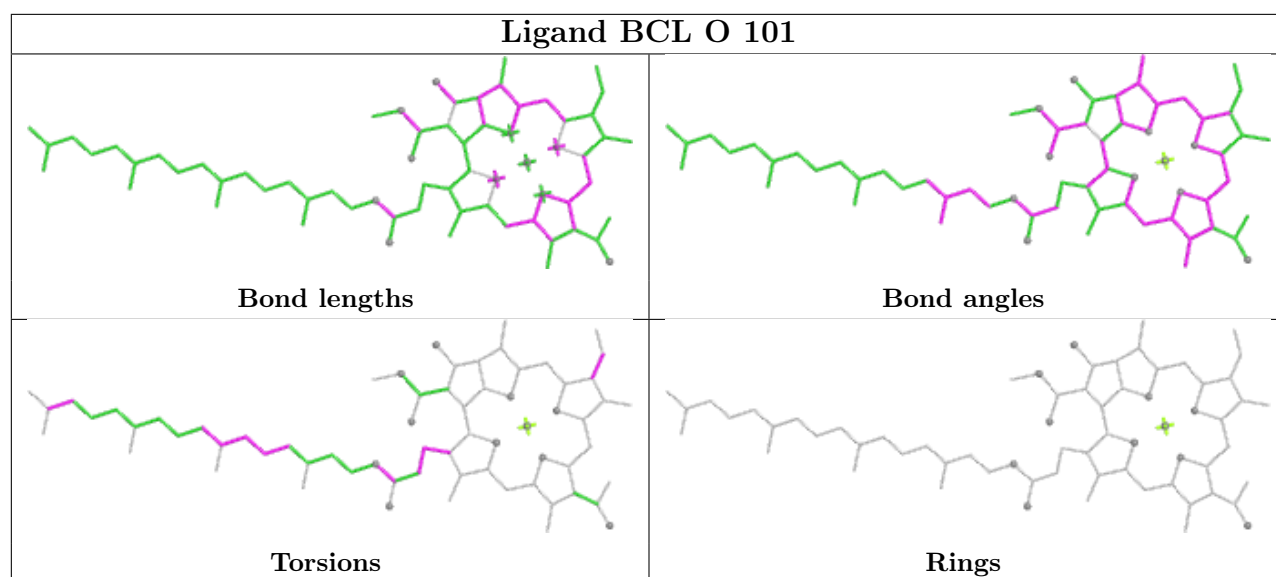


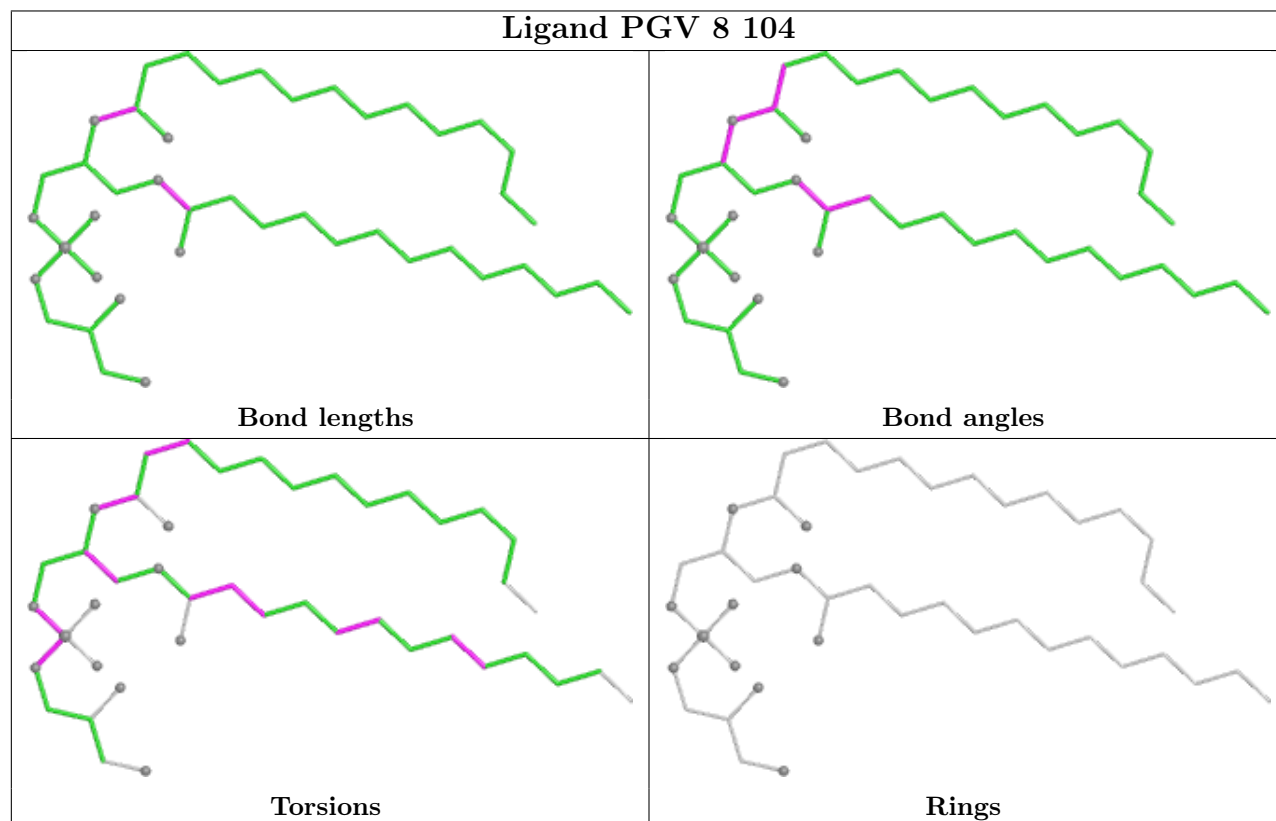
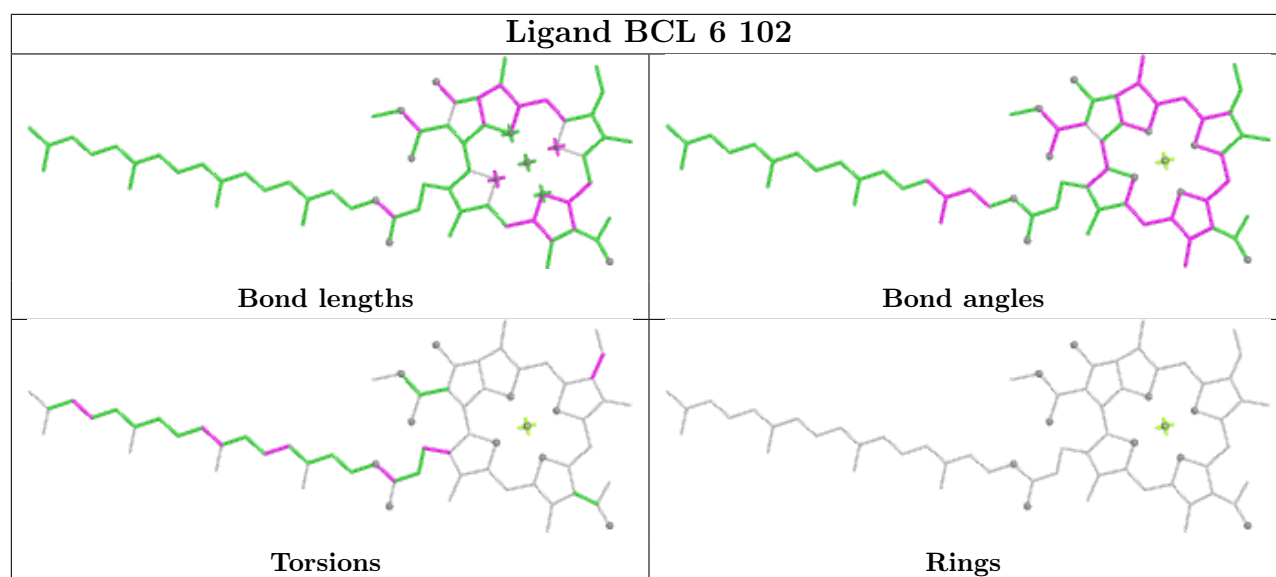


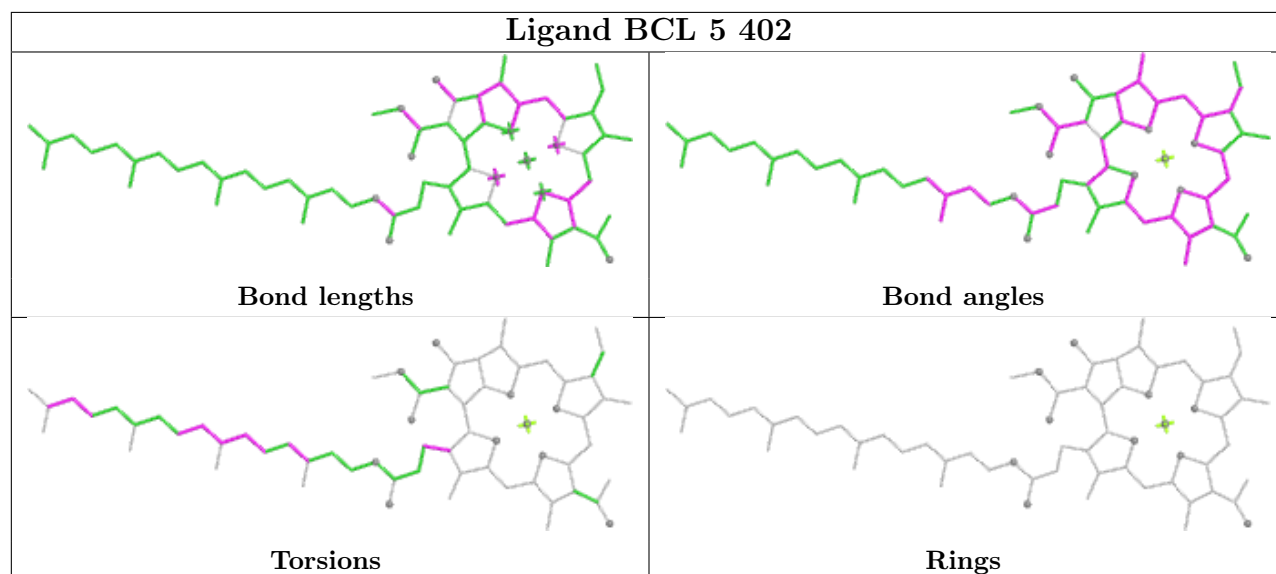
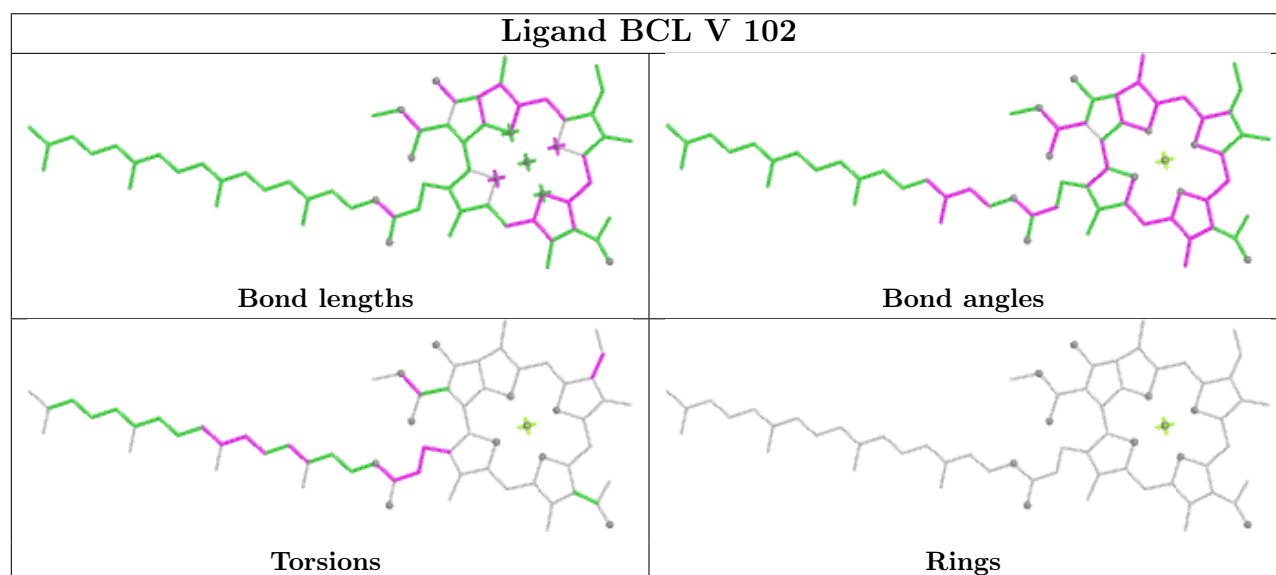
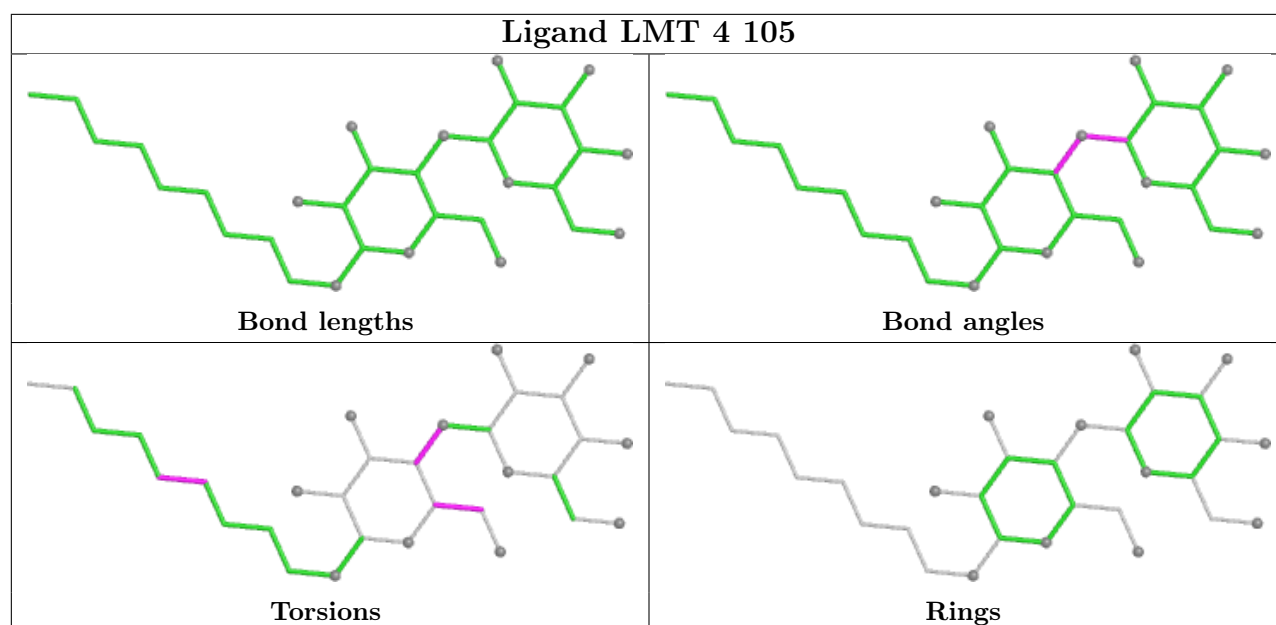


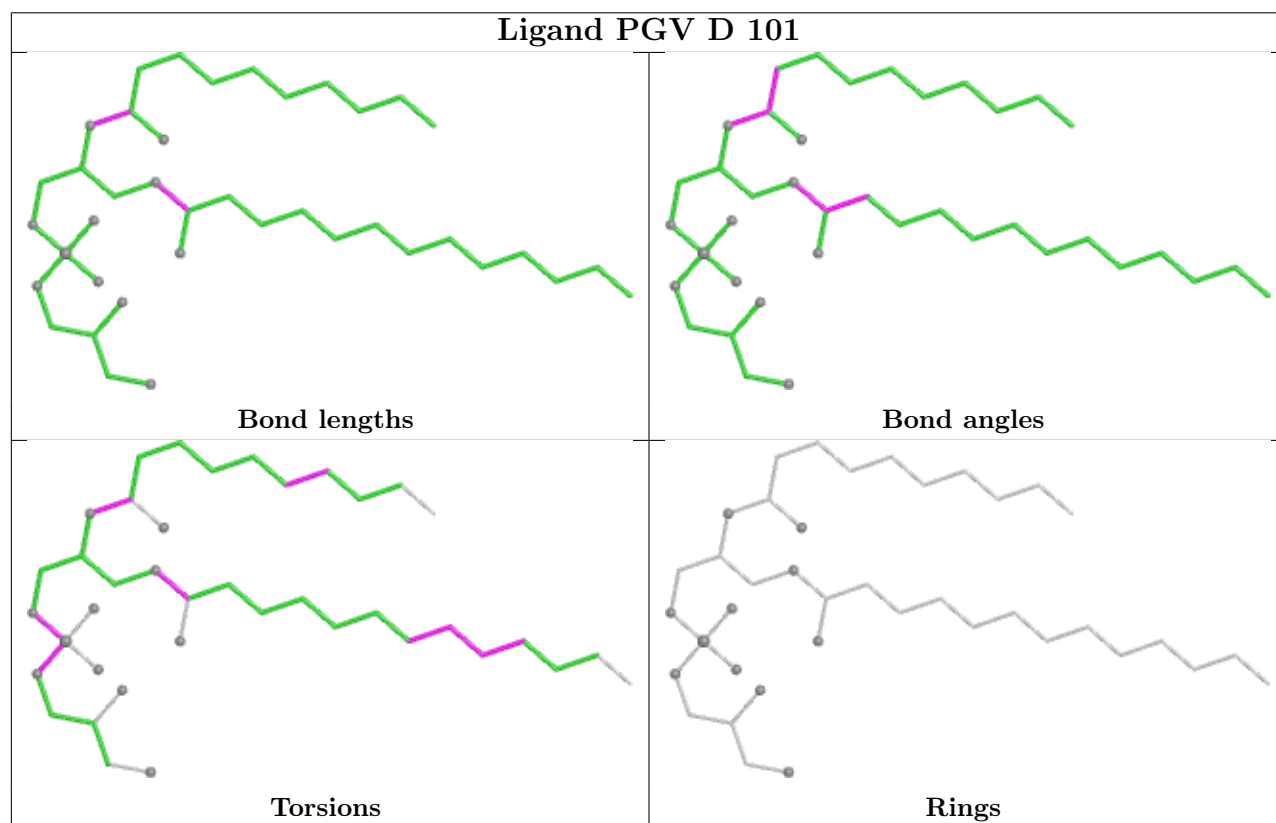
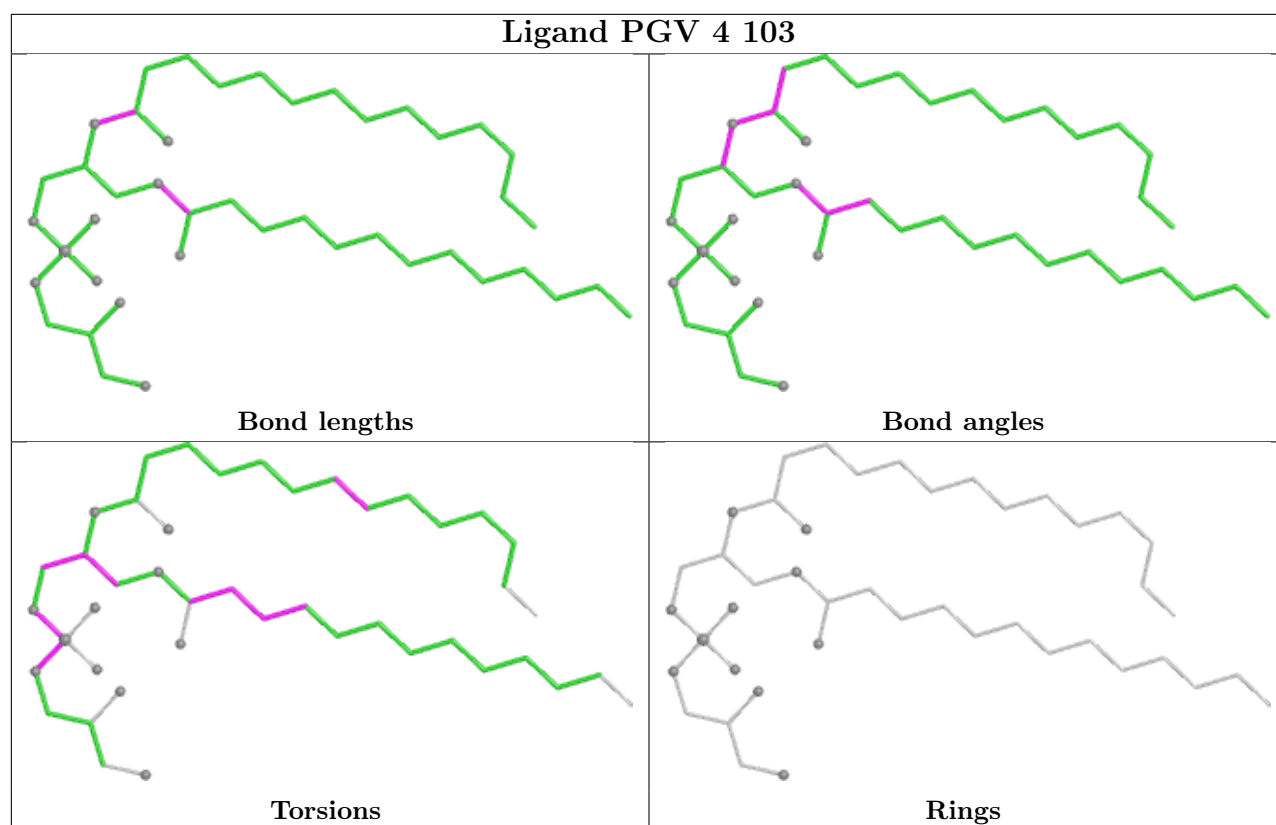


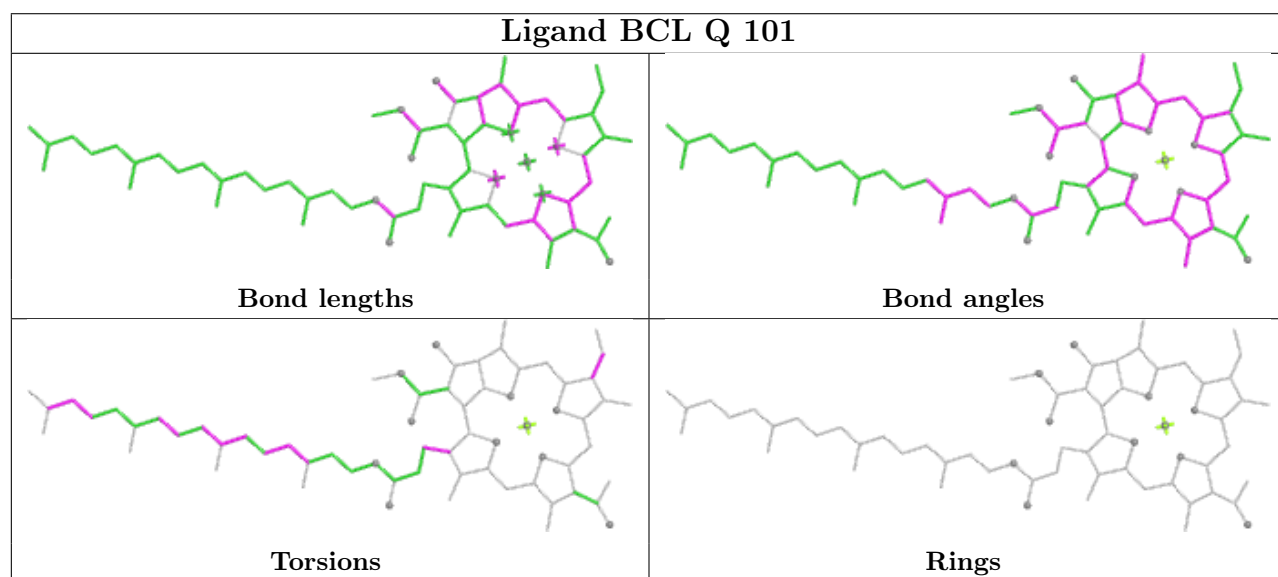
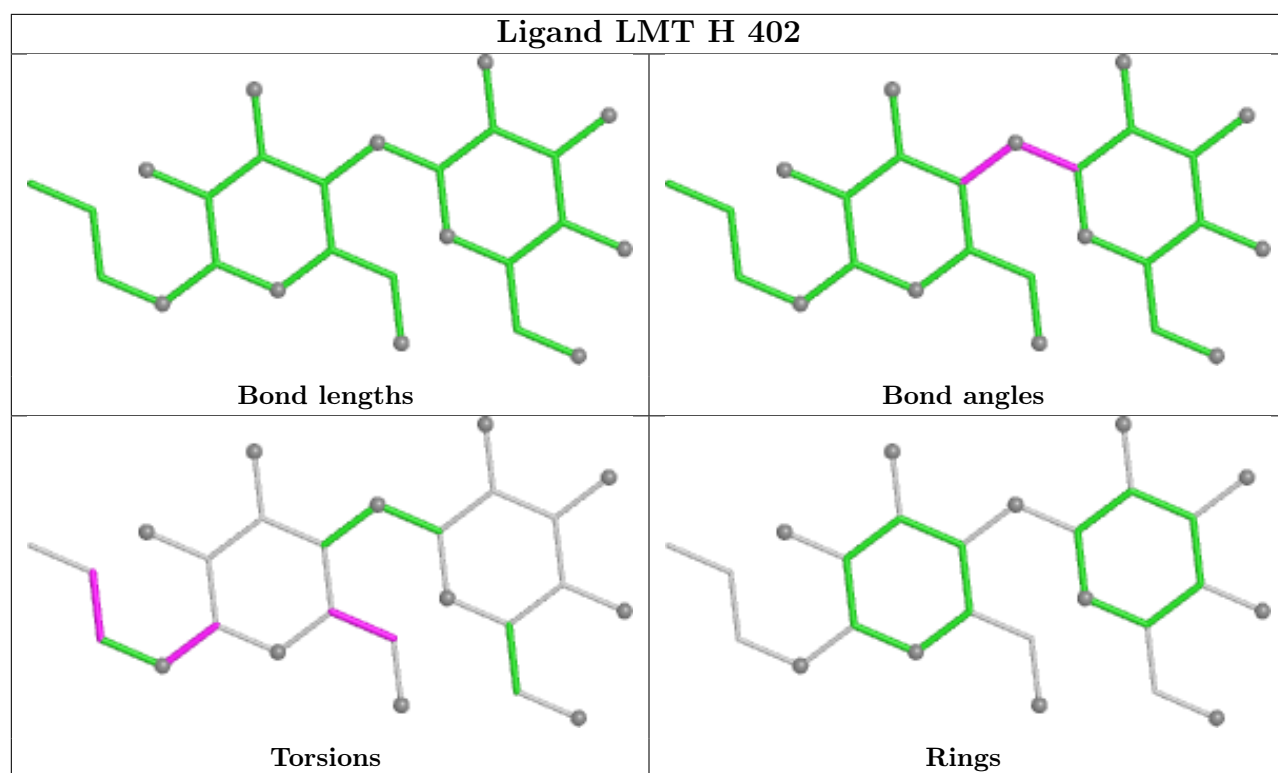


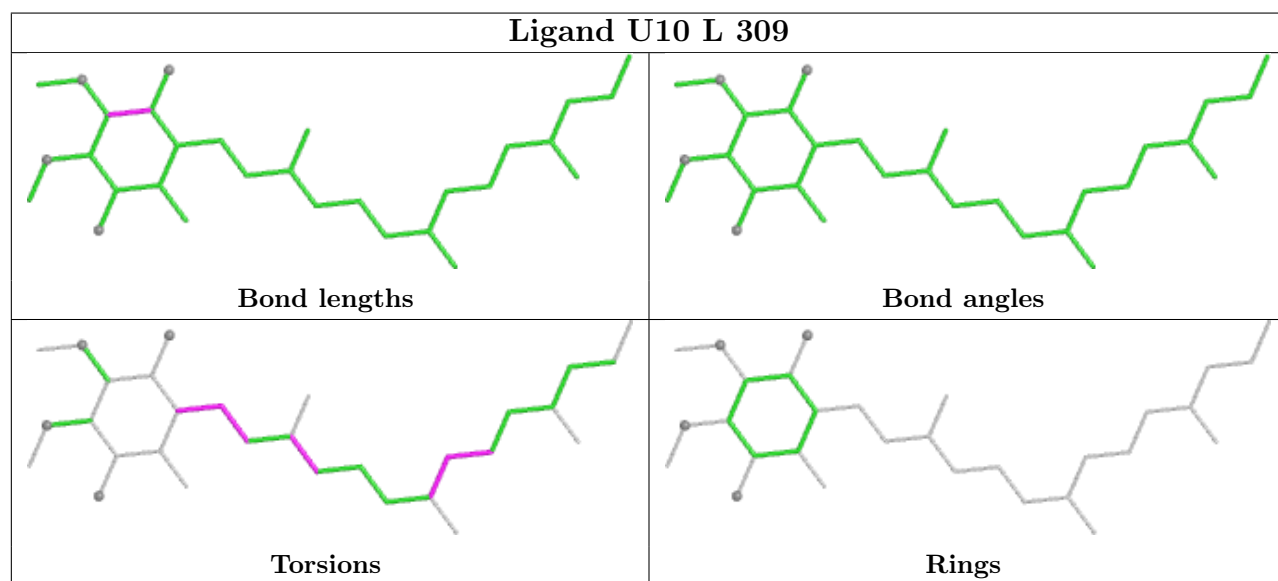
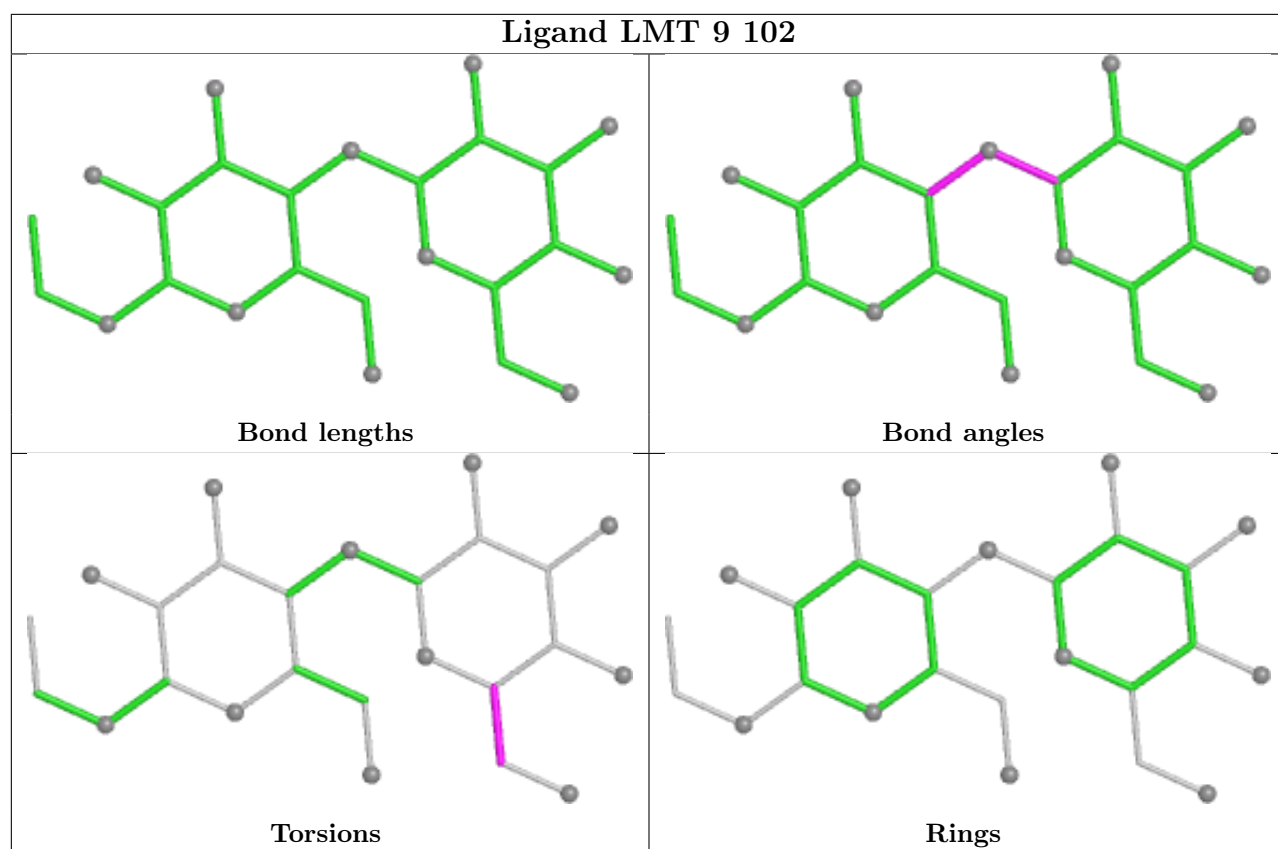


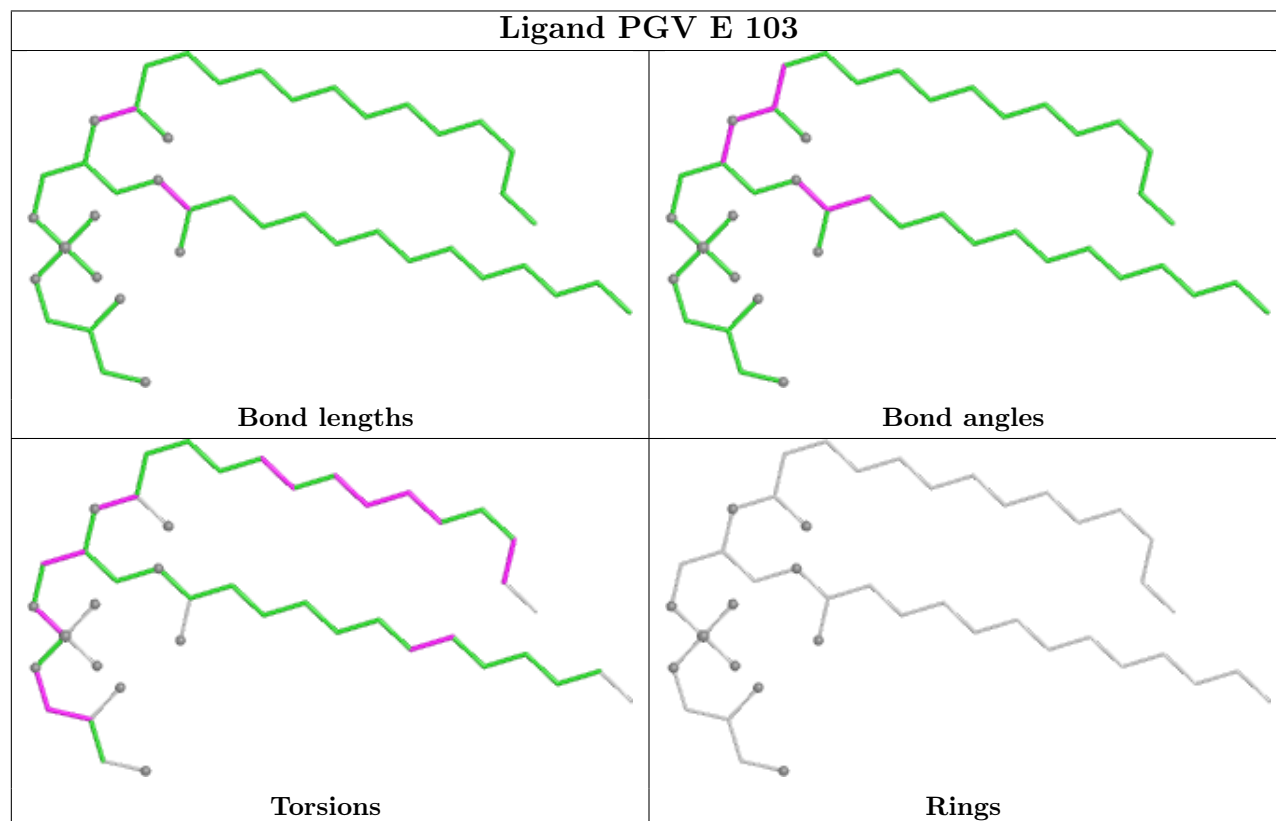
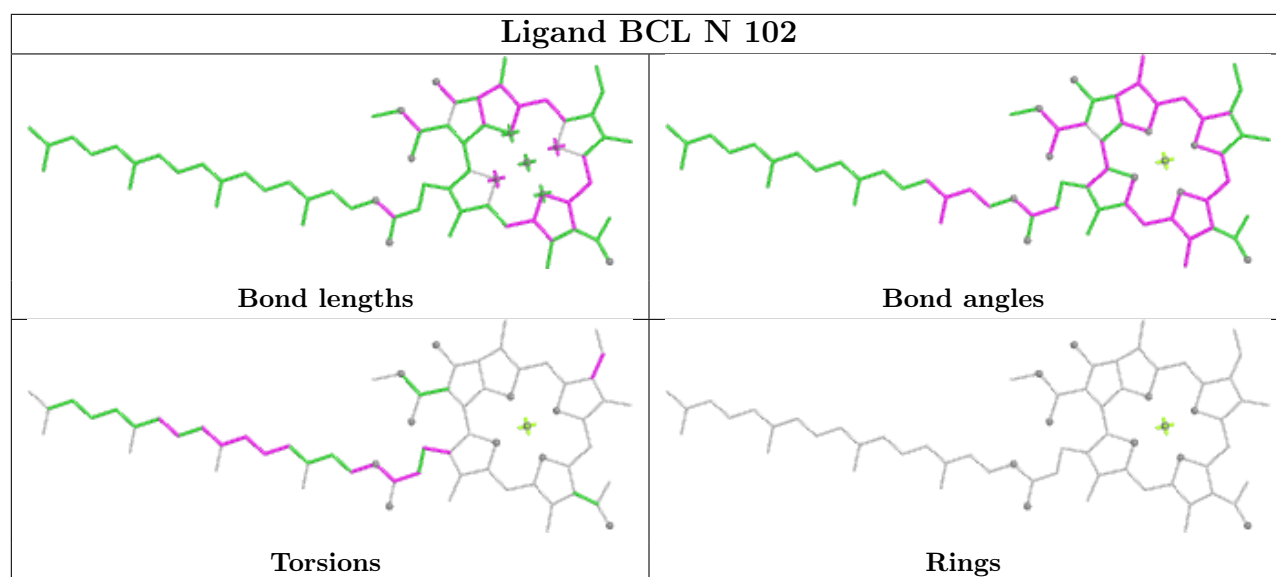


