



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:11 AM UTC

PDB ID : 8IUN / pdb_00008iun
EMDB ID : EMD-35727
Title : Cryo-EM structure of the CRT-LESS RC-LH core complex from *roseiflexus castenholzii*
Authors : Wang, G.-L.; Qi, C.-H.; Yu, L.-J.
Deposited on : 2023-03-24
Resolution : 2.85 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:

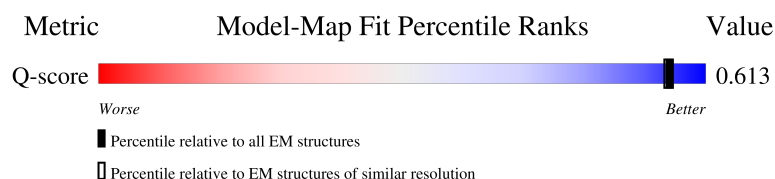
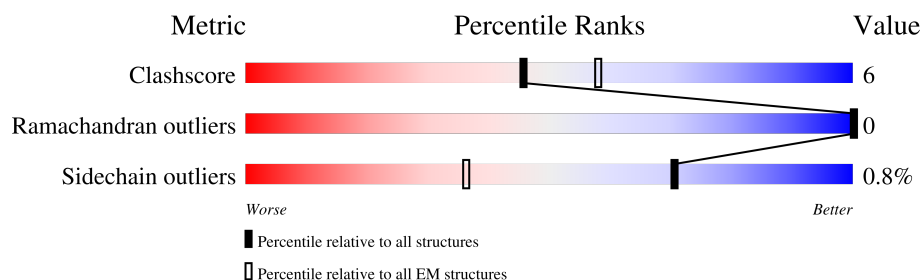
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.85 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.



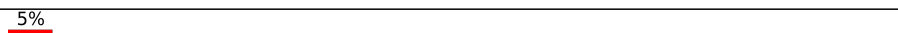
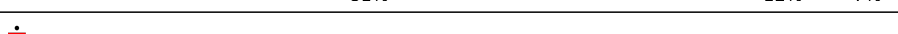
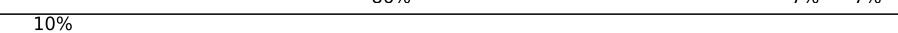
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	0	55	5% 80% 11% 9%
1	2	55	16% 80% 11% 9%
1	4	55	5% 87% • 9%
1	6	55	• 80% 11% 9%

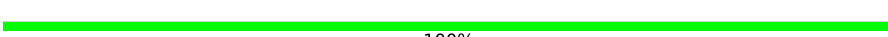
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Mol	Chain	Length	Quality of chain
1	8	55	
1	B	55	
1	E	55	
1	G	55	
1	I	55	
1	K	55	
1	O	55	
1	Q	55	
1	S	55	
1	U	55	
1	W	55	
2	L	641	
2	M	641	
3	1	42	
3	3	42	
3	5	42	
3	7	42	
3	9	42	
3	A	42	
3	D	42	
3	F	42	
3	H	42	
3	J	42	
3	N	42	
3	P	42	

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Mol	Chain	Length	Quality of chain
3	R	42	
3	T	42	
3	V	42	
4	Y	39	
5	h	63	
6	C	320	
7	Z	10	

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
17	UNL	9	103	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 24285 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 Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	W	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	U	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	S	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	Q	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	O	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	K	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	I	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	G	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	E	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	B	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	0	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	8	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	6	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	4	50	Total 416	C 280	N 69	O 66	S 1	0	0
1	2	50	Total 416	C 280	N 69	O 66	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	306	Total	C	N	O	S	0	0
			2488	1673	399	409	7		
2	L	286	Total	C	N	O	S	0	0
			2278	1527	367	376	8		

- Molecule 3 is a protein called Alpha subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	J	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	N	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	P	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	R	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	T	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	V	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	1	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	3	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	5	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	7	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	9	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	A	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
3	D	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
3	F	38	Total	C	N	O	S	0	0
			300	201	51	47	1		

- Molecule 4 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Y	32	Total	C	N	O	S	0	0
			259	181	36	39	3		

- Molecule 5 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	47	Total	C	N	O	S	0	0
			362	242	59	60	1		

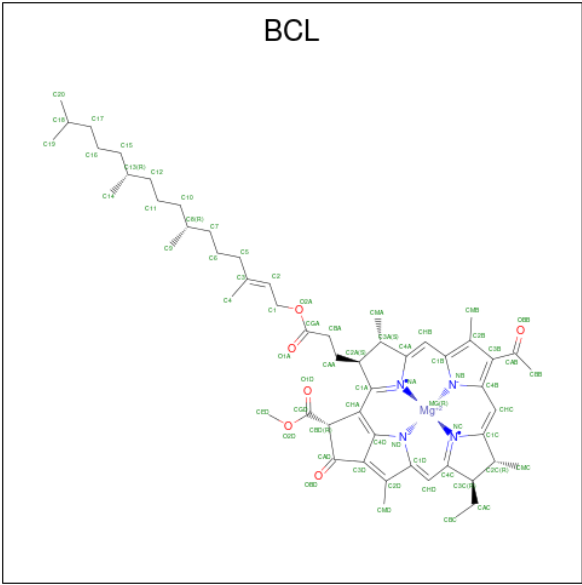
- Molecule 6 is a protein called Cytochrome subunit of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	308	Total	C	N	O	S	0	0
			2347	1492	400	433	22		

- Molecule 7 is a protein called reaction center unknown polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Z	10	Total	C	N	O	0	0
			51	31	10	10		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0

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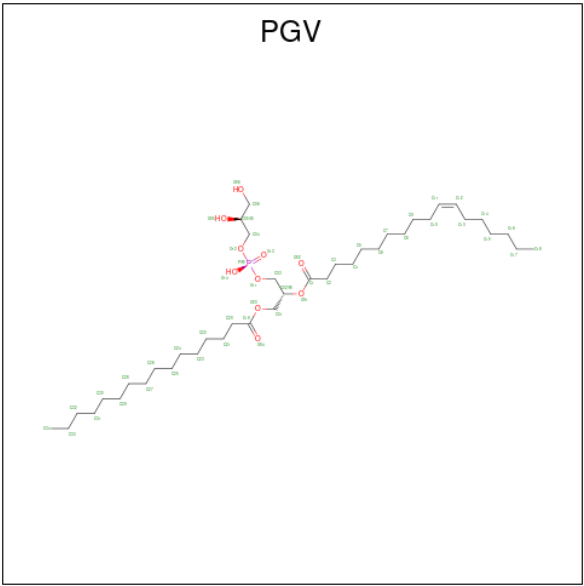
Mol	Chain	Residues	Atoms					AltConf
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



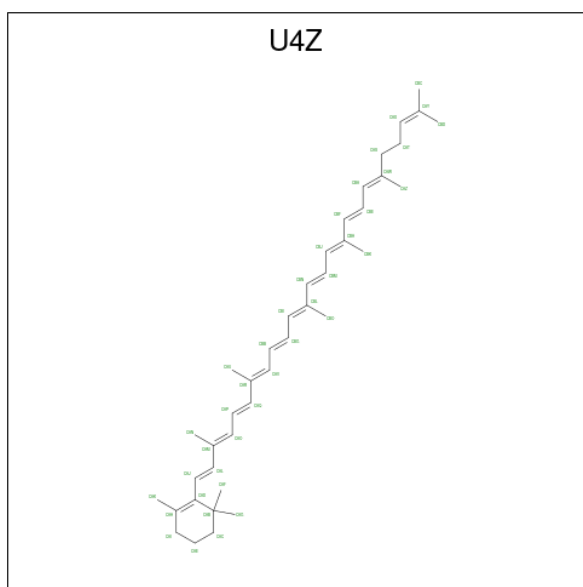
Mol	Chain	Residues	Atoms				AltConf
9	U	1	Total	C	O	P	0
			44	33	10	1	
9	U	1	Total	C	O	P	0
			44	33	10	1	
9	S	1	Total	C	O	P	0
			44	33	10	1	
9	O	1	Total	C	O	P	0
			44	33	10	1	
9	K	1	Total	C	O	P	0
			44	33	10	1	
9	K	1	Total	C	O	P	0
			44	33	10	1	
9	I	1	Total	C	O	P	0
			44	33	10	1	

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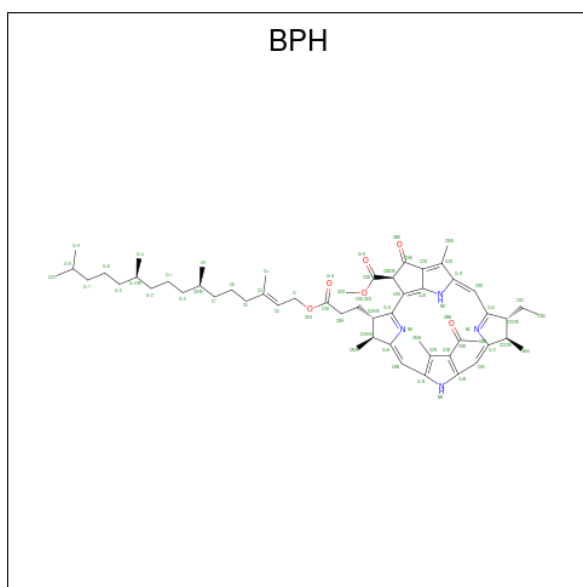
Mol	Chain	Residues	Atoms				AltConf
9	E	1	Total	C	O	P	0
			44	33	10	1	
9	E	1	Total	C	O	P	0
			44	33	10	1	
9	0	1	Total	C	O	P	0
			44	33	10	1	
9	0	1	Total	C	O	P	0
			44	33	10	1	
9	8	1	Total	C	O	P	0
			44	33	10	1	
9	6	1	Total	C	O	P	0
			44	33	10	1	
9	4	1	Total	C	O	P	0
			44	33	10	1	
9	M	1	Total	C	O	P	0
			35	24	10	1	
9	L	1	Total	C	O	P	0
			51	40	10	1	
9	L	1	Total	C	O	P	0
			33	23	9	1	
9	L	1	Total	C	O	P	0
			35	24	10	1	
9	N	1	Total	C	O	P	0
			24	13	10	1	
9	1	1	Total	C	O	P	0
			36	27	8	1	
9	h	1	Total	C	O	P	0
			46	37	8	1	
9	C	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 10 is gamma-Carotene (CCD ID: U4Z) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
10	0	1	Total C 40 40	0
10	J	1	Total C 40 40	0
10	R	1	Total C 40 40	0
10	3	1	Total C 40 40	0
10	D	1	Total C 40 40	0

- Molecule 11 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

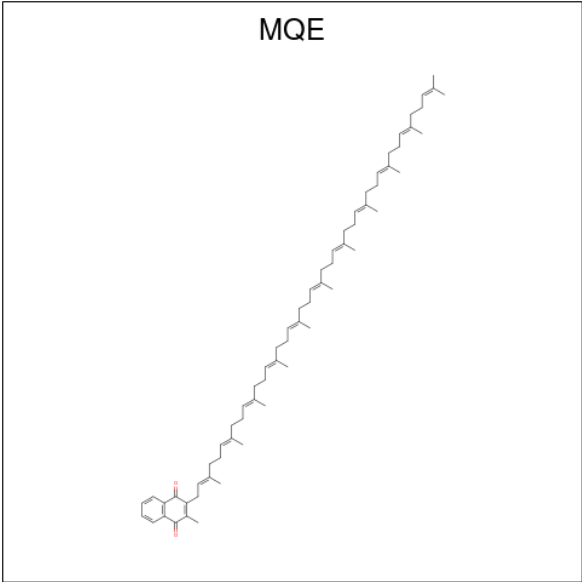


Mol	Chain	Residues	Atoms				AltConf
11	M	1	Total	C	N	O	0
			65	55	4	6	
11	L	1	Total	C	N	O	0
			65	55	4	6	
11	L	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

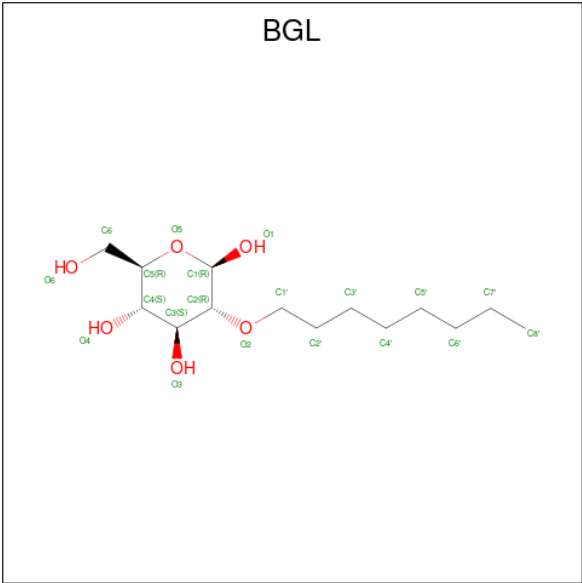
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Mn	0
			1	1	

- Molecule 13 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetraetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaen-1-yl]naphthalene-1,4-dione (CCD ID: MQE) (formula: C₆₆H₉₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			68	66	2	
13	L	1	Total	C	O	0
			53	51	2	

- Molecule 14 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: C₁₄H₂₈O₆).



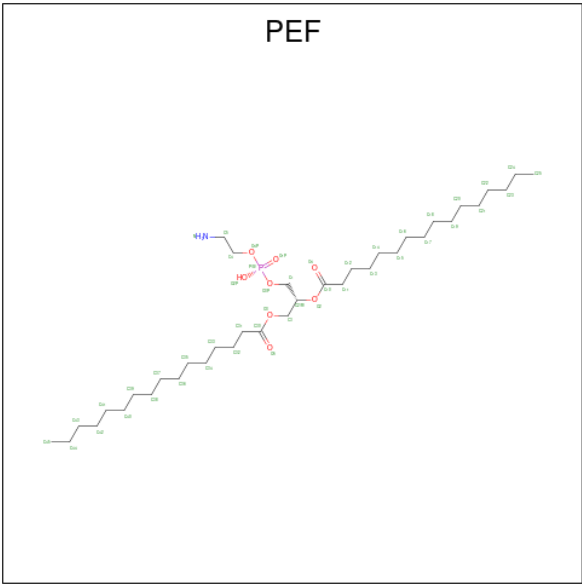
Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			20	14	6	
14	M	1	Total	C	O	0
			20	14	6	

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Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			20	14	6	
14	L	1	Total	C	O	0
			20	14	6	
14	L	1	Total	C	O	0
			20	14	6	
14	L	1	Total	C	O	0
			20	14	6	
14	L	1	Total	C	O	0
			20	14	6	
14	H	1	Total	C	O	0
			20	14	6	
14	Y	1	Total	C	O	0
			20	14	6	
14	Y	1	Total	C	O	0
			20	14	6	
14	C	1	Total	C	O	0
			20	14	6	

- Molecule 15 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P).



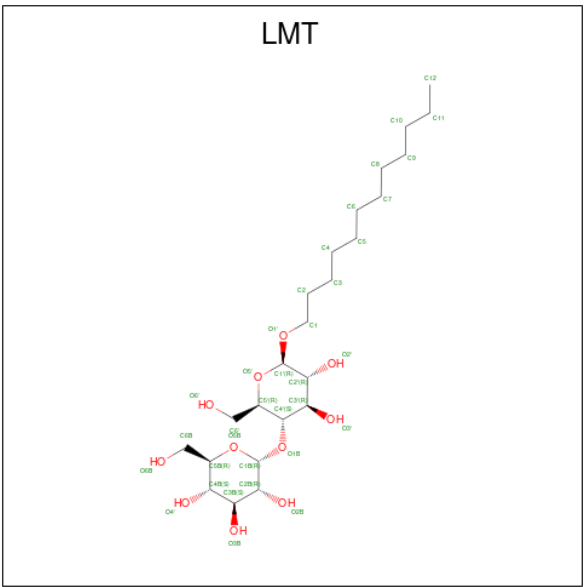
Mol	Chain	Residues	Atoms					AltConf
15	M	1	Total	C	N	O	P	0
			21	11	1	8	1	
15	L	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	N	O	P	0
			41	31	1	8	1	
15	h	1	Total	C	N	O	P	0
			41	31	1	8	1	

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



Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			35	24	11	
16	H	1	Total	C	O	0
			35	24	11	
16	T	1	Total	C	O	0
			35	24	11	
16	1	1	Total	C	O	0
			35	24	11	
16	D	1	Total	C	O	0
			35	24	11	

- Molecule 17 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

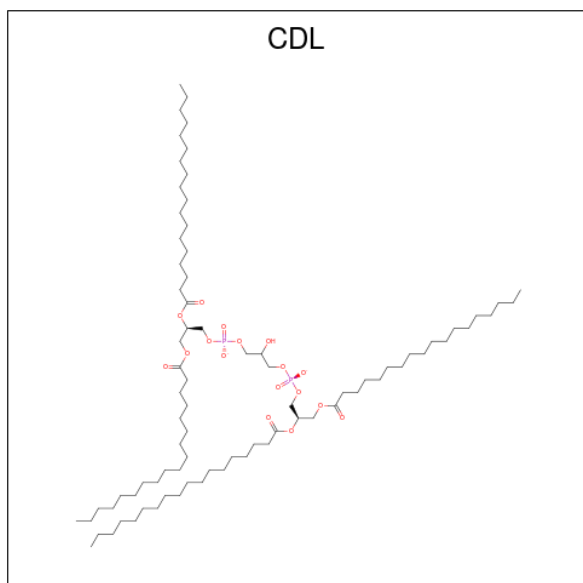
Mol	Chain	Residues	Atoms		AltConf
17	M	3	Total	C	0
			44	44	
17	L	3	Total	C	0
			30	30	

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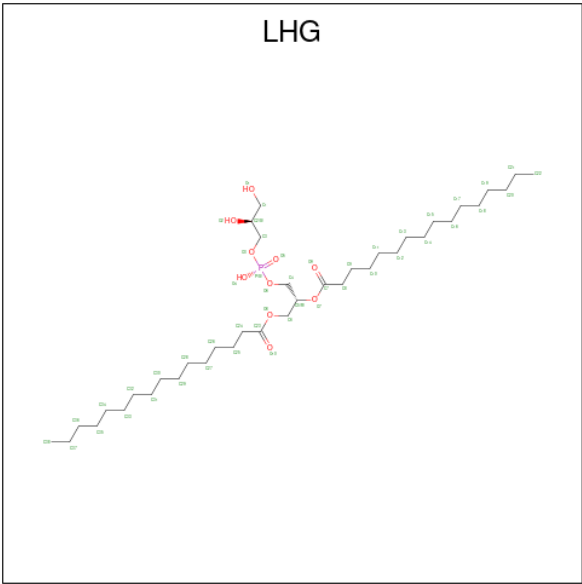
Mol	Chain	Residues	Atoms		AltConf
17	H	1	Total	C	0
			13	13	
17	V	2	Total	C	0
			26	26	
17	1	1	Total	C	0
			18	18	
17	9	2	Total	C	0
			36	36	
17	A	1	Total	C	0
			18	18	
17	D	1	Total	C	0
			12	12	
17	F	1	Total	C	0
			15	15	
17	Y	1	Total	C	0
			14	14	
17	h	2	Total	C	0
			24	24	
17	C	2	Total	C	0
			34	34	

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



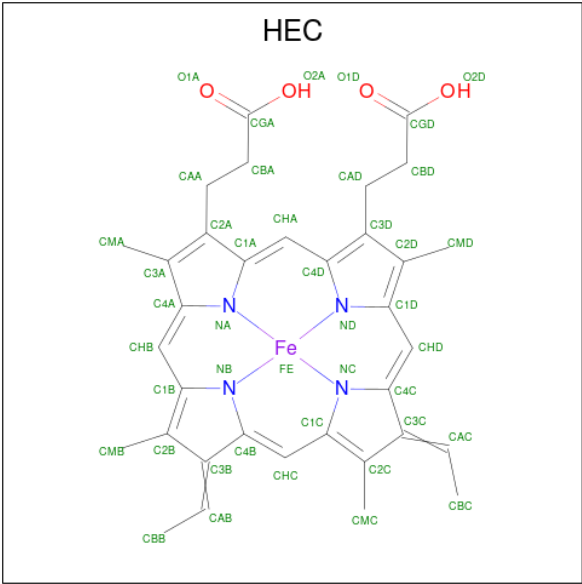
Mol	Chain	Residues	Atoms				AltConf
18	P	1	Total	C	O	P	0
			50	31	17	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	h	1	Total	C	O	0
			24	20	4	

- Molecule 20 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
21	C	1	Total	Ca	0
			1	1	

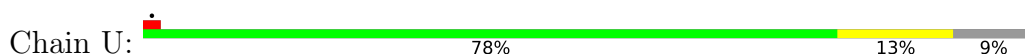
3 Residue-property plots [i](#)

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.

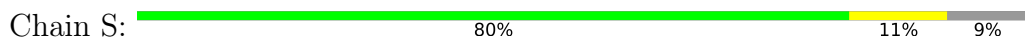
- Molecule 1: Antenna complex alpha/beta subunit



- Molecule 1: Antenna complex alpha/beta subunit



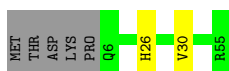
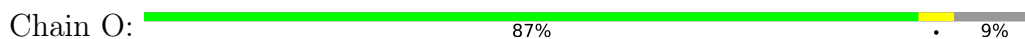
- Molecule 1: Antenna complex alpha/beta subunit



- Molecule 1: Antenna complex alpha/beta subunit

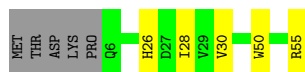


- Molecule 1: Antenna complex alpha/beta subunit



- Molecule 1: Antenna complex alpha/beta subunit

Chain K:  82% 9% 9%



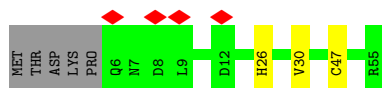
- Molecule 1: Antenna complex alpha/beta subunit

Chain I:  75% 16% 9%



- Molecule 1: Antenna complex alpha/beta subunit

Chain G:  7% 85% 5% 9%



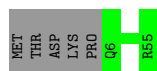
- Molecule 1: Antenna complex alpha/beta subunit

Chain E:  80% 11% 9%



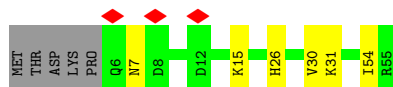
- Molecule 1: Antenna complex alpha/beta subunit

Chain B:  91% 9%



- Molecule 1: Antenna complex alpha/beta subunit

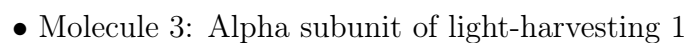
Chain 0:  5% 80% 11% 9%

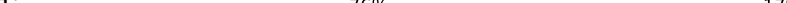


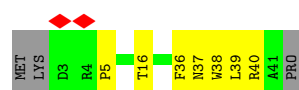
- Molecule 1: Antenna complex alpha/beta subunit

Chain 8:  69% 22% 9%

Opinion	Percentage
Doing a good job	42%
Doing a bad job	55%

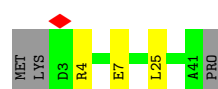


Chain H:  5% 76% 17% 7%



- Molecule 3: Alpha subunit of light-harvesting 1

Chain J: 



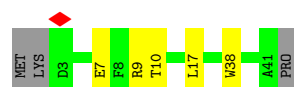
- Molecule 3: Alpha subunit of light-harvesting 1

Chain N: 83% 10% 7%



- Molecule 3: Alpha subunit of light-harvesting 1

Chain P: 81% 12% 7%



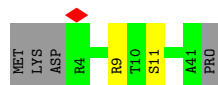
- Molecule 3: Alpha subunit of light-harvesting 1

Chain R:  90% 7%



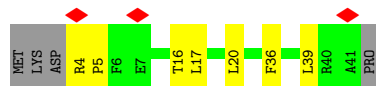
- Molecule 3: Alpha subunit of light-harvesting 1

Chain T:  86% 5% 10%



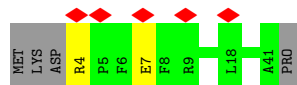
- Molecule 3: Alpha subunit of light-harvesting 1

Chain V:  74% 17% 10% 7%



- Molecule 3: Alpha subunit of light-harvesting 1

Chain 1:  86% 5% 10% 12%



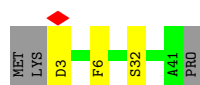
- Molecule 3: Alpha subunit of light-harvesting 1

Chain 3:  81% 12% 7% 5%



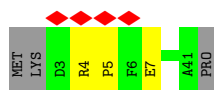
- Molecule 3: Alpha subunit of light-harvesting 1

Chain 5:  86% 7% 7%

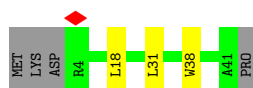
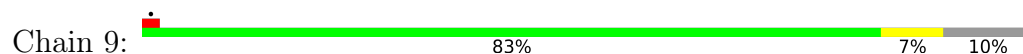


- Molecule 3: Alpha subunit of light-harvesting 1

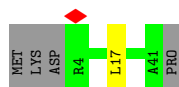
Chain 7:  86% 7% 7% 10%



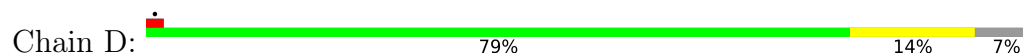
- Molecule 3: Alpha subunit of light-harvesting 1



- Molecule 3: Alpha subunit of light-harvesting 1



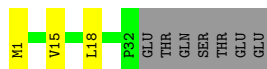
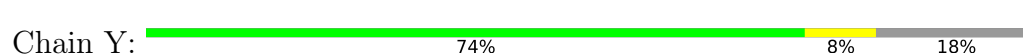
- Molecule 3: Alpha subunit of light-harvesting 1



- Molecule 3: Alpha subunit of light-harvesting 1



- Molecule 4: reaction center small polypeptide

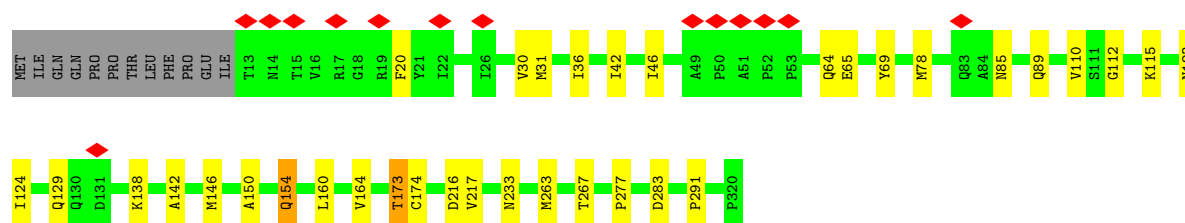


- Molecule 5: reaction center small polypeptide

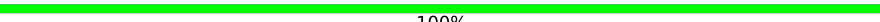


- Molecule 6: Cytochrome subunit of photosynthetic reaction center

Chain C:  85% 10% . .



- Molecule 7: reaction center unknown polypeptide

Chain Z:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	373675	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.500	Depositor
Minimum map value	-1.414	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.307	Depositor
Map size ($\text{\AA}$)	320.4, 320.4, 320.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.89, 0.89, 0.89	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, LHG, CDL, PEF, BPH, U4Z, MQE, BCL, PGV, UNL, HEC, MN, LMT, BGL

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	0	0.20	0/432	0.32	0/597
1	2	0.16	0/432	0.27	0/597
1	4	0.17	0/432	0.28	0/597
1	6	0.18	0/432	0.28	0/597
1	8	0.19	0/432	0.30	0/597
1	B	0.20	0/432	0.37	0/597
1	E	0.20	0/432	0.31	0/597
1	G	0.18	0/432	0.30	0/597
1	I	0.18	0/432	0.29	0/597
1	K	0.20	0/432	0.32	0/597
1	O	0.19	0/432	0.30	0/597
1	Q	0.24	0/432	0.35	0/597
1	S	0.20	0/432	0.31	0/597
1	U	0.21	0/432	0.33	0/597
1	W	0.16	0/432	0.27	0/597
2	L	0.41	0/2360	0.58	1/3220 (0.0%)
2	M	0.66	1/2597 (0.0%)	0.49	2/3566 (0.1%)
3	1	0.16	0/307	0.25	0/417
3	3	0.15	0/315	0.25	0/428
3	5	0.17	0/315	0.37	0/428
3	7	0.19	0/315	0.29	0/428
3	9	0.22	0/307	0.37	0/417
3	A	0.19	0/307	0.29	0/417
3	D	0.18	0/315	0.27	0/428
3	F	0.16	0/307	0.28	0/417
3	H	0.36	0/315	0.48	0/428
3	J	0.18	0/315	0.35	0/428
3	N	0.43	0/315	0.66	0/428
3	P	0.17	0/315	0.32	0/428
3	R	0.18	0/315	0.28	0/428
3	T	0.29	0/307	0.42	0/417
3	V	0.18	0/307	0.35	0/417