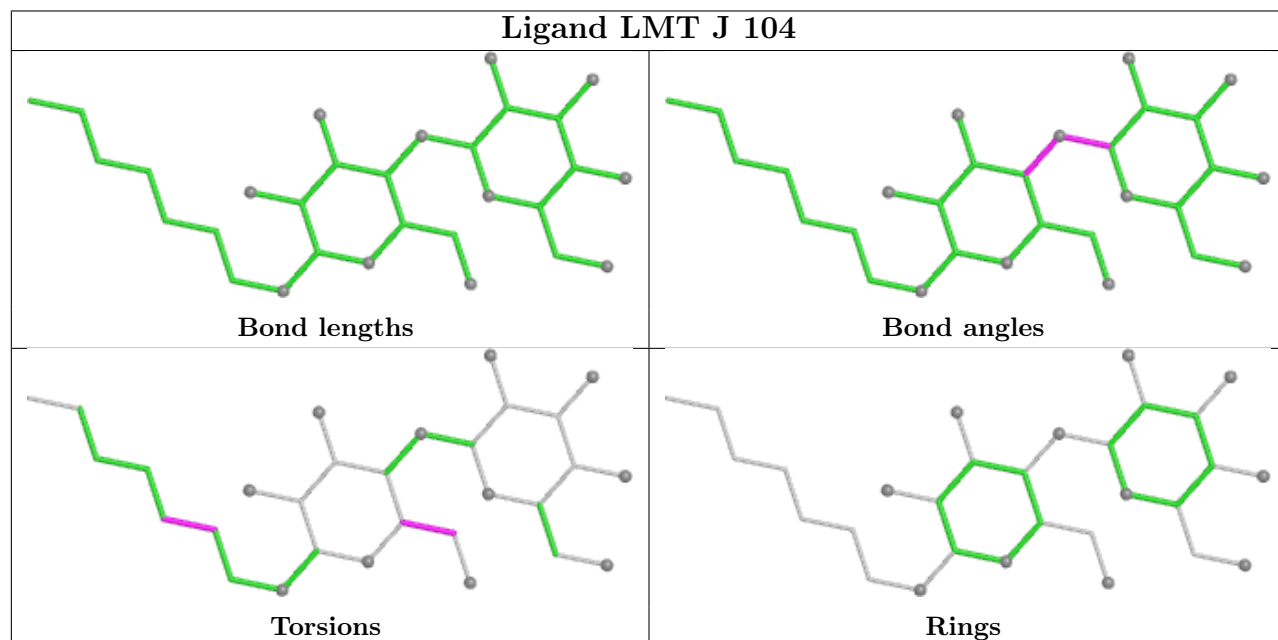
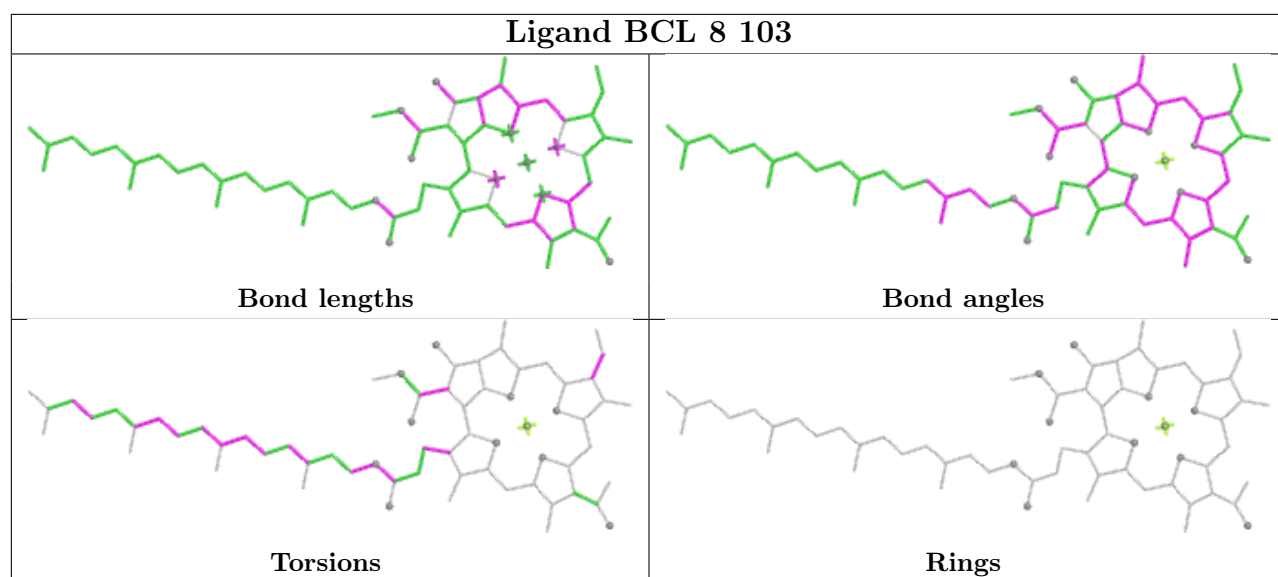


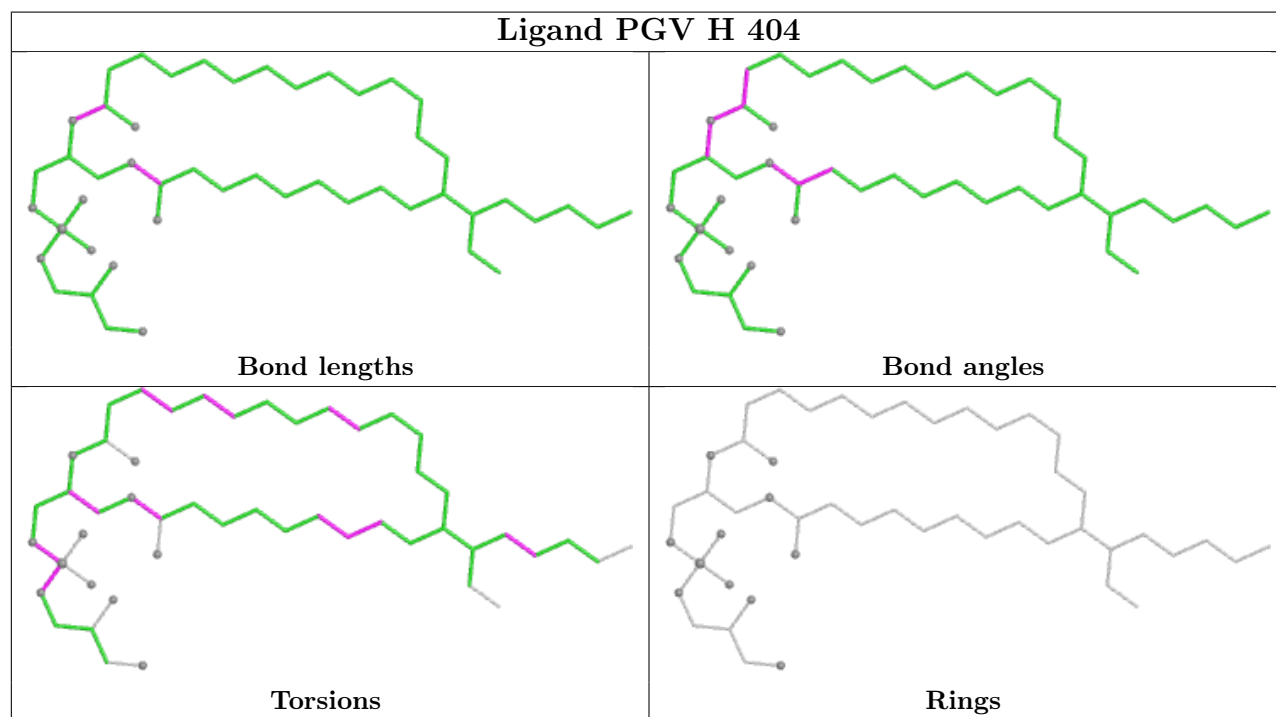
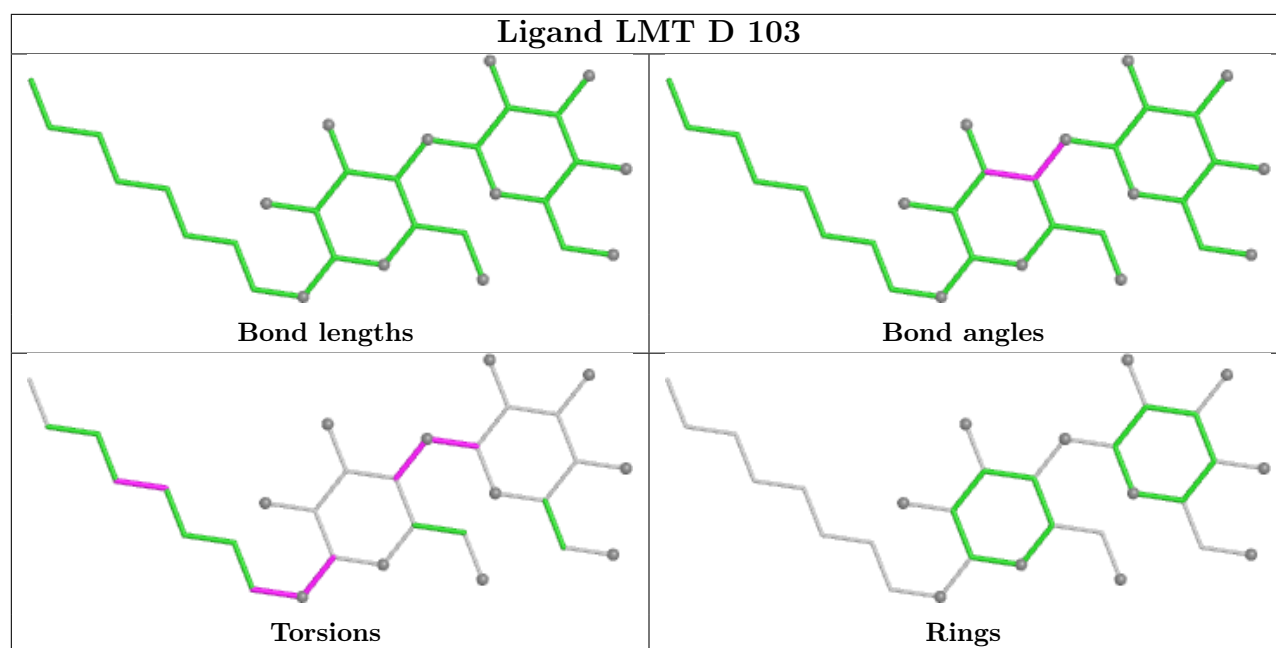


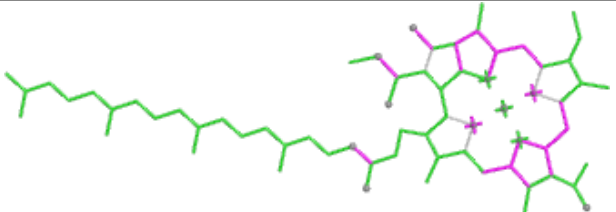
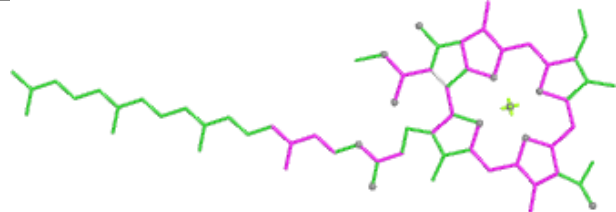
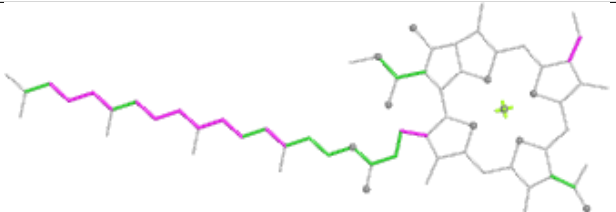
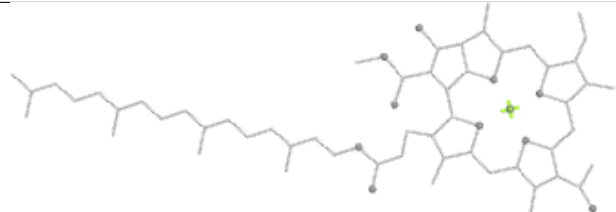


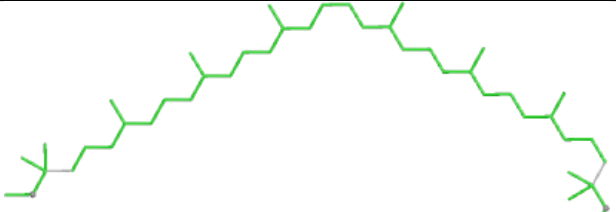
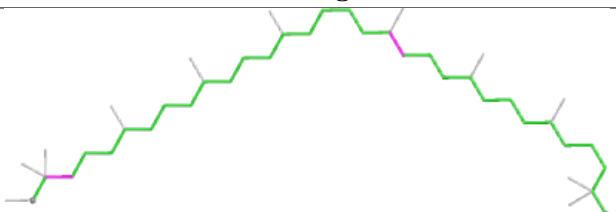
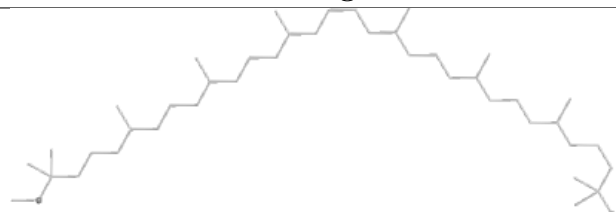


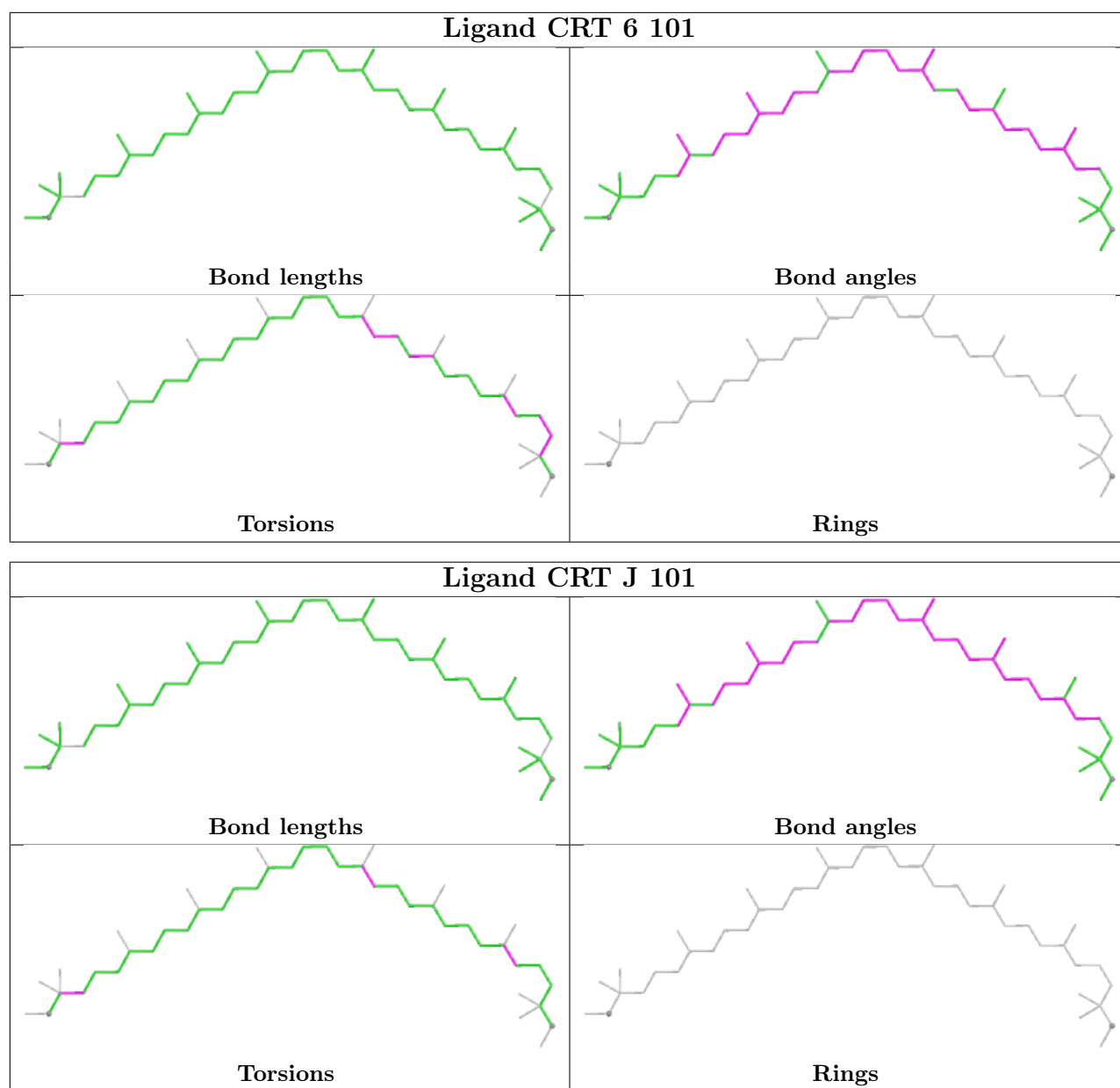


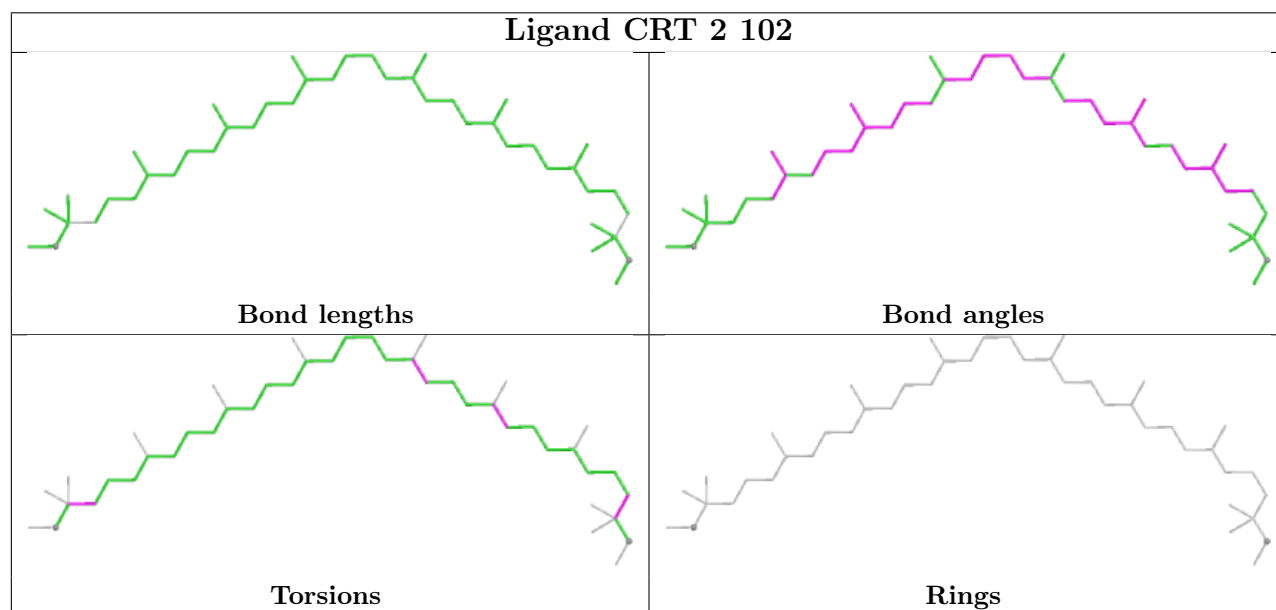
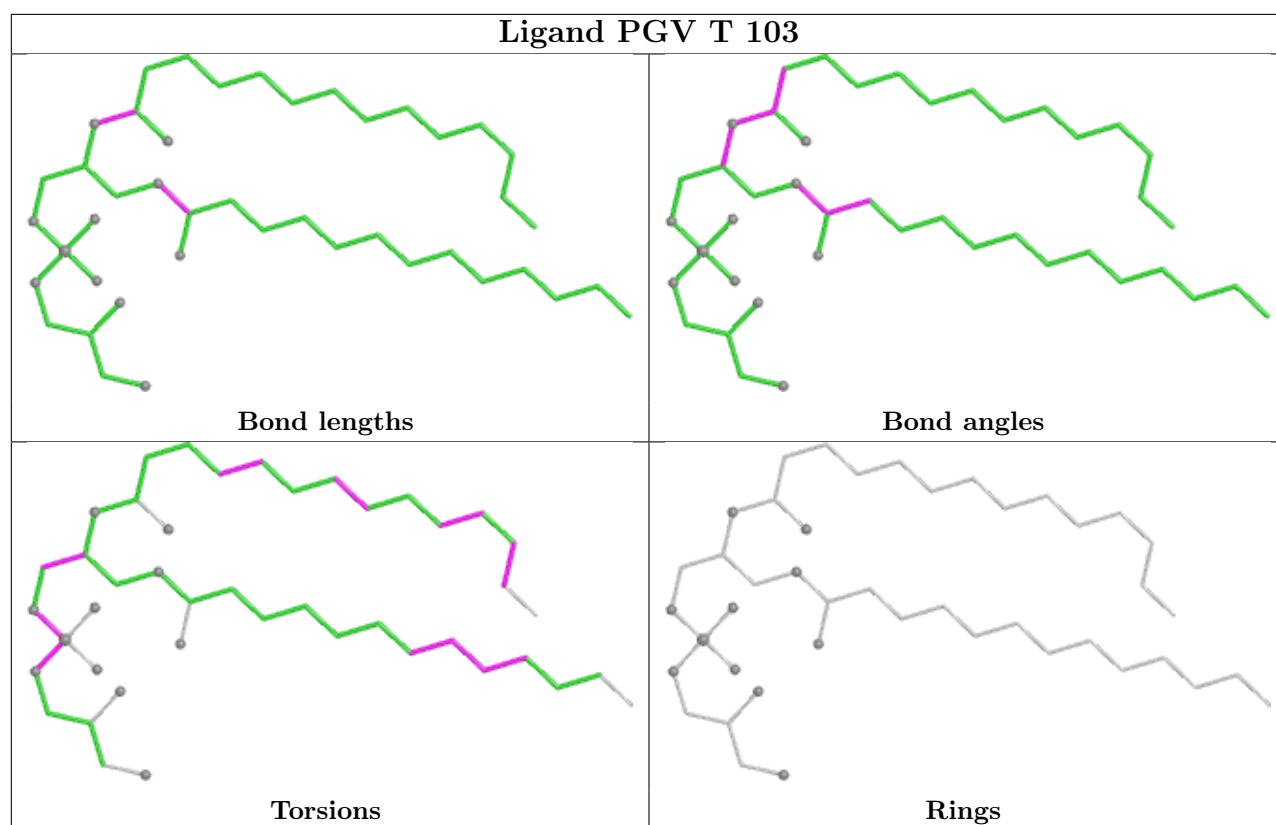


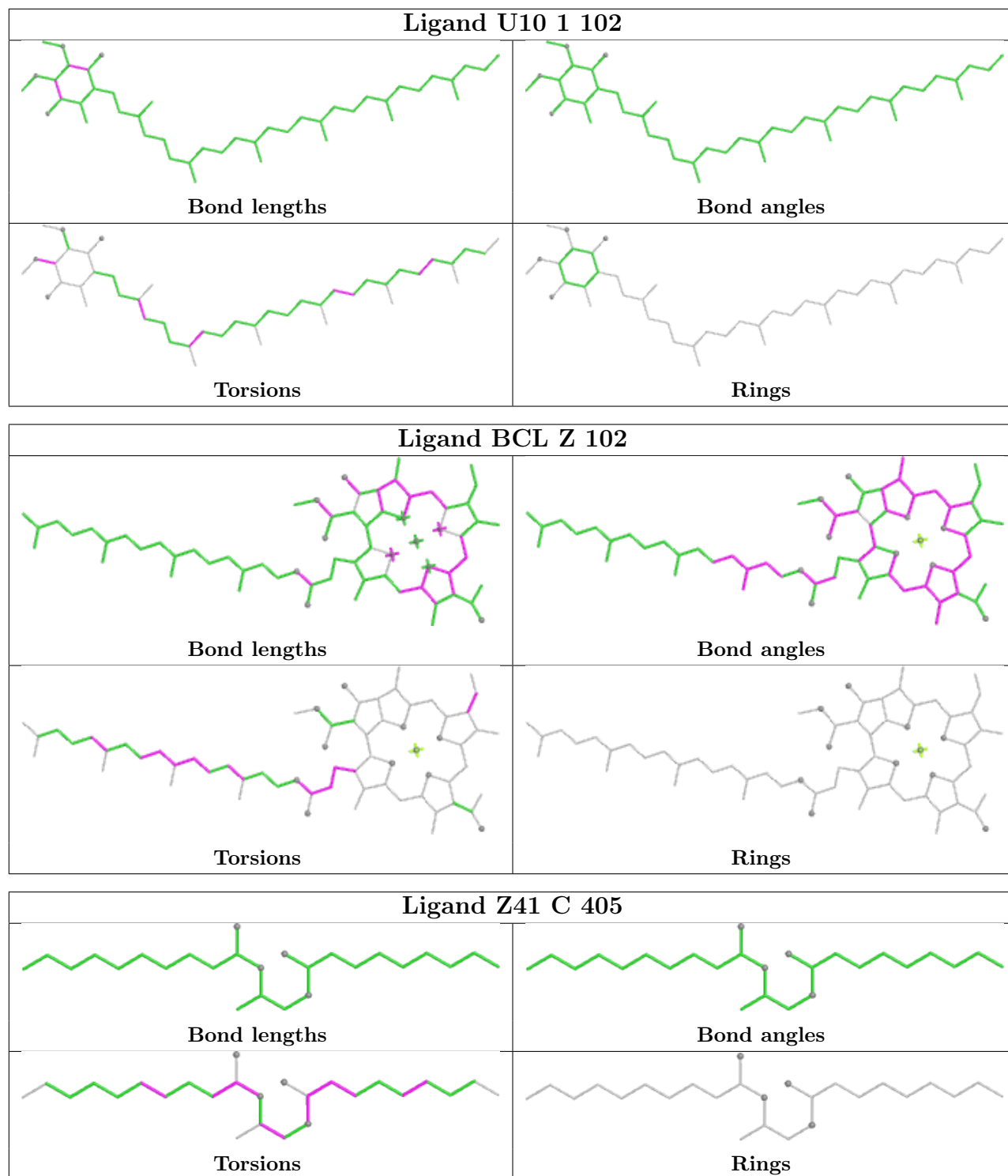


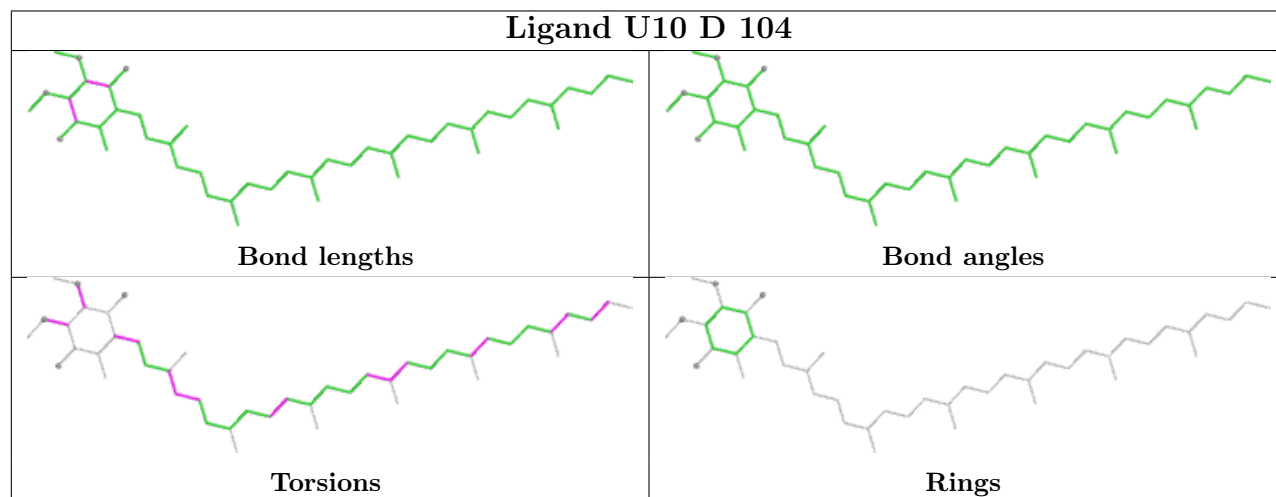
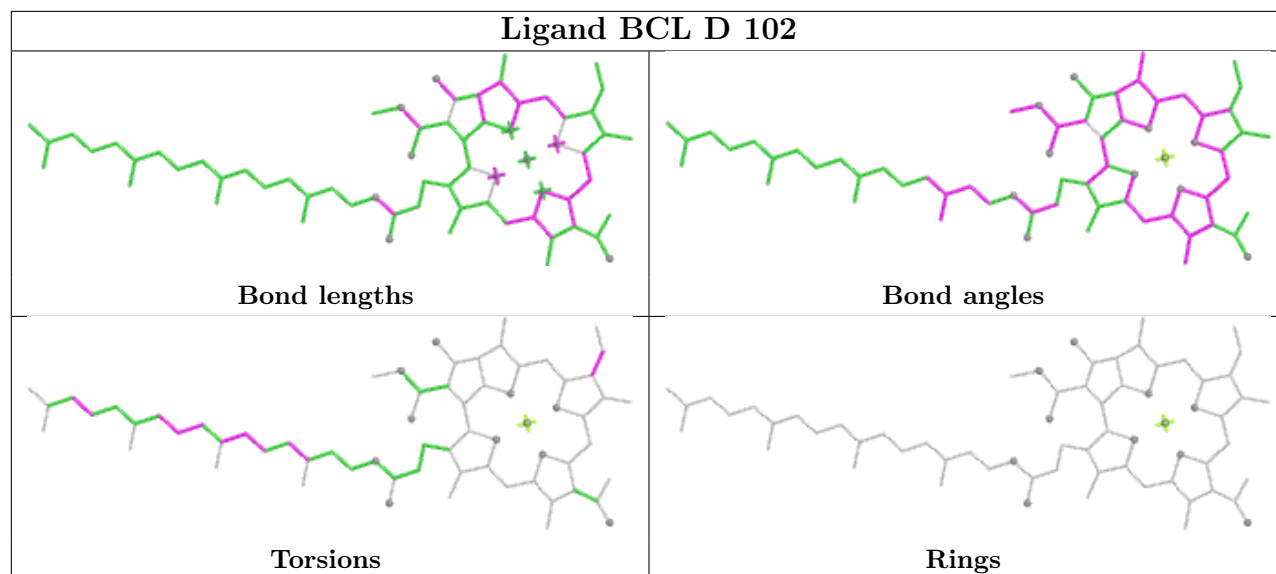
Ligand BCL K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

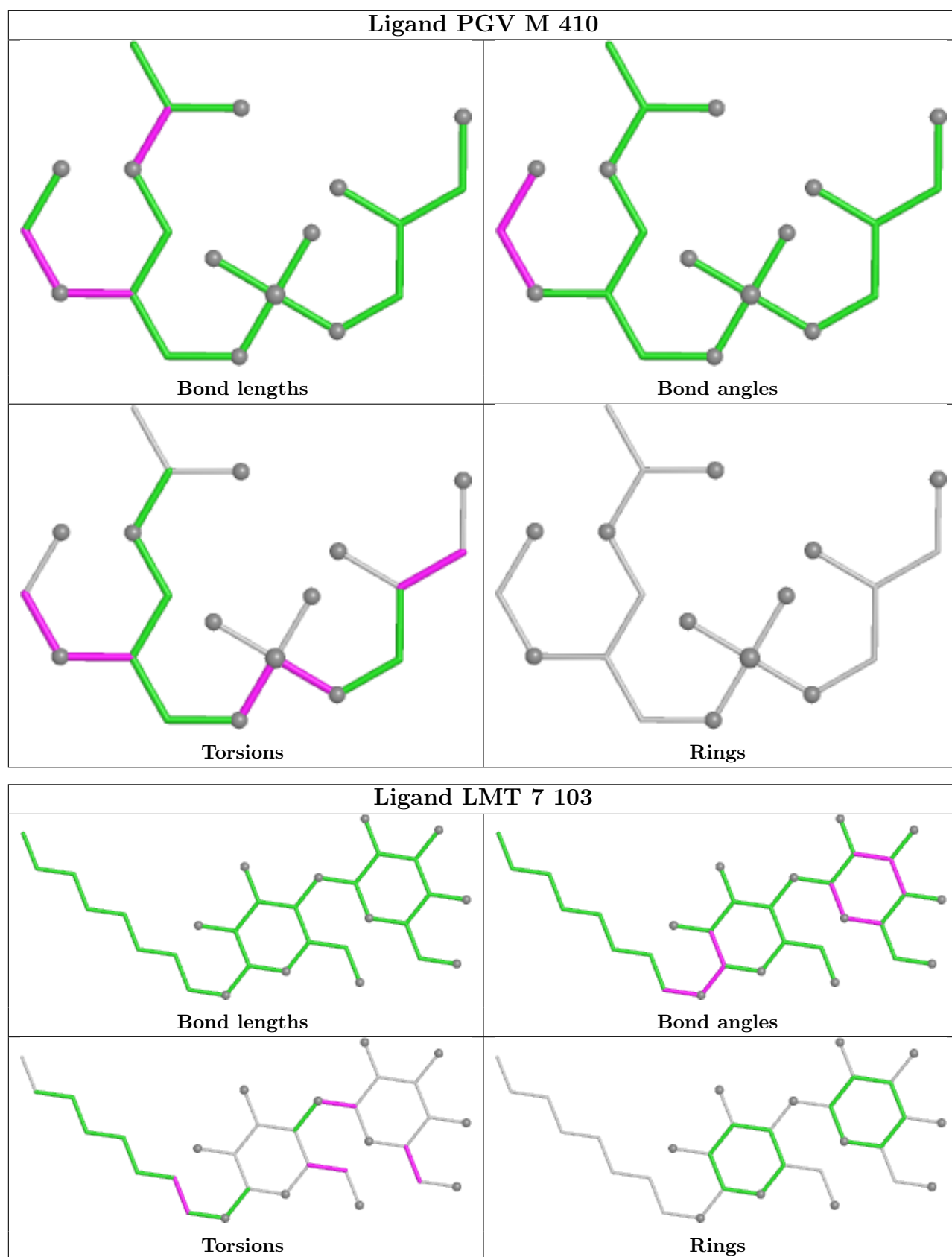
Ligand CRT T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