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	Y	0.20	0/268	0.38	0/370
5	h	0.19	0/374	0.29	0/513
6	C	0.39	0/2409	0.57	0/3288
7	Z	1.30	0/51	1.58	0/70
All	All	0.36	1/19216 (0.0%)	0.43	3/26336 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	355	PRO	N-CD	-29.75	1.06	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	185	PHE	CA-CB-CG	8.63	122.43	113.80
2	M	355	PRO	N-CD-CG	7.76	114.85	103.20
2	M	375	VAL	N-CA-C	-5.22	100.97	108.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	416	0	413	6	0
1	2	416	0	413	3	0
1	4	416	0	413	1	0
1	6	416	0	413	3	0
1	8	416	0	413	12	0
1	B	416	0	413	0	0
1	E	416	0	413	5	0
1	G	416	0	413	2	0
1	I	416	0	413	9	0
1	K	416	0	413	6	0
1	O	416	0	413	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	416	0	413	7	0
1	S	416	0	413	6	0
1	U	416	0	413	5	0
1	W	416	0	413	6	0
2	L	2278	0	2235	16	0
2	M	2488	0	2373	27	0
3	1	300	0	316	2	0
3	3	308	0	320	4	0
3	5	308	0	320	3	0
3	7	308	0	320	2	0
3	9	300	0	316	11	0
3	A	300	0	316	1	0
3	D	308	0	320	8	0
3	F	300	0	316	6	0
3	H	308	0	320	7	0
3	J	308	0	320	2	0
3	N	308	0	320	4	0
3	P	308	0	320	4	0
3	R	308	0	320	1	0
3	T	300	0	316	2	0
3	V	300	0	316	12	0
4	Y	259	0	272	2	0
5	h	362	0	365	2	0
6	C	2347	0	2301	29	0
7	Z	51	0	49	0	0
8	0	132	0	148	8	0
8	1	66	0	74	3	0
8	2	132	0	148	7	0
8	3	132	0	148	0	0
8	4	66	0	74	6	0
8	5	66	0	74	2	0
8	6	132	0	148	4	0
8	7	66	0	74	1	0
8	8	132	0	148	4	0
8	9	66	0	74	0	0
8	A	132	0	148	3	0
8	B	66	0	74	2	0
8	D	66	0	74	3	0
8	E	132	0	148	10	0
8	F	66	0	74	3	0
8	G	132	0	148	3	0
8	H	66	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	132	0	148	3	0
8	J	66	0	74	0	0
8	K	132	0	148	1	0
8	L	132	0	148	8	0
8	M	66	0	74	2	0
8	N	66	0	74	3	0
8	O	132	0	148	4	0
8	P	66	0	74	2	0
8	Q	132	0	148	4	0
8	R	66	0	74	3	0
8	S	132	0	148	4	0
8	T	66	0	74	0	0
8	U	132	0	148	7	0
8	V	66	0	74	8	0
8	W	132	0	148	6	0
9	0	88	0	122	2	0
9	1	36	0	43	1	0
9	4	44	0	61	1	0
9	6	44	0	61	1	0
9	8	44	0	61	1	0
9	C	51	0	76	1	0
9	E	88	0	122	2	0
9	I	44	0	61	3	0
9	K	88	0	122	3	0
9	L	119	0	154	3	0
9	M	35	0	38	5	0
9	N	24	0	18	0	0
9	O	44	0	61	1	0
9	S	44	0	61	1	0
9	U	88	0	122	2	0
9	h	46	0	69	2	0
10	0	40	0	0	0	0
10	3	40	0	0	2	0
10	D	40	0	0	0	0
10	J	40	0	0	0	0
10	R	40	0	0	1	0
11	L	130	0	152	3	0
11	M	65	0	76	2	0
12	M	1	0	0	0	0
13	L	53	0	0	0	0
13	M	68	0	0	1	0
14	C	20	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	20	0	28	0	0
14	L	80	0	112	1	0
14	M	60	0	84	2	0
14	Y	40	0	56	0	0
15	L	88	0	131	3	0
15	M	21	0	15	0	0
15	h	41	0	55	4	0
16	1	35	0	46	1	0
16	D	35	0	46	3	0
16	H	35	0	46	2	0
16	M	35	0	46	2	0
16	T	35	0	46	2	0
17	1	18	0	0	0	0
17	9	36	0	0	10	0
17	A	18	0	0	0	0
17	C	34	0	0	0	0
17	D	12	0	0	0	0
17	F	15	0	0	0	0
17	H	13	0	0	0	0
17	L	30	0	0	0	0
17	M	44	0	0	0	0
17	V	26	0	0	0	0
17	Y	14	0	0	0	0
17	h	24	0	0	0	0
18	P	50	0	44	2	0
19	h	24	0	34	5	0
20	C	172	0	120	5	0
21	C	1	0	0	0	0
All	All	24285	0	24535	302	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 6.

All (302) 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)
3:9:31:LEU:HD23	17:9:103:UNL:C11	1.59	1.32
3:9:31:LEU:HD21	17:9:103:UNL:C14	1.62	1.27
3:9:31:LEU:CD2	17:9:103:UNL:C11	2.23	1.16
8:2:102:BCL:HBB2	6:C:20:PHE:CE1	1.85	1.10
3:V:20:LEU:HD12	8:V:101:BCL:C4	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:37:ASN:HD21	3:H:40:ARG:HD2	1.18	1.04
6:C:164:VAL:HG12	20:C:504:HEC:O1D	1.58	1.03
3:H:37:ASN:ND2	3:H:40:ARG:HD2	1.75	1.02
3:9:31:LEU:CD2	17:9:103:UNL:C14	2.38	1.02
8:2:102:BCL:HBB2	6:C:20:PHE:CZ	1.99	0.98
6:C:164:VAL:CG1	20:C:504:HEC:O1D	2.13	0.95
8:2:102:BCL:CBB	6:C:20:PHE:CZ	2.50	0.94
6:C:64:GLN:HG2	6:C:65:GLU:HG2	1.56	0.88
8:L:702:BCL:CED	19:h:101:LHG:O9	2.24	0.85
3:V:20:LEU:HD12	8:V:101:BCL:H43	1.58	0.84
8:L:702:BCL:HED1	19:h:101:LHG:O9	1.78	0.84
1:0:7:ASN:HB3	1:0:15:LYS:HD2	1.61	0.82
3:V:20:LEU:CD1	8:V:101:BCL:C4	2.59	0.81
1:I:7:ASN:OD1	1:I:7:ASN:O	2.03	0.77
1:8:9:LEU:HD13	1:8:20:ASN:CG	2.10	0.77
2:M:466:GLY:HA2	9:M:705:PGV:H061	1.67	0.75
1:K:55:ARG:HH11	1:K:55:ARG:HG2	1.51	0.74
3:9:31:LEU:HD22	17:9:103:UNL:C11	2.15	0.74
1:K:50:TRP:HB2	9:K:104:PGV:H22	1.72	0.71
1:I:7:ASN:O	1:I:7:ASN:CG	2.34	0.71
8:2:102:BCL:HBB1	6:C:20:PHE:CZ	2.24	0.70
2:M:359:GLY:H	14:M:710:BGL:H4	1.57	0.69
2:L:306:ASN:O	3:5:32:SER:OG	2.09	0.69
13:M:704:MQE:CCP	3:R:22:MET:HG3	2.22	0.68
6:C:150:ALA:O	6:C:154:GLN:HB2	1.93	0.68
3:V:20:LEU:CD1	8:V:101:BCL:H41	2.22	0.68
15:L:713:PEF:H232	15:L:713:PEF:H453	1.75	0.68
1:K:55:ARG:HG2	1:K:55:ARG:NH1	2.10	0.67
1:S:8:ASP:OD1	1:S:9:LEU:CD1	2.44	0.66
2:L:66:ARG:HE	9:L:711:PGV:H061	1.60	0.65
2:L:58:ASP:HB3	2:L:61:ASP:HB2	1.79	0.65
8:B:101:BCL:H43	1:0:31:LYS:HE3	1.80	0.64
8:Q:101:BCL:H51	8:P:101:BCL:H72	1.80	0.64
1:8:9:LEU:HD13	1:8:20:ASN:OD1	1.98	0.63
2:M:461:LYS:NZ	9:M:705:PGV:O05	2.32	0.62
2:M:489:LEU:HD21	3:D:28:PHE:CE2	2.34	0.62
3:9:31:LEU:HD23	17:9:103:UNL:C12	2.26	0.62
9:M:705:PGV:H041	2:L:239:ARG:HH22	1.64	0.62
6:C:164:VAL:HG11	20:C:504:HEC:O1D	1.98	0.62
3:D:28:PHE:HD1	3:D:28:PHE:O	1.83	0.61
2:L:38:ILE:HD12	2:L:38:ILE:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:102:BCL:H2	8:S:102:BCL:HAA2	1.82	0.60
8:2:102:BCL:CBB	6:C:20:PHE:CE1	2.70	0.60
6:C:85:ASN:OD1	6:C:89:GLN:OE1	2.20	0.59
2:L:208:TYR:HA	9:C:506:PGV:H241	1.84	0.59
6:C:123:ASN:ND2	6:C:129:GLN:OE1	2.34	0.59
8:O:102:BCL:CBB	8:O:102:BCL:HMB3	2.32	0.59
1:6:6:GLN:O	1:6:20:ASN:ND2	2.36	0.58
1:U:36:GLY:HA3	8:U:101:BCL:H52	1.85	0.58
1:Q:54:ILE:HG22	9:O:103:PGV:H031	1.86	0.58
2:M:384:ILE:HD12	3:A:17:LEU:HD23	1.86	0.57
3:F:37:ASN:OD1	3:F:40:ARG:NH1	2.37	0.57
16:H:102:LMT:H101	3:J:25:LEU:HD11	1.86	0.57
3:3:4:ARG:NH2	3:3:7:GLU:OE1	2.38	0.57
2:M:438:TRP:O	2:M:442:THR:OG1	2.18	0.57
1:S:8:ASP:OD1	1:S:9:LEU:HD12	2.04	0.56
3:V:36:PHE:O	3:V:39:LEU:N	2.33	0.56
5:h:44:GLN:HG3	9:h:102:PGV:H012	1.87	0.56
1:W:7:ASN:O	1:W:15:LYS:NZ	2.30	0.56
1:I:55:ARG:HB2	3:F:37:ASN:HD22	1.71	0.56
8:O:102:BCL:HMB3	8:O:102:BCL:HBB3	1.87	0.56
6:C:30:VAL:HG23	6:C:31:MET:HE2	1.89	0.55
6:C:142:ALA:O	6:C:146:MET:HG3	2.06	0.55
1:U:9:LEU:HG	1:U:20:ASN:ND2	2.23	0.54
8:L:703:BCL:H151	11:L:704:BPH:H5C2	1.88	0.54
8:8:102:BCL:HBB3	8:8:102:BCL:HMB1	1.88	0.54
1:8:9:LEU:HD12	1:8:9:LEU:N	2.23	0.53
3:N:5:PRO:HD2	3:N:6:PHE:H	1.73	0.53
1:W:36:GLY:HA3	8:W:101:BCL:H52	1.89	0.53
6:C:78:MET:HG3	20:C:501:HEC:HMB3	1.89	0.53
1:I:51:THR:HG23	3:H:36:PHE:CE1	2.44	0.53
8:6:102:BCL:CAB	10:3:102:U4Z:CAE	2.86	0.53
3:N:13:VAL:HG22	8:N:101:BCL:H201	1.90	0.53
16:T:102:LMT:O1B	16:T:102:LMT:O6'	2.27	0.53
1:I:53:TRP:HZ2	9:I:103:PGV:H281	1.73	0.53
1:8:7:ASN:O	1:8:15:LYS:NZ	2.29	0.53
3:P:38:TRP:CZ2	8:P:101:BCL:HHC	2.44	0.53
3:V:16:THR:HG23	8:V:101:BCL:H62	1.91	0.53
2:M:410:ARG:HG2	2:M:411:GLU:HG2	1.91	0.53
3:H:5:PRO:O	3:F:9:ARG:NE	2.38	0.53
3:D:17:LEU:HD11	16:D:104:LMT:H51	1.91	0.53
1:0:7:ASN:HD22	1:0:15:LYS:HG3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:26:HIS:O	1:K:30:VAL:HG13	2.10	0.52
1:I:19:ASN:OD1	1:I:20:ASN:N	2.38	0.52
2:M:609:LEU:HD22	2:M:613:LEU:HD12	1.91	0.52
3:9:31:LEU:HB2	3:9:38:TRP:CZ3	2.45	0.52
2:M:420:PRO:HB3	2:M:430:VAL:HG11	1.92	0.51
8:U:102:BCL:HMB3	8:U:102:BCL:HBB3	1.91	0.51
9:K:103:PGV:H21	1:I:50:TRP:HB2	1.91	0.51
3:H:37:ASN:ND2	3:H:40:ARG:CD	2.61	0.51
6:C:173:THR:O	6:C:174:CYS:HB2	2.11	0.51
2:M:489:LEU:HD21	3:D:28:PHE:CZ	2.46	0.51
6:C:277:PRO:HG2	6:C:283:ASP:HB2	1.93	0.51
8:U:102:BCL:HMB3	8:U:102:BCL:CBB	2.41	0.51
3:5:3:ASP:N	3:5:3:ASP:OD1	2.44	0.50
3:T:9:ARG:HH22	3:V:5:PRO:HG2	1.74	0.50
9:K:103:PGV:O12	9:K:103:PGV:O06	2.27	0.50
2:M:358:VAL:HG13	14:M:710:BGL:H2	1.93	0.50
2:L:54:PHE:HE1	3:V:17:LEU:HD12	1.76	0.50
2:M:557:GLU:O	2:M:561:MET:HG3	2.11	0.50
1:S:55:ARG:HG3	1:S:55:ARG:HH11	1.77	0.49
1:Q:7:ASN:ND2	1:Q:18:PHE:O	2.45	0.49
3:V:20:LEU:HD13	8:V:101:BCL:H41	1.94	0.49
1:S:26:HIS:O	1:S:30:VAL:HG13	2.12	0.49
8:S:102:BCL:HBB3	8:S:102:BCL:HMB1	1.94	0.49
6:C:233:ASN:C	6:C:233:ASN:OD1	2.55	0.49
2:L:90:GLU:HG2	2:L:105:ILE:HG23	1.93	0.49
8:O:102:BCL:HMB3	8:O:102:BCL:CBB	2.41	0.49
1:G:26:HIS:O	1:G:30:VAL:HG13	2.13	0.49
8:K:102:BCL:HBD	8:K:102:BCL:HBA1	1.94	0.49
2:M:367:GLU:OE1	2:M:368:GLY:N	2.46	0.48
8:E:101:BCL:H111	8:E:101:BCL:H142	1.67	0.48
1:Q:6:GLN:N	1:Q:8:ASP:OD1	2.46	0.48
8:A:102:BCL:H141	8:A:102:BCL:H161	1.74	0.48
1:E:19:ASN:HB3	1:E:22:GLU:HG3	1.95	0.48
8:S:102:BCL:H112	1:Q:32:THR:HA	1.96	0.48
9:S:103:PGV:H21	1:Q:50:TRP:HB2	1.95	0.47
3:9:31:LEU:CD2	17:9:103:UNL:C13	2.91	0.47
9:I:103:PGV:H61	1:G:47:CYS:SG	2.54	0.47
8:E:101:BCL:H111	8:E:101:BCL:H91	1.69	0.47
1:8:27:ASP:OD2	1:8:31:LYS:NZ	2.35	0.47
2:L:38:ILE:HD12	2:L:38:ILE:H	1.76	0.47
3:D:9:ARG:HD3	16:D:104:LMT:H2B	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2:102:BCL:H143	8:2:102:BCL:H162	1.75	0.47
2:M:529:ILE:HD13	8:L:702:BCL:HMD3	1.94	0.47
9:0:104:PGV:H21	1:8:50:TRP:HB2	1.96	0.47
8:2:102:BCL:H62	8:2:102:BCL:H2	1.50	0.47
16:M:709:LMT:H22	3:F:29:VAL:HG22	1.95	0.47
1:W:26:HIS:O	1:W:30:VAL:HG13	2.15	0.47
8:0:102:BCL:H62	8:0:102:BCL:H93	1.66	0.47
2:M:557:GLU:OE2	2:M:589:HIS:HE1	1.97	0.47
2:M:603:GLY:HA2	8:M:701:BCL:HED3	1.97	0.47
8:7:101:BCL:H192	8:7:101:BCL:H162	1.75	0.47
8:F:101:BCL:H161	8:F:101:BCL:H202	1.60	0.47
8:G:101:BCL:H91	8:G:101:BCL:H111	1.79	0.46
8:I:102:BCL:H122	8:I:102:BCL:H162	1.66	0.46
8:E:101:BCL:H41	8:E:101:BCL:H62	1.60	0.46
16:H:102:LMT:H1B	16:H:102:LMT:H3'	1.52	0.46
3:N:5:PRO:CD	3:N:6:PHE:H	2.28	0.46
1:6:27:ASP:OD1	1:6:31:LYS:HE3	2.15	0.46
9:1:102:PGV:H132	6:C:36:ILE:HG12	1.96	0.46
9:L:711:PGV:H222	9:L:711:PGV:H251	1.74	0.46
9:E:103:PGV:O12	9:E:103:PGV:O06	2.28	0.46
3:H:16:THR:HG22	8:H:101:BCL:H172	1.97	0.46
8:D:102:BCL:H141	3:F:11:SER:HB2	1.97	0.46
1:8:9:LEU:HD13	1:8:20:ASN:ND2	2.29	0.46
2:M:467:THR:HG23	9:M:705:PGV:H062	1.97	0.46
9:U:103:PGV:H21	1:S:50:TRP:HB2	1.96	0.46
3:1:4:ARG:NH1	3:3:4:ARG:O	2.49	0.46
8:S:102:BCL:H111	8:S:102:BCL:H151	1.36	0.46
8:G:102:BCL:H72	1:E:32:THR:HA	1.98	0.46
8:E:102:BCL:H162	8:E:102:BCL:H121	1.45	0.46
3:9:31:LEU:HD23	17:9:103:UNL:C14	2.40	0.45
1:2:12:ASP:HA	1:2:15:LYS:HG3	1.98	0.45
8:B:101:BCL:H91	8:B:101:BCL:H111	1.80	0.45
8:1:101:BCL:H62	8:1:101:BCL:H93	1.66	0.45
2:L:38:ILE:H	2:L:38:ILE:CD1	2.29	0.45
2:M:584:ASN:HB3	2:M:586:TYR:H	1.82	0.45
15:h:103:PEF:H181	15:h:103:PEF:H372	1.98	0.45
8:U:101:BCL:H41	8:U:101:BCL:H61	1.77	0.45
2:L:54:PHE:CE1	3:V:17:LEU:HD12	2.51	0.45
2:L:38:ILE:N	2:L:38:ILE:CD1	2.80	0.45
1:Q:19:ASN:HB3	1:Q:22:GLU:HG3	1.99	0.45
8:O:102:BCL:H2	1:K:28:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:104:LMT:H1B	16:1:104:LMT:H3'	1.72	0.45
8:5:101:BCL:H142	8:5:101:BCL:H111	1.72	0.45
2:M:541:MET:O	2:M:545:THR:HG22	2.17	0.45
8:W:102:BCL:CAB	10:R:101:U4Z:CAC	2.94	0.44
8:8:102:BCL:HHD	8:8:102:BCL:HAC2	1.81	0.44
1:4:26:HIS:O	1:4:30:VAL:HG13	2.17	0.44
1:2:11:PRO:HG2	1:2:14:TRP:HE3	1.82	0.44
8:W:101:BCL:HBA2	8:W:101:BCL:HBD	1.98	0.44
8:W:102:BCL:H151	1:U:39:ILE:HD12	1.99	0.44
8:I:101:BCL:HAA1	9:I:103:PGV:H331	2.00	0.44
8:6:102:BCL:H62	8:6:102:BCL:H41	1.59	0.44
2:M:378:TRP:HE1	16:D:104:LMT:H6D	1.81	0.44
8:L:702:BCL:HED1	19:h:101:LHG:C7	2.46	0.44
3:1:7:GLU:OE1	3:1:7:GLU:N	2.46	0.44
3:9:31:LEU:HD22	17:9:103:UNL:C10	2.48	0.44
8:4:101:BCL:OBB	8:4:101:BCL:HHC	2.17	0.44
1:K:55:ARG:HH11	1:K:55:ARG:CG	2.26	0.44
8:0:102:BCL:H91	1:8:35:GLY:HA3	1.98	0.44
2:M:452:TRP:HZ3	11:M:702:BPH:H102	1.81	0.44
2:M:487:HIS:HB3	2:M:488:PRO:HD3	2.00	0.44
8:N:101:BCL:H111	8:N:101:BCL:H142	1.77	0.44
6:C:267:THR:HG22	6:C:291:PRO:HG2	2.00	0.44
8:0:102:BCL:H2	1:8:28:ILE:HG23	2.00	0.44
1:8:26:HIS:O	1:8:30:VAL:HG13	2.18	0.44
8:4:101:BCL:H171	8:4:101:BCL:H13	1.76	0.44
3:7:4:ARG:HH21	3:7:7:GLU:HG3	1.81	0.44