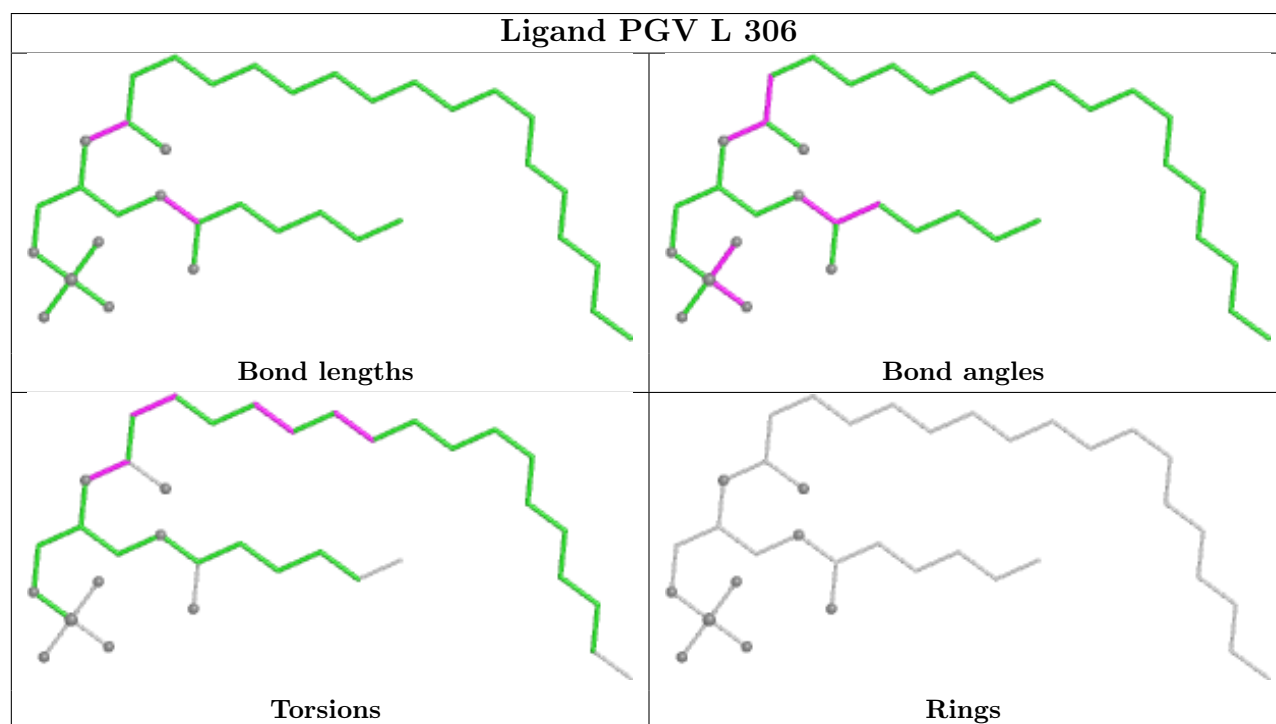
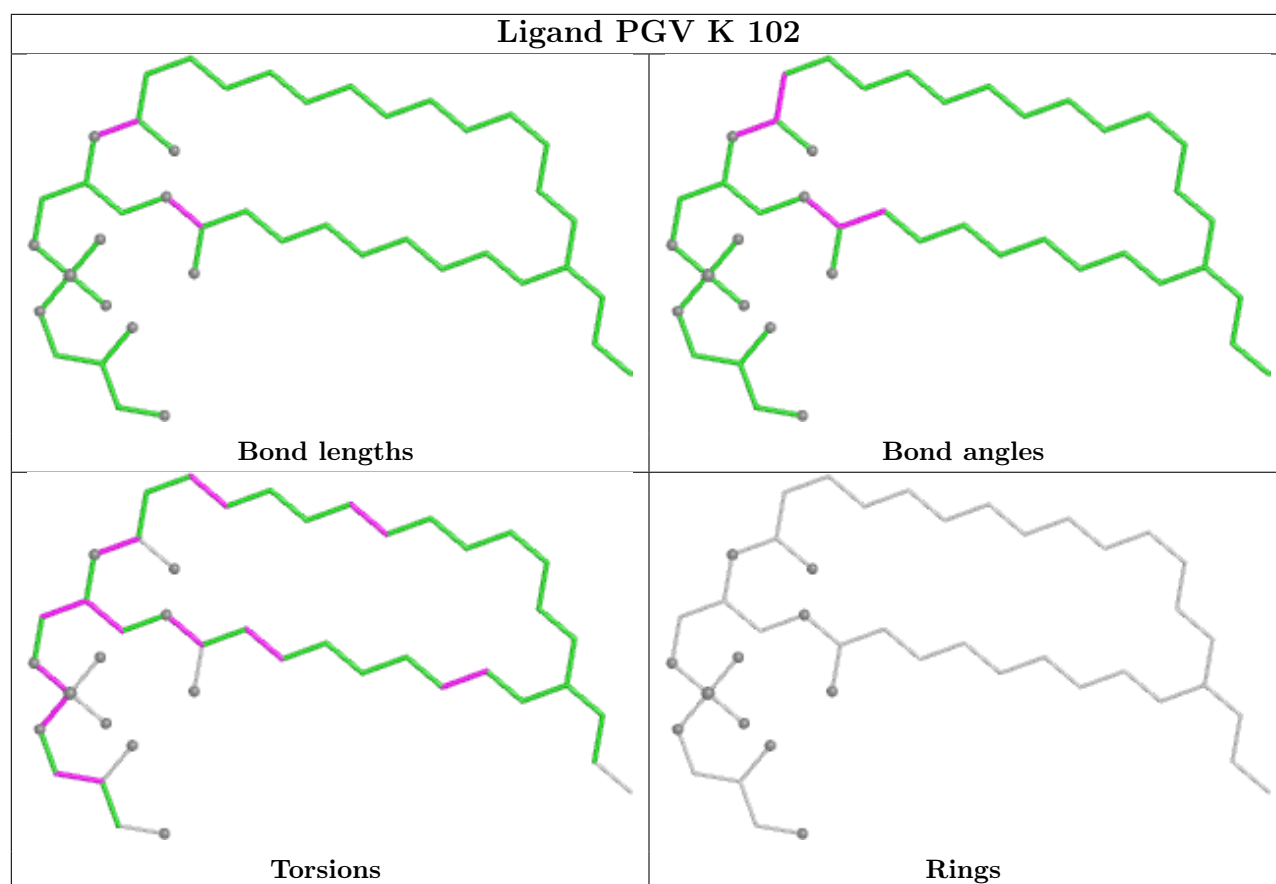


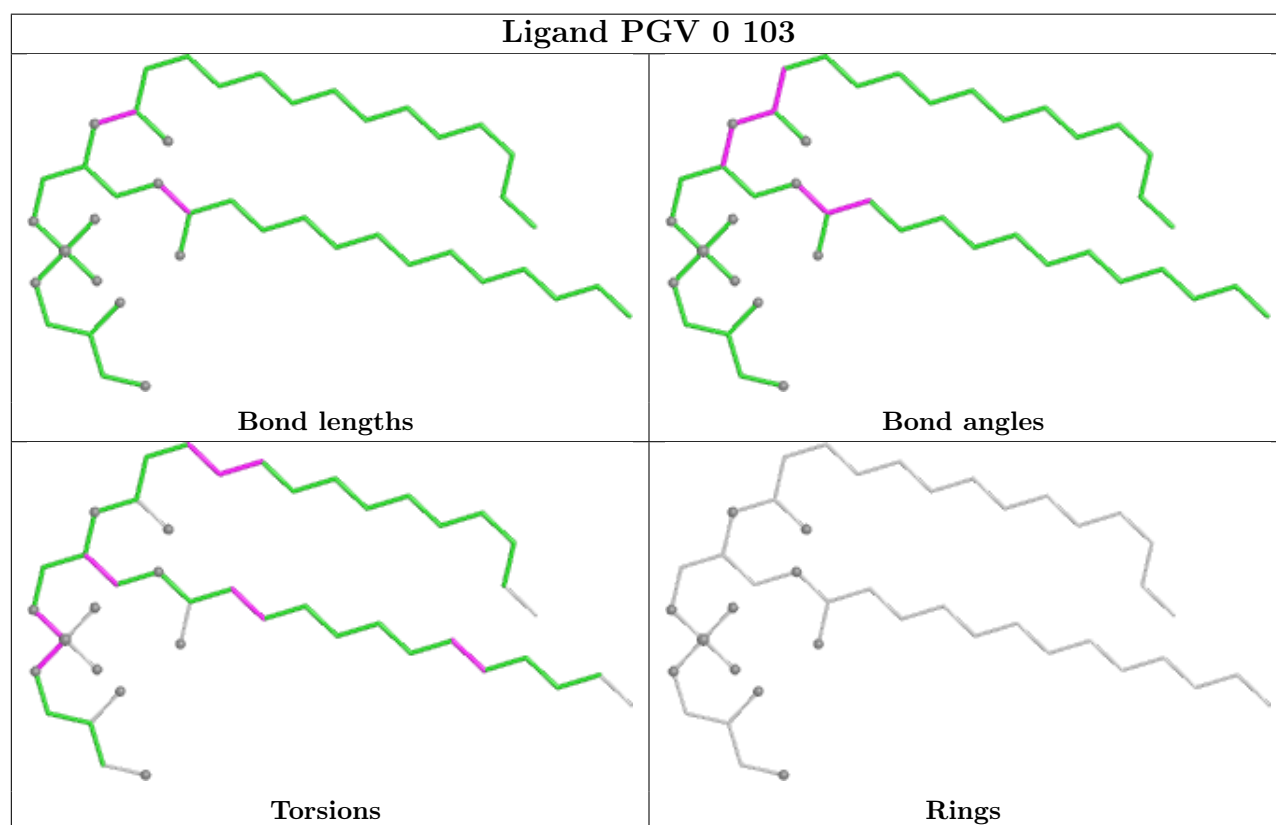
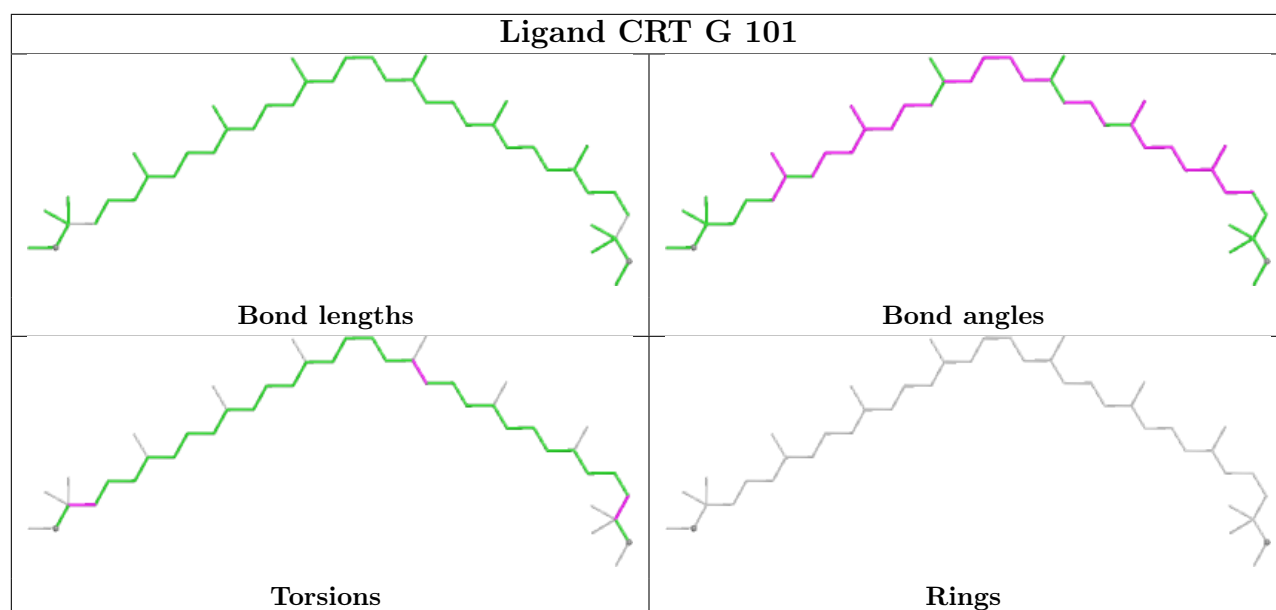


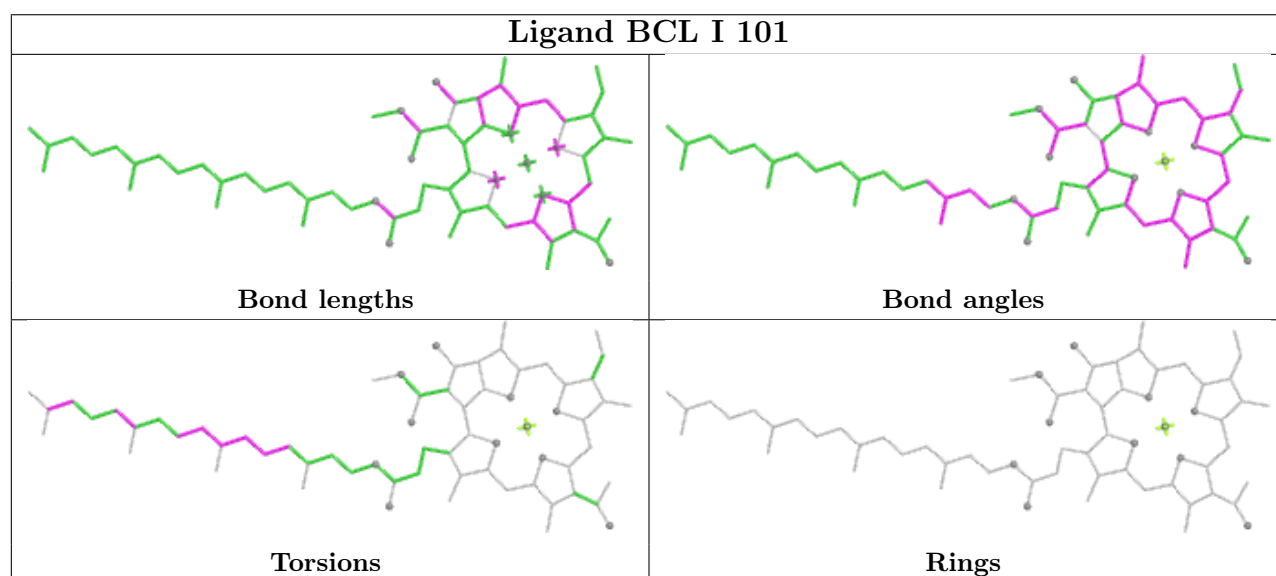
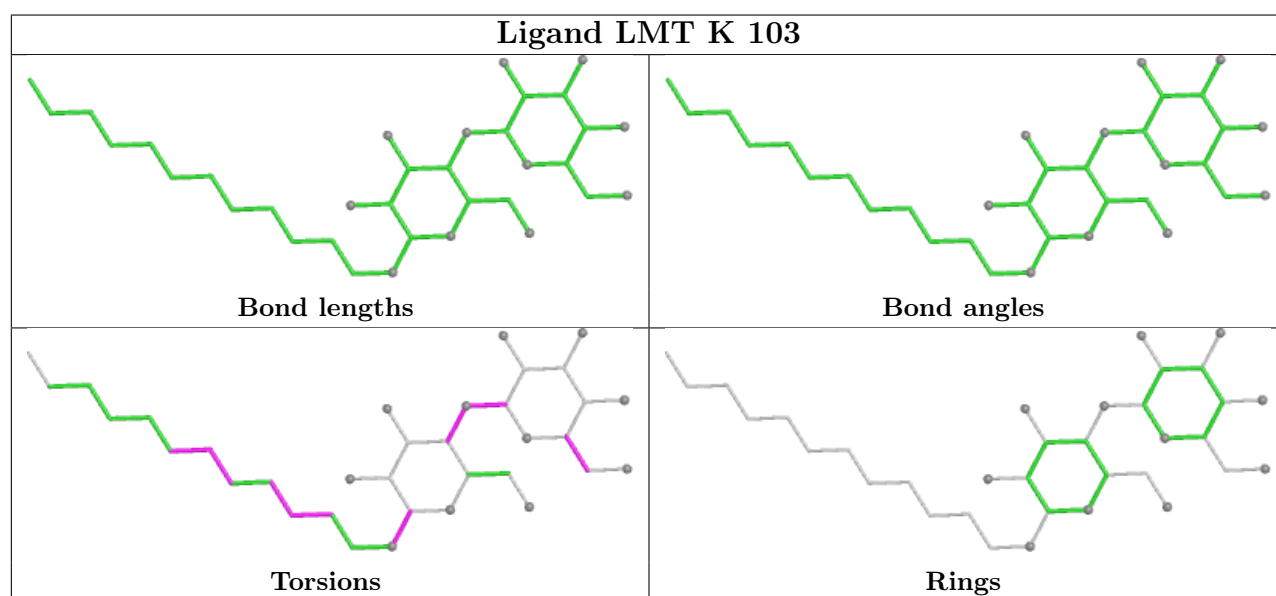
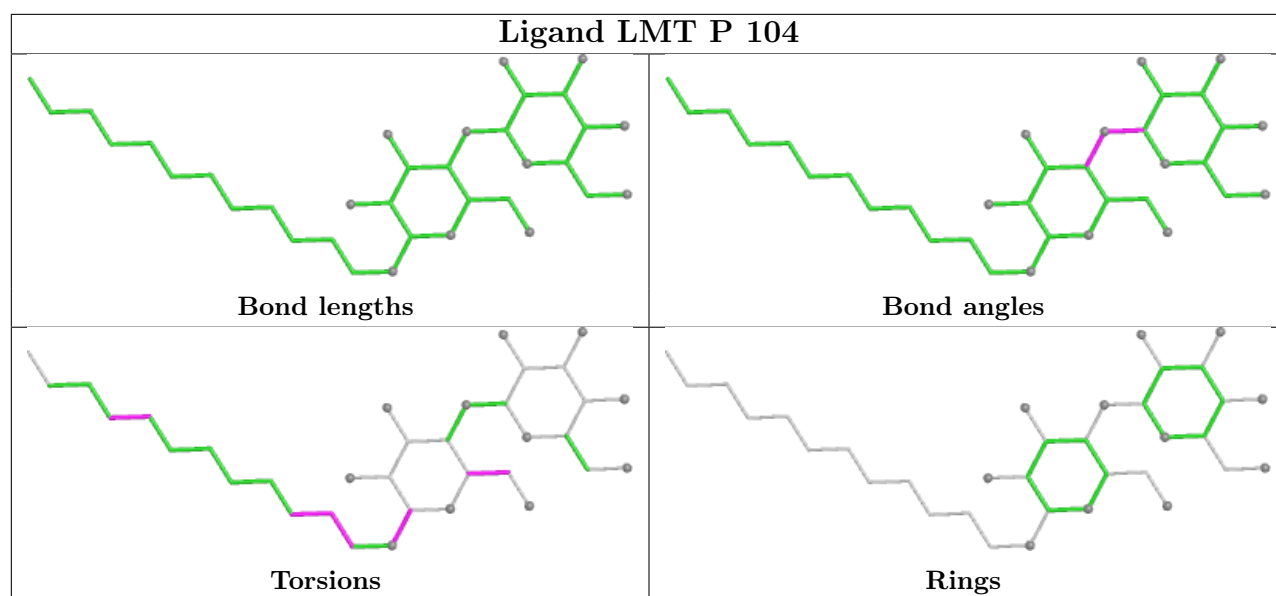




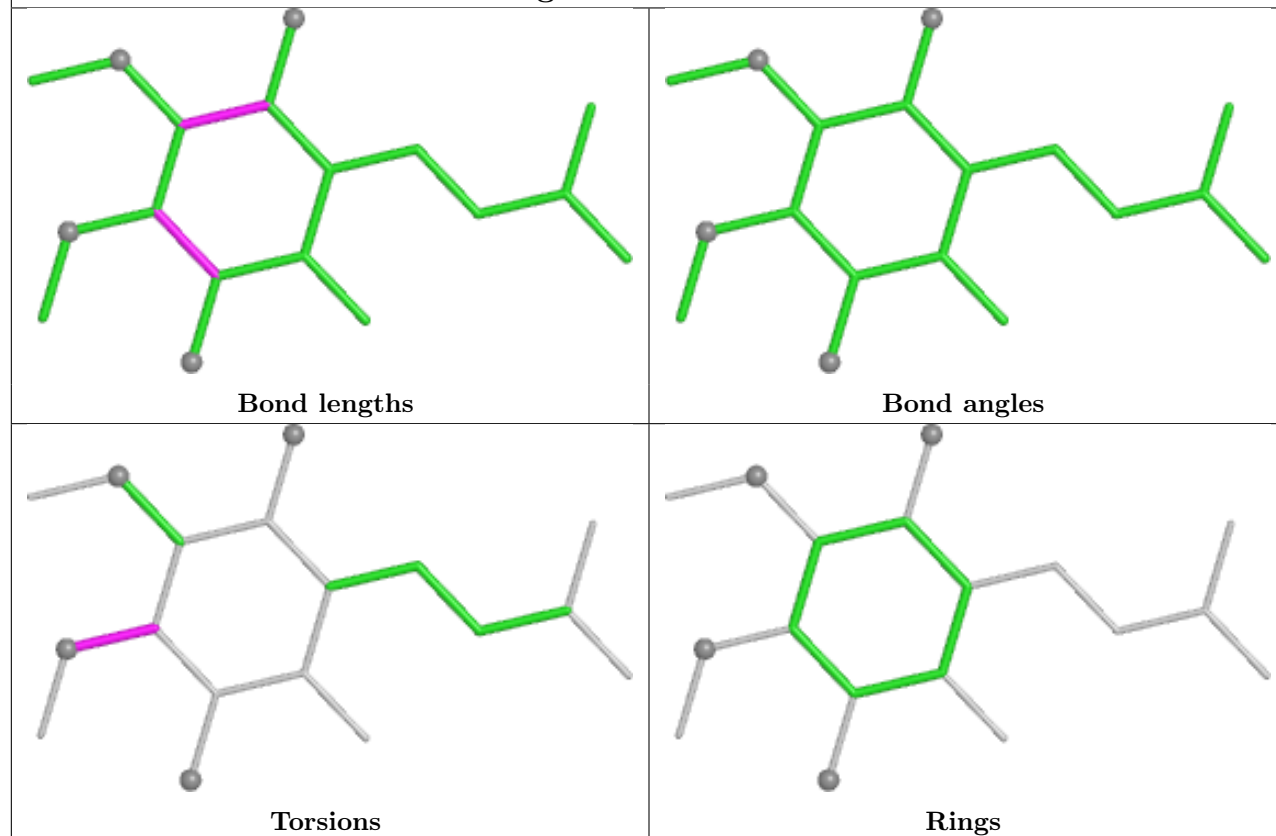




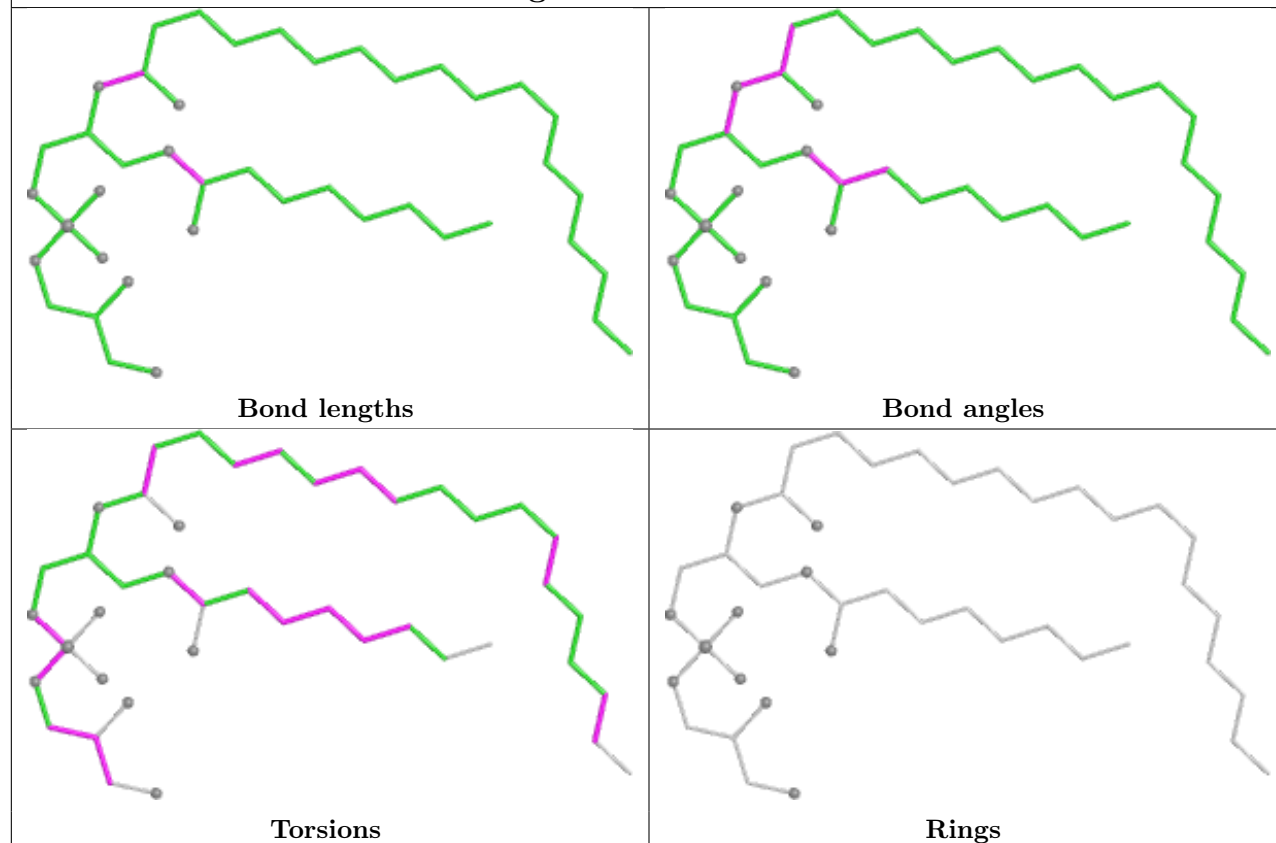


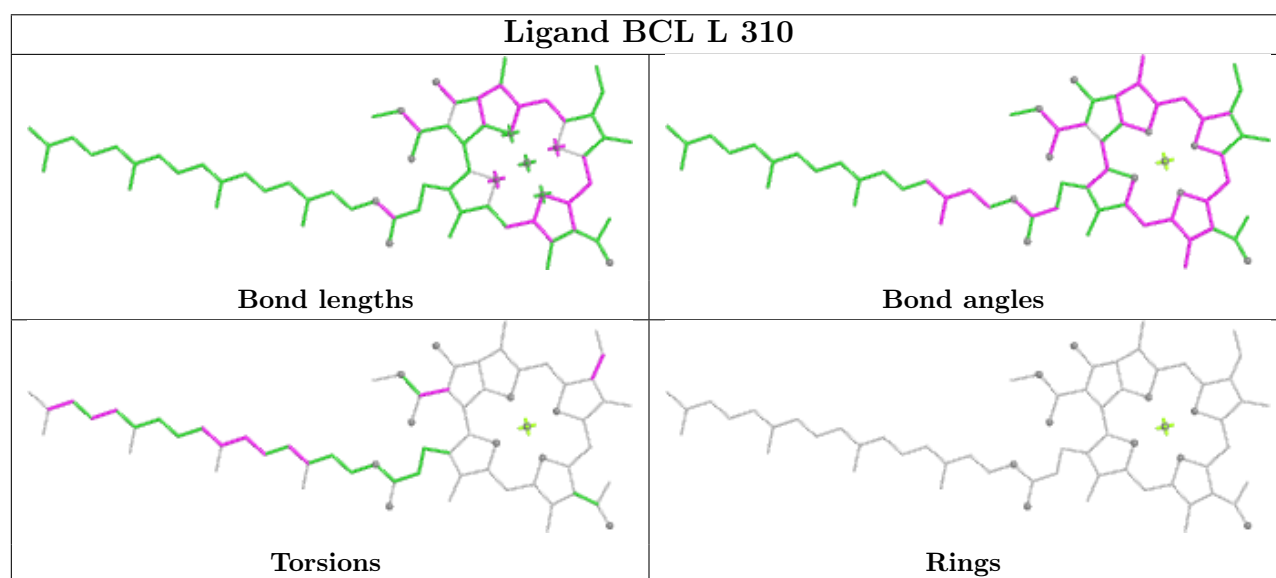
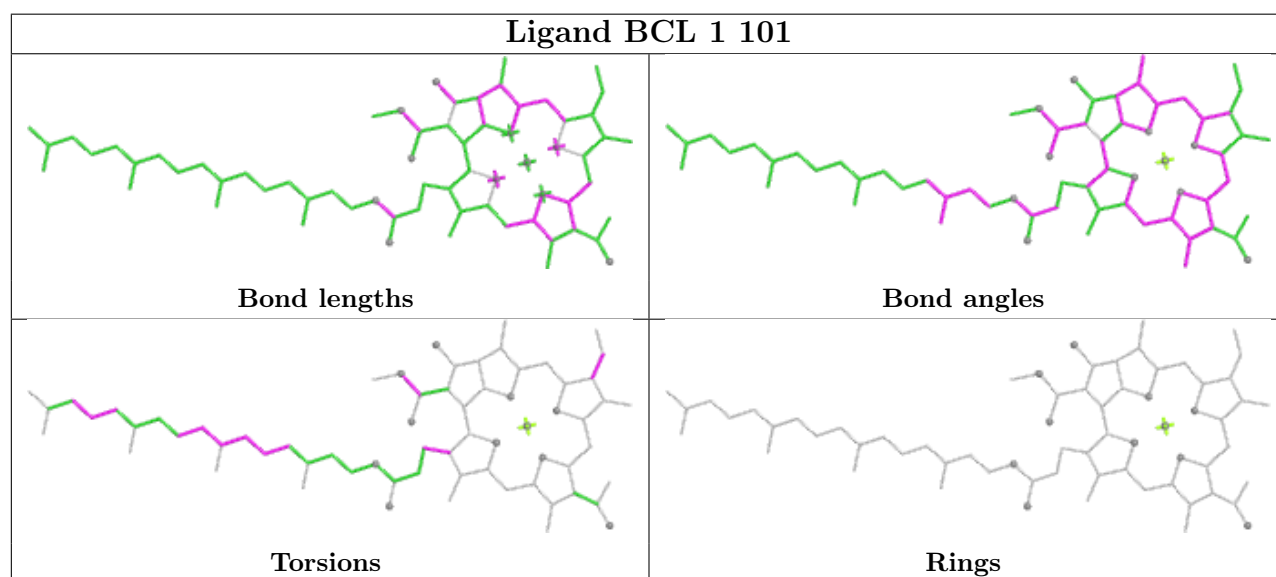
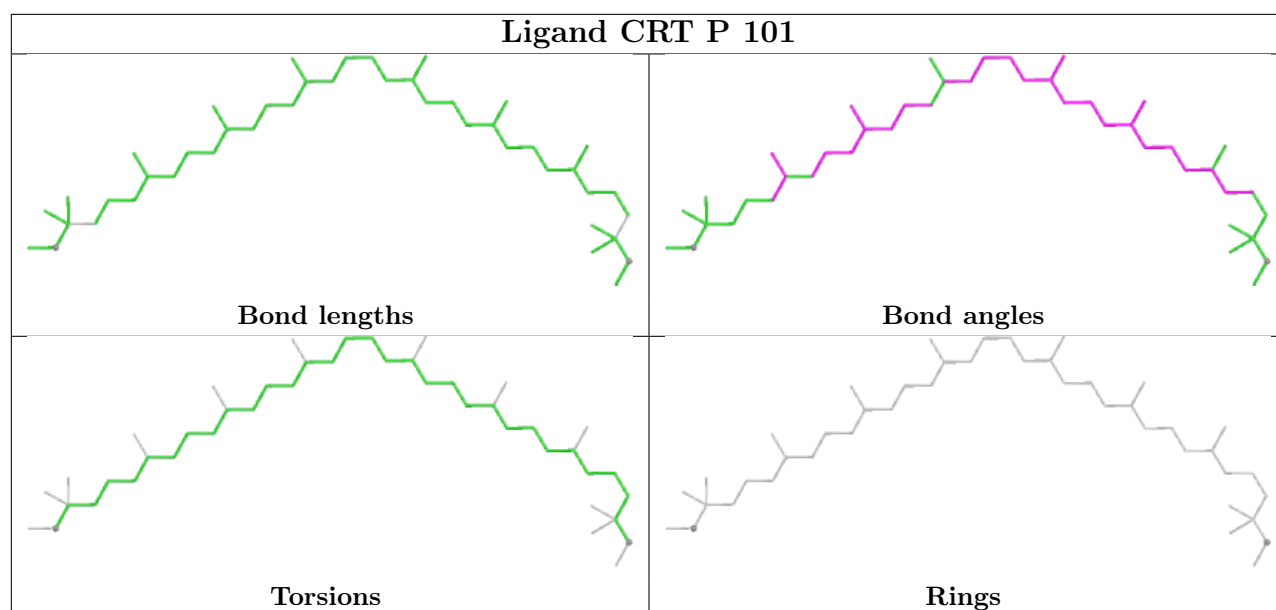


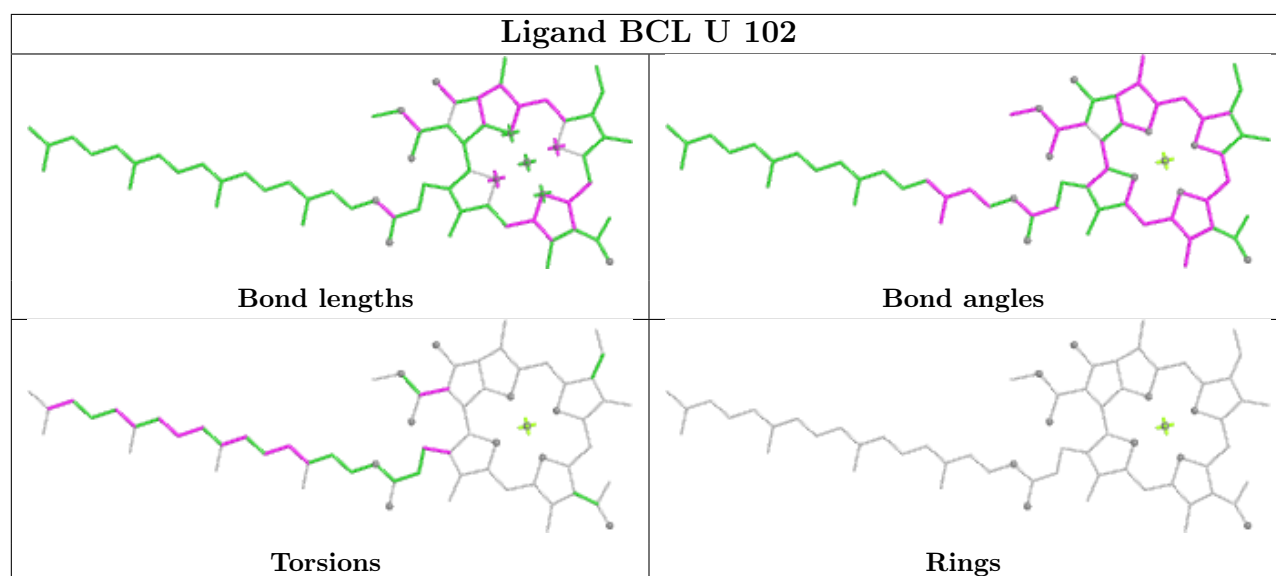
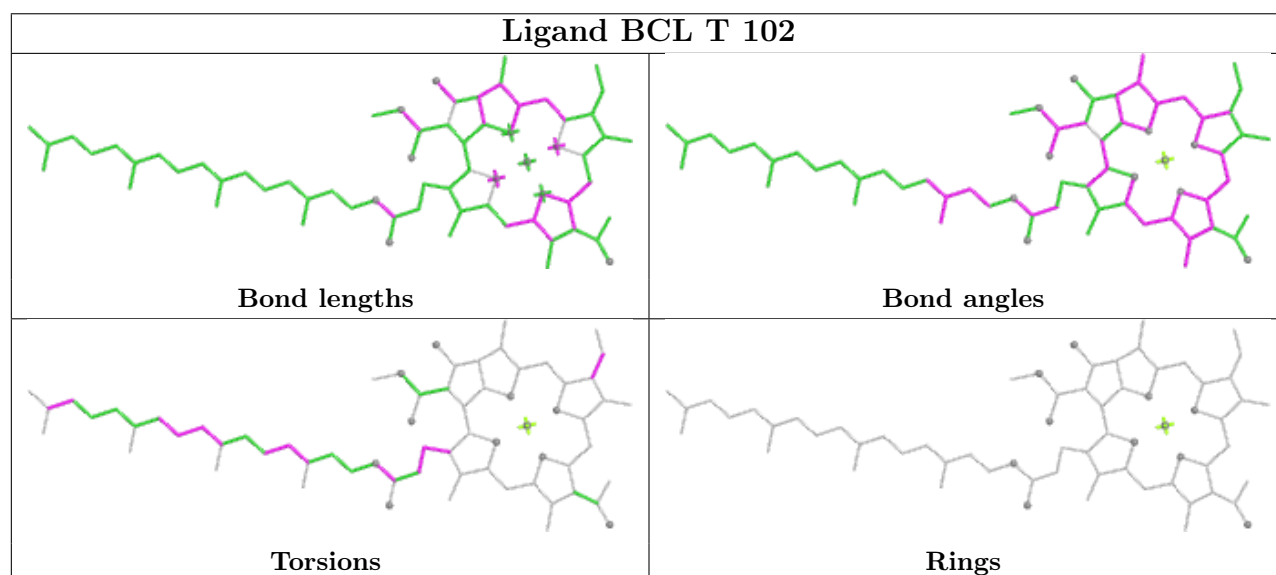
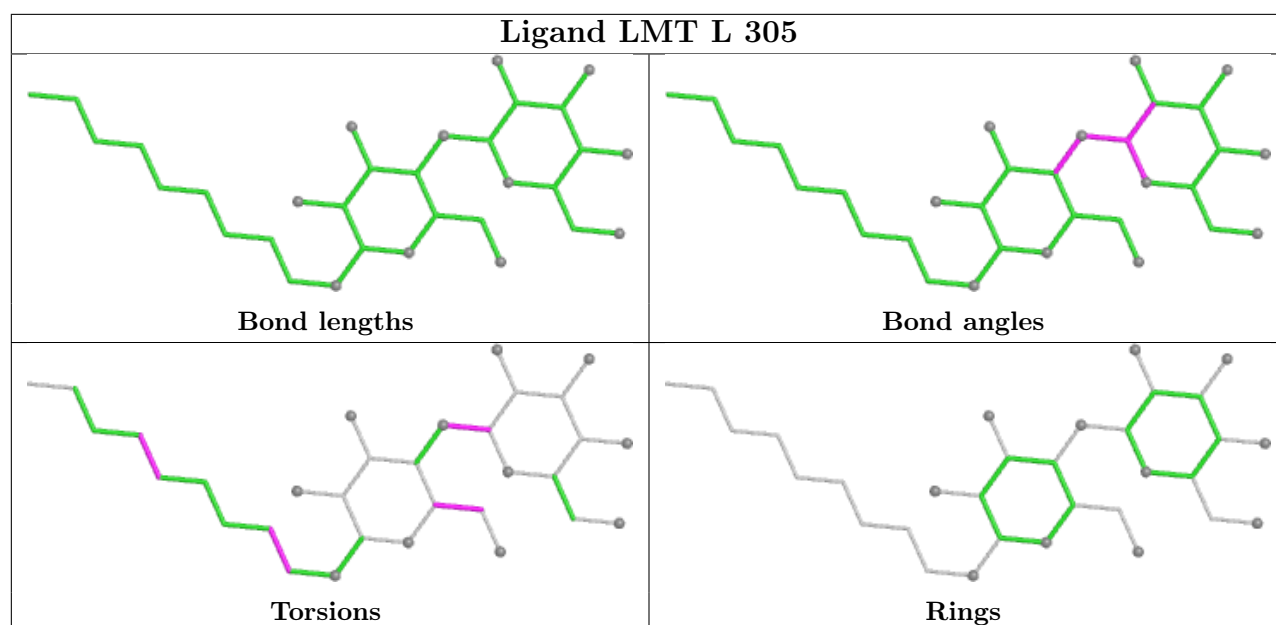
Ligand U10 U 101