1:0:54:ILE:HG21	9:0:104:PGV:O02	2.17	0.44
8:O:102:BCL:HBB3	8:O:102:BCL:CMB	2.48	0.44
8:F:101:BCL:H93	8:F:101:BCL:H112	1.74	0.44
3:3:31:LEU:HB2	3:3:38:TRP:CZ3	2.53	0.43
8:U:101:BCL:H141	8:U:101:BCL:H161	1.86	0.43
1:I:27:ASP:OD2	1:I:31:LYS:NZ	2.50	0.43
8:6:102:BCL:C3B	10:3:102:U4Z:CAC	2.96	0.43
6:C:69:TYR:CE2	6:C:115:LYS:HD2	2.53	0.43
16:M:709:LMT:H1B	16:M:709:LMT:H3'	1.72	0.43
1:E:50:TRP:CG	1:E:51:THR:HG23	2.53	0.43
6:C:110:VAL:C	6:C:112:GLY:H	2.25	0.43
8:Q:102:BCL:H91	8:Q:102:BCL:H111	1.75	0.43
8:G:102:BCL:H41	8:G:102:BCL:H61	1.63	0.43
1:0:26:HIS:O	1:0:30:VAL:HG13	2.19	0.43
8:1:101:BCL:H152	8:1:101:BCL:H112	1.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:101:BCL:HAA1	9:8:103:PGV:H342	2.01	0.43
1:E:50:TRP:CD1	1:E:51:THR:HG23	2.54	0.43
8:0:102:BCL:H91	8:0:102:BCL:H111	1.86	0.43
2:M:526:MET:SD	19:h:101:LHG:HC61	2.59	0.43
9:M:705:PGV:H041	2:L:239:ARG:NH2	2.32	0.43
8:A:102:BCL:H142	8:A:102:BCL:H111	1.93	0.43
2:M:354:PRO:HA	2:M:355:PRO:HD3	1.72	0.42
4:Y:1:MET:HE2	4:Y:1:MET:HB2	1.82	0.42
6:C:138:LYS:HA	6:C:138:LYS:HD3	1.71	0.42
8:Q:101:BCL:H142	8:Q:101:BCL:H111	1.77	0.42
8:4:101:BCL:H13	8:4:101:BCL:H102	1.72	0.42
3:P:9:ARG:H	3:P:9:ARG:HG3	1.62	0.42
8:R:102:BCL:H111	8:R:102:BCL:H143	1.75	0.42
3:P:7:GLU:HB2	3:P:10:THR:HG23	2.00	0.42
3:V:20:LEU:CD1	8:V:101:BCL:H43	2.35	0.42
8:U:102:BCL:H101	8:U:102:BCL:H162	2.01	0.42
2:M:482:VAL:HG12	2:M:607:LEU:HD23	2.02	0.42
8:1:101:BCL:H121	8:1:101:BCL:H8	1.85	0.42
8:4:101:BCL:H61	8:4:101:BCL:H41	1.44	0.42
9:h:102:PGV:H332	9:h:102:PGV:H301	1.83	0.42
1:O:26:HIS:O	1:O:30:VAL:HG13	2.19	0.42
8:0:102:BCL:H12	1:8:31:LYS:HE2	2.02	0.42
8:4:101:BCL:H2	1:2:28:ILE:HG12	2.02	0.42
6:C:30:VAL:HG23	6:C:31:MET:CE	2.50	0.42
8:M:701:BCL:H112	8:M:701:BCL:H72	1.99	0.42
11:L:704:BPH:HMB1	11:L:704:BPH:HBB3	2.01	0.42
3:P:17:LEU:CD1	18:P:102:CDL:H531	2.49	0.42
3:9:31:LEU:CD2	17:9:103:UNL:C12	2.93	0.42
5:h:31:ILE:O	5:h:35:ILE:HG12	2.20	0.42
8:W:102:BCL:H203	8:W:102:BCL:H161	1.89	0.42
8:E:101:BCL:H203	8:E:101:BCL:H161	1.87	0.42
8:0:102:BCL:HMB3	8:0:102:BCL:HBB3	2.02	0.42
9:L:711:PGV:H031	15:h:103:PEF:H31	2.01	0.42
1:E:36:GLY:HA3	8:E:101:BCL:H52	2.01	0.42
3:J:4:ARG:NH2	3:J:7:GLU:OE1	2.53	0.42
3:N:9:ARG:HH21	15:h:103:PEF:H21	1.84	0.42
8:Q:102:BCL:H193	8:Q:102:BCL:H162	1.76	0.42
8:4:101:BCL:H61	8:4:101:BCL:H92	1.84	0.42
2:L:174:ARG:HB3	2:L:175:PRO:HD3	2.01	0.42
1:W:27:ASP:O	1:W:31:LYS:HG2	2.20	0.41
8:E:102:BCL:H41	8:E:102:BCL:H62	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:11:PRO:O	1:8:15:LYS:HG2	2.19	0.41
1:S:55:ARG:HG3	1:S:55:ARG:NH1	2.33	0.41
2:M:459:ARG:HB2	2:L:253:ILE:HD11	2.01	0.41
3:V:4:ARG:HB3	3:V:5:PRO:HD3	2.02	0.41
3:D:28:PHE:C	3:D:28:PHE:CD1	2.98	0.41
8:E:102:BCL:H142	8:E:102:BCL:H112	1.82	0.41
8:L:702:BCL:H92	8:L:702:BCL:H62	1.79	0.41
15:L:717:PEF:H331	4:Y:18:LEU:HD23	2.02	0.41
8:U:102:BCL:H41	8:U:102:BCL:H62	1.76	0.41
2:L:253:ILE:HG22	2:L:254:LEU:HG	2.02	0.41
8:N:101:BCL:H2	8:N:101:BCL:H61	1.90	0.41
8:E:101:BCL:H93	8:E:101:BCL:H61	1.77	0.41
1:0:7:ASN:ND2	1:0:15:LYS:HG3	2.35	0.41
11:M:702:BPH:H6C1	11:M:702:BPH:H4C1	1.71	0.41
3:H:38:TRP:O	3:H:39:LEU:C	2.63	0.41
3:D:16:THR:HG23	8:D:102:BCL:H61	2.03	0.41
8:D:102:BCL:H41	8:D:102:BCL:H62	1.80	0.41
6:C:42:ILE:O	6:C:46:ILE:HG12	2.21	0.41
1:U:26:HIS:O	1:U:30:VAL:HG13	2.21	0.41
8:E:101:BCL:CBB	9:E:103:PGV:H91	2.50	0.41
2:M:350:THR:HB	2:M:372:PRO:HB2	2.03	0.41
6:C:124:ILE:HD13	6:C:124:ILE:HA	1.93	0.41
8:W:101:BCL:H161	8:W:101:BCL:H192	1.88	0.41
9:4:102:PGV:H272	9:4:102:PGV:H241	1.86	0.41
8:L:702:BCL:HED2	19:h:101:LHG:O9	2.16	0.41
15:L:713:PEF:H252	15:L:717:PEF:H371	2.03	0.41
18:P:102:CDL:H141	18:P:102:CDL:H111	1.89	0.41
15:h:103:PEF:H381	15:h:103:PEF:H351	1.76	0.41
8:0:102:BCL:H61	8:0:102:BCL:H41	1.49	0.41
1:6:22:GLU:HG3	3:7:5:PRO:HG3	2.02	0.41
8:V:101:BCL:H41	8:V:101:BCL:H61	1.40	0.41
3:3:9:ARG:HG3	3:5:6:PHE:CE1	2.56	0.41
8:A:102:BCL:H122	8:A:102:BCL:H8	1.78	0.41
1:U:54:ILE:HG21	9:U:103:PGV:O02	2.21	0.40
1:I:55:ARG:HB2	3:F:37:ASN:ND2	2.34	0.40
8:6:101:BCL:HAA1	9:6:103:PGV:H342	2.03	0.40
8:5:101:BCL:H203	8:5:101:BCL:H161	1.82	0.40
8:F:101:BCL:H142	8:F:101:BCL:H111	1.96	0.40
1:W:53:TRP:CD1	1:W:54:ILE:HG13	2.57	0.40
8:I:102:BCL:HHD	8:I:102:BCL:HAC2	1.87	0.40
6:C:216:ASP:OD1	6:C:216:ASP:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:15:LYS:N	1:Q:16:PRO:HD2	2.37	0.40
14:L:715:BGL:O1	16:T:102:LMT:O2'	2.34	0.40
8:R:102:BCL:H171	3:T:11:SER:HA	2.03	0.40
6:C:78:MET:HG3	20:C:501:HEC:CMB	2.49	0.40
6:C:160:LEU:HD11	6:C:263:MET:HE3	2.03	0.40
1:W:8:ASP:N	1:W:8:ASP:OD1	2.52	0.40
8:8:102:BCL:H8	8:8:102:BCL:H122	1.69	0.40
8:L:703:BCL:H52	11:L:704:BPH:HBB2	2.04	0.40
8:R:102:BCL:H13	8:R:102:BCL:H172	1.95	0.40
3:D:37:ASN:OD1	3:D:40:ARG:HG3	2.22	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	0	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	2	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
1	4	48/55 (87%)	48 (100%)	0	0	100	100
1	6	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	8	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
1	B	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	E	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	G	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
1	I	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	K	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	O	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	Q	48/55 (87%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	U	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	W	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
2	L	284/641 (44%)	272 (96%)	12 (4%)	0	100	100
2	M	304/641 (47%)	294 (97%)	10 (3%)	0	100	100
3	1	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
3	3	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
3	5	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
3	7	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
3	9	36/42 (86%)	36 (100%)	0	0	100	100
3	A	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
3	D	37/42 (88%)	37 (100%)	0	0	100	100
3	F	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
3	H	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
3	J	37/42 (88%)	35 (95%)	2 (5%)	0	100	100
3	N	37/42 (88%)	37 (100%)	0	0	100	100
3	P	37/42 (88%)	37 (100%)	0	0	100	100
3	R	37/42 (88%)	37 (100%)	0	0	100	100
3	T	36/42 (86%)	36 (100%)	0	0	100	100
3	V	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
4	Y	30/39 (77%)	29 (97%)	1 (3%)	0	100	100
5	h	45/63 (71%)	45 (100%)	0	0	100	100
6	C	306/320 (96%)	290 (95%)	16 (5%)	0	100	100
7	Z	8/10 (80%)	8 (100%)	0	0	100	100
All	All	2246/3169 (71%)	2166 (96%)	80 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	44/49 (90%)	44 (100%)	0	100	100
1	2	44/49 (90%)	43 (98%)	1 (2%)	44	68
1	4	44/49 (90%)	44 (100%)	0	100	100
1	6	44/49 (90%)	43 (98%)	1 (2%)	44	68
1	8	44/49 (90%)	44 (100%)	0	100	100
1	B	44/49 (90%)	44 (100%)	0	100	100
1	E	44/49 (90%)	44 (100%)	0	100	100
1	G	44/49 (90%)	44 (100%)	0	100	100
1	I	44/49 (90%)	44 (100%)	0	100	100
1	K	44/49 (90%)	44 (100%)	0	100	100
1	O	44/49 (90%)	44 (100%)	0	100	100
1	Q	44/49 (90%)	44 (100%)	0	100	100
1	S	44/49 (90%)	44 (100%)	0	100	100
1	U	44/49 (90%)	44 (100%)	0	100	100
1	W	44/49 (90%)	44 (100%)	0	100	100
2	L	232/511 (45%)	229 (99%)	3 (1%)	61	79
2	M	244/511 (48%)	240 (98%)	4 (2%)	55	76
3	1	33/37 (89%)	33 (100%)	0	100	100
3	3	34/37 (92%)	34 (100%)	0	100	100
3	5	34/37 (92%)	34 (100%)	0	100	100
3	7	34/37 (92%)	34 (100%)	0	100	100
3	9	33/37 (89%)	32 (97%)	1 (3%)	36	61
3	A	33/37 (89%)	33 (100%)	0	100	100
3	D	34/37 (92%)	34 (100%)	0	100	100
3	F	33/37 (89%)	33 (100%)	0	100	100
3	H	34/37 (92%)	34 (100%)	0	100	100
3	J	34/37 (92%)	34 (100%)	0	100	100
3	N	34/37 (92%)	34 (100%)	0	100	100
3	P	34/37 (92%)	34 (100%)	0	100	100
3	R	34/37 (92%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	33/37 (89%)	33 (100%)	0	100	100
3	V	33/37 (89%)	33 (100%)	0	100	100
4	Y	29/36 (81%)	28 (97%)	1 (3%)	32	58
5	h	36/50 (72%)	35 (97%)	1 (3%)	38	62
6	C	250/262 (95%)	247 (99%)	3 (1%)	63	80
7	Z	1/1 (100%)	1 (100%)	0	100	100
All	All	1956/2661 (74%)	1941 (99%)	15 (1%)	70	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6	7	ASN
1	2	10	VAL
2	M	353	LYS
2	M	375	VAL
2	M	401	VAL
2	M	442	THR
2	L	93	VAL
2	L	281	CYS
2	L	308	VAL
3	9	18	LEU
4	Y	15	VAL
5	h	18	SER
6	C	154	GLN
6	C	173	THR
6	C	217	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	6	GLN
1	O	13	GLN
2	M	414	ASN
2	M	493	ASN
2	M	525	HIS
2	L	115	ASN
2	L	212	HIS
3	H	37	ASN
3	J	37	ASN

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Mol	Chain	Res	Type
3	R	27	HIS
3	A	37	ASN
5	h	44	GLN
6	C	55	GLN
6	C	83	GLN
6	C	89	GLN
6	C	168	GLN
6	C	225	ASN
6	C	226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 2 are monoatomic and 20 are unknown - leaving 106 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	$\# Z > 2$
8	BCL	3	101	-	69,74,74	1.82	18 (26%)	79,115,115	2.28	26 (32%)
8	BCL	L	703	-	69,74,74	1.80	17 (24%)	79,115,115	2.35	24 (30%)
8	BCL	F	101	-	69,74,74	1.78	19 (27%)	79,115,115	2.21	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PGV	6	103	-	43,43,50	0.99	2 (4%)	46,49,56	1.16	4 (8%)
8	BCL	M	701	-	69,74,74	1.82	17 (24%)	79,115,115	2.41	23 (29%)
10	U4Z	D	101	-	40,40,40	1.46	6 (15%)	51,51,51	1.51	12 (23%)
8	BCL	H	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.33	22 (27%)
8	BCL	3	103	-	69,74,74	1.79	18 (26%)	79,115,115	2.25	20 (25%)
15	PEF	M	708	-	20,20,46	1.54	2 (10%)	23,25,51	1.64	3 (13%)
8	BCL	O	101	-	69,74,74	1.82	18 (26%)	79,115,115	2.15	21 (26%)
9	PGV	L	712	-	34,34,50	1.09	2 (5%)	37,40,56	1.22	4 (10%)
20	HEC	C	501	6	46,50,50	1.82	5 (10%)	58,82,82	1.86	4 (6%)
9	PGV	h	102	-	45,45,50	0.98	2 (4%)	48,50,56	1.21	5 (10%)
8	BCL	E	102	-	69,74,74	1.80	18 (26%)	79,115,115	2.32	23 (29%)
8	BCL	4	101	-	69,74,74	1.76	20 (28%)	79,115,115	2.27	25 (31%)
8	BCL	5	101	-	69,74,74	1.77	16 (23%)	79,115,115	2.22	24 (30%)
9	PGV	N	102	-	23,23,50	1.32	2 (8%)	26,29,56	1.36	3 (11%)
14	BGL	M	707	-	20,20,20	0.35	0	24,25,25	0.85	1 (4%)
14	BGL	C	507	-	20,20,20	0.37	0	24,25,25	0.64	0
8	BCL	6	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.09	23 (29%)
9	PGV	E	104	-	43,43,50	0.97	2 (4%)	46,49,56	1.10	4 (8%)
14	BGL	L	714	-	20,20,20	0.37	0	24,25,25	0.56	0
8	BCL	7	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.28	24 (30%)
14	BGL	L	708	-	20,20,20	0.41	0	24,25,25	0.76	0
8	BCL	W	101	-	69,74,74	1.82	19 (27%)	79,115,115	2.10	20 (25%)
14	BGL	Y	103	-	20,20,20	0.40	0	24,25,25	0.64	0
10	U4Z	R	101	-	40,40,40	1.45	7 (17%)	51,51,51	1.49	13 (25%)
14	BGL	H	103	-	20,20,20	0.36	0	24,25,25	0.60	0
9	PGV	4	102	-	43,43,50	0.98	2 (4%)	46,49,56	1.08	4 (8%)
10	U4Z	J	101	-	40,40,40	1.47	7 (17%)	51,51,51	1.59	15 (29%)
8	BCL	G	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.18	28 (35%)
11	BPH	L	701	-	59,70,70	0.78	2 (3%)	59,101,101	1.00	3 (5%)
8	BCL	0	101	-	69,74,74	1.80	16 (23%)	79,115,115	2.18	25 (31%)
8	BCL	V	101	-	69,74,74	1.75	18 (26%)	79,115,115	2.16	19 (24%)
16	LMT	H	102	-	36,36,36	0.41	0	47,47,47	0.73	1 (2%)
8	BCL	8	101	-	69,74,74	1.81	17 (24%)	79,115,115	2.05	23 (29%)
14	BGL	M	706	-	20,20,20	0.44	0	24,25,25	0.63	0
16	LMT	D	104	-	36,36,36	0.40	0	47,47,47	0.77	0
8	BCL	B	101	-	69,74,74	1.86	19 (27%)	79,115,115	2.24	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PGV	I	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.28	4 (8%)
9	PGV	U	104	-	43,43,50	0.98	2 (4%)	46,49,56	1.11	4 (8%)
19	LHG	h	101	-	23,23,48	0.30	0	24,24,54	0.73	1 (4%)
8	BCL	L	702	-	69,74,74	1.80	16 (23%)	79,115,115	2.29	22 (27%)
8	BCL	Q	102	-	69,74,74	1.80	18 (26%)	79,115,115	2.20	21 (26%)
9	PGV	K	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.04	4 (8%)
8	BCL	8	102	-	69,74,74	1.72	18 (26%)	79,115,115	2.32	25 (31%)
8	BCL	W	102	-	69,74,74	1.78	18 (26%)	79,115,115	2.37	26 (32%)
8	BCL	R	102	-	69,74,74	1.80	17 (24%)	79,115,115	2.27	21 (26%)
20	HEC	C	502	6	46,50,50	1.83	3 (6%)	58,82,82	1.89	4 (6%)
8	BCL	U	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.82	30 (37%)
8	BCL	S	101	-	69,74,74	1.80	17 (24%)	79,115,115	2.06	22 (27%)
8	BCL	2	102	-	69,74,74	1.77	19 (27%)	79,115,115	2.43	28 (35%)
8	BCL	0	102	-	69,74,74	1.76	21 (30%)	79,115,115	2.27	24 (30%)
9	PGV	L	711	-	32,32,50	0.85	1 (3%)	34,37,56	1.10	2 (5%)
13	MQE	M	704	-	69,69,69	0.39	0	85,87,87	0.44	1 (1%)
8	BCL	E	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.08	22 (27%)
8	BCL	D	102	-	69,74,74	1.79	18 (26%)	79,115,115	2.29	24 (30%)
9	PGV	U	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.10	4 (8%)
14	BGL	L	715	-	20,20,20	0.35	0	24,25,25	0.94	1 (4%)
9	PGV	K	104	-	43,43,50	0.98	2 (4%)	46,49,56	1.04	2 (4%)
8	BCL	2	101	-	69,74,74	1.81	17 (24%)	79,115,115	2.06	23 (29%)
9	PGV	L	706	-	50,50,50	0.91	2 (4%)	53,56,56	1.00	2 (3%)
8	BCL	1	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.27	21 (26%)
9	PGV	O	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.16	3 (6%)
9	PGV	1	102	-	35,35,50	1.12	2 (5%)	38,40,56	1.21	4 (10%)
8	BCL	A	102	-	69,74,74	1.79	18 (26%)	79,115,115	2.20	22 (27%)
8	BCL	K	102	-	69,74,74	1.80	20 (28%)	79,115,115	2.17	23 (29%)
9	PGV	E	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.14	3 (6%)
9	PGV	0	104	-	43,43,50	0.98	2 (4%)	46,49,56	1.18	4 (8%)
8	BCL	N	101	-	69,74,74	1.75	17 (24%)	79,115,115	2.25	20 (25%)
8	BCL	P	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.25	22 (27%)
11	BPH	L	704	-	59,70,70	0.88	3 (5%)	59,101,101	0.95	2 (3%)
8	BCL	A	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.20	23 (29%)
20	HEC	C	503	6	46,50,50	1.83	4 (8%)	58,82,82	1.93	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PEF	h	103	-	40,40,46	1.02	2 (5%)	43,45,51	1.14	3 (6%)
8	BCL	G	102	-	69,74,74	1.80	19 (27%)	79,115,115	2.35	22 (27%)
8	BCL	Q	101	-	69,74,74	1.78	16 (23%)	79,115,115	2.14	21 (26%)
8	BCL	S	102	-	69,74,74	1.80	22 (31%)	79,115,115	2.32	24 (30%)
8	BCL	O	102	-	69,74,74	1.75	18 (26%)	79,115,115	2.33	25 (31%)
15	PEF	L	713	-	46,46,46	0.95	2 (4%)	49,51,51	1.10	4 (8%)
10	U4Z	0	103	-	40,40,40	1.47	6 (15%)	51,51,51	1.53	13 (25%)
8	BCL	U	101	-	69,74,74	1.80	18 (26%)	79,115,115	2.14	24 (30%)
14	BGL	Y	101	-	20,20,20	0.38	0	24,25,25	0.78	0
8	BCL	9	101	-	69,74,74	1.79	18 (26%)	79,115,115	2.26	23 (29%)
8	BCL	I	101	-	69,74,74	1.81	17 (24%)	79,115,115	2.14	23 (29%)
9	PGV	C	506	21	50,50,50	0.87	2 (4%)	53,56,56	1.12	4 (7%)
11	BPH	M	702	-	59,70,70	0.85	2 (3%)	59,101,101	0.99	3 (5%)
15	PEF	L	717	-	40,40,46	1.01	2 (5%)	43,45,51	1.08	2 (4%)
8	BCL	T	101	-	69,74,74	1.77	20 (28%)	79,115,115	2.27	20 (25%)
8	BCL	6	102	-	69,74,74	1.82	18 (26%)	79,115,115	2.31	22 (27%)
9	PGV	0	105	-	43,43,50	0.97	2 (4%)	46,49,56	1.18	4 (8%)
8	BCL	J	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.22	21 (26%)
16	LMT	M	709	-	36,36,36	0.37	0	47,47,47	0.97	3 (6%)
14	BGL	M	710	-	20,20,20	0.39	0	24,25,25	0.60	0
20	HEC	C	504	6	46,50,50	1.86	4 (8%)	58,82,82	1.84	5 (8%)
8	BCL	I	102	-	69,74,74	1.77	20 (28%)	79,115,115	2.23	20 (25%)
10	U4Z	3	102	-	40,40,40	1.47	9 (22%)	51,51,51	1.57	14 (27%)
8	BCL	K	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.10	23 (29%)
9	PGV	S	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.13	5 (10%)
9	PGV	8	103	-	43,43,50	0.98	2 (4%)	46,49,56	1.17	4 (8%)
16	LMT	T	102	-	36,36,36	0.51	1 (2%)	47,47,47	1.05	3 (6%)
14	BGL	L	709	-	20,20,20	0.39	0	24,25,25	0.49	0
13	MQE	L	705	-	54,54,69	0.35	0	67,69,87	0.72	2 (2%)
16	LMT	1	104	-	36,36,36	0.39	0	47,47,47	0.80	1 (2%)
18	CDL	P	102	-	49,49,99	1.29	4 (8%)	55,61,111	1.31	6 (10%)
9	PGV	M	705	-	34,34,50	1.12	2 (5%)	37,40,56	1.11	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	3	101	-	-	11/41/137/137	-
8	BCL	L	703	-	-	17/41/137/137	-
8	BCL	F	101	-	-	20/41/137/137	-
9	PGV	6	103	-	-	15/48/48/55	-
8	BCL	M	701	-	-	18/41/137/137	-
10	U4Z	D	101	-	-	4/36/53/53	0/1/1/1
8	BCL	H	101	-	-	16/41/137/137	-
8	BCL	3	103	-	-	14/41/137/137	-
15	PEF	M	708	-	-	9/23/23/50	-
8	BCL	O	101	-	-	12/41/137/137	-
9	PGV	L	712	-	-	15/39/39/55	-
20	HEC	C	501	6	-	5/14/54/54	-
9	PGV	h	102	-	-	11/47/47/55	-
8	BCL	E	102	-	-	22/41/137/137	-
8	BCL	4	101	-	-	16/41/137/137	-
8	BCL	5	101	-	-	14/41/137/137	-
9	PGV	N	102	-	-	0/28/28/55	-
14	BGL	M	707	-	-	1/11/31/31	0/1/1/1
14	BGL	C	507	-	-	1/11/31/31	0/1/1/1
8	BCL	6	101	-	-	10/41/137/137	-
9	PGV	E	104	-	-	10/48/48/55	-
14	BGL	L	714	-	-	2/11/31/31	0/1/1/1
8	BCL	7	101	-	-	12/41/137/137	-
14	BGL	L	708	-	-	3/11/31/31	0/1/1/1
8	BCL	W	101	-	-	17/41/137/137	-
14	BGL	Y	103	-	-	3/11/31/31	0/1/1/1
10	U4Z	R	101	-	-	4/36/53/53	0/1/1/1
14	BGL	H	103	-	-	2/11/31/31	0/1/1/1
9	PGV	4	102	-	-	16/48/48/55	-
10	U4Z	J	101	-	-	4/36/53/53	0/1/1/1
8	BCL	G	101	-	-	15/41/137/137	-
11	BPH	L	701	-	-	14/37/105/105	0/5/6/6
8	BCL	0	101	-	-	11/41/137/137	-
8	BCL	V	101	-	-	19/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMT	H	102	-	-	6/21/61/61	0/2/2/2
8	BCL	8	101	-	-	14/41/137/137	-
14	BGL	M	706	-	-	3/11/31/31	0/1/1/1
16	LMT	D	104	-	-	10/21/61/61	0/2/2/2
8	BCL	B	101	-	-	15/41/137/137	-
9	PGV	I	103	-	-	10/48/48/55	-
9	PGV	U	104	-	-	12/48/48/55	-
19	LHG	h	101	-	-	19/23/23/53	-
8	BCL	L	702	-	-	14/41/137/137	-
8	BCL	Q	102	-	-	19/41/137/137	-
9	PGV	K	103	-	-	13/48/48/55	-
8	BCL	8	102	-	-	11/41/137/137	-
8	BCL	W	102	-	-	19/41/137/137	-
8	BCL	R	102	-	-	12/41/137/137	-
20	HEC	C	502	6	-	4/14/54/54	-
8	BCL	U	102	-	-	21/41/137/137	-
8	BCL	S	101	-	-	17/41/137/137	-
8	BCL	2	102	-	-	21/41/137/137	-
8	BCL	0	102	-	-	20/41/137/137	-
9	PGV	L	711	-	-	9/36/36/55	-
13	MQE	M	704	-	-	10/65/85/85	0/2/2/2
8	BCL	E	101	-	-	15/41/137/137	-
8	BCL	D	102	-	-	13/41/137/137	-
9	PGV	U	103	-	-	11/48/48/55	-
14	BGL	L	715	-	-	1/11/31/31	0/1/1/1
9	PGV	K	104	-	-	15/48/48/55	-
8	BCL	2	101	-	-	13/41/137/137	-
9	PGV	L	706	-	-	14/55/55/55	-
8	BCL	1	101	-	-	13/41/137/137	-
9	PGV	O	103	-	-	17/48/48/55	-
9	PGV	1	102	-	-	12/37/37/55	-
8	BCL	A	102	-	-	10/41/137/137	-
8	BCL	K	102	-	-	20/41/137/137	-
9	PGV	E	103	-	-	13/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PGV	0	104	-	-	15/48/48/55	-
8	BCL	N	101	-	-	17/41/137/137	-
8	BCL	P	101	-	-	8/41/137/137	-
11	BPH	L	704	-	-	11/37/105/105	0/5/6/6
8	BCL	A	101	-	-	15/41/137/137	-
20	HEC	C	503	6	-	4/14/54/54	-
15	PEF	h	103	-	-	18/44/44/50	-
8	BCL	G	102	-	-	24/41/137/137	-
8	BCL	Q	101	-	-	14/41/137/137	-
8	BCL	S	102	-	-	19/41/137/137	-
8	BCL	O	102	-	-	18/41/137/137	-
15	PEF	L	713	-	-	14/50/50/50	-
10	U4Z	0	103	-	-	2/36/53/53	0/1/1/1
8	BCL	U	101	-	-	10/41/137/137	-
14	BGL	Y	101	-	-	2/11/31/31	0/1/1/1
8	BCL	9	101	-	-	13/41/137/137	-
8	BCL	I	101	-	-	10/41/137/137	-
9	PGV	C	506	21	-	20/55/55/55	-
11	BPH	M	702	-	-	22/37/105/105	0/5/6/6
15	PEF	L	717	-	-	11/44/44/50	-
8	BCL	T	101	-	-	15/41/137/137	-
8	BCL	6	102	-	-	20/41/137/137	-
9	PGV	0	105	-	-	10/48/48/55	-
8	BCL	J	102	-	-	14/41/137/137	-
16	LMT	M	709	-	-	13/21/61/61	0/2/2/2
14	BGL	M	710	-	-	1/11/31/31	0/1/1/1
20	HEC	C	504	6	-	6/14/54/54	-
8	BCL	I	102	-	-	23/41/137/137	-
10	U4Z	3	102	-	-	4/36/53/53	0/1/1/1
8	BCL	K	101	-	-	15/41/137/137	-
9	PGV	S	103	-	-	10/48/48/55	-
9	PGV	8	103	-	-	14/48/48/55	-
16	LMT	T	102	-	-	8/21/61/61	0/2/2/2
14	BGL	L	709	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MQE	L	705	-	-	6/47/67/85	0/2/2/2
16	LMT	1	104	-	-	3/21/61/61	0/2/2/2
18	CDL	P	102	-	-	24/60/60/110	-
9	PGV	M	705	-	-	10/39/39/55	-