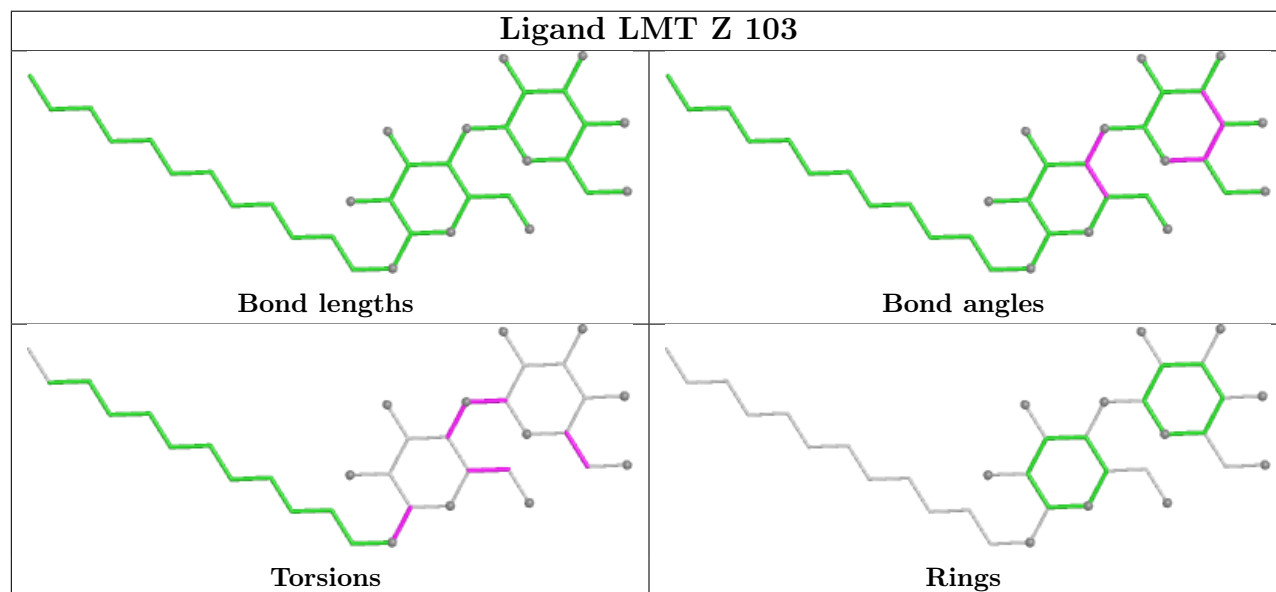
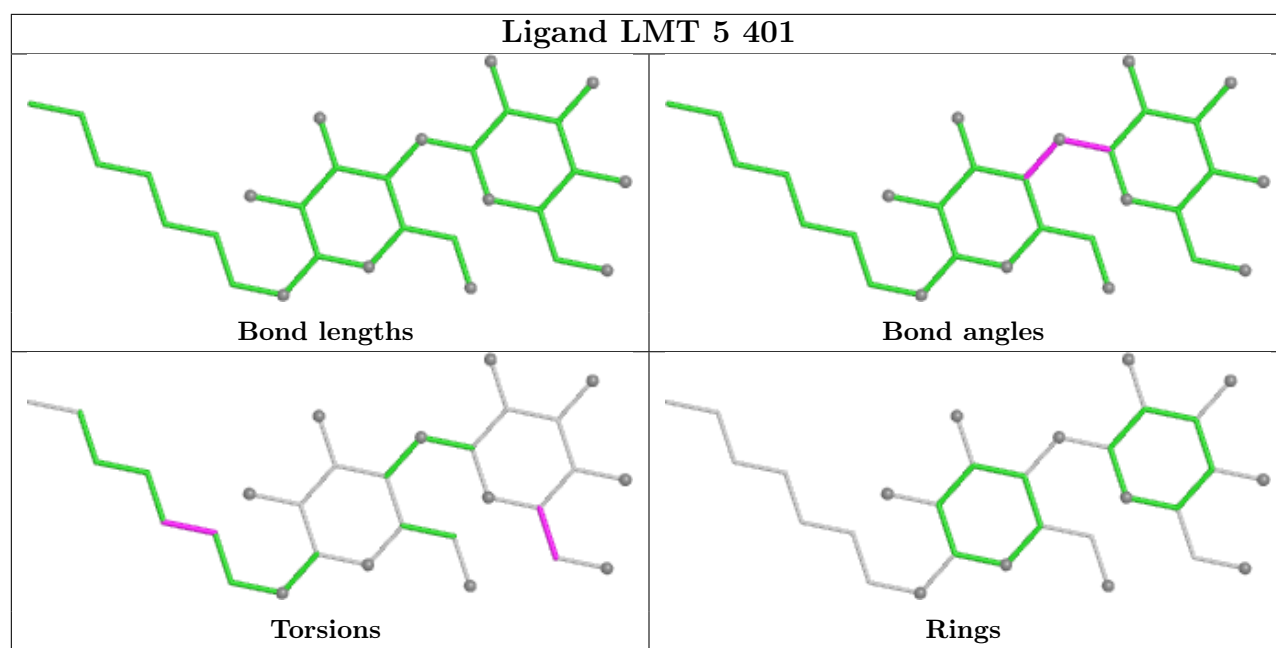


Ligand PGV H 403

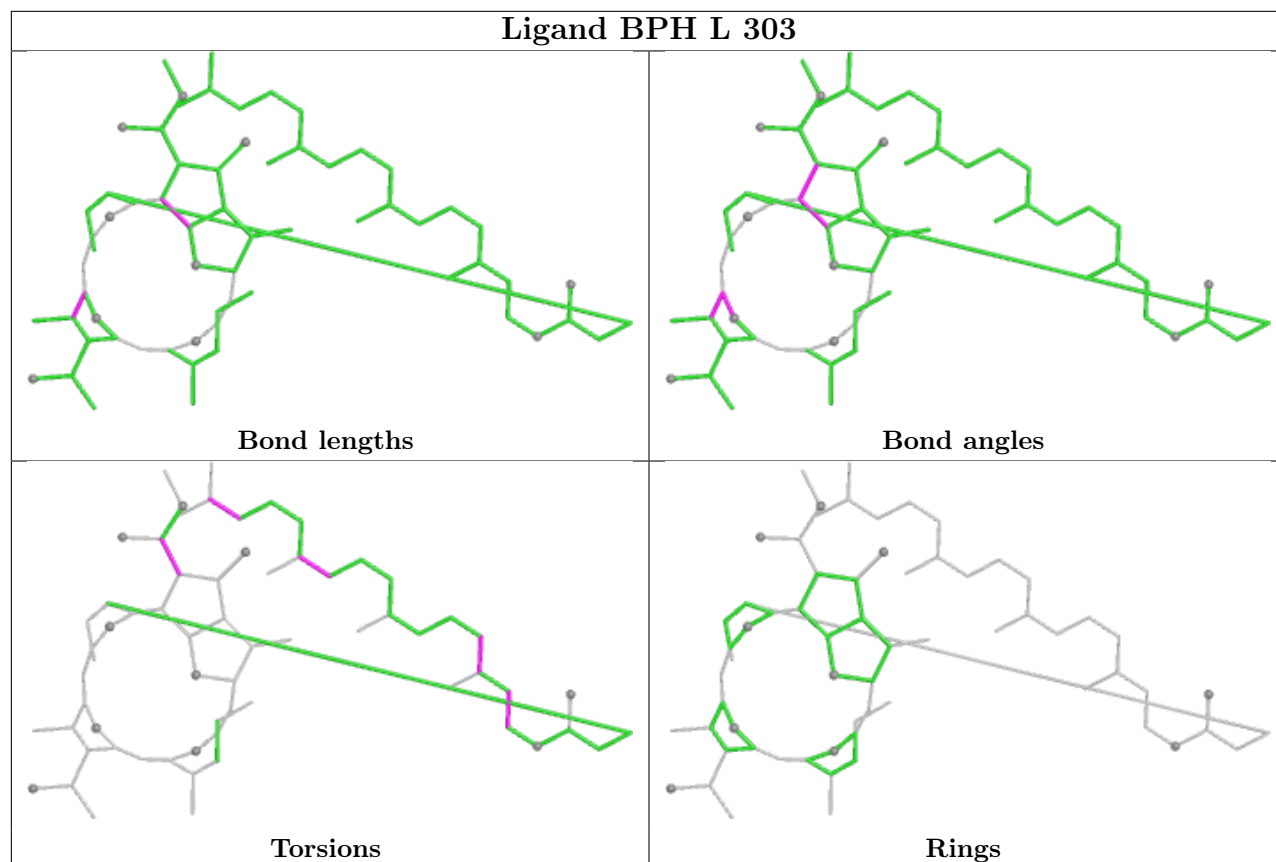




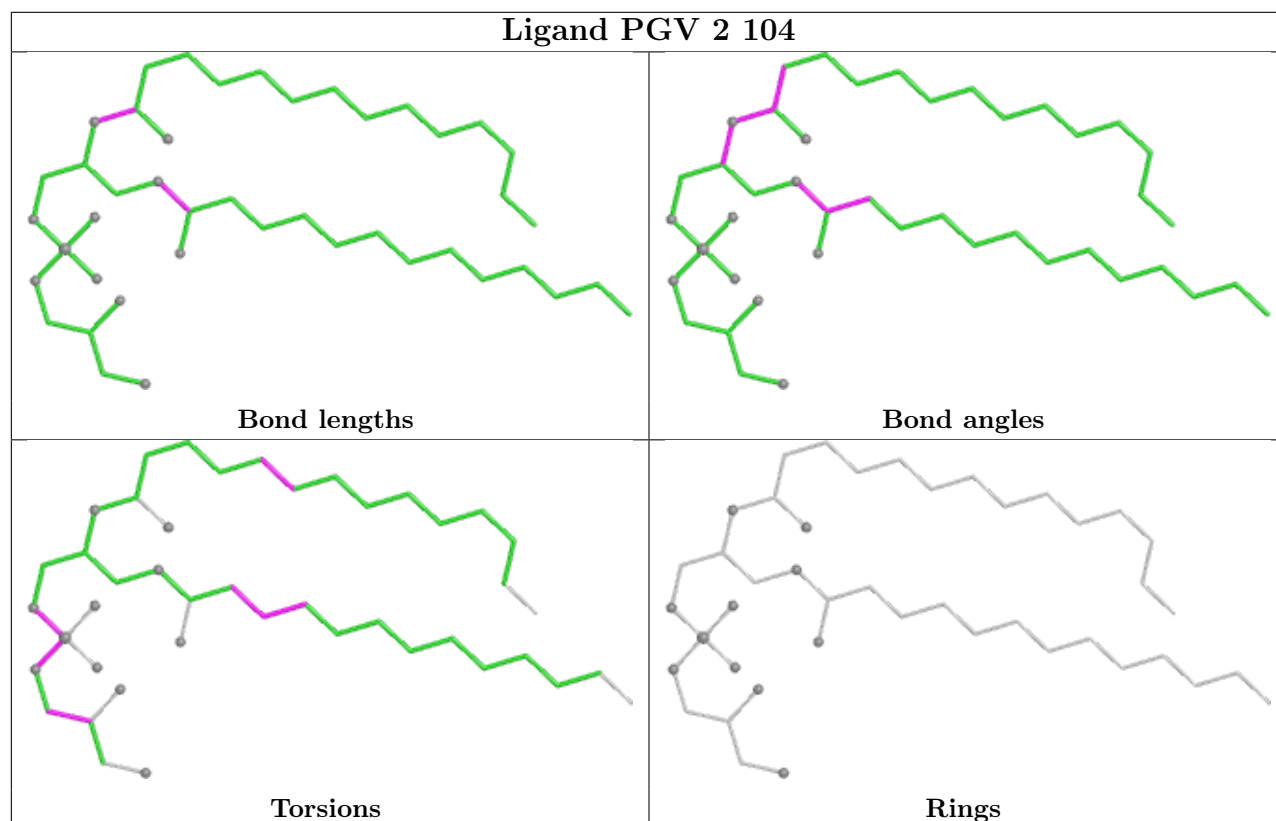


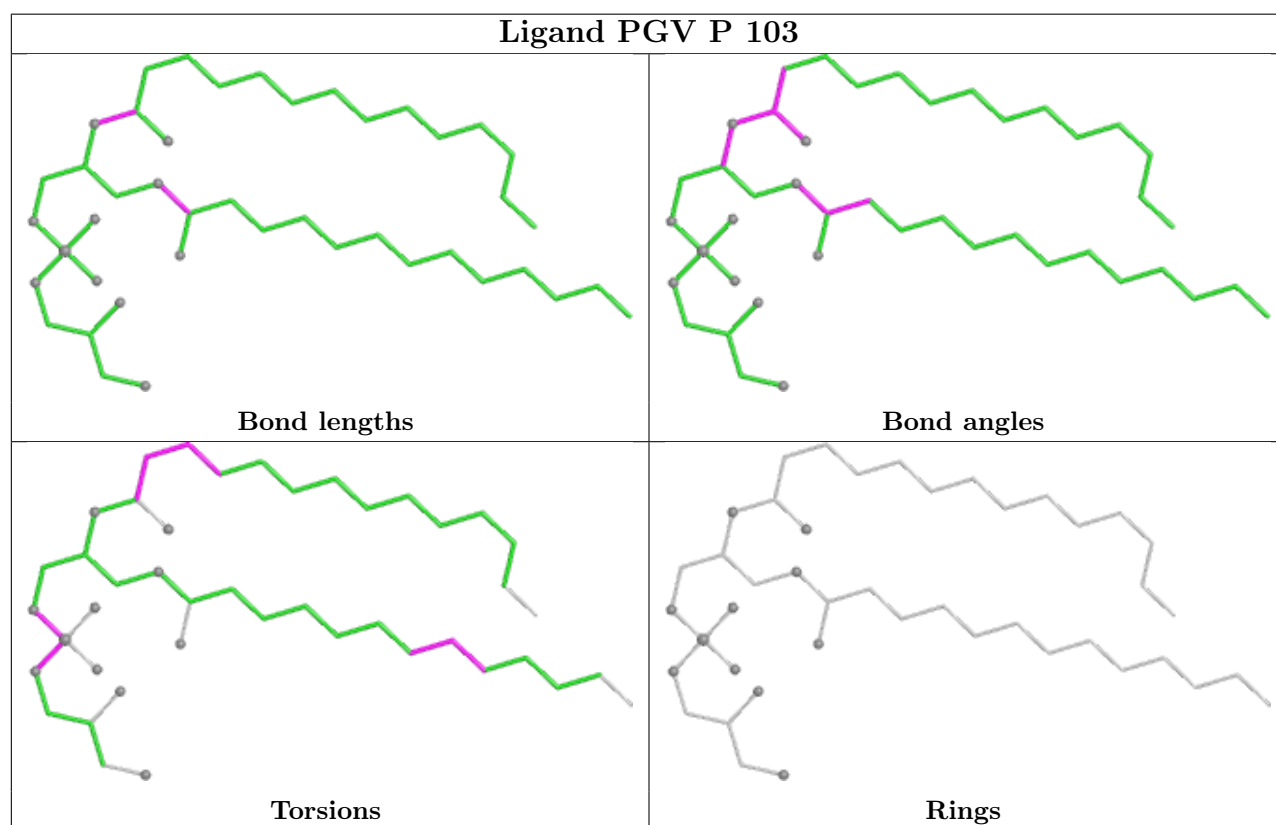
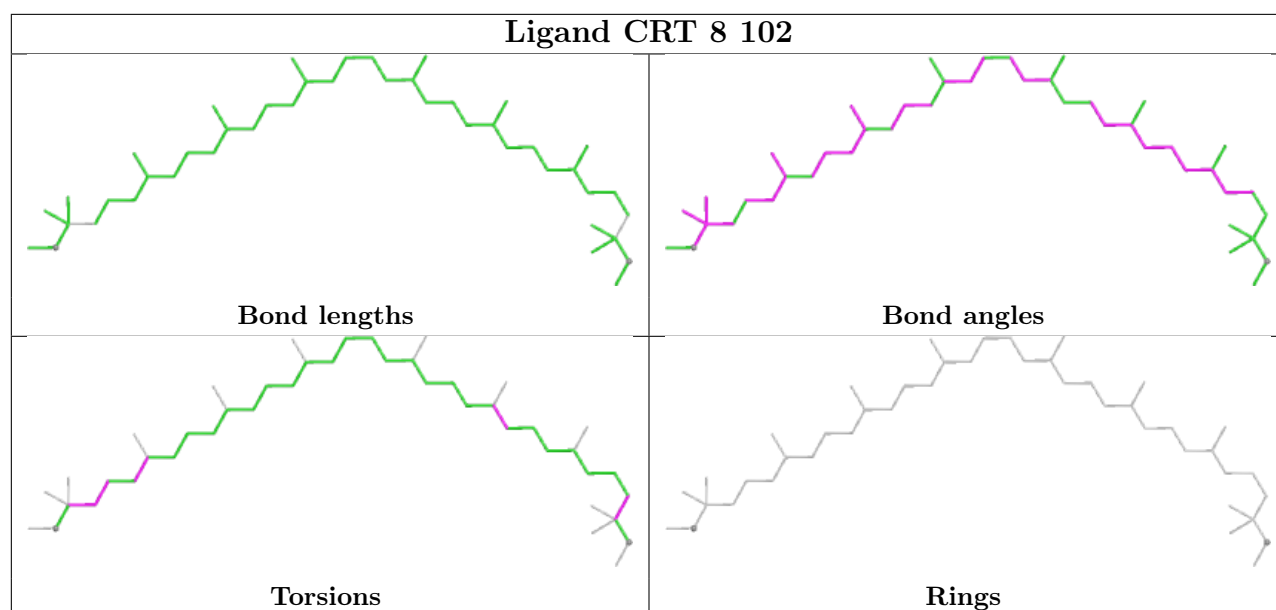


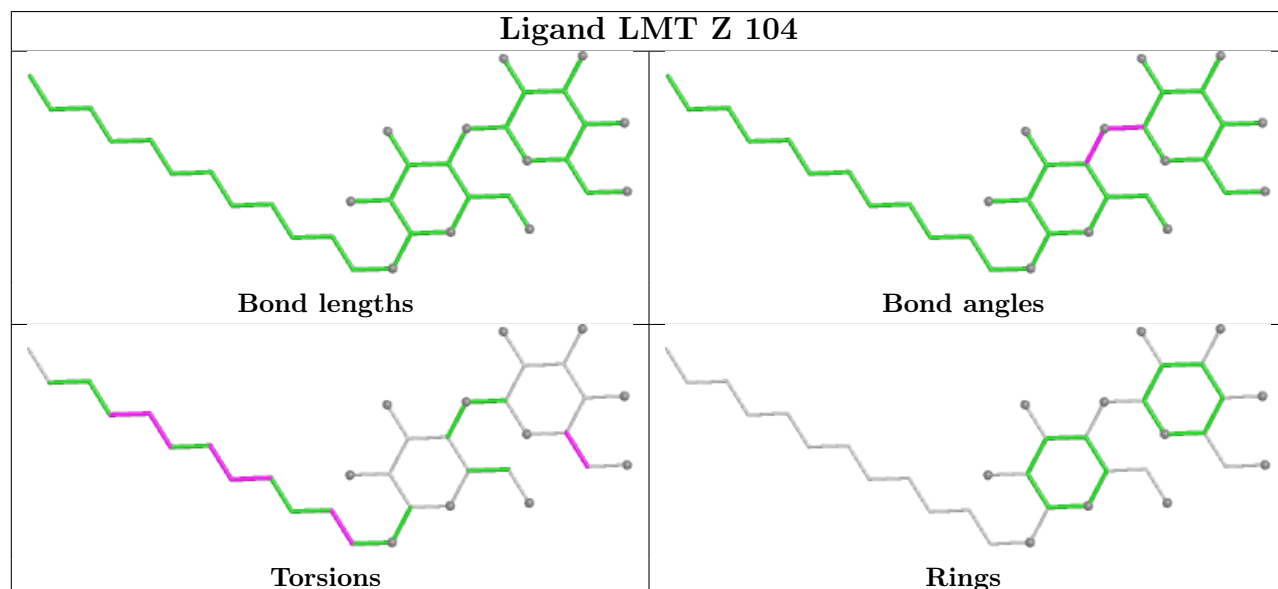
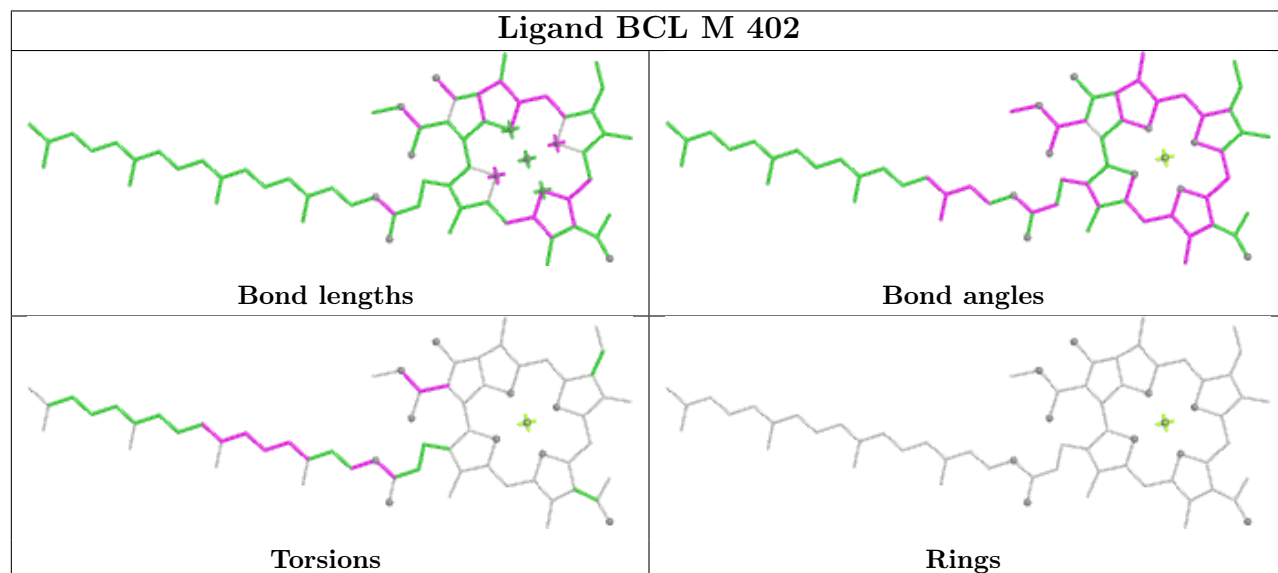
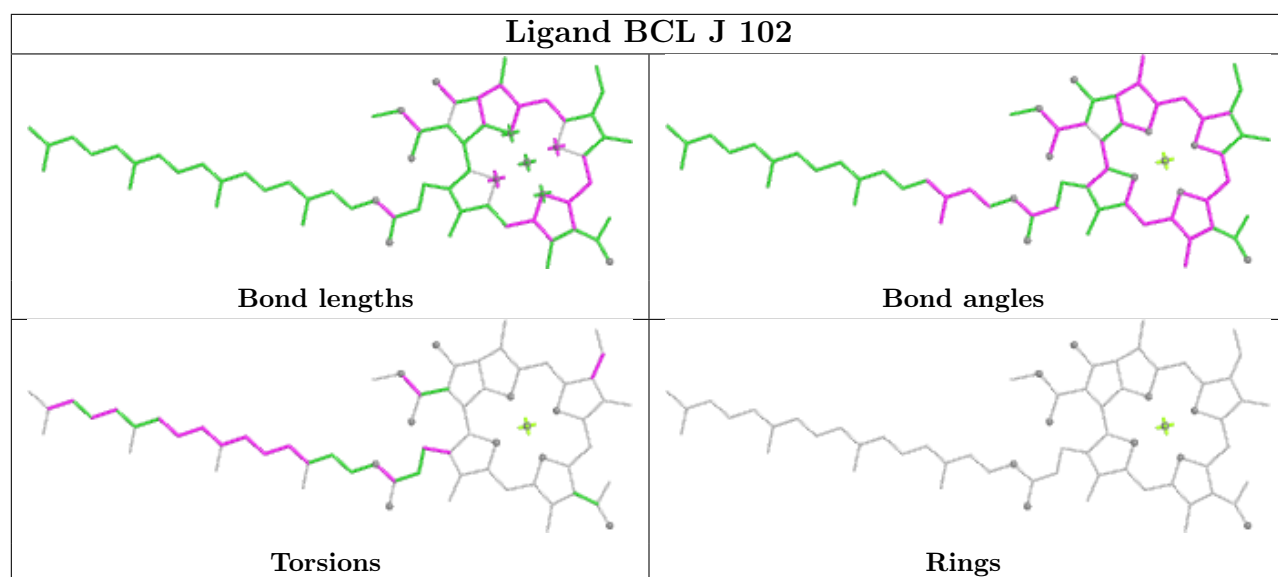
Ligand BPH L 303

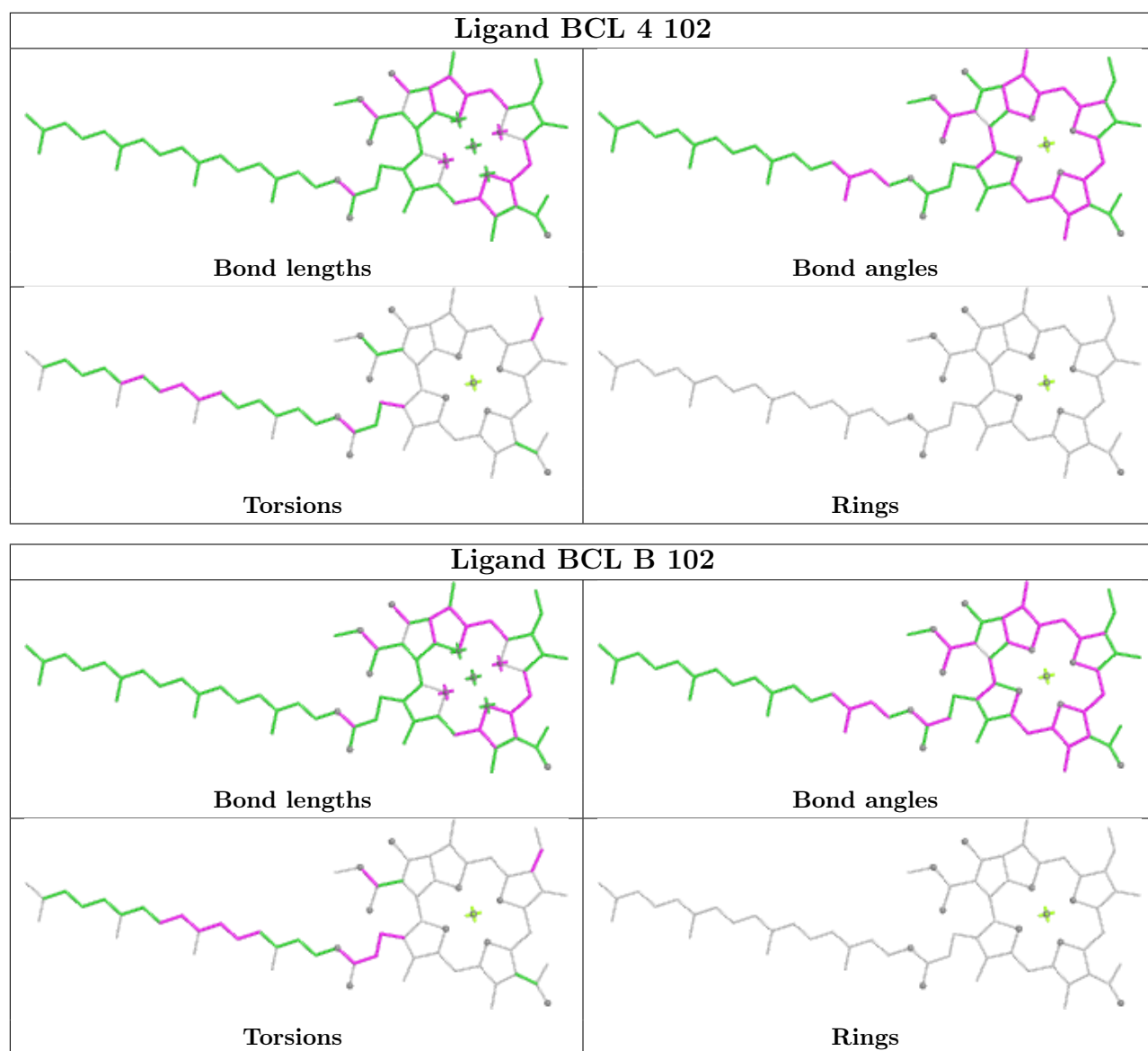


Ligand PGV 2 104

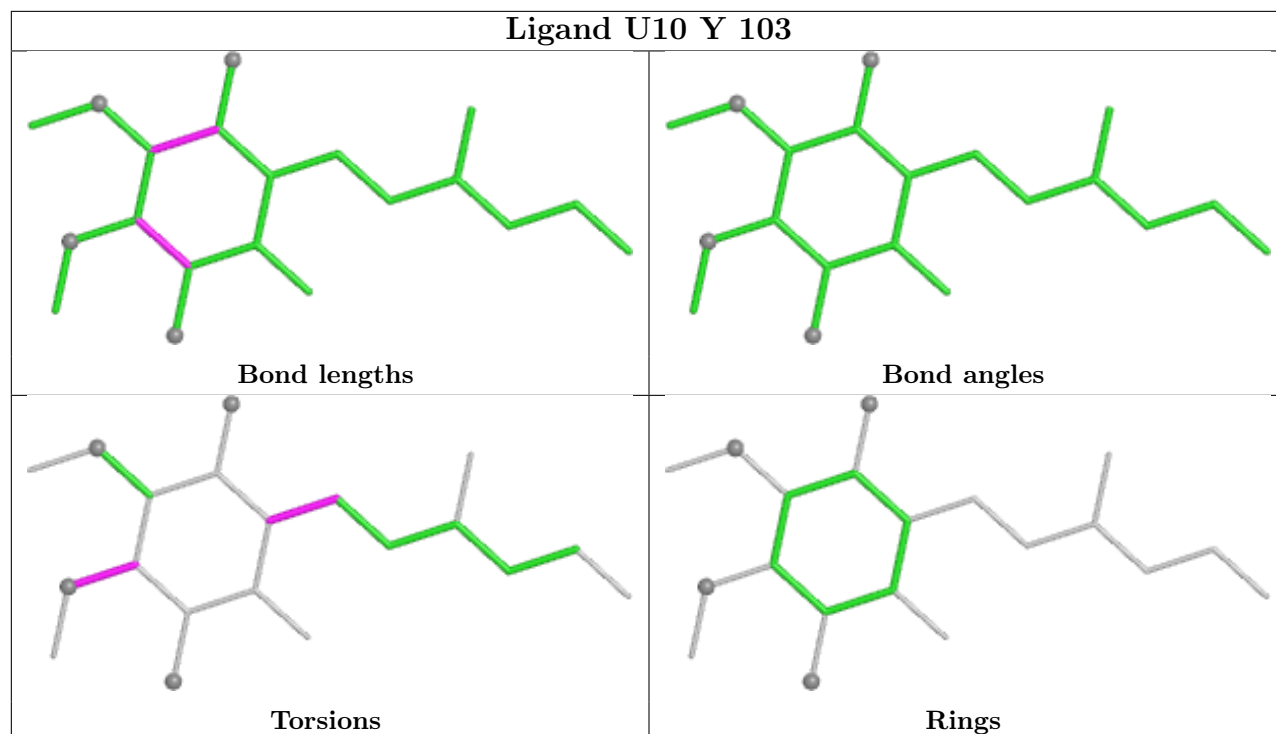




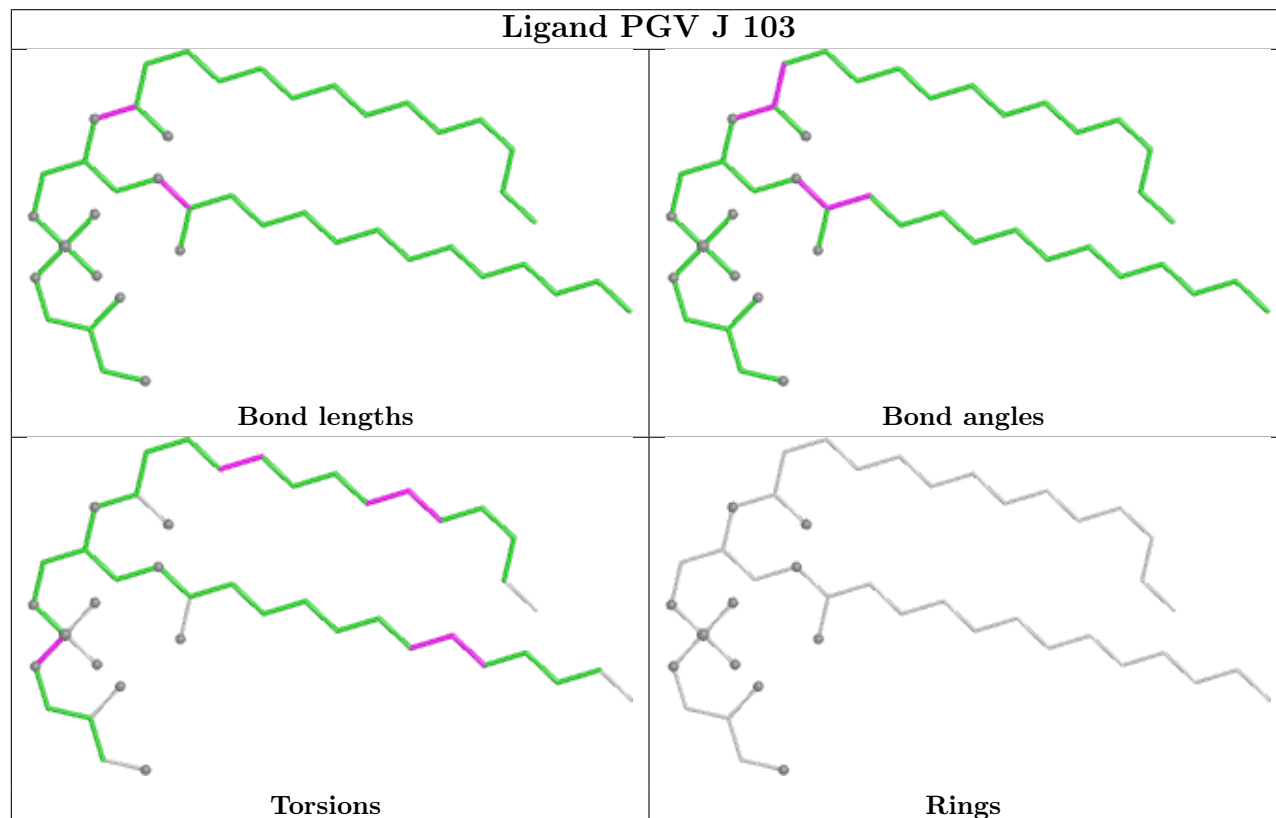


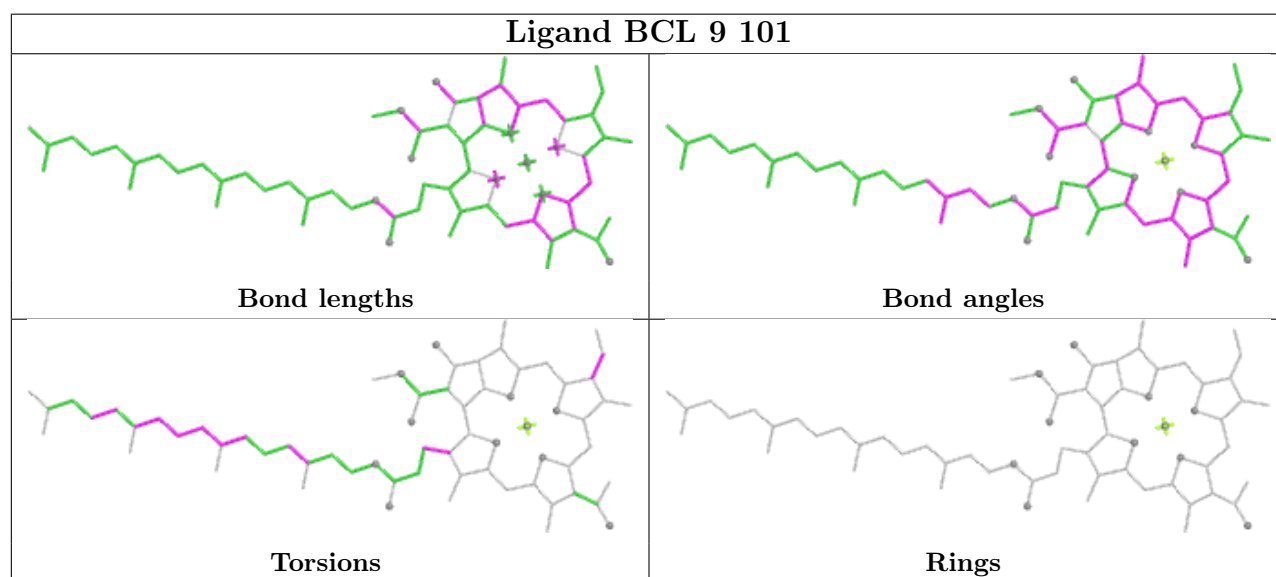
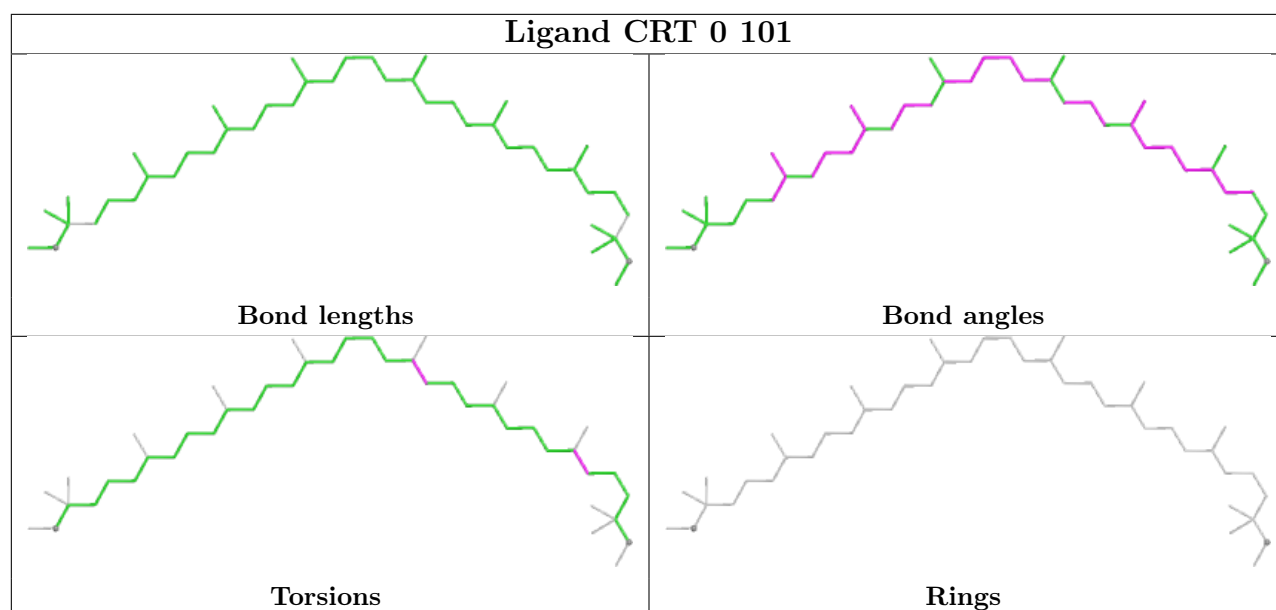


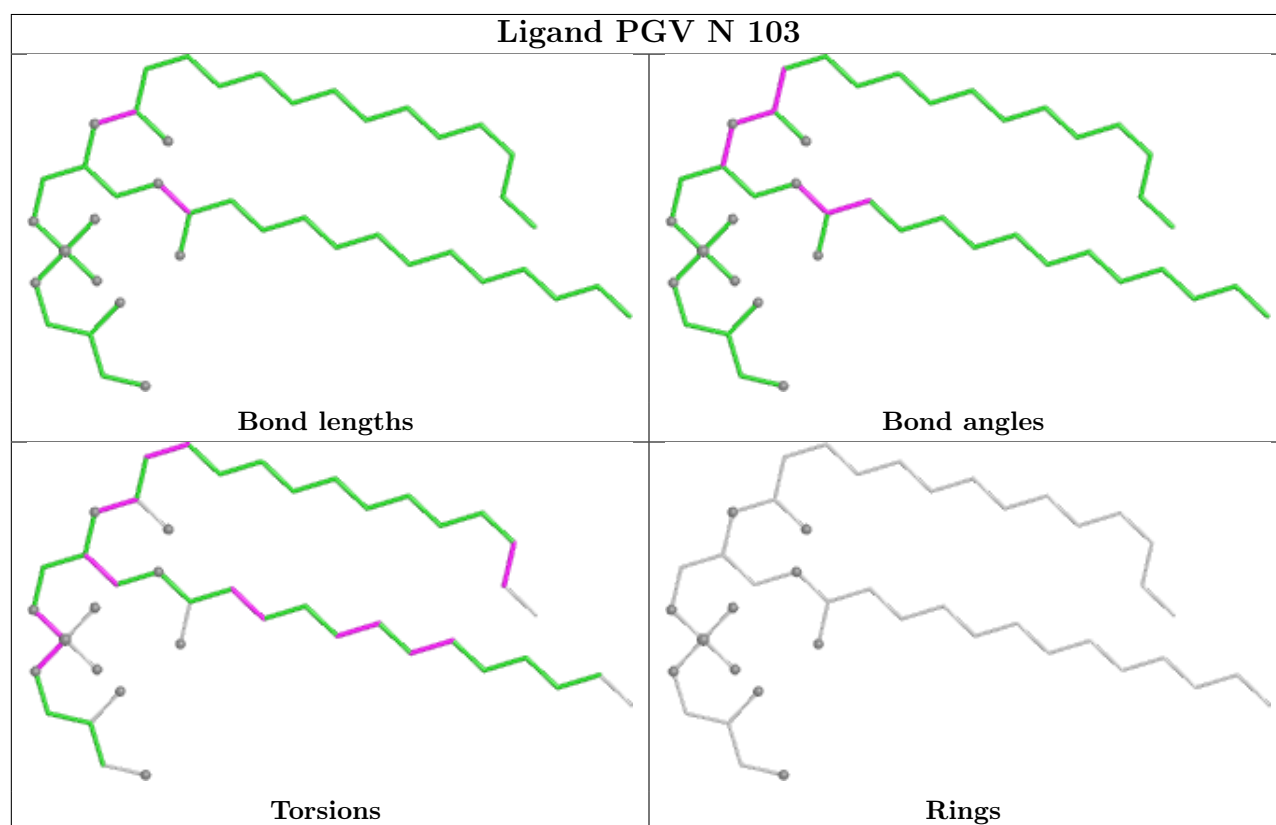
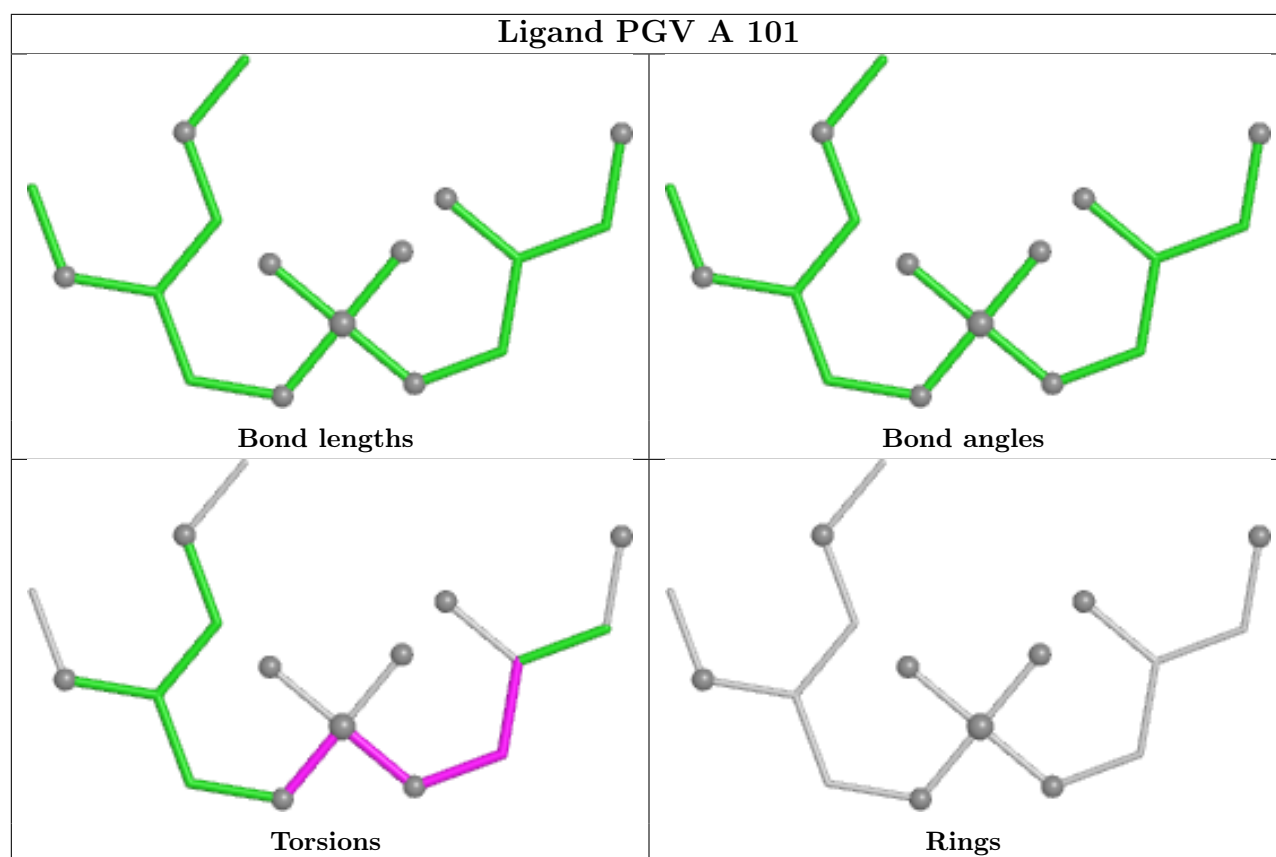
Ligand U10 Y 103



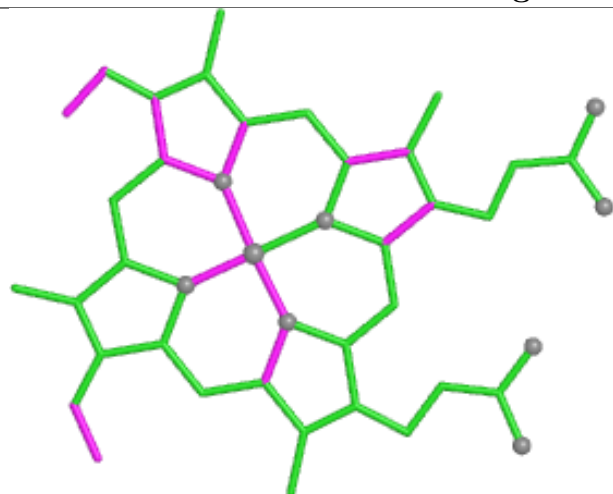
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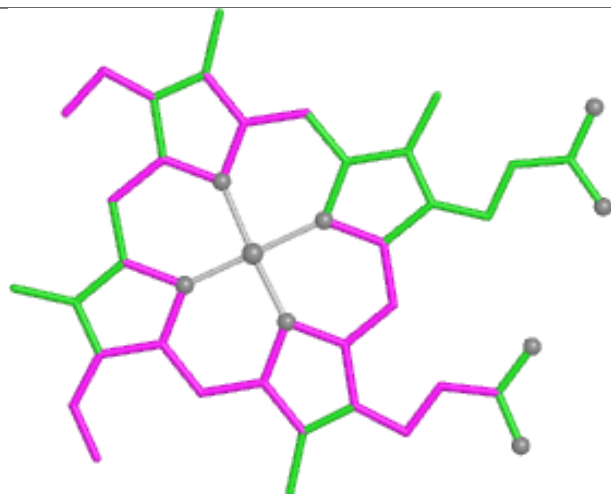




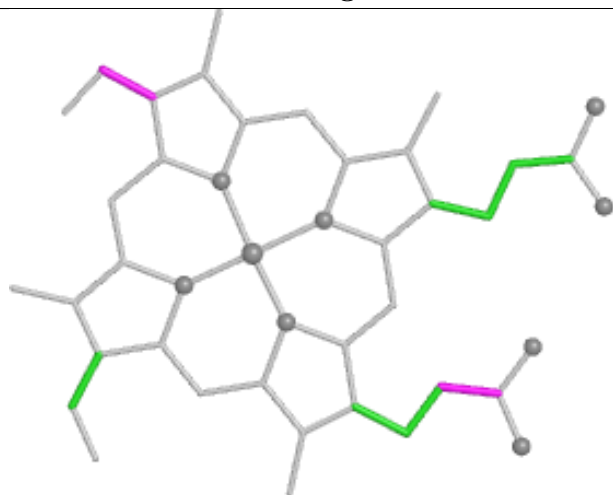
Ligand HEC C 404



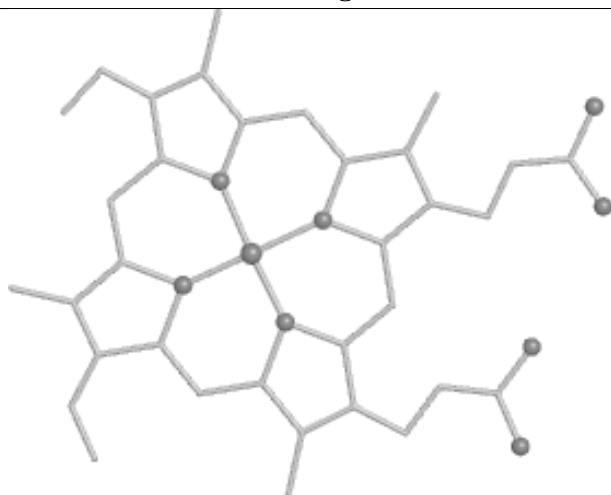
Bond lengths



Bond angles

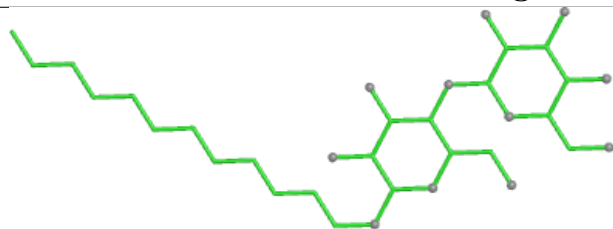


Torsions

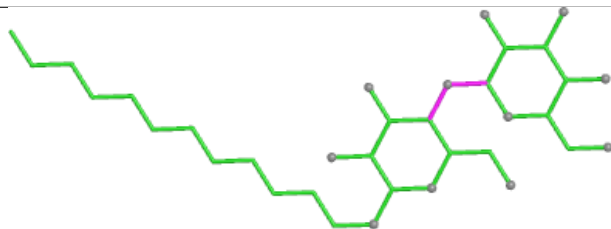


Rings

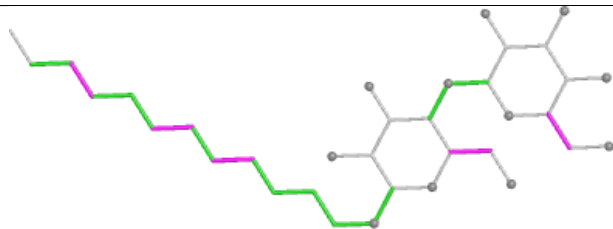
Ligand LMT E 104



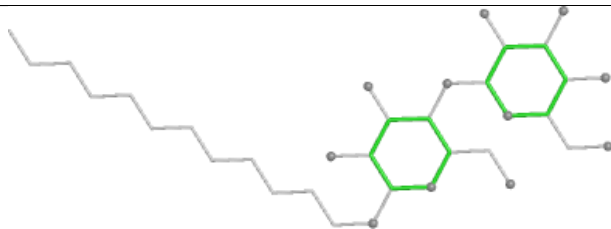
Bond lengths



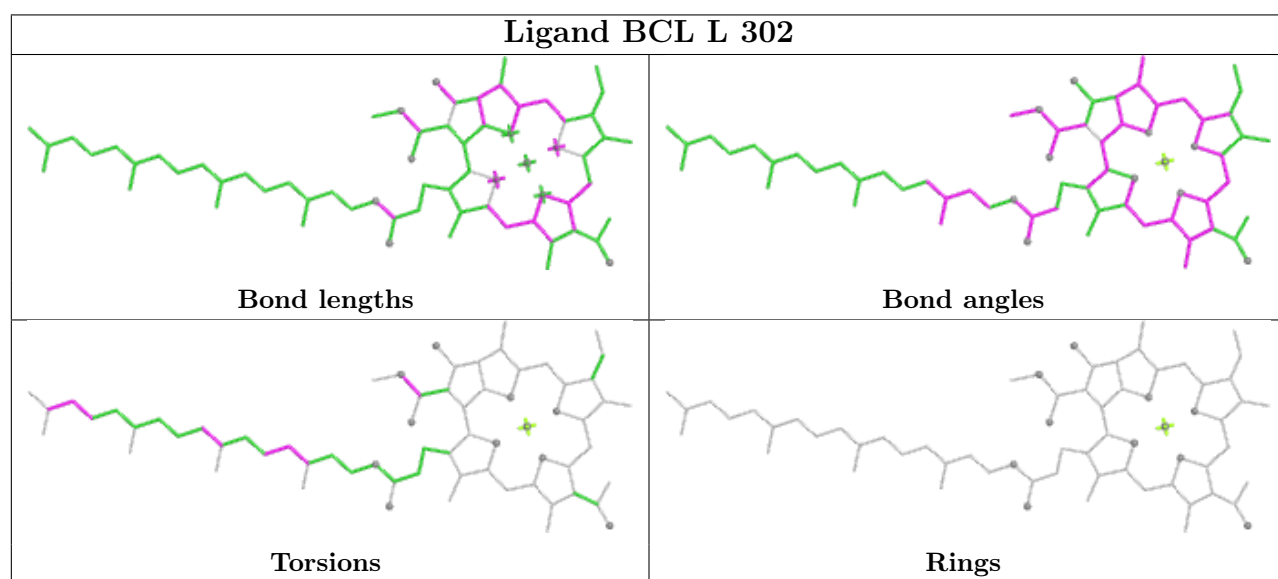
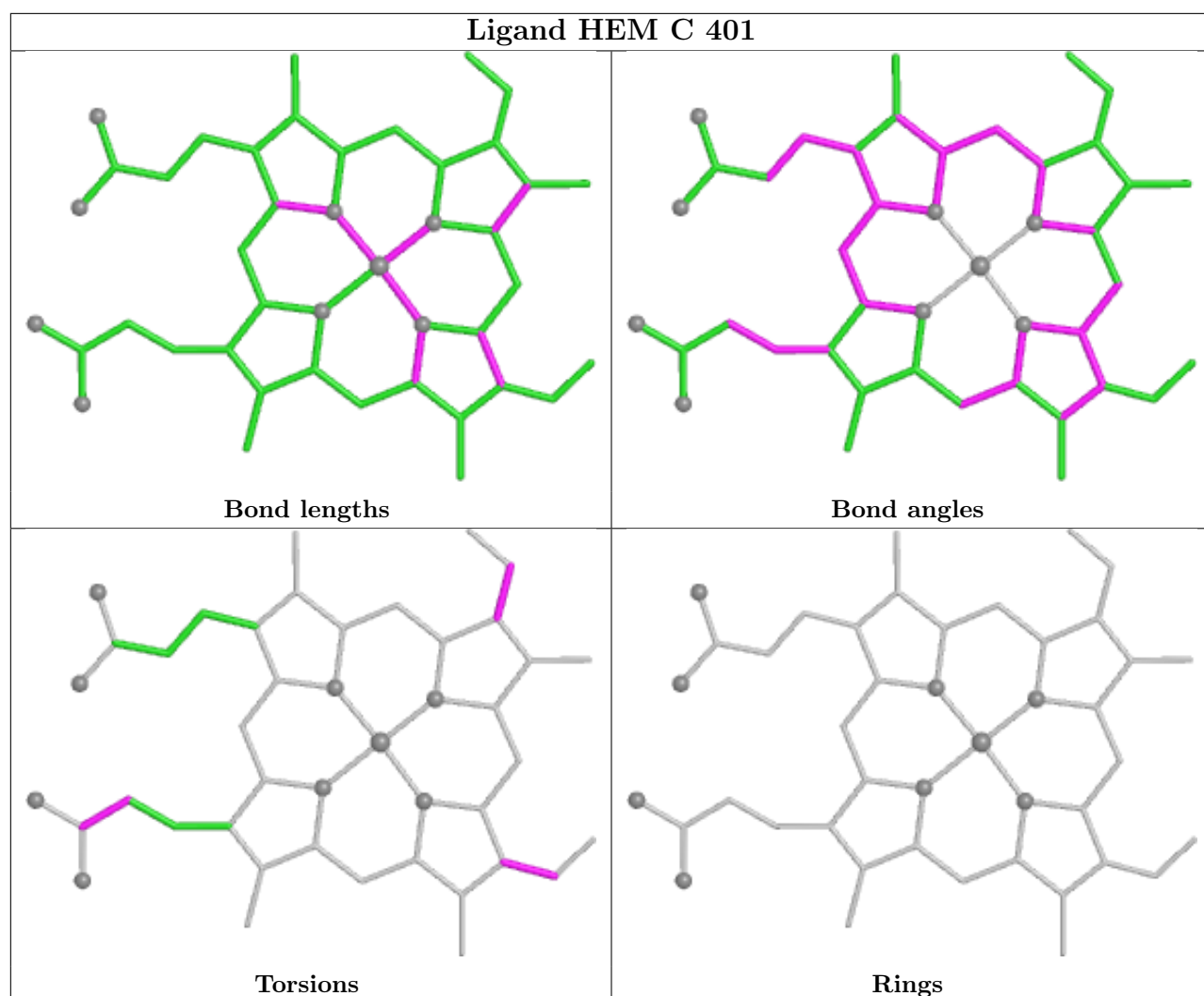
Bond angles