All (974) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	503	HEC	CAC-C3C	6.46	1.56	1.35
20	C	504	HEC	CAC-C3C	6.40	1.55	1.35
20	C	502	HEC	CAC-C3C	6.39	1.55	1.35
20	C	501	HEC	CAC-C3C	6.29	1.55	1.35
20	C	504	HEC	CAB-C3B	6.26	1.55	1.35
20	C	502	HEC	CAB-C3B	6.24	1.55	1.35
20	C	501	HEC	CAB-C3B	6.10	1.54	1.35
20	C	503	HEC	CAB-C3B	6.03	1.54	1.35
20	C	504	HEC	C3D-C2D	5.86	1.54	1.38
20	C	502	HEC	C3D-C2D	5.57	1.53	1.38
20	C	501	HEC	C3D-C2D	5.56	1.53	1.38
20	C	503	HEC	C3D-C2D	5.54	1.53	1.38
8	G	102	BCL	O2D-CGD	5.12	1.45	1.33
8	B	101	BCL	C3D-C4D	-5.11	1.32	1.44
8	L	703	BCL	O2D-CGD	5.07	1.45	1.33
8	L	702	BCL	C3D-C4D	-5.03	1.32	1.44
8	G	102	BCL	C3D-C4D	-5.02	1.32	1.44
8	M	701	BCL	O2D-CGD	5.01	1.45	1.33
8	I	102	BCL	C3D-C4D	-5.00	1.32	1.44
8	O	102	BCL	O2D-CGD	5.00	1.45	1.33
8	K	102	BCL	C3D-C4D	-5.00	1.32	1.44
8	Q	102	BCL	C3D-C4D	-4.99	1.33	1.44
8	O	102	BCL	C3D-C4D	-4.98	1.33	1.44
8	E	102	BCL	C3D-C4D	-4.97	1.33	1.44
8	W	102	BCL	O2D-CGD	4.95	1.45	1.33
8	R	102	BCL	O2D-CGD	4.93	1.45	1.33
8	9	101	BCL	O2D-CGD	4.93	1.45	1.33
8	S	102	BCL	C3D-C4D	-4.93	1.33	1.44
8	U	101	BCL	O2D-CGD	4.92	1.45	1.33
8	A	102	BCL	C3D-C4D	-4.92	1.33	1.44
8	8	102	BCL	O2D-CGD	4.91	1.45	1.33
8	S	101	BCL	O2D-CGD	4.90	1.45	1.33
8	I	101	BCL	O2D-CGD	4.90	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	101	BCL	O2D-CGD	4.89	1.45	1.33
8	T	101	BCL	O2D-CGD	4.88	1.45	1.33
8	U	102	BCL	O2D-CGD	4.88	1.45	1.33
8	0	101	BCL	O2D-CGD	4.88	1.45	1.33
8	6	102	BCL	C3D-C4D	-4.88	1.33	1.44
8	2	101	BCL	O2D-CGD	4.88	1.45	1.33
8	2	102	BCL	O2D-CGD	4.86	1.45	1.33
8	V	101	BCL	O2D-CGD	4.86	1.45	1.33
8	4	101	BCL	C3D-C4D	-4.85	1.33	1.44
8	O	101	BCL	O2D-CGD	4.85	1.45	1.33
8	S	102	BCL	O2D-CGD	4.84	1.45	1.33
8	V	101	BCL	C3D-C4D	-4.84	1.33	1.44
8	8	102	BCL	C3D-C4D	-4.84	1.33	1.44
8	7	101	BCL	O2D-CGD	4.83	1.45	1.33
8	O	102	BCL	C3D-C4D	-4.83	1.33	1.44
8	4	101	BCL	O2D-CGD	4.83	1.45	1.33
8	5	101	BCL	C3D-C4D	-4.83	1.33	1.44
8	P	101	BCL	O2D-CGD	4.82	1.45	1.33
8	6	102	BCL	O2D-CGD	4.82	1.45	1.33
8	F	101	BCL	O2D-CGD	4.81	1.45	1.33
8	D	102	BCL	O2D-CGD	4.81	1.45	1.33
8	N	101	BCL	O2D-CGD	4.81	1.45	1.33
8	W	102	BCL	C3D-C4D	-4.80	1.33	1.44
8	J	102	BCL	C3D-C4D	-4.80	1.33	1.44
8	Q	101	BCL	C3D-C4D	-4.79	1.33	1.44
8	A	102	BCL	O2D-CGD	4.79	1.45	1.33
8	A	101	BCL	O2D-CGD	4.79	1.45	1.33
8	3	103	BCL	O2D-CGD	4.79	1.45	1.33
8	8	101	BCL	C3D-C4D	-4.79	1.33	1.44
8	9	101	BCL	C3D-C4D	-4.78	1.33	1.44
8	8	101	BCL	O2D-CGD	4.78	1.45	1.33
8	R	102	BCL	C3D-C4D	-4.78	1.33	1.44
8	3	103	BCL	C3D-C4D	-4.78	1.33	1.44
8	3	101	BCL	O2D-CGD	4.77	1.45	1.33
8	5	101	BCL	O2D-CGD	4.77	1.45	1.33
8	Q	101	BCL	O2D-CGD	4.77	1.45	1.33
15	M	708	PEF	O2-C10	4.76	1.45	1.35
8	M	701	BCL	C3D-C4D	-4.76	1.33	1.44
8	A	101	BCL	C3D-C4D	-4.76	1.33	1.44
8	U	101	BCL	C3D-C4D	-4.76	1.33	1.44
8	K	101	BCL	O2D-CGD	4.76	1.44	1.33
8	G	101	BCL	O2D-CGD	4.76	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	101	BCL	C3D-C4D	-4.76	1.33	1.44
8	0	101	BCL	C3D-C4D	-4.75	1.33	1.44
8	T	101	BCL	C3D-C4D	-4.74	1.33	1.44
8	H	101	BCL	C3D-C4D	-4.74	1.33	1.44
8	E	101	BCL	O2D-CGD	4.74	1.44	1.33
8	P	101	BCL	C3D-C4D	-4.73	1.33	1.44
8	F	101	BCL	C3D-C4D	-4.73	1.33	1.44
8	D	102	BCL	C3D-C4D	-4.73	1.33	1.44
8	H	101	BCL	O2D-CGD	4.73	1.44	1.33
8	J	102	BCL	O2D-CGD	4.72	1.44	1.33
8	7	101	BCL	C3D-C4D	-4.72	1.33	1.44
8	6	101	BCL	O2D-CGD	4.72	1.44	1.33
8	S	101	BCL	C3D-C4D	-4.71	1.33	1.44
8	3	101	BCL	C3D-C4D	-4.71	1.33	1.44
8	O	102	BCL	O2D-CGD	4.70	1.44	1.33
8	W	101	BCL	C3D-C4D	-4.70	1.33	1.44
8	O	101	BCL	C3D-C4D	-4.69	1.33	1.44
8	2	102	BCL	C3D-C4D	-4.69	1.33	1.44
8	K	102	BCL	O2D-CGD	4.68	1.44	1.33
8	N	101	BCL	C3D-C4D	-4.68	1.33	1.44
8	U	102	BCL	C3D-C4D	-4.67	1.33	1.44
8	G	101	BCL	C3D-C4D	-4.67	1.33	1.44
8	2	101	BCL	C3D-C4D	-4.66	1.33	1.44
8	K	101	BCL	C3D-C4D	-4.66	1.33	1.44
8	I	101	BCL	C3D-C4D	-4.65	1.33	1.44
8	L	703	BCL	C3D-C4D	-4.64	1.33	1.44
8	6	101	BCL	C3D-C4D	-4.64	1.33	1.44
8	1	101	BCL	C3D-C4D	-4.63	1.33	1.44
8	E	102	BCL	O2D-CGD	4.63	1.44	1.33
8	I	102	BCL	O2D-CGD	4.59	1.44	1.33
8	Q	102	BCL	O2D-CGD	4.57	1.44	1.33
8	B	101	BCL	O2D-CGD	4.52	1.44	1.33
8	M	701	BCL	O2A-CGA	4.51	1.46	1.33
8	E	101	BCL	O2A-CGA	4.49	1.46	1.33
8	K	102	BCL	O2A-CGA	4.49	1.46	1.33
8	U	102	BCL	C1B-NB	-4.46	1.32	1.37
8	L	703	BCL	O2A-CGA	4.46	1.46	1.33
8	2	102	BCL	O2A-CGA	4.45	1.46	1.33
8	1	101	BCL	O2D-CGD	4.44	1.44	1.33
8	2	101	BCL	C3B-C4B	4.42	1.49	1.41
8	Q	102	BCL	C3B-C4B	4.41	1.49	1.41
8	L	702	BCL	C3B-C4B	4.41	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	102	BCL	O2A-CGA	4.40	1.46	1.33
8	B	101	BCL	O2A-CGA	4.40	1.46	1.33
8	W	102	BCL	O2A-CGA	4.39	1.46	1.33
8	0	101	BCL	C3B-C4B	4.37	1.49	1.41
8	O	102	BCL	O2A-CGA	4.36	1.46	1.33
8	L	703	BCL	C3B-C4B	4.36	1.49	1.41
9	M	705	PGV	O03-C19	4.36	1.46	1.33
8	L	702	BCL	O2D-CGD	4.34	1.43	1.33
8	8	101	BCL	O2A-CGA	4.33	1.46	1.33
8	U	101	BCL	O2A-CGA	4.32	1.45	1.33
8	I	102	BCL	O2A-CGA	4.31	1.45	1.33
8	V	101	BCL	O2A-CGA	4.31	1.45	1.33
9	0	104	PGV	O03-C19	4.31	1.45	1.33
9	U	104	PGV	O03-C19	4.30	1.45	1.33
8	3	101	BCL	C3B-C4B	4.29	1.49	1.41
9	1	102	PGV	O03-C19	4.29	1.45	1.33
9	O	103	PGV	O03-C19	4.28	1.45	1.33
18	P	102	CDL	OB8-CB7	4.28	1.45	1.33
8	W	102	BCL	C3B-C4B	4.28	1.49	1.41
8	M	701	BCL	C3B-C4B	4.28	1.49	1.41
9	8	103	PGV	O03-C19	4.28	1.45	1.33
15	L	713	PEF	O3-C30	4.27	1.45	1.33
15	h	103	PEF	O3-C30	4.27	1.45	1.33
9	6	103	PGV	O03-C19	4.26	1.45	1.33
8	8	101	BCL	C1D-ND	-4.26	1.32	1.37
8	I	101	BCL	C3B-C4B	4.26	1.49	1.41
8	7	101	BCL	C3B-C4B	4.26	1.49	1.41
8	G	102	BCL	C3B-C4B	4.25	1.49	1.41
9	K	103	PGV	O03-C19	4.25	1.45	1.33
9	U	103	PGV	O03-C19	4.25	1.45	1.33
9	E	104	PGV	O03-C19	4.25	1.45	1.33
8	S	102	BCL	O2A-CGA	4.24	1.45	1.33
9	I	103	PGV	O03-C19	4.24	1.45	1.33
9	4	102	PGV	O03-C19	4.24	1.45	1.33
9	0	105	PGV	O03-C19	4.24	1.45	1.33
8	A	101	BCL	C3B-C4B	4.24	1.49	1.41
8	A	102	BCL	O2A-CGA	4.24	1.45	1.33
8	1	101	BCL	O2A-CGA	4.24	1.45	1.33
9	E	103	PGV	O03-C19	4.23	1.45	1.33
8	O	101	BCL	C3B-C4B	4.23	1.49	1.41
8	6	102	BCL	O2A-CGA	4.22	1.45	1.33
9	S	103	PGV	O03-C19	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	102	PGV	O03-C19	4.22	1.45	1.33
8	S	101	BCL	C3B-C4B	4.21	1.49	1.41
15	M	708	PEF	O3-C30	4.21	1.45	1.33
9	K	104	PGV	O03-C19	4.21	1.45	1.33
9	L	711	PGV	O03-C19	4.21	1.45	1.33
15	L	717	PEF	O3-C30	4.20	1.45	1.33
9	6	103	PGV	O01-C1	4.19	1.46	1.34
18	P	102	CDL	OA8-CA7	4.19	1.45	1.33
8	K	101	BCL	O2A-CGA	4.19	1.45	1.33
8	J	102	BCL	C3B-C4B	4.18	1.49	1.41
8	6	101	BCL	O2A-CGA	4.18	1.45	1.33
9	K	104	PGV	O01-C1	4.17	1.46	1.34
18	P	102	CDL	OB6-CB5	4.17	1.46	1.34
8	4	101	BCL	O2A-CGA	4.17	1.45	1.33
8	6	101	BCL	C3B-C4B	4.16	1.49	1.41
8	2	101	BCL	O2A-CGA	4.16	1.45	1.33
8	6	102	BCL	C3B-C4B	4.16	1.49	1.41
8	A	101	BCL	O2A-CGA	4.14	1.45	1.33
8	R	102	BCL	C3B-C4B	4.14	1.49	1.41
9	S	103	PGV	O01-C1	4.14	1.46	1.34
8	1	101	BCL	C3B-C4B	4.13	1.49	1.41
8	G	101	BCL	C3B-C4B	4.13	1.49	1.41
8	J	102	BCL	O2A-CGA	4.13	1.45	1.33
9	U	104	PGV	O01-C1	4.13	1.45	1.34
8	I	101	BCL	O2A-CGA	4.13	1.45	1.33
8	Q	102	BCL	O2A-CGA	4.13	1.45	1.33
8	F	101	BCL	O2A-CGA	4.12	1.45	1.33
9	0	105	PGV	O01-C1	4.12	1.45	1.34
8	K	101	BCL	C3B-C4B	4.11	1.49	1.41
9	O	103	PGV	O01-C1	4.11	1.45	1.34
9	h	102	PGV	O01-C1	4.11	1.45	1.34
9	h	102	PGV	O03-C19	4.11	1.45	1.33
9	M	705	PGV	O01-C1	4.10	1.45	1.34
9	L	712	PGV	O03-C19	4.10	1.45	1.33
8	Q	101	BCL	O2A-CGA	4.10	1.45	1.33
9	L	706	PGV	O03-C19	4.10	1.45	1.33
8	H	101	BCL	O2A-CGA	4.10	1.45	1.33
8	G	102	BCL	O2A-CGA	4.09	1.45	1.33
9	K	103	PGV	O01-C1	4.09	1.45	1.34
8	0	101	BCL	O2A-CGA	4.09	1.45	1.33
9	U	103	PGV	O01-C1	4.09	1.45	1.34
9	8	103	PGV	O01-C1	4.09	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	101	BCL	O2A-CGA	4.08	1.45	1.33
9	E	103	PGV	O01-C1	4.08	1.45	1.34
9	L	706	PGV	O01-C1	4.07	1.45	1.34
9	I	103	PGV	O01-C1	4.07	1.45	1.34
9	L	712	PGV	O01-C1	4.07	1.45	1.34
8	E	102	BCL	C3B-C4B	4.06	1.49	1.41
8	U	101	BCL	C3B-C4B	4.06	1.49	1.41
9	0	104	PGV	O01-C1	4.06	1.45	1.34
15	h	103	PEF	O2-C10	4.06	1.45	1.34
8	N	101	BCL	O2A-CGA	4.06	1.45	1.33
8	5	101	BCL	O2A-CGA	4.06	1.45	1.33
9	N	102	PGV	O01-C1	4.05	1.45	1.34
9	C	506	PGV	O03-C19	4.05	1.45	1.33
9	4	102	PGV	O01-C1	4.04	1.45	1.34
8	3	103	BCL	O2A-CGA	4.04	1.45	1.33
8	R	102	BCL	O2A-CGA	4.04	1.45	1.33
8	L	702	BCL	O2A-CGA	4.04	1.45	1.33
15	L	717	PEF	O2-C10	4.03	1.45	1.34
8	U	102	BCL	O2A-CGA	4.03	1.45	1.33
8	8	101	BCL	C3B-C4B	4.03	1.49	1.41
8	3	103	BCL	C3B-C4B	4.03	1.49	1.41
8	W	101	BCL	O2A-CGA	4.03	1.45	1.33
8	0	102	BCL	O2A-CGA	4.03	1.45	1.33
8	S	101	BCL	O2A-CGA	4.03	1.45	1.33
8	W	101	BCL	C3B-C4B	4.02	1.49	1.41
9	E	104	PGV	O01-C1	4.02	1.45	1.34
8	8	102	BCL	O2A-CGA	4.01	1.45	1.33
8	7	101	BCL	O2A-CGA	4.01	1.45	1.33
8	P	101	BCL	O2A-CGA	4.00	1.45	1.33
8	D	102	BCL	O2A-CGA	4.00	1.45	1.33
8	O	101	BCL	O2A-CGA	3.99	1.45	1.33
18	P	102	CDL	OA6-CA5	3.98	1.45	1.34
8	G	101	BCL	O2A-CGA	3.98	1.45	1.33
8	H	101	BCL	C3B-C4B	3.94	1.48	1.41
8	B	101	BCL	C3B-C4B	3.93	1.48	1.41
9	1	102	PGV	O01-C1	3.93	1.45	1.34
15	L	713	PEF	O2-C10	3.93	1.45	1.34
8	6	101	BCL	C1D-ND	-3.92	1.32	1.37
8	U	102	BCL	C4B-NB	-3.91	1.32	1.37
8	2	101	BCL	C1D-ND	-3.91	1.32	1.37
8	F	101	BCL	C3B-C4B	3.90	1.48	1.41
8	K	101	BCL	C1D-ND	-3.90	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	101	BCL	C3B-C4B	3.88	1.48	1.41
8	3	101	BCL	O2A-CGA	3.87	1.44	1.33
8	Q	101	BCL	C1D-ND	-3.86	1.32	1.37
8	U	102	BCL	C3B-C4B	3.86	1.48	1.41
8	U	101	BCL	C1D-ND	-3.86	1.32	1.37
8	D	102	BCL	C3B-C4B	3.85	1.48	1.41
8	T	101	BCL	O2A-CGA	3.85	1.44	1.33
8	A	101	BCL	C1D-ND	-3.85	1.32	1.37
8	I	101	BCL	C1D-ND	-3.84	1.32	1.37
8	G	101	BCL	C1D-ND	-3.83	1.32	1.37
8	S	101	BCL	C1D-ND	-3.81	1.32	1.37
8	Q	101	BCL	C3B-C4B	3.81	1.48	1.41
8	B	101	BCL	C4B-NB	-3.76	1.32	1.37
8	T	101	BCL	C3B-C4B	3.74	1.48	1.41
8	N	101	BCL	C3B-C4B	3.74	1.48	1.41
8	5	101	BCL	C3B-C4B	3.74	1.48	1.41
8	E	101	BCL	C3B-C4B	3.73	1.48	1.41
8	0	101	BCL	C1D-ND	-3.73	1.33	1.37
8	O	101	BCL	C1D-ND	-3.73	1.33	1.37
8	A	102	BCL	C3B-C4B	3.73	1.48	1.41
8	6	102	BCL	CHB-C1B	3.72	1.47	1.39
8	W	101	BCL	C1D-ND	-3.72	1.33	1.37
8	P	101	BCL	C3B-C4B	3.72	1.48	1.41
8	E	101	BCL	C1D-ND	-3.71	1.33	1.37
8	3	101	BCL	C1D-ND	-3.64	1.33	1.37
8	V	101	BCL	C3B-C4B	3.63	1.48	1.41
8	O	102	BCL	C3B-C4B	3.60	1.48	1.41
8	8	102	BCL	C3B-C4B	3.58	1.48	1.41
9	C	506	PGV	O01-C1	3.56	1.44	1.34
8	S	102	BCL	C3B-C4B	3.51	1.48	1.41
8	2	102	BCL	C4B-NB	-3.48	1.33	1.37
8	4	101	BCL	C4B-NB	-3.46	1.33	1.37
10	0	103	U4Z	CAL-CAM	-3.45	1.38	1.46
8	K	102	BCL	C3B-C4B	3.44	1.47	1.41
8	K	102	BCL	CHD-C1D	3.43	1.45	1.38
8	L	702	BCL	CHC-C4B	3.43	1.47	1.39
8	A	102	BCL	CHD-C1D	3.41	1.45	1.38
8	O	101	BCL	CHC-C4B	3.40	1.47	1.39
8	P	101	BCL	C4B-NB	-3.40	1.33	1.37
8	I	102	BCL	C3B-C4B	3.39	1.47	1.41
8	L	703	BCL	CHD-C1D	3.39	1.45	1.38
8	I	101	BCL	CHC-C4B	3.38	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3	103	BCL	CHB-C1B	3.38	1.47	1.39
8	I	102	BCL	CHB-C1B	3.37	1.47	1.39
8	0	102	BCL	CHD-C1D	3.37	1.45	1.38
8	2	102	BCL	C3B-C4B	3.37	1.47	1.41
8	H	101	BCL	CHB-C1B	3.36	1.46	1.39
8	Q	102	BCL	C4B-NB	-3.35	1.33	1.37
10	J	101	U4Z	CAL-CAM	-3.34	1.38	1.46
8	G	102	BCL	C4B-NB	-3.34	1.33	1.37
10	D	101	U4Z	CAL-CAM	-3.32	1.38	1.46
8	K	102	BCL	C4B-NB	-3.32	1.33	1.37
8	U	102	BCL	CHD-C1D	3.32	1.44	1.38
8	0	102	BCL	C3B-C4B	3.31	1.47	1.41
8	7	101	BCL	CHC-C4B	3.31	1.46	1.39
8	5	101	BCL	C4B-NB	-3.31	1.33	1.37
8	V	101	BCL	CHD-C1D	3.31	1.44	1.38
8	H	101	BCL	C1D-ND	-3.30	1.33	1.37
8	O	102	BCL	C4B-NB	-3.30	1.33	1.37