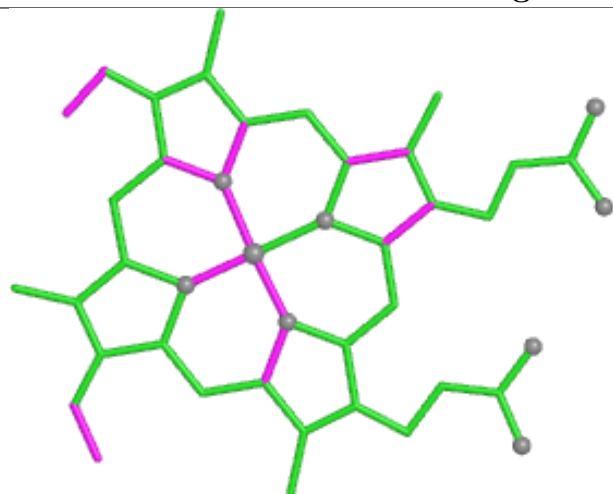
Torsions



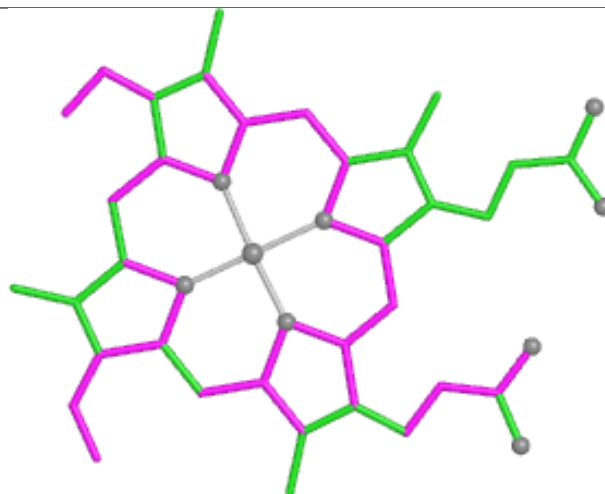
Rings



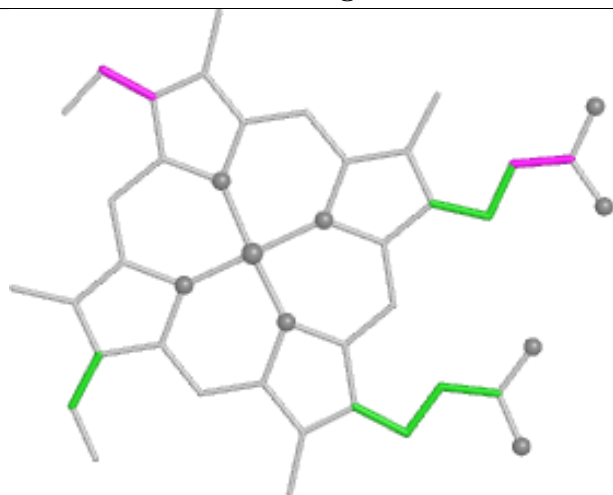
Ligand HEC C 402



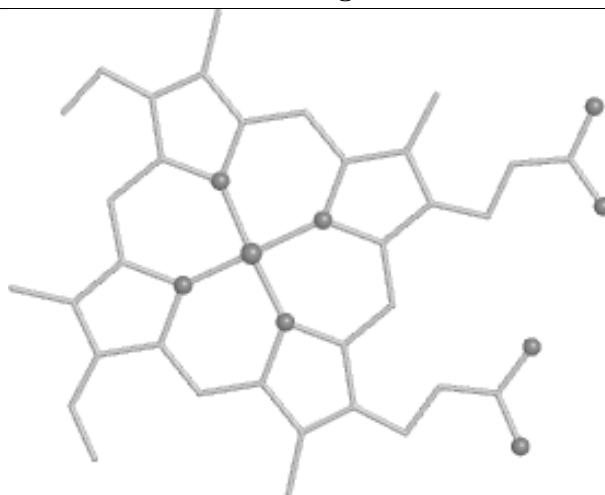
Bond lengths



Bond angles

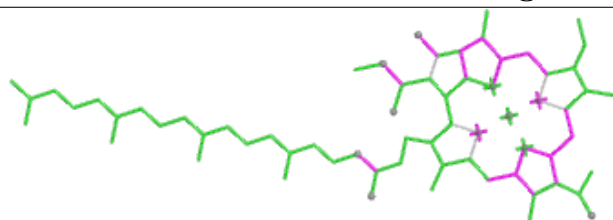


Torsions

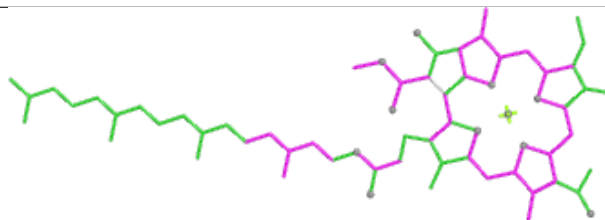


Rings

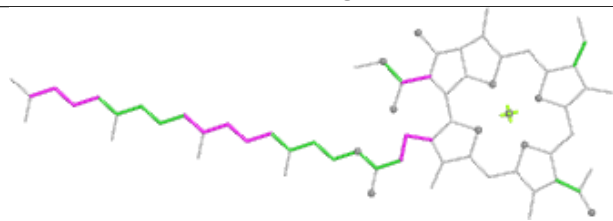
Ligand BCL S 101



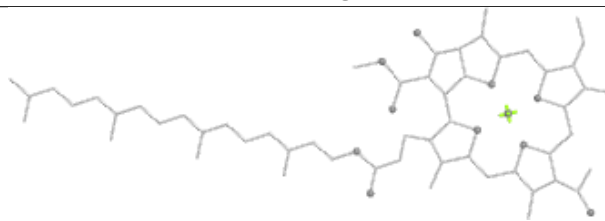
Bond lengths



Bond angles

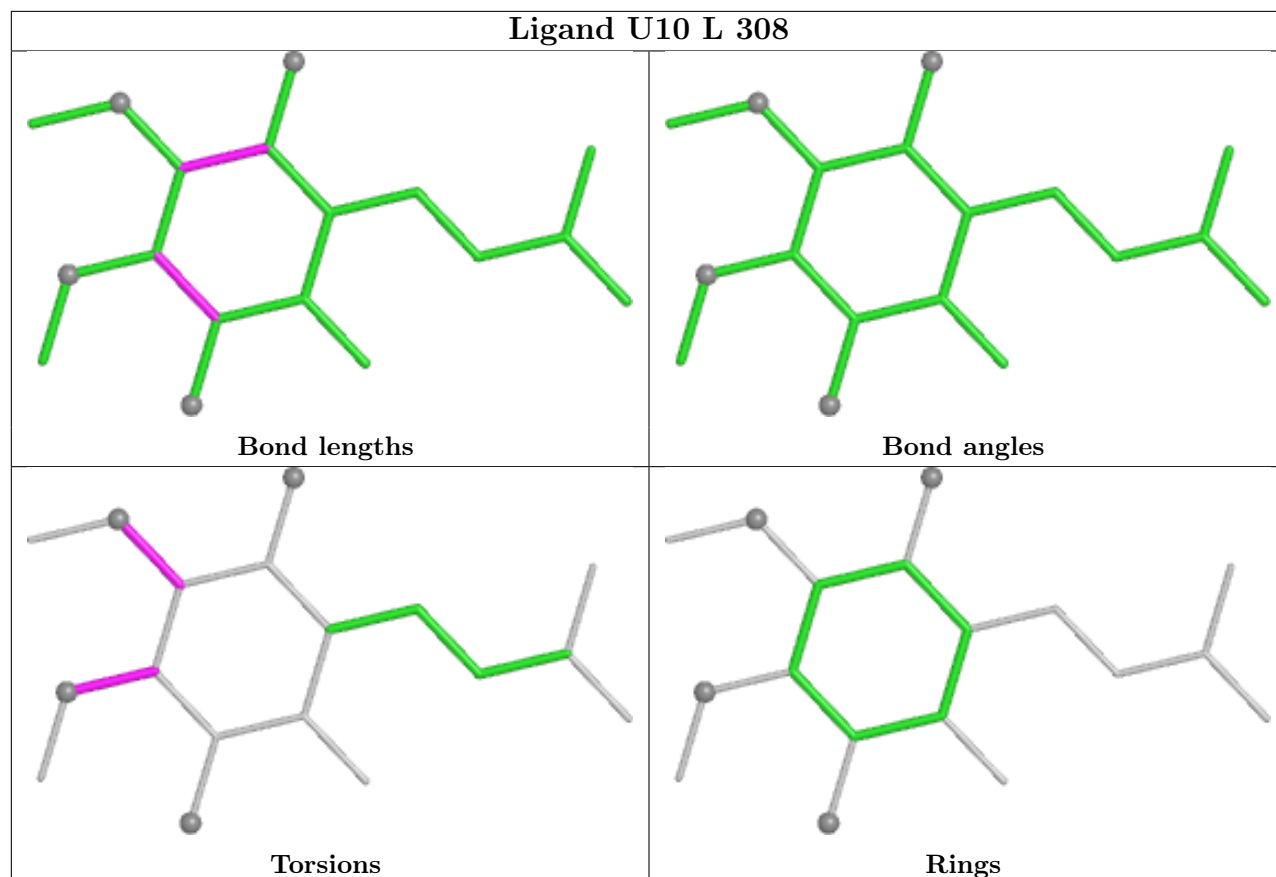


Torsions

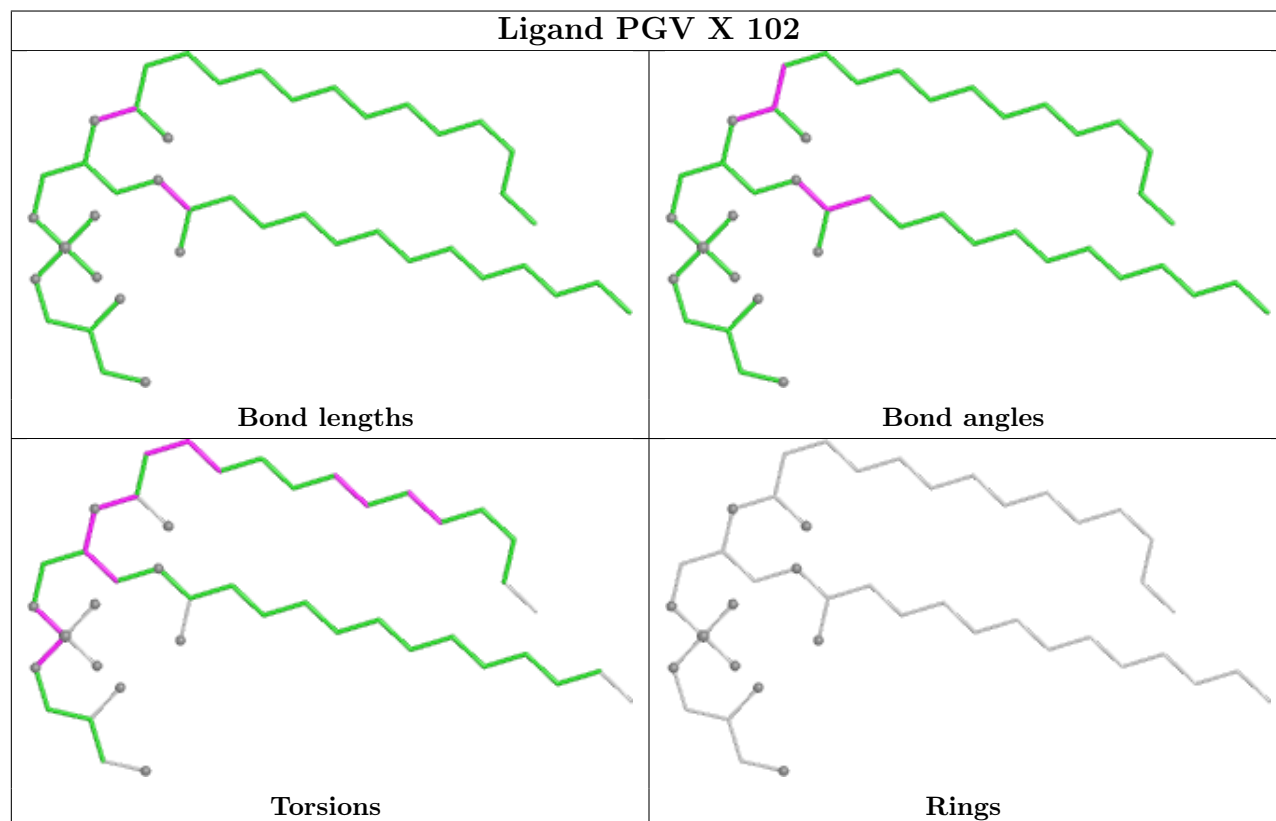


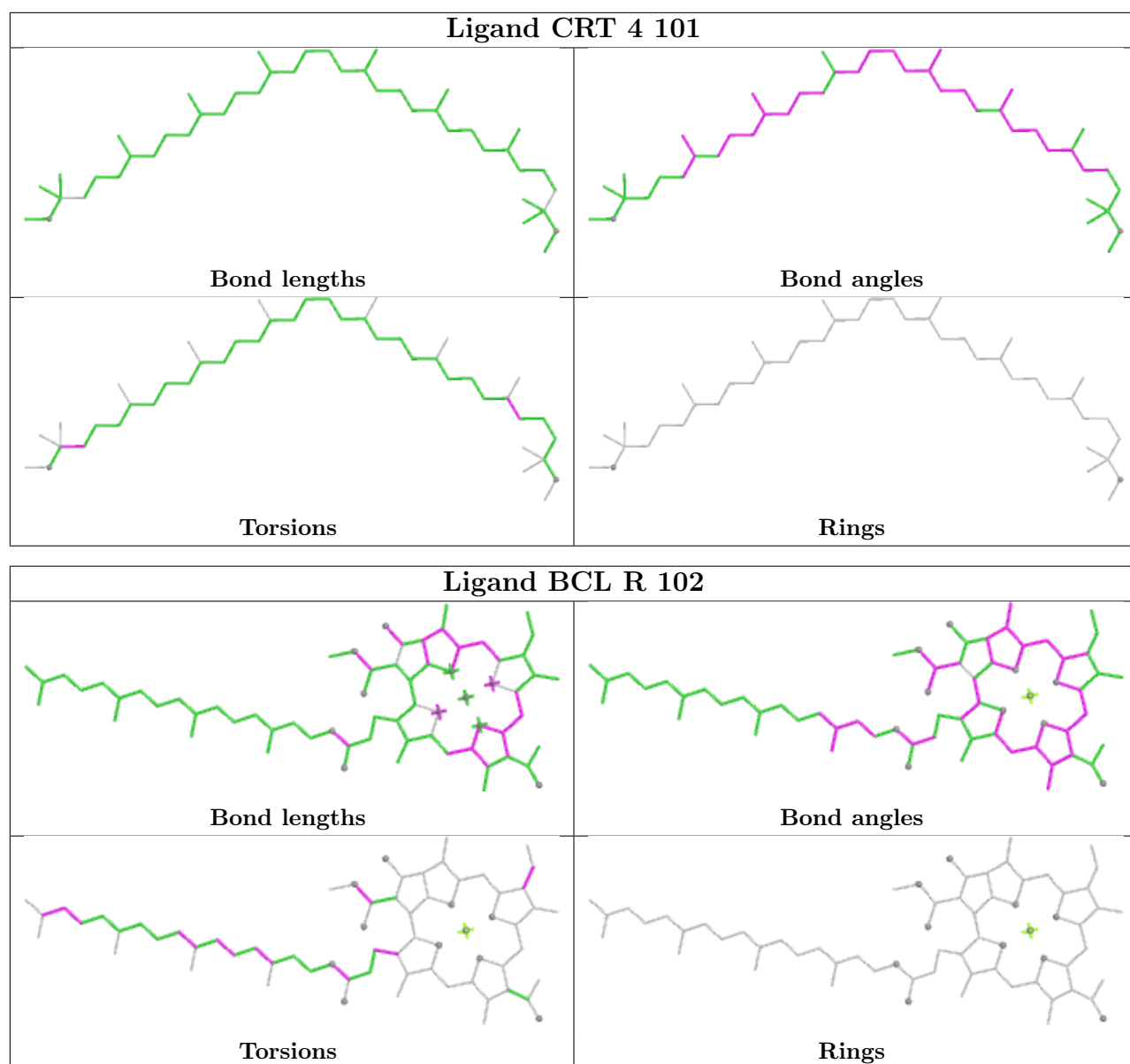
Rings

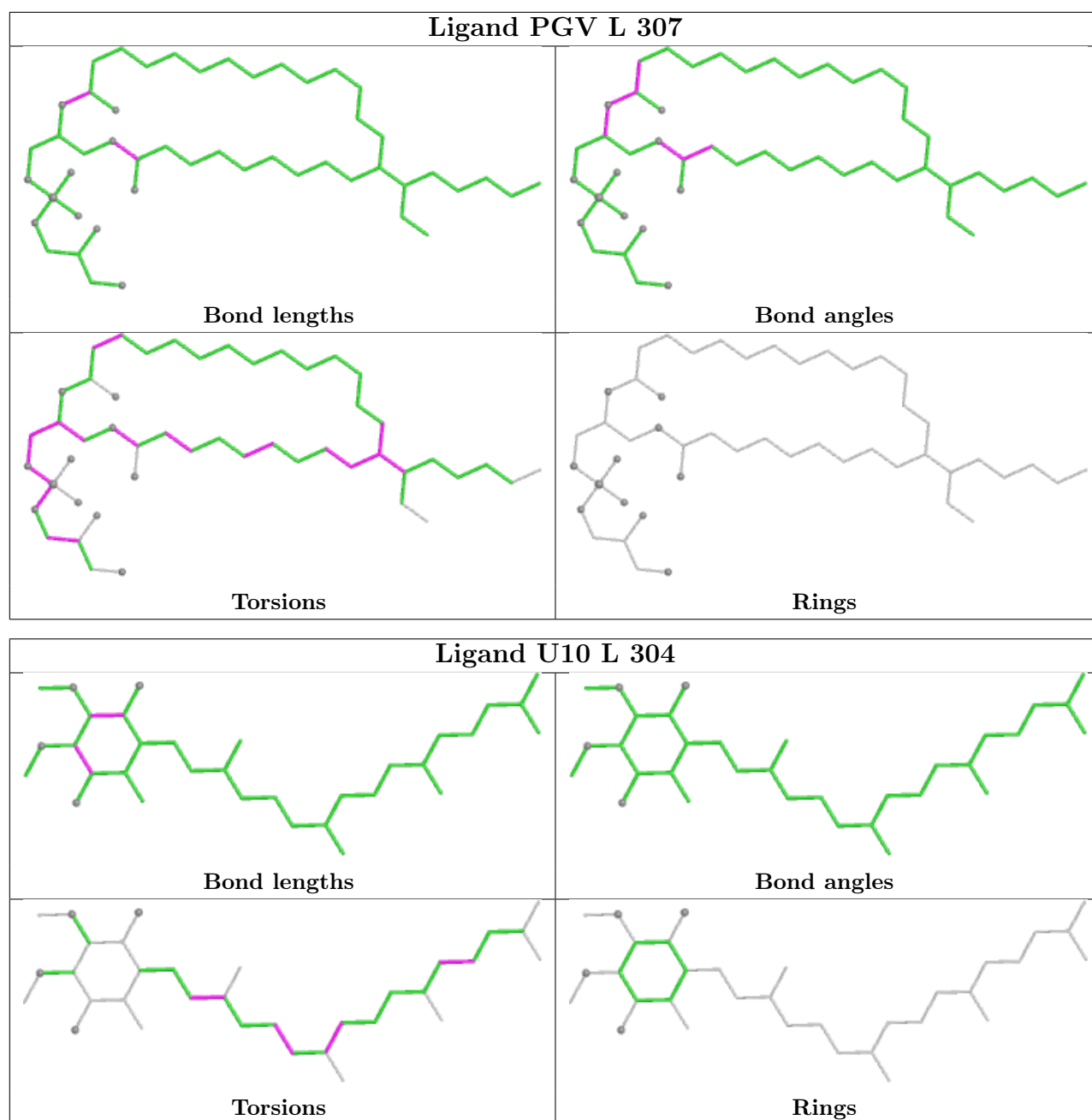
Ligand U10 L 308

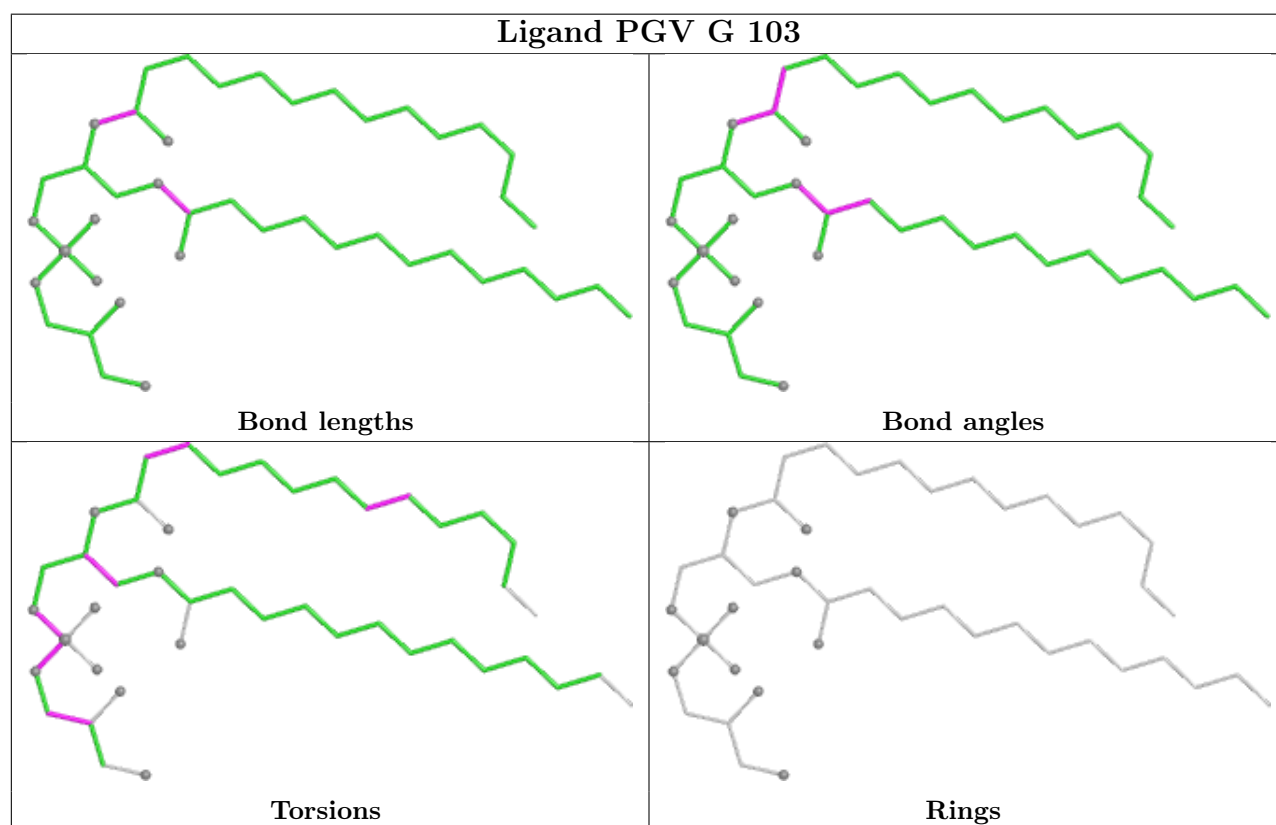
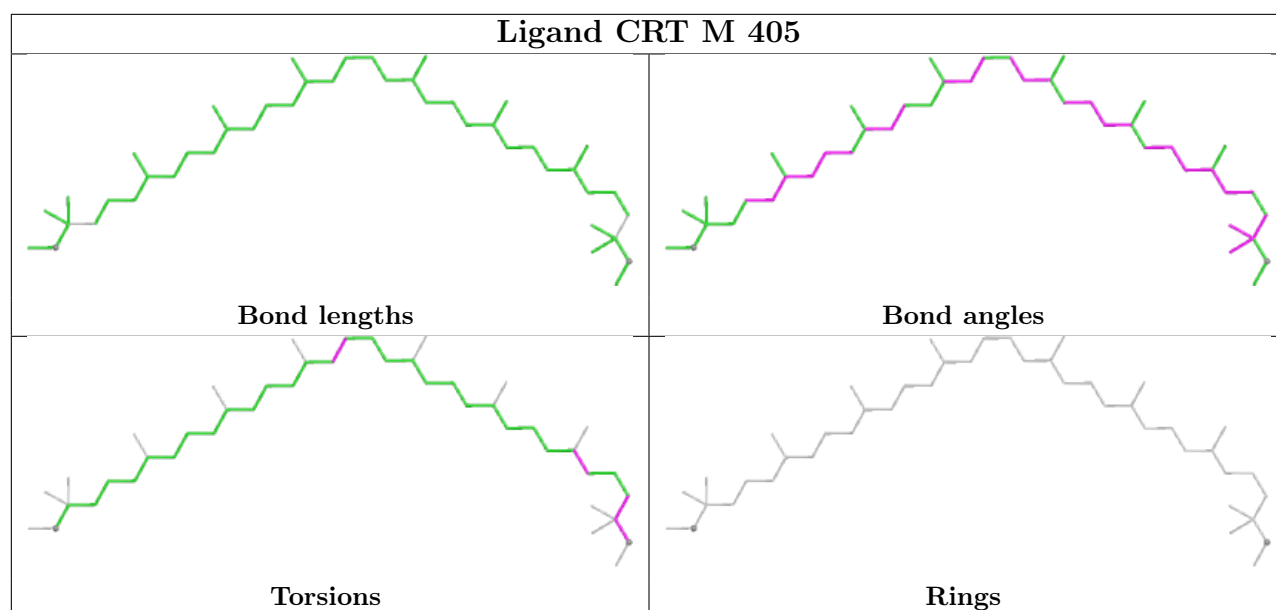


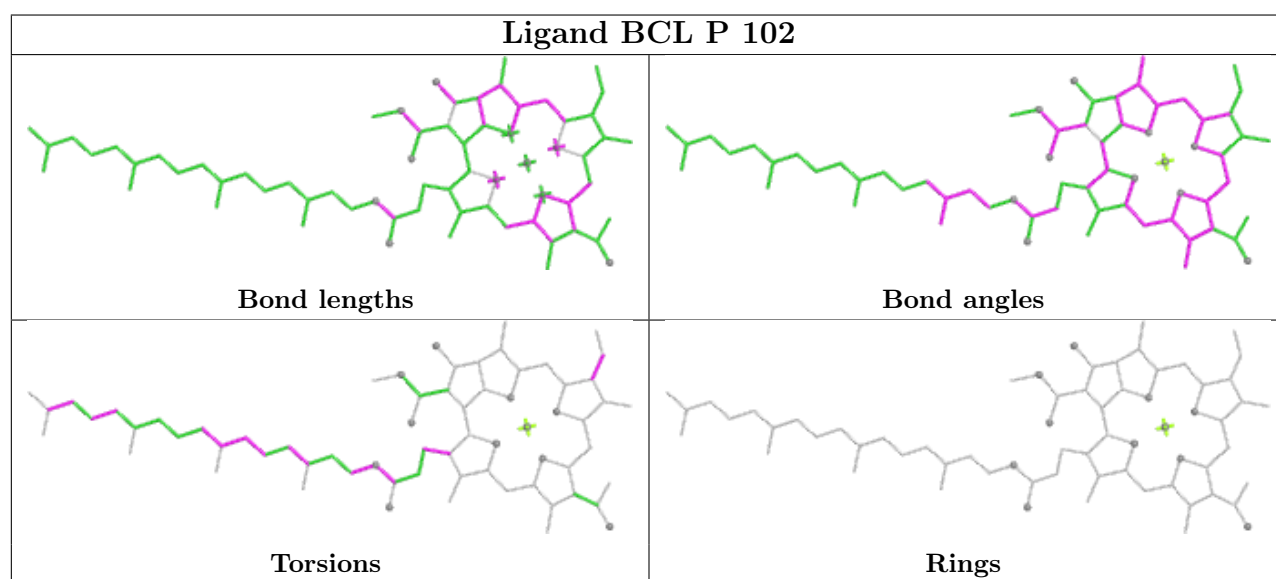
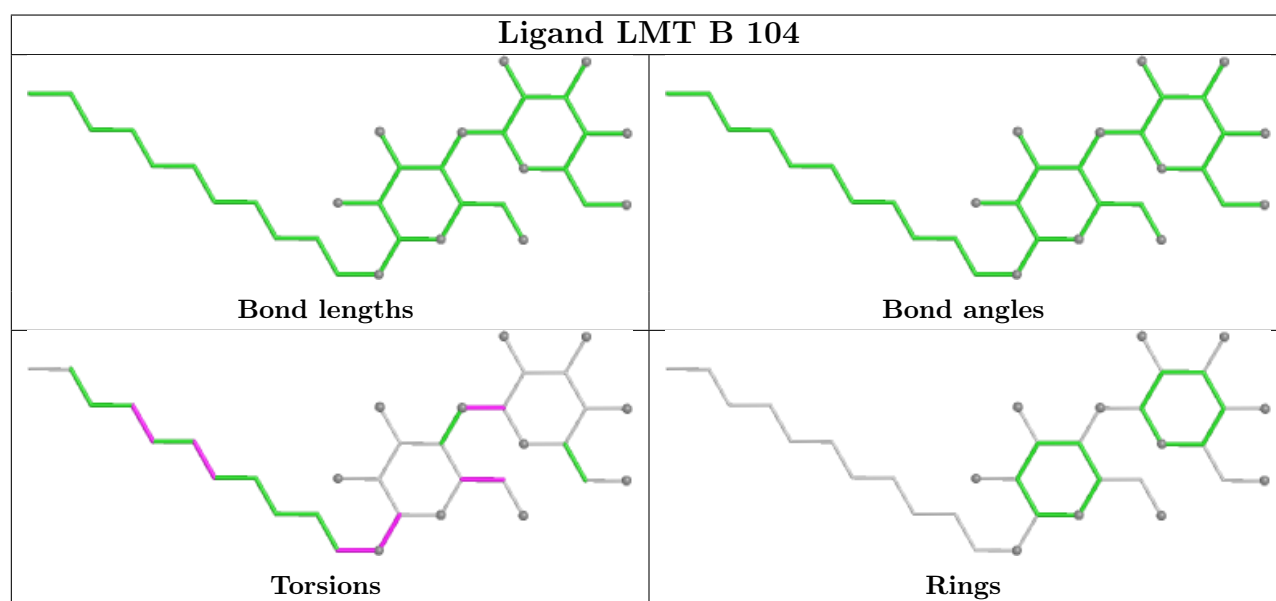
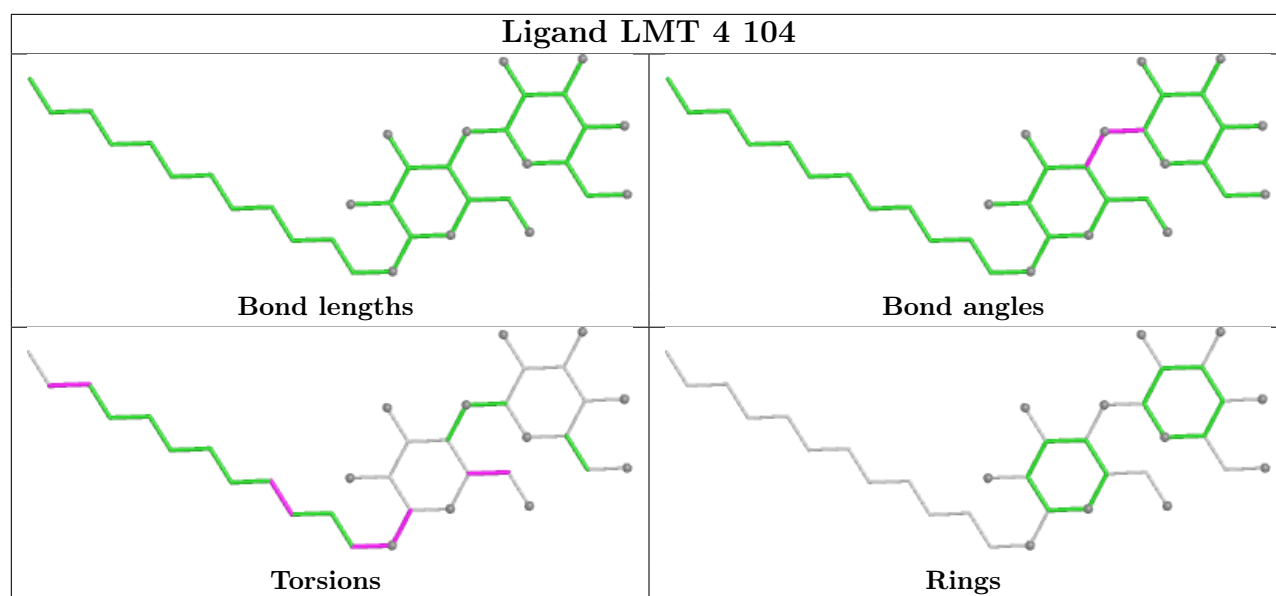
Ligand PGV X 102

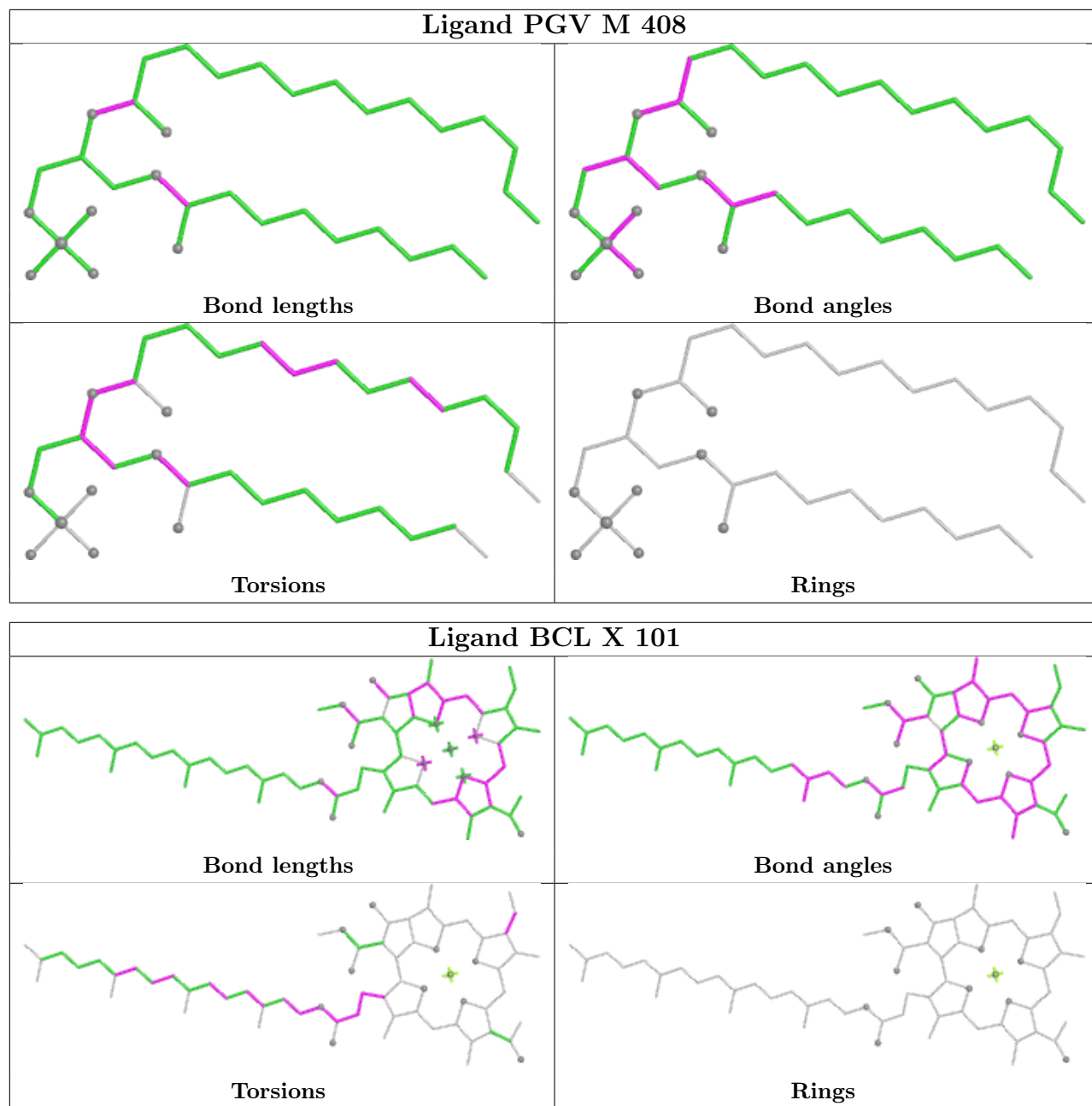


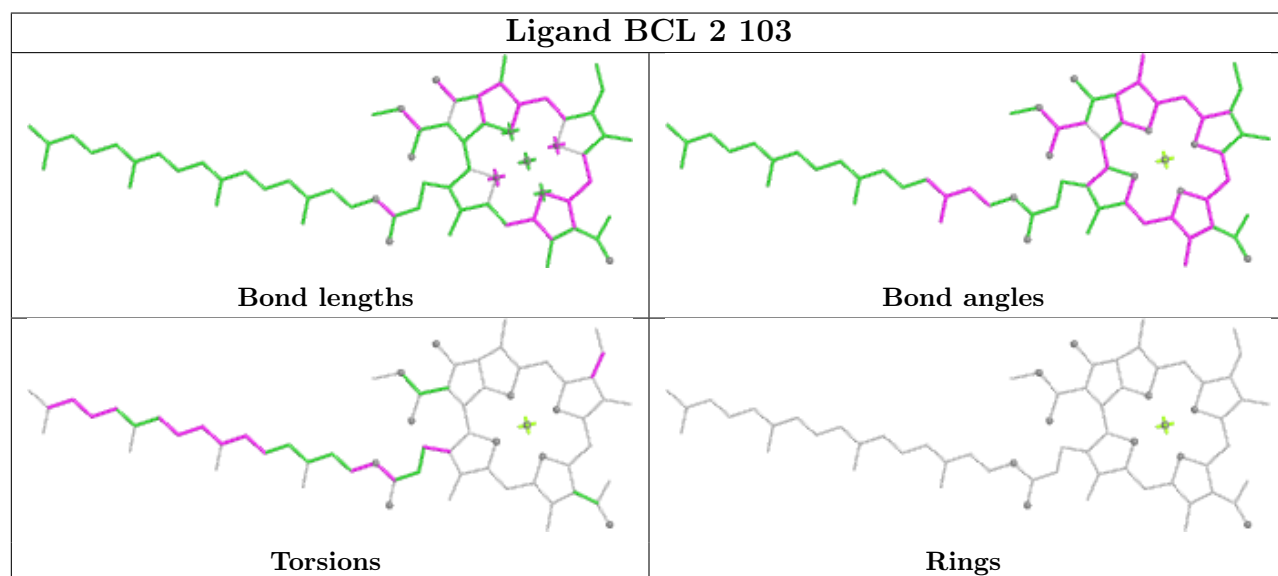
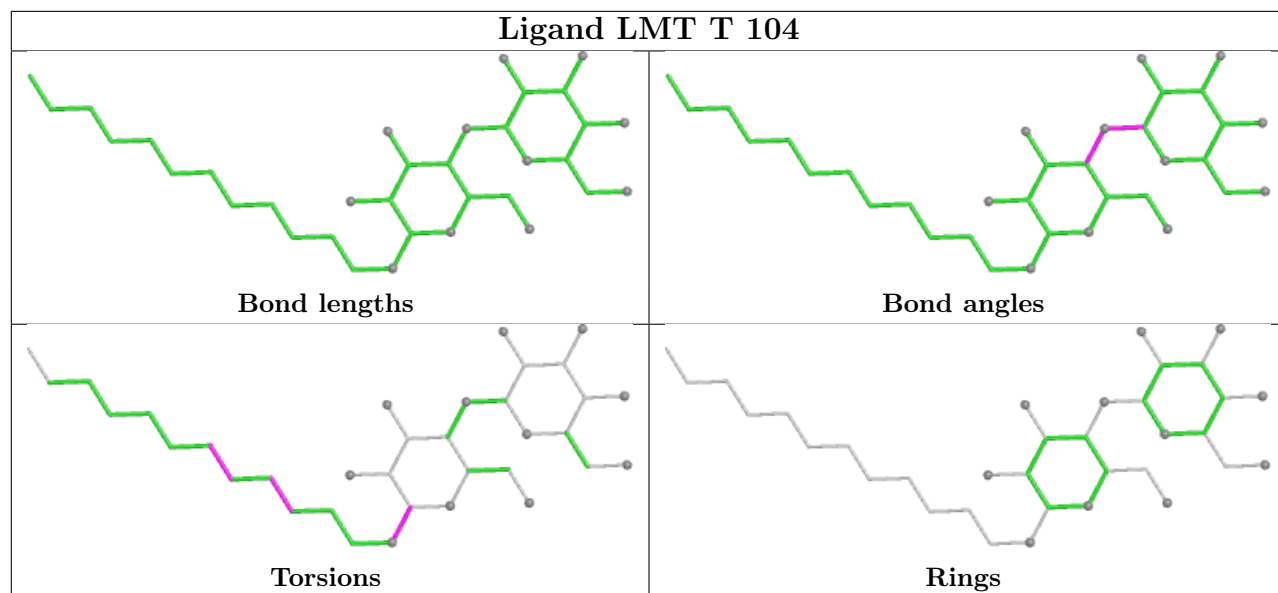




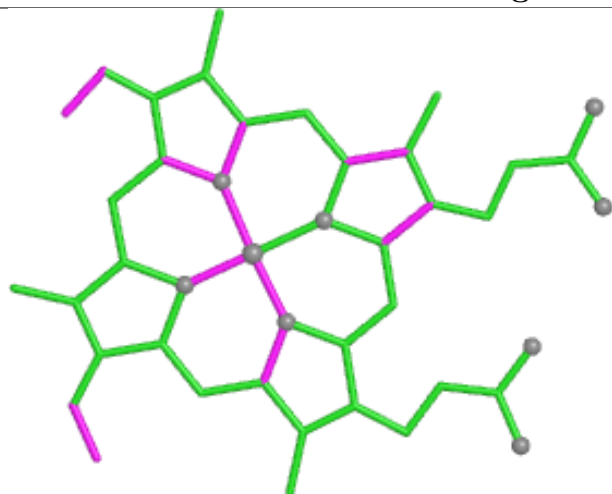




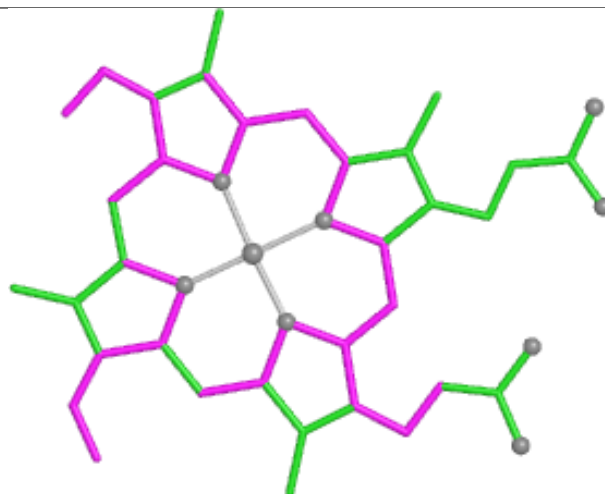




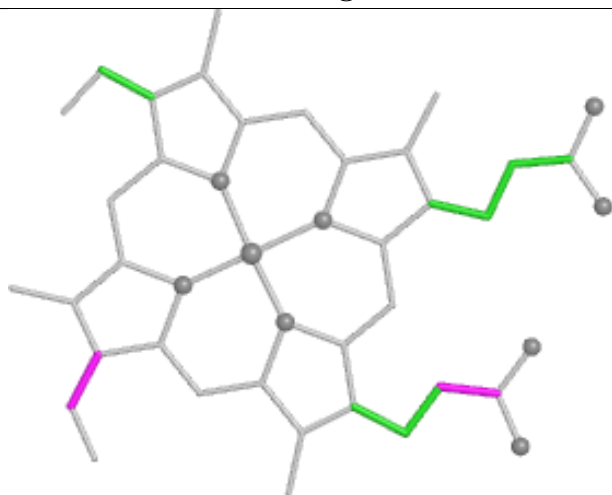
Ligand HEC C 403



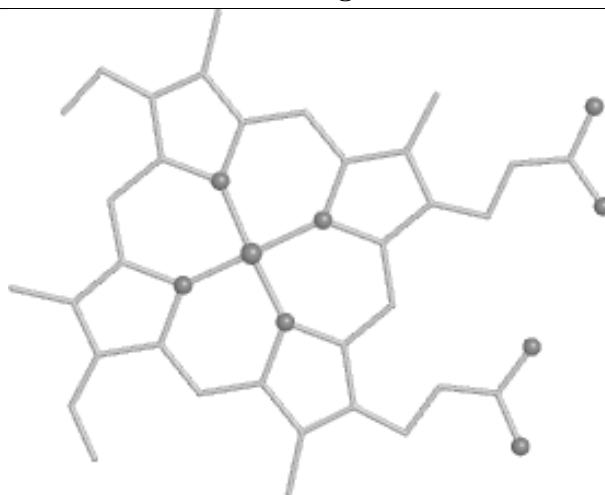
Bond lengths



Bond angles

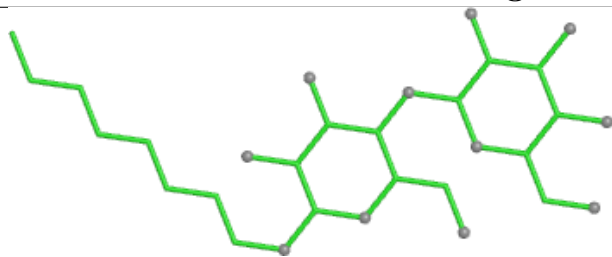


Torsions

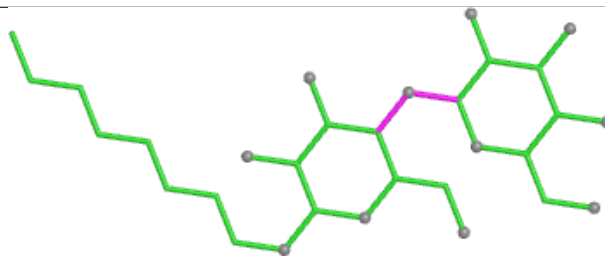


Rings

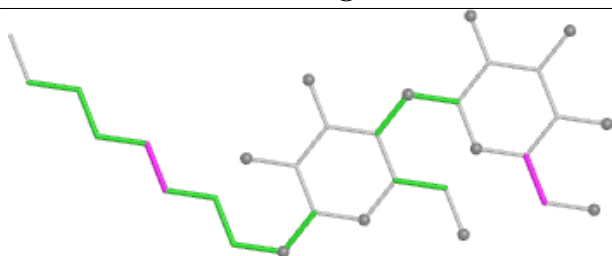
Ligand LMT M 409



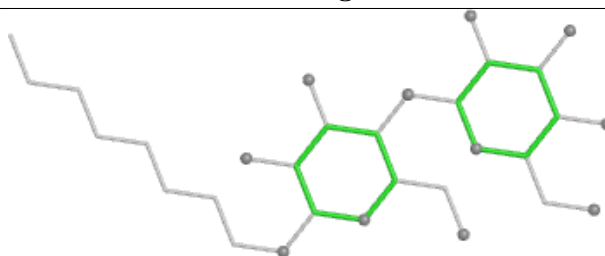
Bond lengths



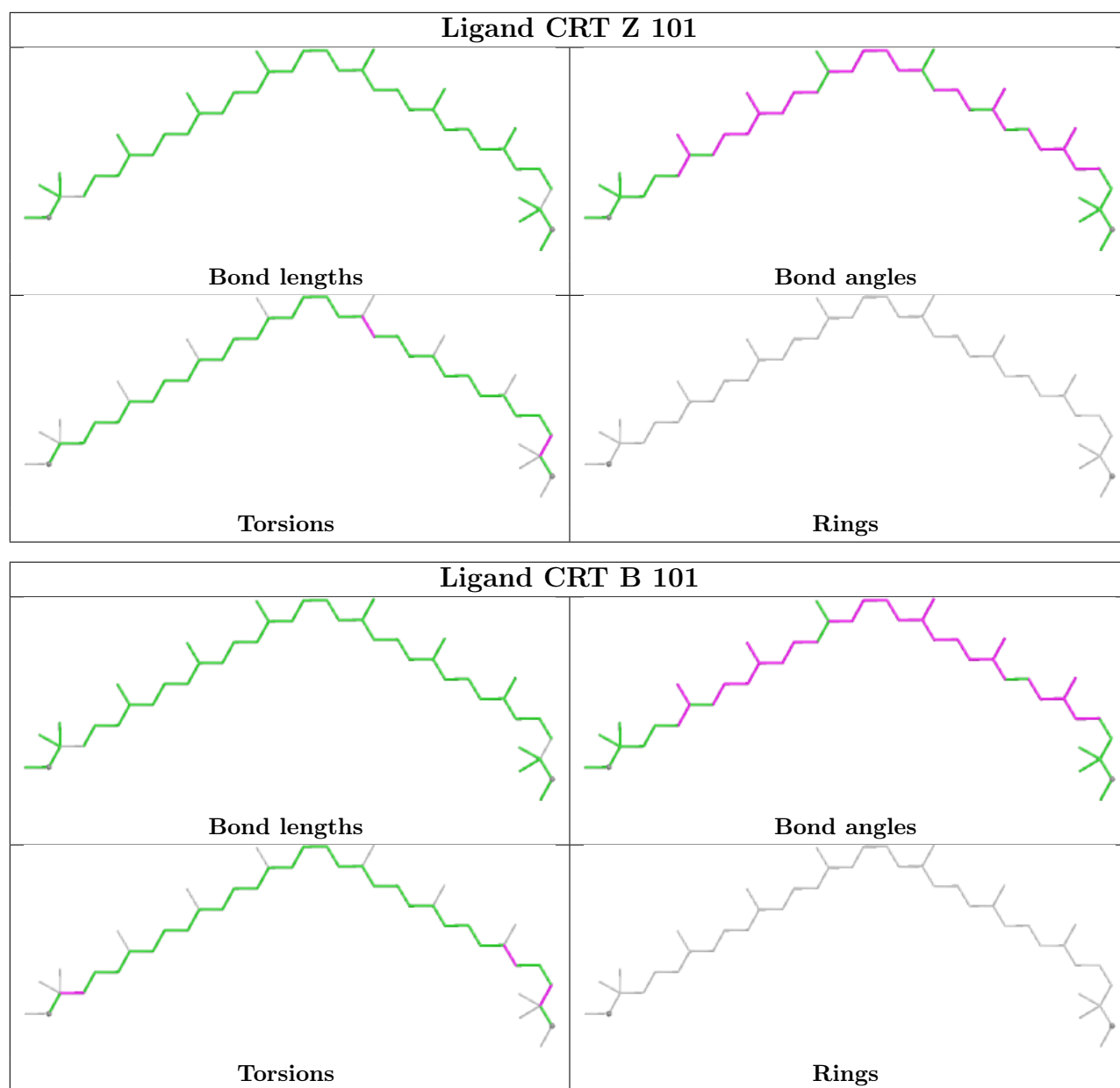
Bond angles

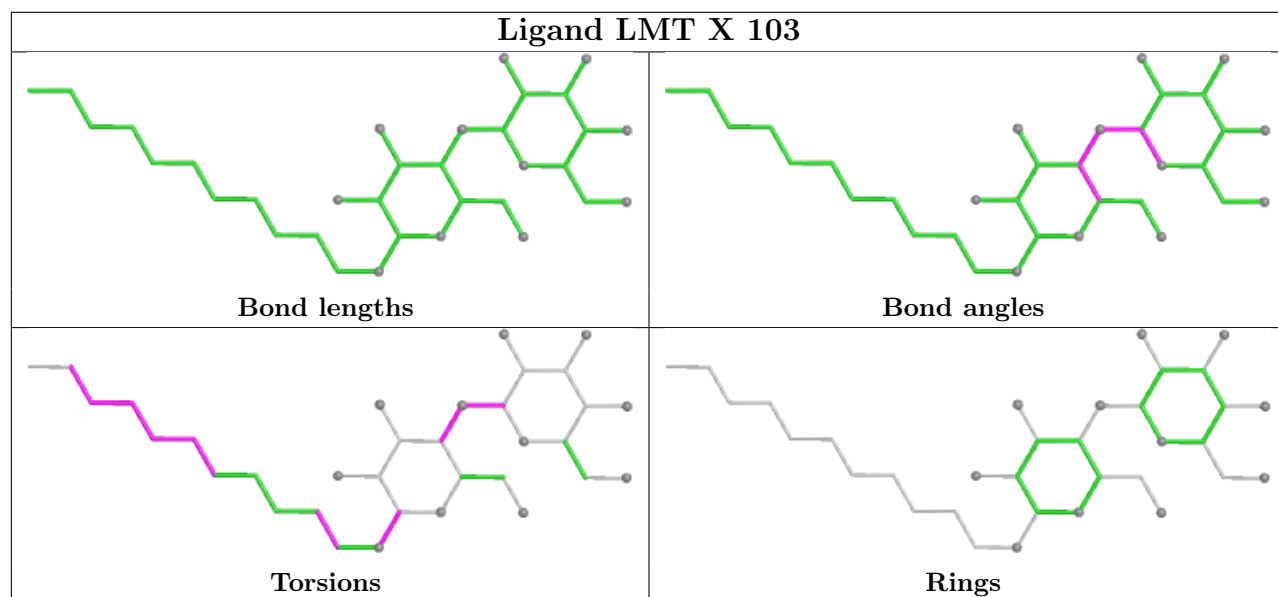
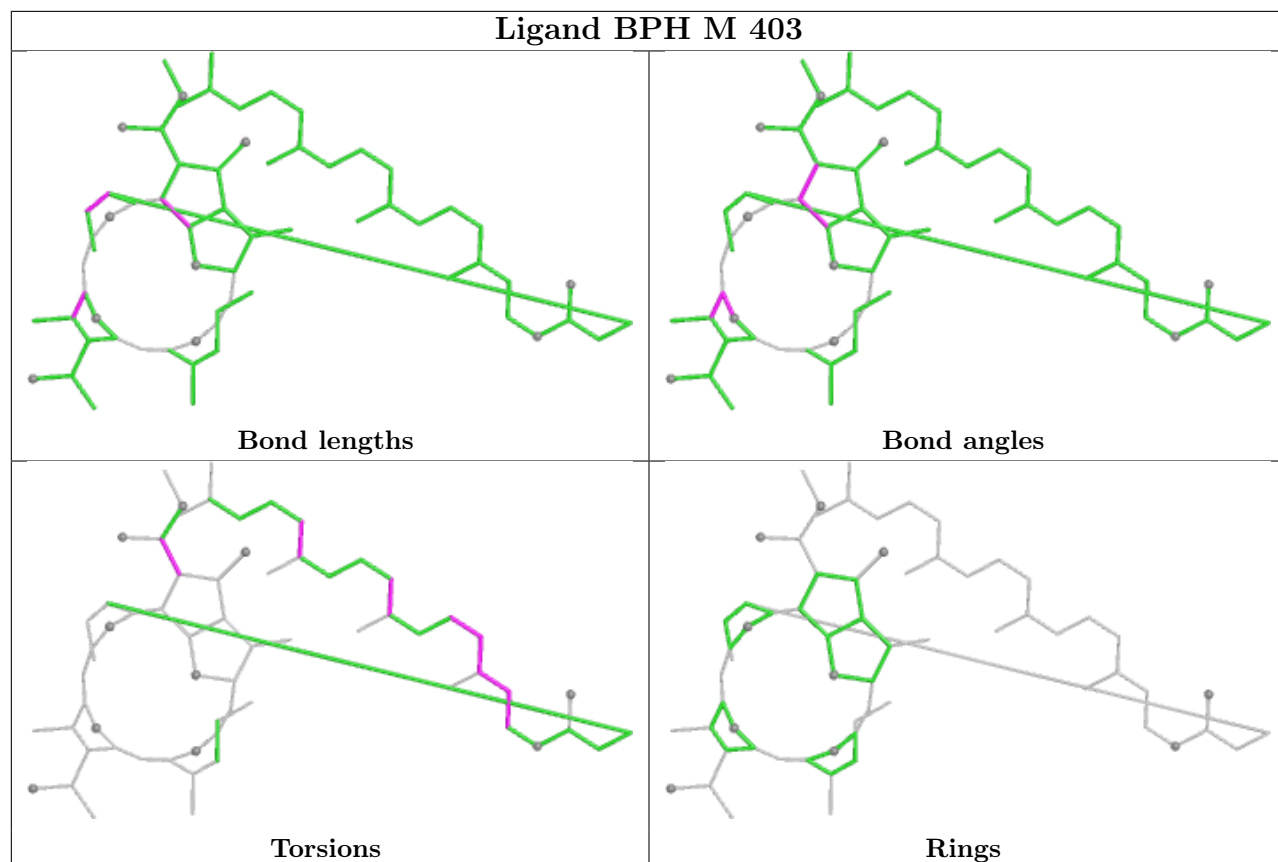


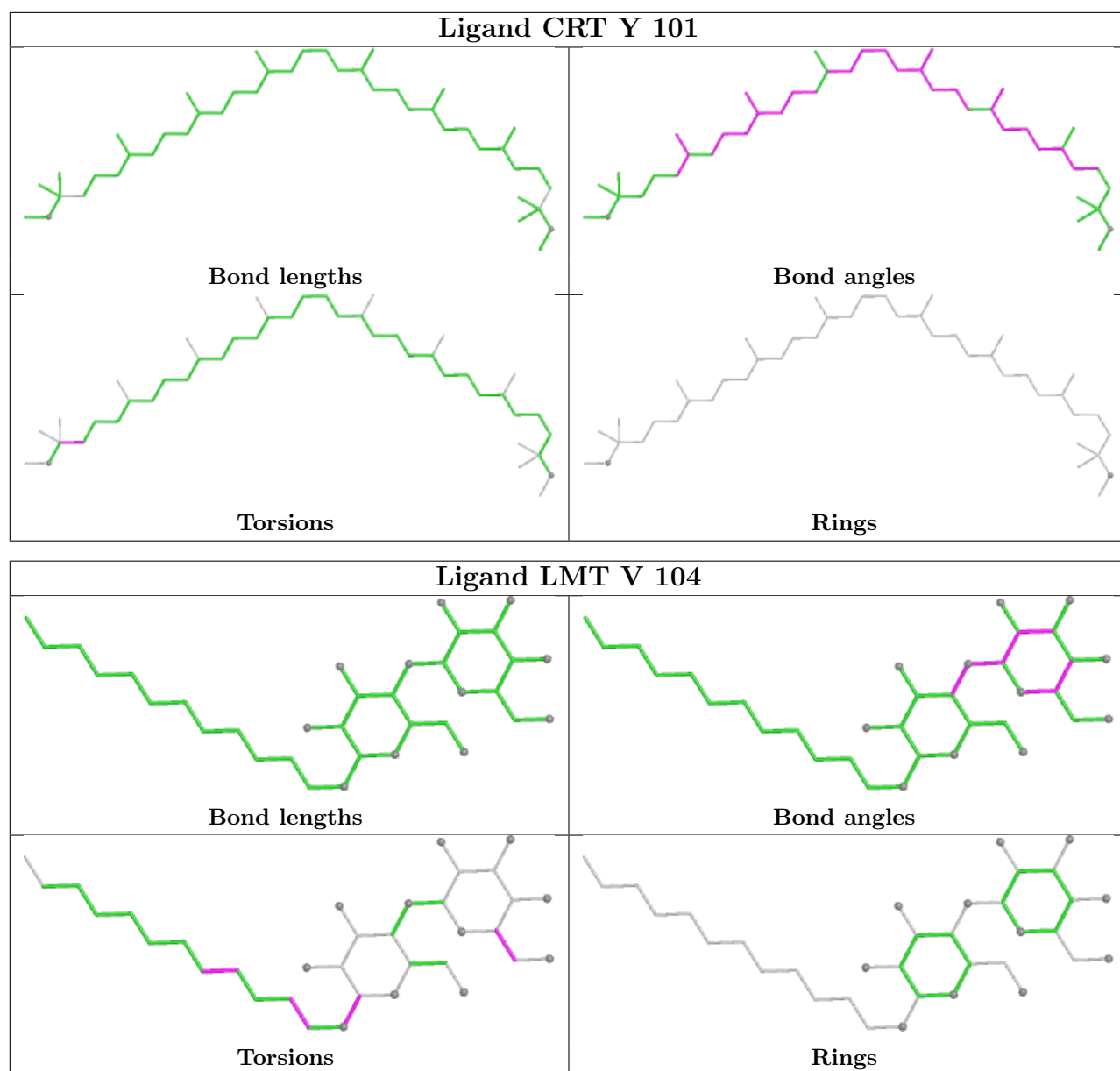
Torsions

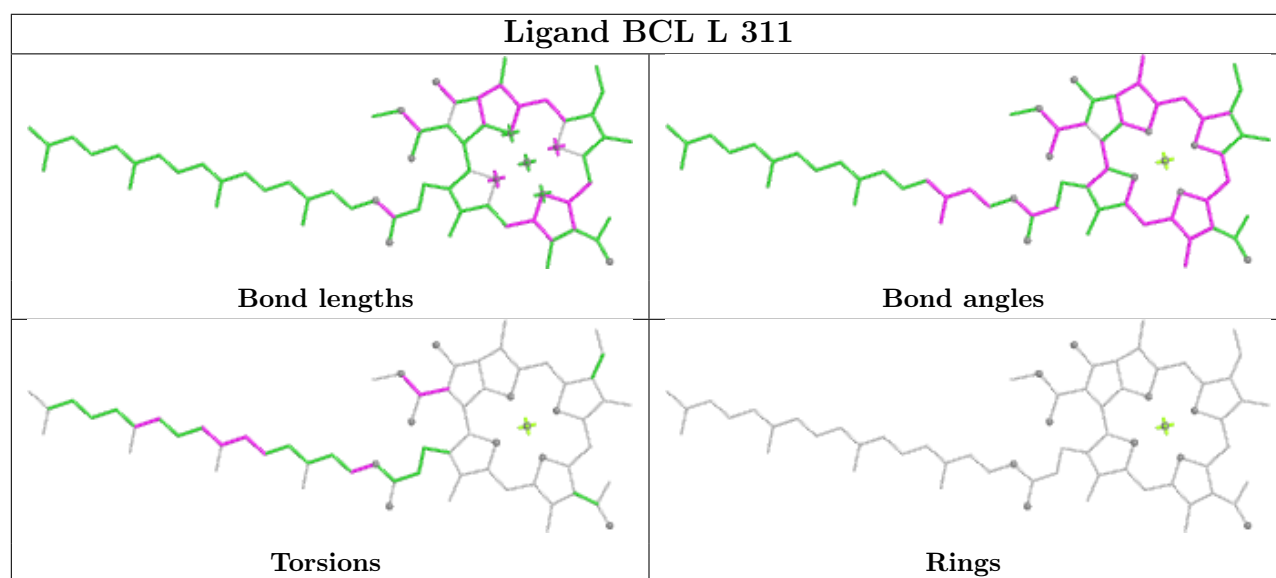
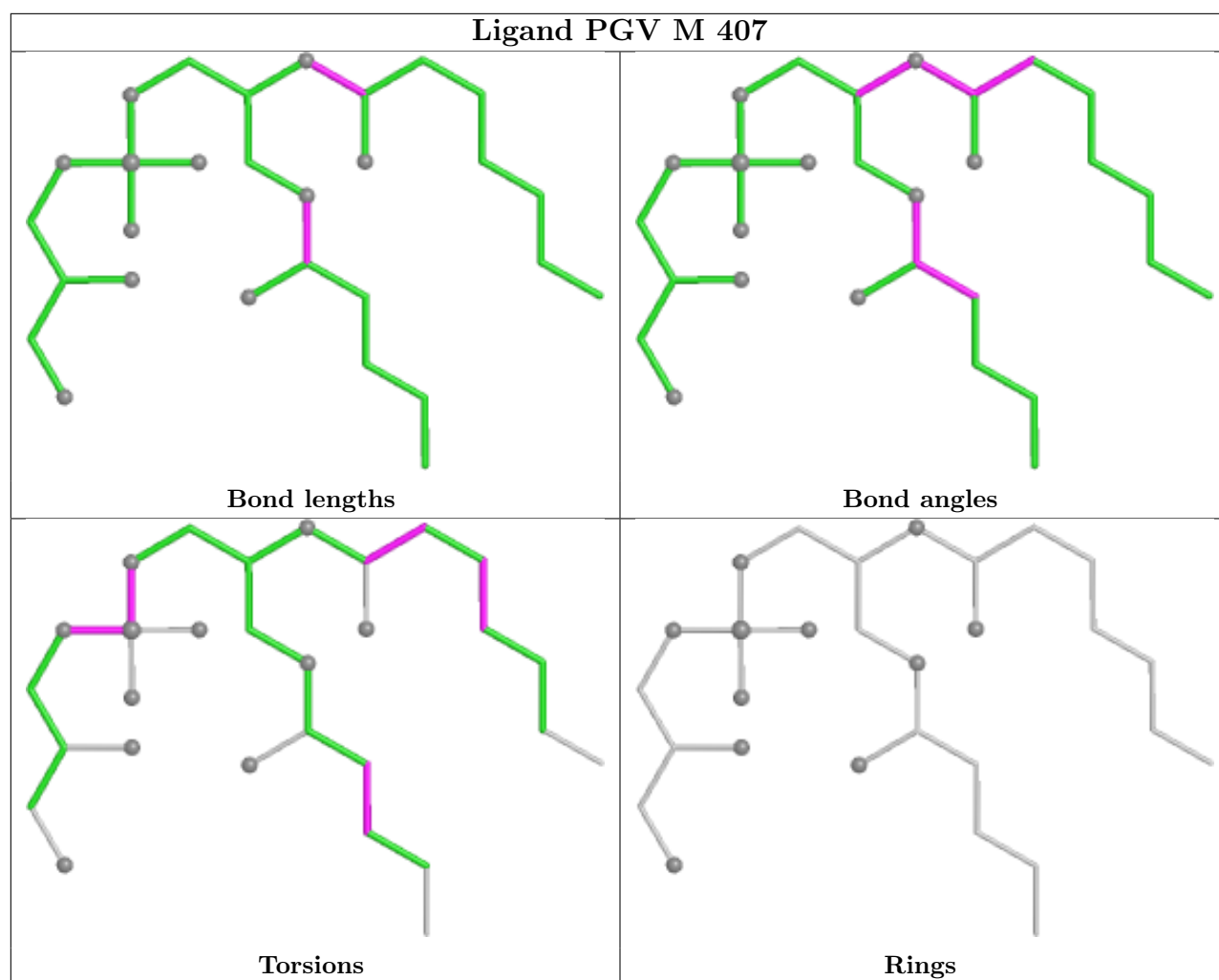


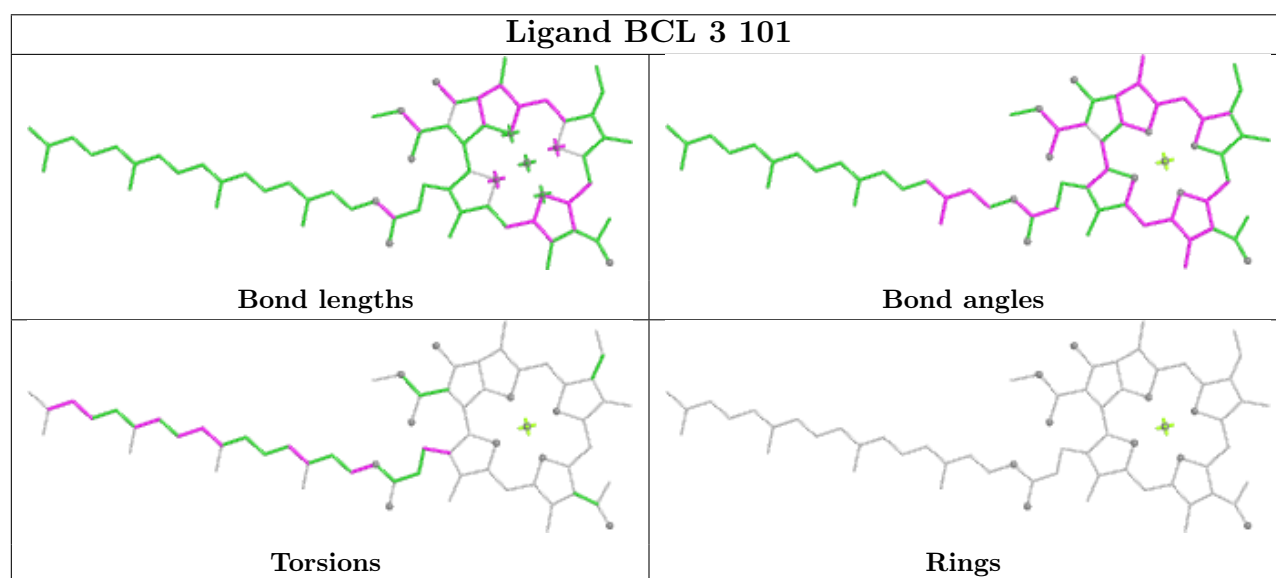
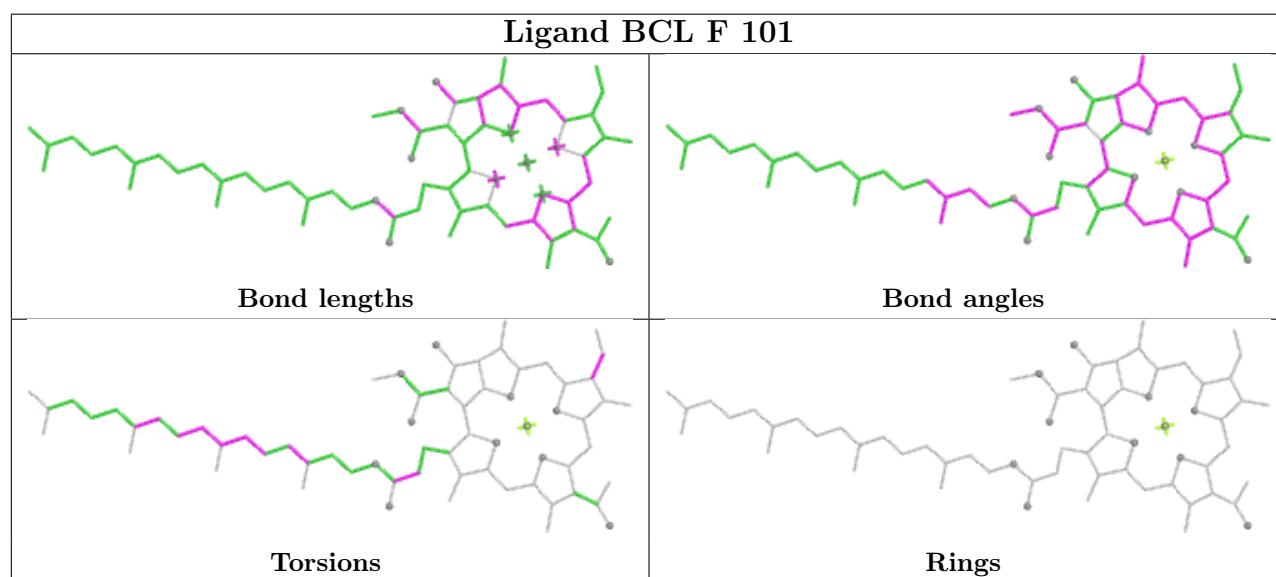
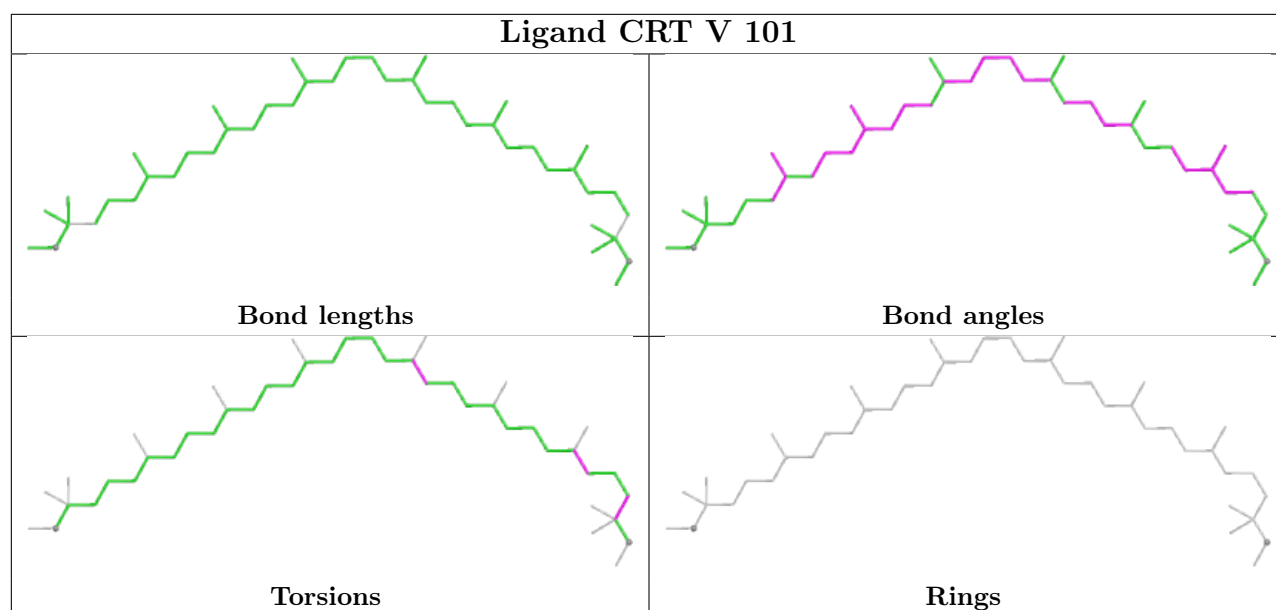
Rings

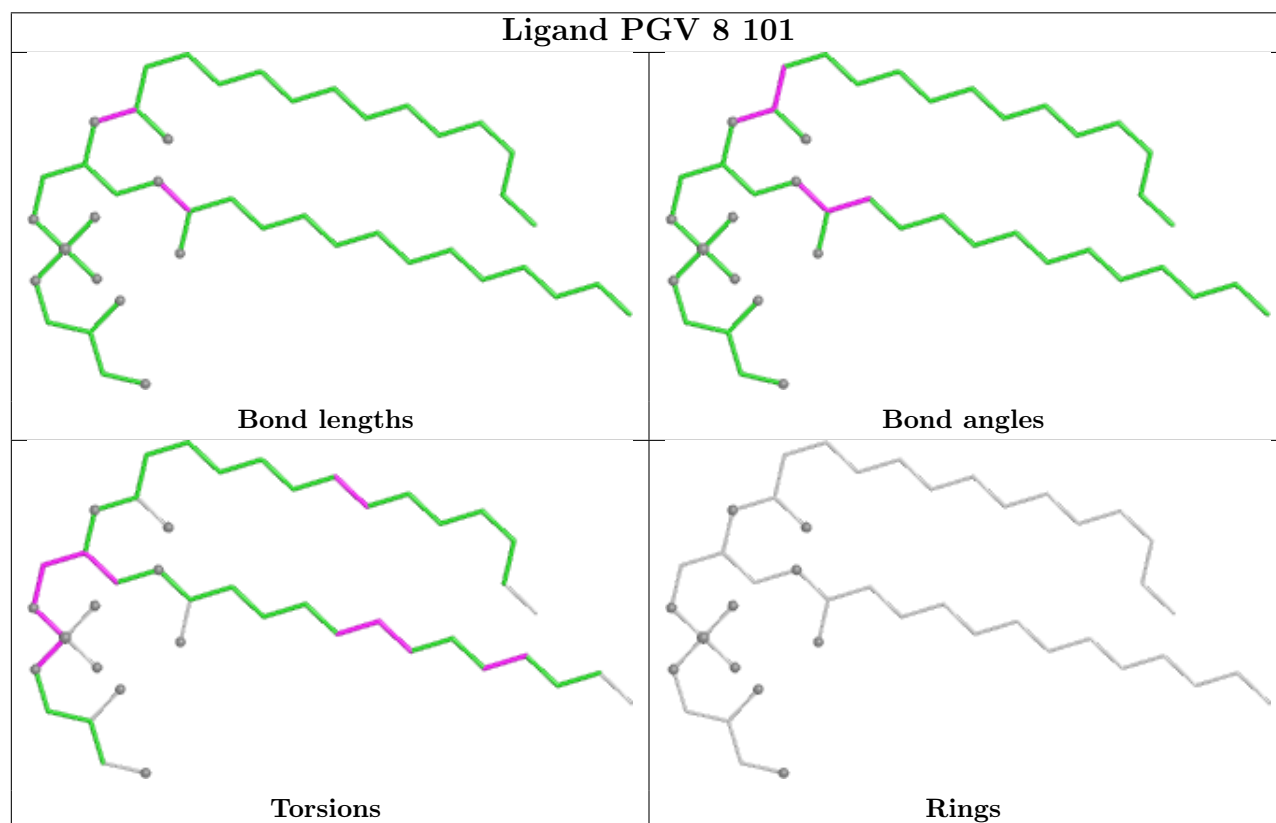
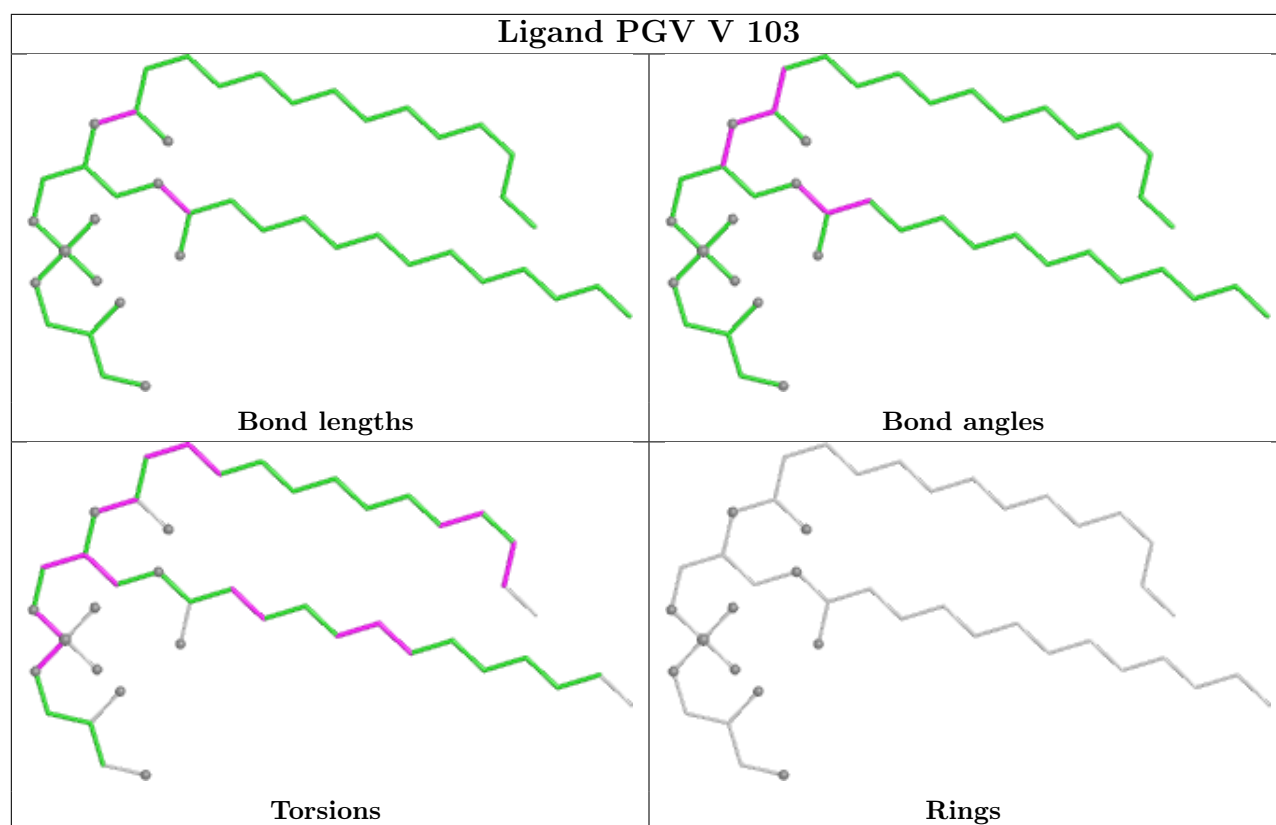












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

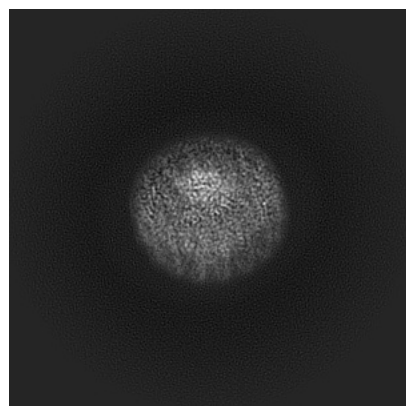
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63714. These allow visual inspection of the internal detail of the map and identification of artifacts.

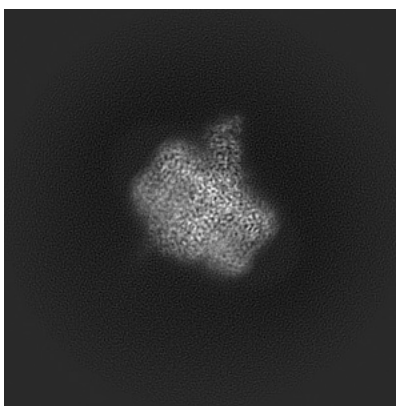
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

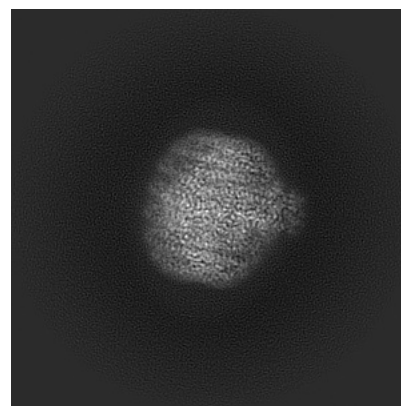
6.1.1 Primary map



X

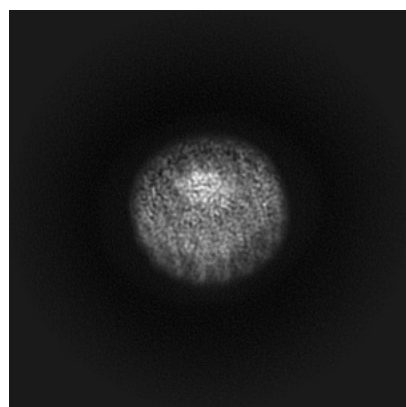


Y

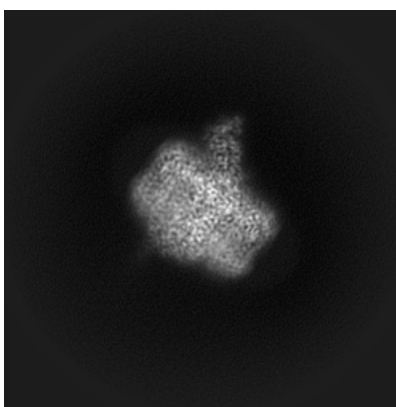


Z

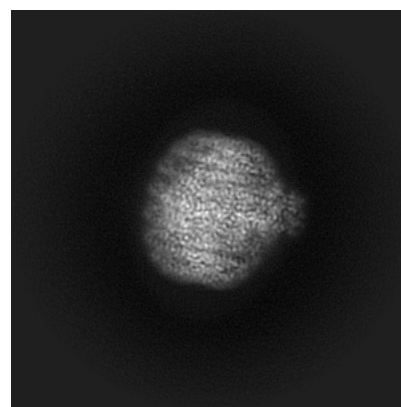
6.1.2 Raw map



X



Y

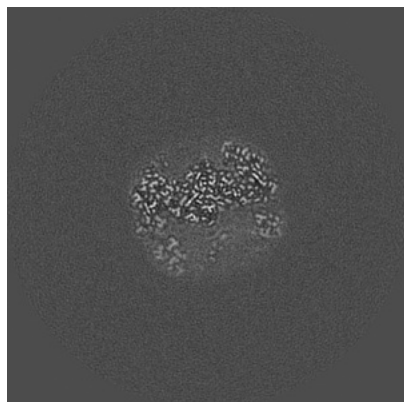


Z

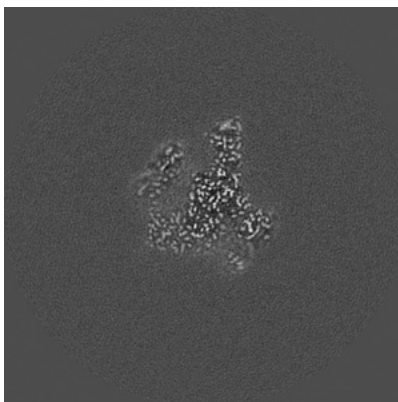
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

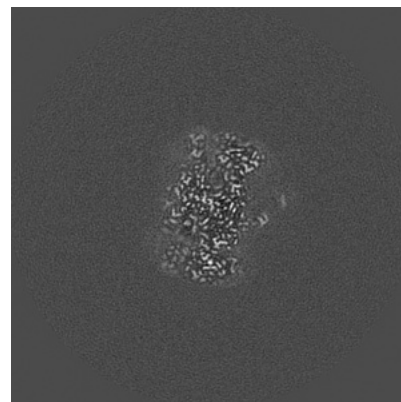
6.2.1 Primary map



X Index: 190

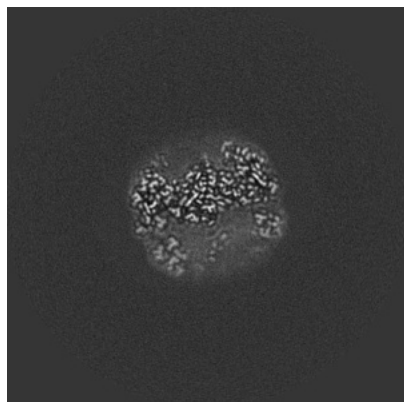


Y Index: 190

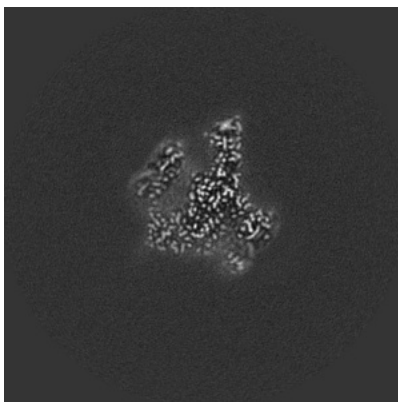


Z Index: 190

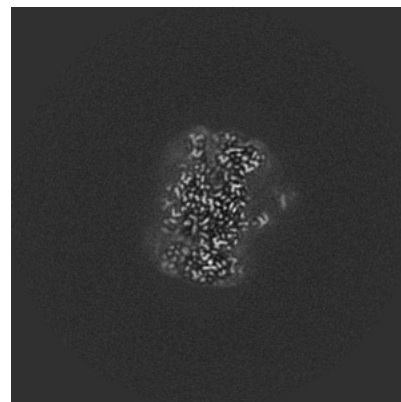
6.2.2 Raw map



X Index: 190



Y Index: 190

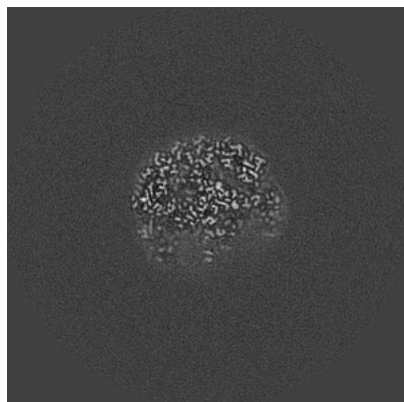


Z Index: 190

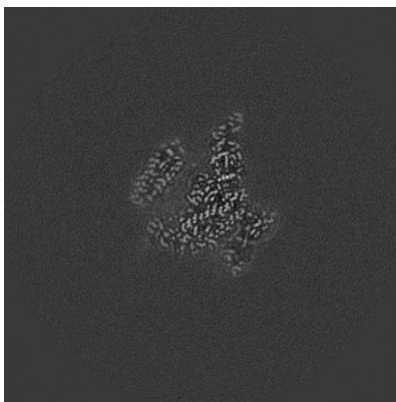
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

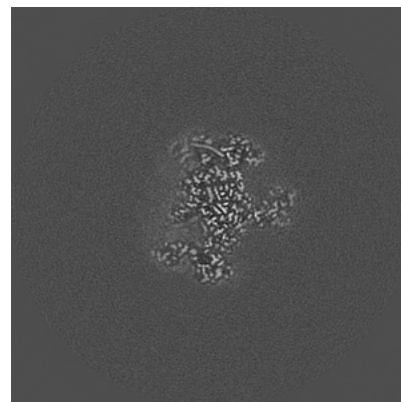
6.3.1 Primary map



X Index: 182

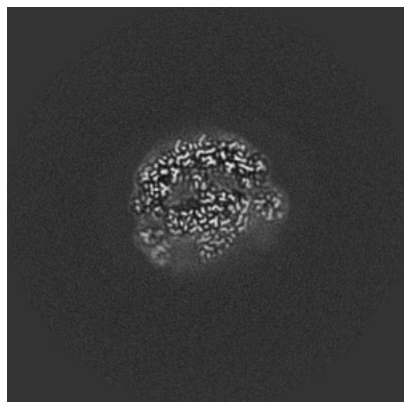


Y Index: 184

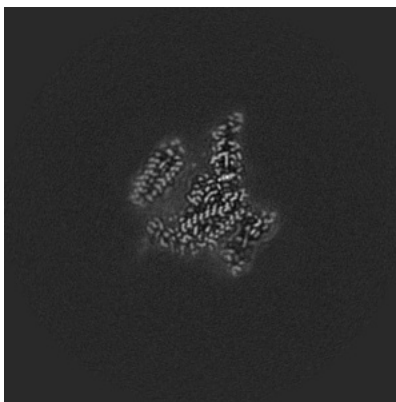


Z Index: 198

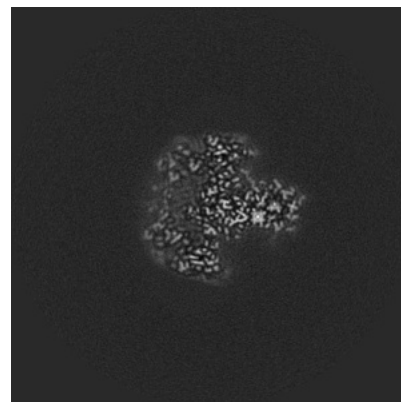
6.3.2 Raw map



X Index: 177



Y Index: 184

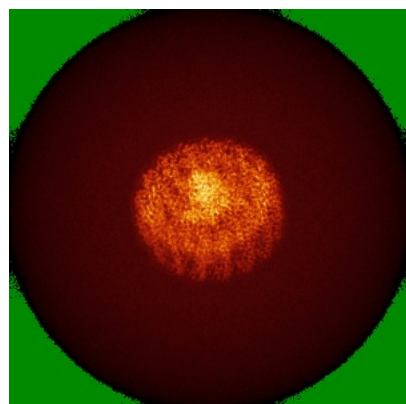


Z Index: 210

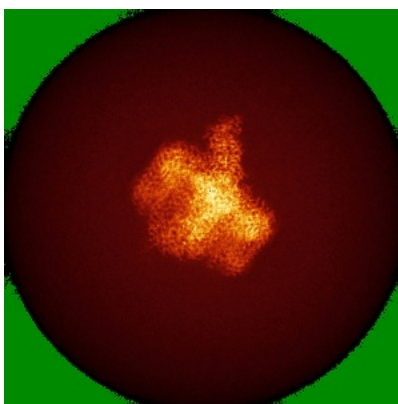
The images above show the largest variance slices of the map in three orthogonal directions.

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

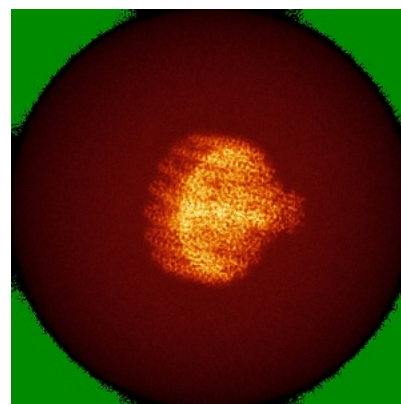
6.4.1 Primary map



X

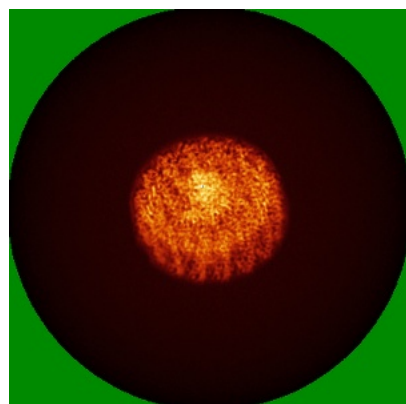


Y

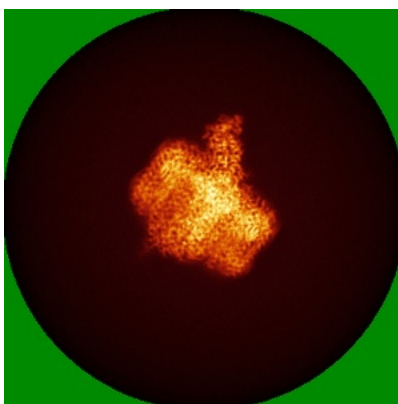


Z

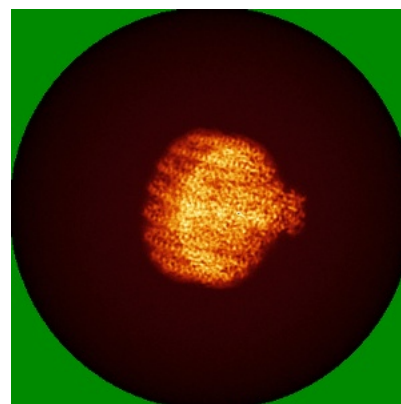
6.4.2 Raw map



X



Y

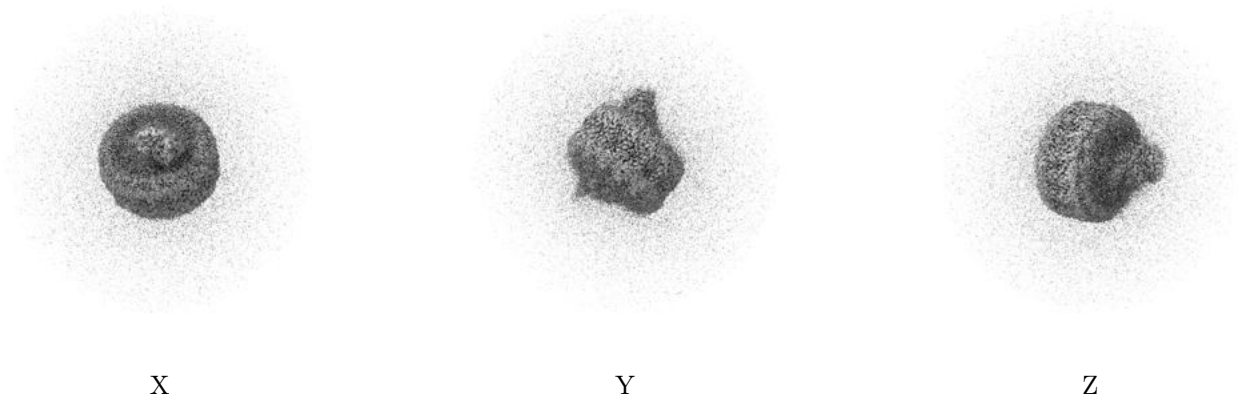


Z

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

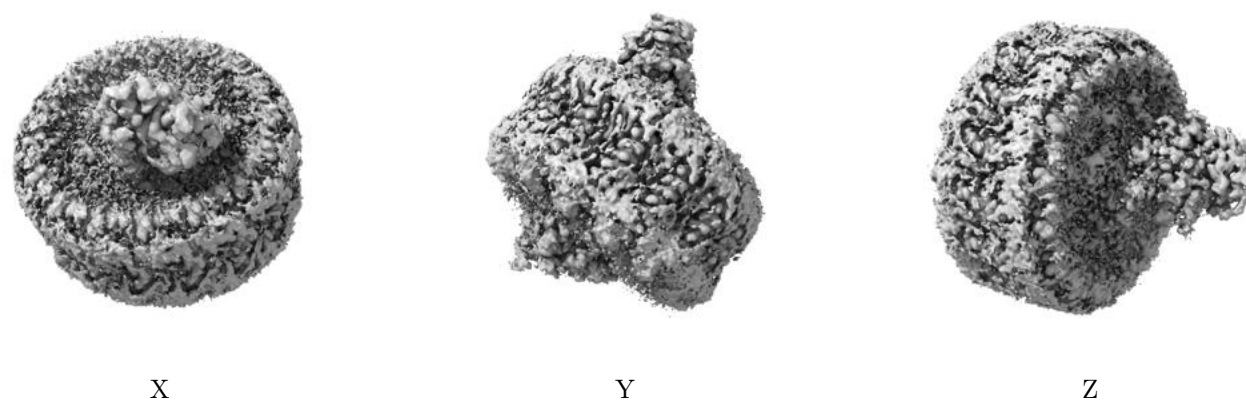
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

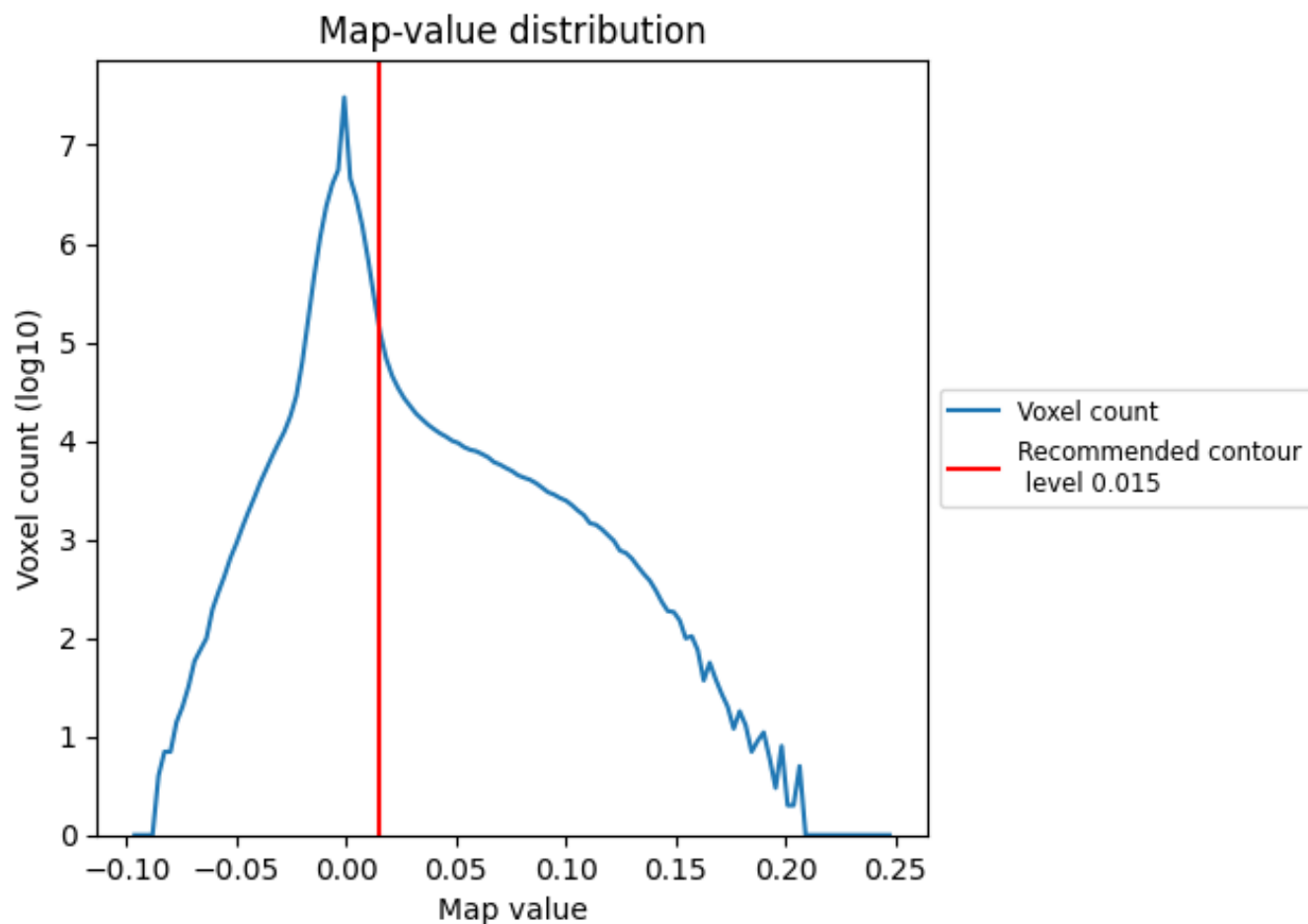
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

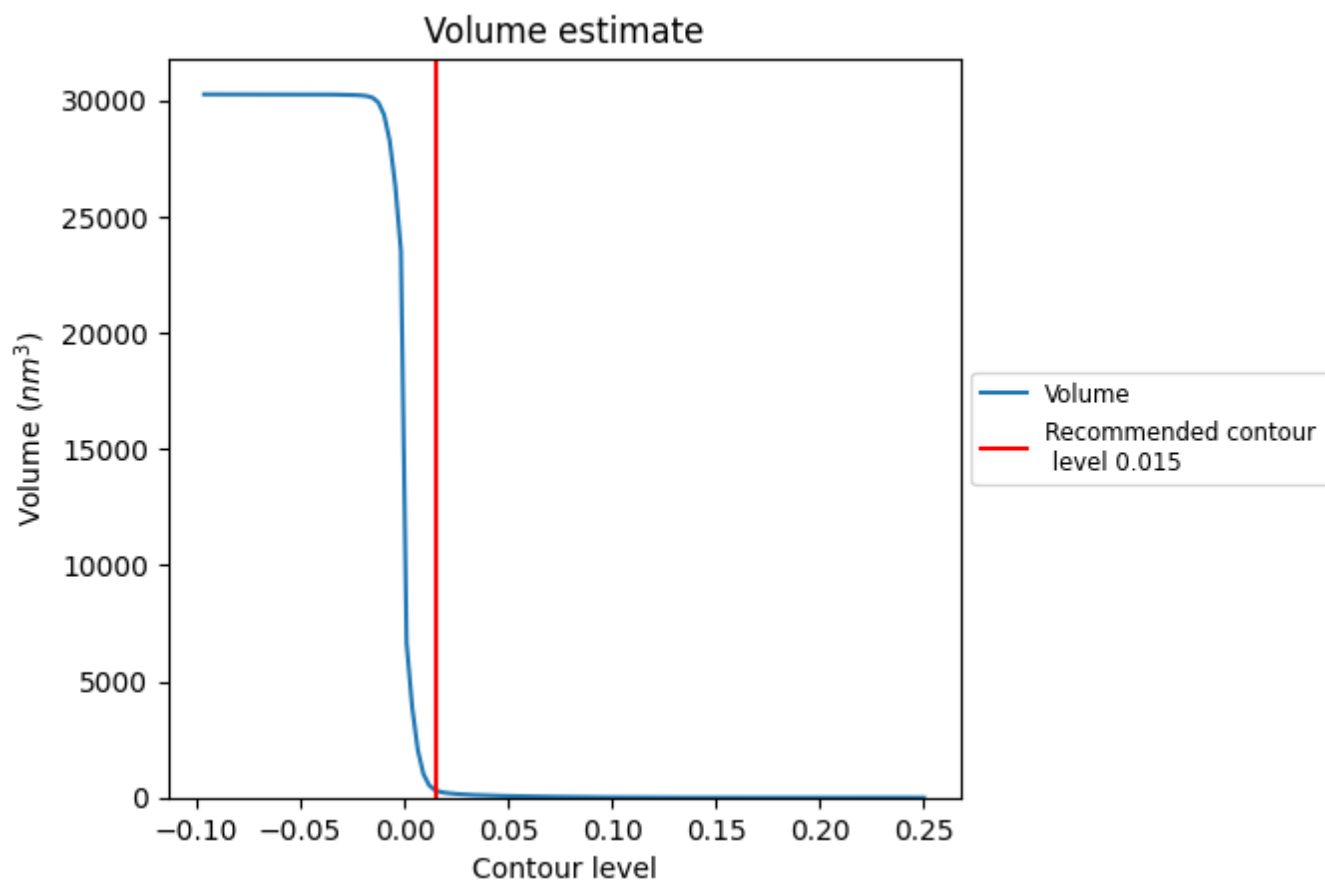
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

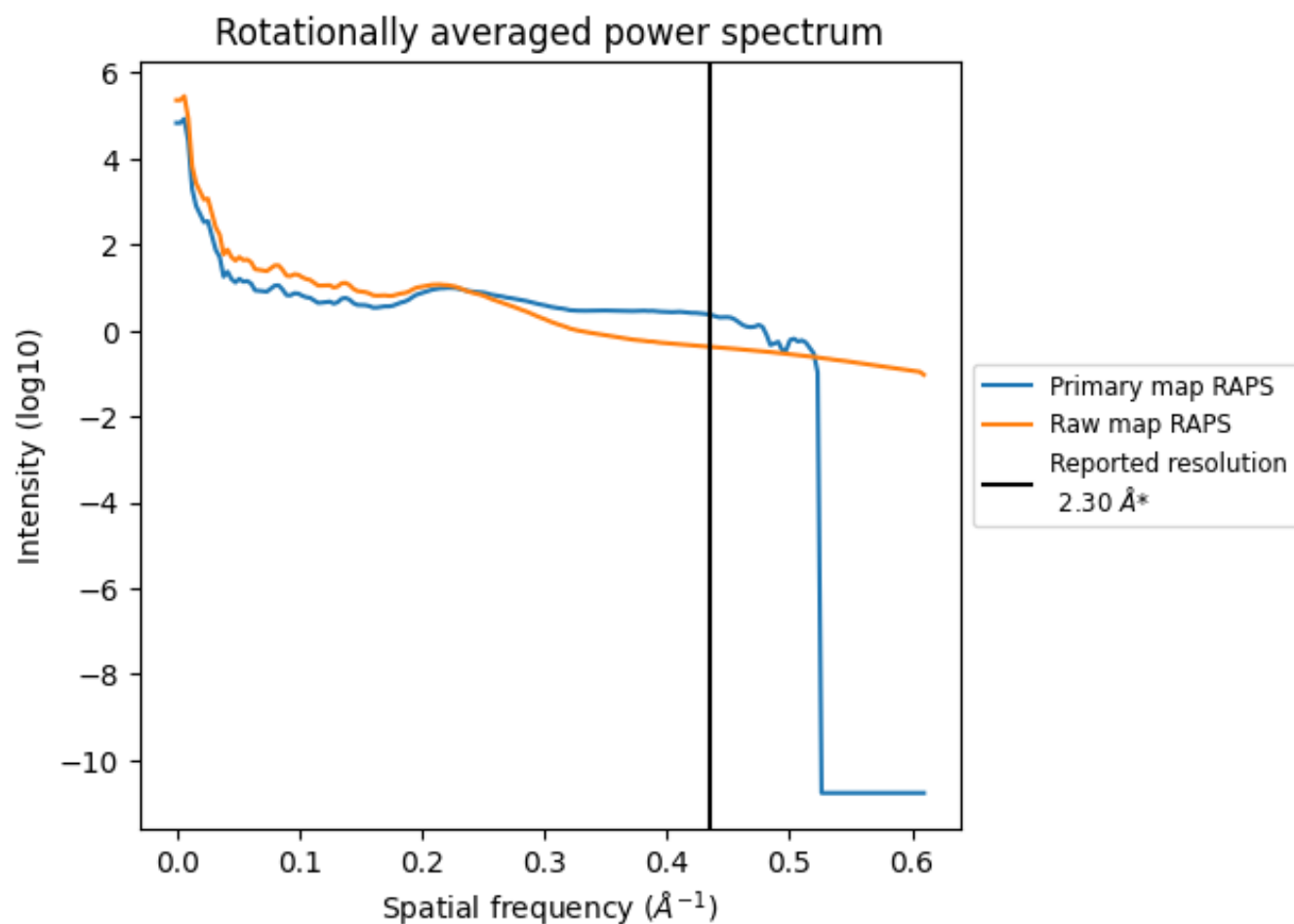
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 318 nm³; this corresponds to an approximate mass of 287 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 ⓘ

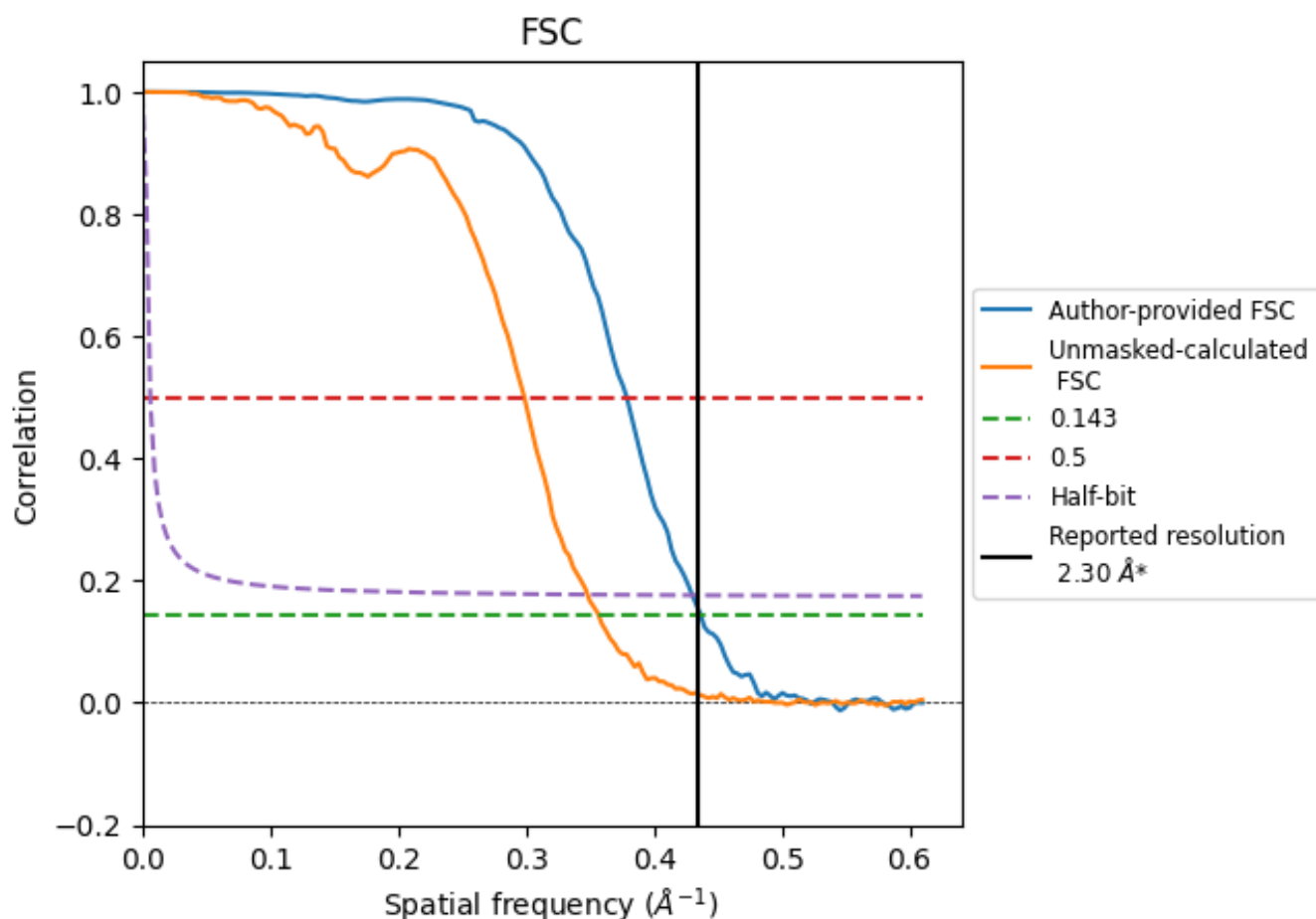


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

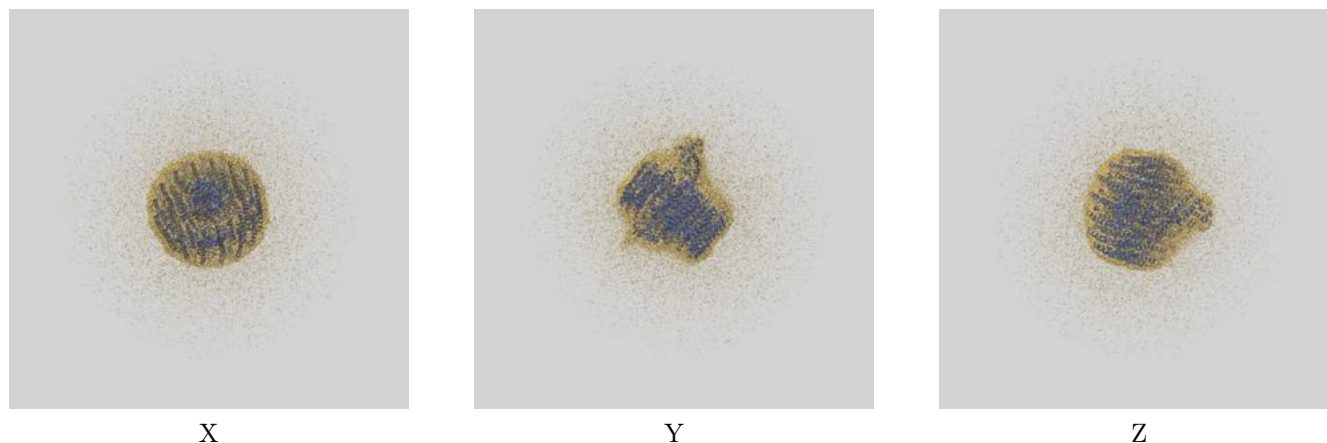
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.29	2.64	2.33
Unmasked-calculated*	2.80	3.35	2.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.80 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

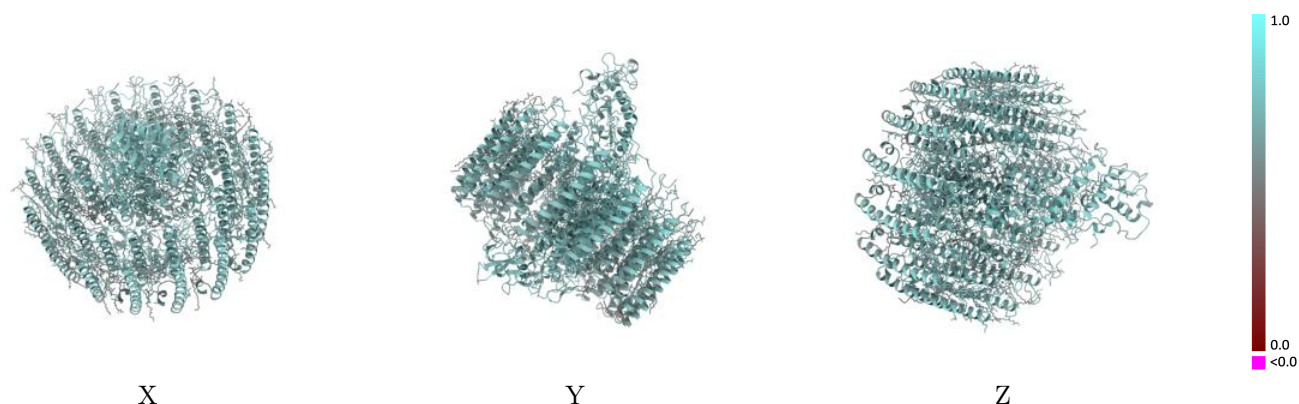
This section contains information regarding the fit between EMDB map EMD-63714 and PDB model 9M8M. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



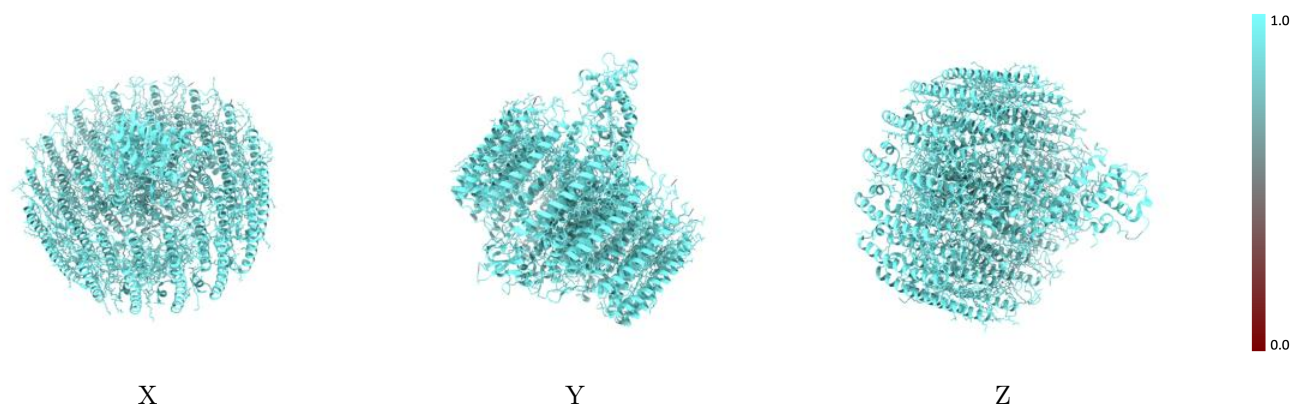
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



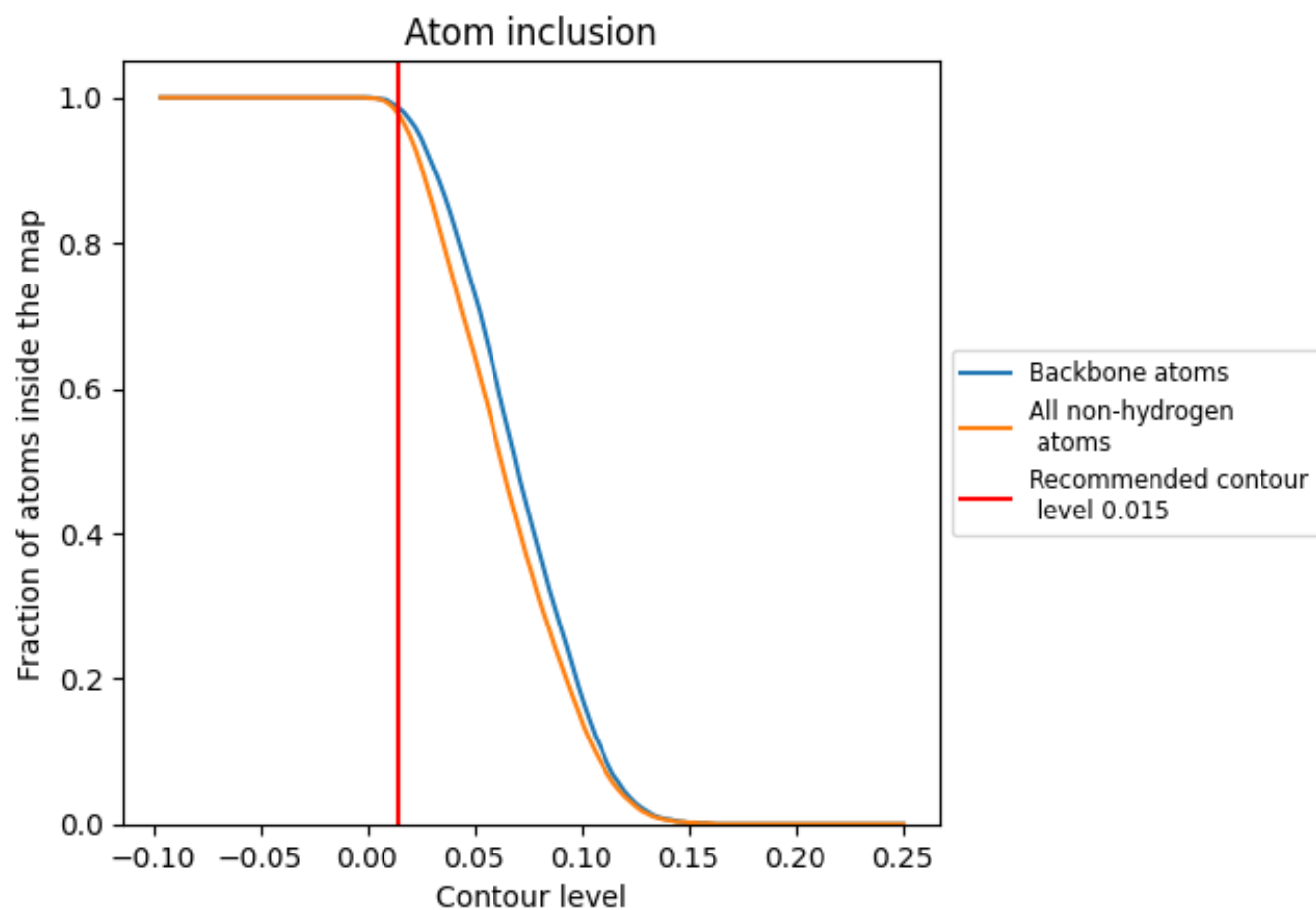
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9770	 0.6660
0	 0.9770	 0.6730
1	 0.9800	 0.6490
2	 0.9540	 0.6320
3	 0.9870	 0.6560
4	 0.9460	 0.6250
5	 0.9760	 0.6340
6	 0.9630	 0.6240
7	 0.9640	 0.6190
8	 0.9550	 0.6220
9	 0.9880	 0.6790
A	 0.9860	 0.6770
B	 0.9640	 0.6410
C	 0.9830	 0.6820
D	 0.9710	 0.6410
E	 0.9730	 0.6430
F	 0.9840	 0.6680
G	 0.9750	 0.6640
H	 0.9700	 0.6590
I	 0.9940	 0.6770
J	 0.9670	 0.6390
K	 0.9710	 0.6380
L	 0.9860	 0.7090
M	 0.9910	 0.7120
N	 0.9570	 0.6320
O	 0.9680	 0.6470
P	 0.9670	 0.6290
Q	 0.9830	 0.6870
R	 0.9710	 0.6630
S	 0.9830	 0.6730
T	 0.9730	 0.6540
U	 0.9860	 0.6780
V	 0.9590	 0.6370
W	 0.9870	 0.6750
X	 0.9670	 0.6330



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.9850	 0.6670
Z	 0.9440	 0.6300