8	0	101	BCL	CHC-C4B	3.30	1.46	1.39
8	1	101	BCL	CHD-C1D	3.29	1.44	1.38
8	G	101	BCL	C1B-NB	-3.28	1.33	1.37
8	I	102	BCL	C4B-NB	-3.28	1.33	1.37
8	D	102	BCL	OBD-CAD	3.28	1.28	1.22
8	U	101	BCL	CHB-C1B	3.28	1.46	1.39
8	I	101	BCL	C1B-NB	-3.28	1.33	1.37
8	L	702	BCL	C1D-ND	-3.27	1.33	1.37
8	7	101	BCL	CHD-C1D	3.27	1.44	1.38
8	W	101	BCL	CHC-C4B	3.26	1.46	1.39
10	R	101	U4Z	CAL-CAM	-3.26	1.39	1.46
8	L	703	BCL	CHC-C4B	3.26	1.46	1.39
8	R	102	BCL	CHD-C1D	3.26	1.44	1.38
8	S	102	BCL	CHB-C1B	3.25	1.46	1.39
8	W	102	BCL	C4B-NB	-3.25	1.33	1.37
8	Q	101	BCL	CHC-C4B	3.24	1.46	1.39
8	D	102	BCL	CHB-C1B	3.24	1.46	1.39
8	U	101	BCL	CHC-C4B	3.24	1.46	1.39
8	L	702	BCL	C3D-C2D	3.24	1.47	1.39
8	9	101	BCL	CHB-C1B	3.23	1.46	1.39
11	L	704	BPH	C4D-CHA	3.23	1.44	1.39
8	M	701	BCL	CHC-C4B	3.23	1.46	1.39
8	M	701	BCL	CHD-C1D	3.22	1.44	1.38
8	B	101	BCL	CHC-C4B	3.22	1.46	1.39
8	S	101	BCL	CHC-C4B	3.22	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	101	BCL	CHB-C1B	3.22	1.46	1.39
8	Q	101	BCL	CHB-C1B	3.22	1.46	1.39
8	K	101	BCL	C1B-NB	-3.22	1.33	1.37
8	M	701	BCL	CHB-C1B	3.21	1.46	1.39
8	6	101	BCL	CHB-C1B	3.21	1.46	1.39
8	Q	102	BCL	CHD-C1D	3.21	1.44	1.38
8	S	102	BCL	CHD-C1D	3.21	1.44	1.38
10	3	102	U4Z	CAL-CAM	-3.20	1.39	1.46
8	O	102	BCL	CHD-C1D	3.20	1.44	1.38
8	3	103	BCL	C1D-ND	-3.19	1.33	1.37
8	2	102	BCL	C1B-NB	-3.19	1.33	1.37
8	B	101	BCL	C1B-NB	-3.19	1.33	1.37
8	V	101	BCL	CHC-C4B	3.19	1.46	1.39
8	M	701	BCL	C1D-ND	-3.19	1.33	1.37
8	J	102	BCL	CHC-C4B	3.18	1.46	1.39
8	O	101	BCL	OBD-CAD	3.18	1.28	1.22
8	T	101	BCL	CHC-C4B	3.18	1.46	1.39
8	A	101	BCL	CHC-C4B	3.18	1.46	1.39
8	2	101	BCL	CHC-C4B	3.17	1.46	1.39
8	R	102	BCL	CHB-C1B	3.17	1.46	1.39
8	W	101	BCL	CHB-C1B	3.17	1.46	1.39
8	P	101	BCL	C1D-ND	-3.17	1.33	1.37
8	B	101	BCL	CHD-C1D	3.17	1.44	1.38
8	9	101	BCL	CHC-C4B	3.17	1.46	1.39
8	D	102	BCL	C4B-NB	-3.17	1.33	1.37
8	N	101	BCL	CHD-C1D	3.17	1.44	1.38
8	N	101	BCL	CHB-C1B	3.17	1.46	1.39
8	J	102	BCL	C1D-ND	-3.16	1.33	1.37
8	J	102	BCL	CHD-C1D	3.16	1.44	1.38
8	J	102	BCL	OBD-CAD	3.16	1.27	1.22
8	G	102	BCL	CHB-C1B	3.16	1.46	1.39
8	6	102	BCL	C4B-NB	-3.16	1.33	1.37
8	2	101	BCL	CHB-C1B	3.16	1.46	1.39
8	V	101	BCL	CHB-C1B	3.16	1.46	1.39
8	F	101	BCL	C1D-ND	-3.16	1.33	1.37
8	5	101	BCL	CHB-C1B	3.15	1.46	1.39
8	G	101	BCL	CHC-C4B	3.15	1.46	1.39
8	S	102	BCL	OBD-CAD	3.15	1.27	1.22
8	R	102	BCL	CHC-C4B	3.15	1.46	1.39
8	S	102	BCL	C4B-NB	-3.15	1.33	1.37
8	N	101	BCL	CHC-C4B	3.15	1.46	1.39
8	F	101	BCL	CHD-C1D	3.15	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	101	BCL	CHD-C1D	3.15	1.44	1.38
8	4	101	BCL	CHB-C1B	3.14	1.46	1.39
8	L	702	BCL	CHD-C1D	3.14	1.44	1.38
8	9	101	BCL	CHD-C1D	3.14	1.44	1.38
8	D	102	BCL	CHD-C1D	3.14	1.44	1.38
8	H	101	BCL	C4B-NB	-3.14	1.33	1.37
8	F	101	BCL	CHC-C4B	3.13	1.46	1.39
8	O	101	BCL	CHB-C1B	3.13	1.46	1.39
8	4	101	BCL	CHD-C1D	3.13	1.44	1.38
8	3	101	BCL	CHC-C4B	3.13	1.46	1.39
8	P	101	BCL	CHD-C1D	3.13	1.44	1.38
8	D	102	BCL	CHC-C4B	3.13	1.46	1.39
8	A	101	BCL	CHB-C1B	3.13	1.46	1.39
8	T	101	BCL	C4B-NB	-3.12	1.33	1.37
8	5	101	BCL	CHC-C4B	3.12	1.46	1.39
8	3	101	BCL	OBD-CAD	3.12	1.27	1.22
8	I	102	BCL	CHD-C1D	3.11	1.44	1.38
8	K	101	BCL	C4B-NB	-3.11	1.33	1.37
8	Q	102	BCL	CHC-C4B	3.11	1.46	1.39
8	6	101	BCL	CHC-C4B	3.11	1.46	1.39
8	8	101	BCL	CHC-C4B	3.11	1.46	1.39
8	A	102	BCL	CHB-C1B	3.11	1.46	1.39
8	9	101	BCL	C4B-NB	-3.11	1.33	1.37
8	2	102	BCL	CHD-C1D	3.11	1.44	1.38
8	J	102	BCL	CHB-C1B	3.10	1.46	1.39
8	5	101	BCL	CHD-C1D	3.10	1.44	1.38
8	E	101	BCL	CHB-C1B	3.10	1.46	1.39
8	1	101	BCL	OBD-CAD	3.10	1.27	1.22
8	B	101	BCL	C1D-ND	-3.10	1.33	1.37
8	5	101	BCL	C1D-ND	-3.10	1.33	1.37
8	8	102	BCL	C4B-NB	-3.10	1.33	1.37
8	G	102	BCL	CHD-C1D	3.10	1.44	1.38
8	3	103	BCL	OBD-CAD	3.09	1.27	1.22
8	0	102	BCL	C4B-NB	-3.09	1.33	1.37
8	T	101	BCL	CHB-C1B	3.09	1.46	1.39
8	R	102	BCL	C3D-C2D	3.09	1.47	1.39
11	L	701	BPH	C4D-CHA	3.09	1.44	1.39
8	3	101	BCL	C1B-NB	-3.09	1.33	1.37
8	6	101	BCL	OBD-CAD	3.08	1.27	1.22
8	G	101	BCL	C4B-NB	-3.08	1.33	1.37
8	K	102	BCL	CHB-C1B	3.08	1.46	1.39
8	8	101	BCL	CHB-C1B	3.08	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	101	BCL	OBD-CAD	3.08	1.27	1.22
8	W	102	BCL	CHC-C4B	3.07	1.46	1.39
8	6	102	BCL	C1B-C2B	3.07	1.50	1.43
8	Q	101	BCL	C4B-NB	-3.07	1.33	1.37
8	A	102	BCL	C3D-C2D	3.07	1.47	1.39
8	F	101	BCL	OBD-CAD	3.07	1.27	1.22
8	E	102	BCL	C4B-NB	-3.06	1.33	1.37
8	O	101	BCL	C3D-C2D	3.06	1.47	1.39
8	G	102	BCL	C1B-NB	-3.06	1.33	1.37
8	W	102	BCL	CHD-C1D	3.06	1.44	1.38
8	1	101	BCL	CHC-C4B	3.06	1.46	1.39
8	U	101	BCL	C3D-C2D	3.06	1.47	1.39
11	M	702	BPH	C4D-CHA	3.06	1.44	1.39
8	3	103	BCL	CHC-C4B	3.06	1.46	1.39
8	R	102	BCL	C4B-NB	-3.05	1.33	1.37
8	2	101	BCL	C3D-C2D	3.05	1.47	1.39
8	2	102	BCL	OBD-CAD	3.05	1.27	1.22
8	1	101	BCL	C3D-C2D	3.05	1.47	1.39
8	P	101	BCL	CHB-C1B	3.05	1.46	1.39
8	Q	101	BCL	OBD-CAD	3.05	1.27	1.22
8	N	101	BCL	C4B-NB	-3.05	1.33	1.37
8	1	101	BCL	C1D-ND	-3.05	1.33	1.37
8	E	102	BCL	CHD-C1D	3.05	1.44	1.38
8	R	102	BCL	OBD-CAD	3.05	1.27	1.22
8	O	101	BCL	C4B-NB	-3.05	1.33	1.37
8	F	101	BCL	C4B-NB	-3.04	1.33	1.37
8	3	103	BCL	CHD-C1D	3.04	1.44	1.38
8	A	102	BCL	C4B-NB	-3.04	1.33	1.37
8	S	101	BCL	CHB-C1B	3.04	1.46	1.39
8	W	101	BCL	C1B-NB	-3.04	1.33	1.37
8	I	101	BCL	CHB-C1B	3.03	1.46	1.39
8	0	102	BCL	CHB-C1B	3.03	1.46	1.39
8	8	102	BCL	CHD-C1D	3.03	1.44	1.38
8	8	101	BCL	C1B-NB	-3.03	1.33	1.37
8	N	101	BCL	OBD-CAD	3.03	1.27	1.22
8	S	101	BCL	C3D-C2D	3.03	1.47	1.39
8	K	102	BCL	CHC-C4B	3.02	1.46	1.39
8	A	102	BCL	CHC-C4B	3.02	1.46	1.39
8	W	102	BCL	C1B-NB	-3.02	1.33	1.37
8	3	101	BCL	CHB-C1B	3.01	1.46	1.39
8	E	102	BCL	C1B-NB	-3.01	1.33	1.37
8	0	101	BCL	C3D-C2D	3.00	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	101	BCL	C1D-ND	-3.00	1.33	1.37
8	7	101	BCL	OBD-CAD	3.00	1.27	1.22
8	8	101	BCL	C3D-C2D	3.00	1.47	1.39
8	Q	102	BCL	C3D-C2D	3.00	1.47	1.39
8	W	101	BCL	C3D-C2D	2.99	1.47	1.39
8	1	101	BCL	C4B-NB	-2.99	1.33	1.37
8	A	102	BCL	C1B-NB	-2.99	1.33	1.37
8	Q	102	BCL	C1D-ND	-2.99	1.33	1.37
8	D	102	BCL	C1D-ND	-2.99	1.33	1.37
8	3	103	BCL	C3D-C2D	2.99	1.47	1.39
8	6	101	BCL	C1B-NB	-2.99	1.33	1.37
8	7	101	BCL	CHB-C1B	2.98	1.46	1.39
8	E	101	BCL	C3D-C2D	2.98	1.47	1.39
8	M	701	BCL	OBD-CAD	2.98	1.27	1.22
8	8	101	BCL	C4B-NB	-2.98	1.33	1.37
8	M	701	BCL	C1B-NB	-2.98	1.33	1.37
8	E	102	BCL	OBD-CAD	2.98	1.27	1.22
8	K	101	BCL	CHC-C4B	2.98	1.46	1.39
8	K	101	BCL	OBD-CAD	2.98	1.27	1.22
8	9	101	BCL	C3D-C2D	2.98	1.47	1.39
11	L	704	BPH	C3A-C2A	-2.98	1.52	1.54
8	S	101	BCL	C1B-NB	-2.98	1.33	1.37
8	Q	101	BCL	C3D-C2D	2.98	1.47	1.39
8	H	101	BCL	OBD-CAD	2.97	1.27	1.22
8	I	101	BCL	OBD-CAD	2.97	1.27	1.22
8	3	101	BCL	C4B-NB	-2.97	1.34	1.37
8	2	101	BCL	OBD-CAD	2.97	1.27	1.22
8	N	101	BCL	C3D-C2D	2.96	1.47	1.39
8	G	101	BCL	OBD-CAD	2.96	1.27	1.22
8	F	101	BCL	C3D-C2D	2.96	1.47	1.39
8	0	101	BCL	C4B-NB	-2.96	1.34	1.37
8	Q	102	BCL	CHB-C1B	2.96	1.46	1.39
8	U	101	BCL	OBD-CAD	2.96	1.27	1.22
8	G	101	BCL	CHB-C1B	2.95	1.46	1.39
8	0	101	BCL	CHB-C1B	2.95	1.46	1.39
11	M	702	BPH	C3A-C2A	-2.95	1.52	1.54
8	4	101	BCL	C3B-C4B	2.95	1.46	1.41
8	I	101	BCL	C4B-NB	-2.95	1.34	1.37
8	A	101	BCL	C3D-C2D	2.95	1.47	1.39
8	A	101	BCL	OBD-CAD	2.95	1.27	1.22
8	K	101	BCL	C3D-C2D	2.95	1.47	1.39
8	L	702	BCL	C4B-NB	-2.95	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	6	101	BCL	C3D-C2D	2.95	1.47	1.39
8	1	101	BCL	CHB-C1B	2.94	1.46	1.39
8	R	102	BCL	C1D-ND	-2.94	1.34	1.37
8	O	101	BCL	C1B-NB	-2.94	1.34	1.37
8	D	102	BCL	C3D-C2D	2.94	1.47	1.39
8	H	101	BCL	CHC-C4B	2.93	1.46	1.39
8	B	101	BCL	C3D-C2D	2.93	1.47	1.39
8	V	101	BCL	C3D-C2D	2.93	1.47	1.39
8	3	101	BCL	C3D-C2D	2.93	1.47	1.39
8	E	102	BCL	CHB-C1B	2.93	1.46	1.39
8	8	102	BCL	CHC-C4B	2.93	1.46	1.39
8	I	102	BCL	CHC-C4B	2.93	1.46	1.39
8	E	101	BCL	OBD-CAD	2.92	1.27	1.22
8	I	101	BCL	C3D-C2D	2.92	1.47	1.39
8	2	101	BCL	C4B-NB	-2.92	1.34	1.37
8	6	102	BCL	CHD-C1D	2.92	1.44	1.38
8	L	702	BCL	OBD-CAD	2.92	1.27	1.22
8	N	101	BCL	C1D-ND	-2.92	1.34	1.37
8	L	702	BCL	CHB-C1B	2.92	1.46	1.39
8	P	101	BCL	C3D-C2D	2.91	1.46	1.39
8	L	703	BCL	C3D-C2D	2.91	1.46	1.39
8	A	102	BCL	C1D-ND	-2.91	1.34	1.37
8	Q	102	BCL	C1B-NB	-2.91	1.34	1.37
8	P	101	BCL	OBD-CAD	2.91	1.27	1.22
8	U	101	BCL	C1B-NB	-2.91	1.34	1.37
8	E	101	BCL	C4B-NB	-2.91	1.34	1.37
8	7	101	BCL	C3D-C2D	2.90	1.46	1.39
8	E	102	BCL	CHC-C4B	2.90	1.45	1.39
8	1	101	BCL	C1B-NB	-2.90	1.34	1.37
8	6	101	BCL	C4B-NB	-2.90	1.34	1.37
8	5	101	BCL	C3D-C2D	2.89	1.46	1.39
8	V	101	BCL	OBD-CAD	2.89	1.27	1.22
8	5	101	BCL	OBD-CAD	2.89	1.27	1.22
8	P	101	BCL	C1B-NB	-2.89	1.34	1.37
8	6	102	BCL	CHC-C4B	2.89	1.45	1.39
8	0	101	BCL	C1B-NB	-2.89	1.34	1.37
8	J	102	BCL	C4B-NB	-2.89	1.34	1.37
8	O	102	BCL	C1B-NB	-2.89	1.34	1.37
8	H	101	BCL	CHD-C1D	2.89	1.44	1.38
8	U	102	BCL	OBD-CAD	2.89	1.27	1.22
8	J	102	BCL	C3D-C2D	2.89	1.46	1.39
8	V	101	BCL	C1D-ND	-2.88	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	101	BCL	MG-NA	-2.88	1.99	2.06
8	O	102	BCL	C3D-C2D	2.88	1.46	1.39
8	K	102	BCL	C3D-C2D	2.88	1.46	1.39
8	L	703	BCL	C1B-NB	-2.88	1.34	1.37
8	8	101	BCL	OBD-CAD	2.88	1.27	1.22
8	L	703	BCL	OBD-CAD	2.88	1.27	1.22
8	L	702	BCL	C1B-NB	-2.88	1.34	1.37
8	O	102	BCL	OBD-CAD	2.88	1.27	1.22
8	H	101	BCL	C3D-C2D	2.87	1.46	1.39
8	E	101	BCL	C1B-NB	-2.87	1.34	1.37
8	M	701	BCL	C3D-C2D	2.87	1.46	1.39
8	U	102	BCL	C3D-C2D	2.87	1.46	1.39
8	T	101	BCL	OBD-CAD	2.87	1.27	1.22
8	H	101	BCL	MG-NA	-2.87	1.99	2.06
10	3	102	U4Z	CAH-CAD	2.87	1.39	1.34
8	T	101	BCL	C1D-ND	-2.87	1.34	1.37
8	0	102	BCL	C3D-C2D	2.87	1.46	1.39
8	Q	101	BCL	C1B-NB	-2.87	1.34	1.37
8	2	101	BCL	CHD-C1D	2.86	1.44	1.38
8	S	102	BCL	CHC-C4B	2.86	1.45	1.39
8	T	101	BCL	C3D-C2D	2.86	1.46	1.39
8	0	102	BCL	CHC-C4B	2.86	1.45	1.39
8	O	102	BCL	C1D-ND	-2.86	1.34	1.37
8	3	103	BCL	C4B-NB	-2.85	1.34	1.37
8	E	101	BCL	CHC-C4B	2.85	1.45	1.39
8	P	101	BCL	CHC-C4B	2.84	1.45	1.39
10	J	101	U4Z	CAH-CAD	2.84	1.39	1.34
8	W	101	BCL	C4B-NB	-2.84	1.34	1.37
8	J	102	BCL	C1B-NB	-2.84	1.34	1.37
8	4	101	BCL	C3D-C2D	2.83	1.46	1.39
8	7	101	BCL	C4B-NB	-2.83	1.34	1.37
10	D	101	U4Z	CAQ-CAR	-2.83	1.39	1.46
8	6	102	BCL	CHB-C4A	-2.83	1.30	1.37
10	0	103	U4Z	CAQ-CAR	-2.82	1.39	1.46
8	S	101	BCL	CHD-C1D	2.82	1.43	1.38
8	K	101	BCL	CHB-C1B	2.81	1.45	1.39
8	O	102	BCL	CHC-C4B	2.80	1.45	1.39
8	G	102	BCL	C3D-C2D	2.80	1.46	1.39
8	B	101	BCL	CHB-C1B	2.80	1.45	1.39
8	G	101	BCL	C3D-C2D	2.80	1.46	1.39
8	W	102	BCL	OBD-CAD	2.80	1.27	1.22
8	I	102	BCL	C1D-ND	-2.79	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	101	BCL	CHD-C1D	2.79	1.43	1.38
8	8	102	BCL	CHB-C1B	2.79	1.45	1.39
8	S	102	BCL	C3D-C2D	2.78	1.46	1.39
8	2	102	BCL	C3D-C2D	2.78	1.46	1.39
8	0	101	BCL	OBD-CAD	2.78	1.27	1.22
8	I	102	BCL	C3D-C2D	2.77	1.46	1.39
8	6	102	BCL	C3D-C2D	2.77	1.46	1.39
8	W	102	BCL	CHB-C1B	2.77	1.45	1.39
8	S	101	BCL	OBD-CAD	2.76	1.27	1.22
8	S	101	BCL	C4B-NB	-2.76	1.34	1.37
8	4	101	BCL	OBD-CAD	2.76	1.27	1.22
8	S	102	BCL	C1D-ND	-2.76	1.34	1.37
8	L	703	BCL	C1D-ND	-2.75	1.34	1.37
8	E	102	BCL	C1D-ND	-2.75	1.34	1.37
8	W	101	BCL	OBD-CAD	2.75	1.27	1.22
8	G	102	BCL	CHC-C4B	2.74	1.45	1.39
8	L	703	BCL	CHB-C1B	2.74	1.45	1.39
10	R	101	U4Z	CAQ-CAR	-2.74	1.40	1.46
8	6	102	BCL	C1B-NB	-2.74	1.34	1.37
8	K	102	BCL	C1B-NB	-2.73	1.34	1.37
8	8	102	BCL	C1D-ND	-2.73	1.34	1.37
8	8	102	BCL	C1B-NB	-2.72	1.34	1.37
8	4	101	BCL	C1B-NB	-2.72	1.34	1.37
8	B	101	BCL	CHD-C4C	2.71	1.46	1.39
8	A	101	BCL	CHD-C1D	2.71	1.43	1.38
8	0	102	BCL	C1B-NB	-2.71	1.34	1.37
8	E	102	BCL	C3D-C2D	2.71	1.46	1.39
8	4	101	BCL	C1D-ND	-2.70	1.34	1.37
8	U	101	BCL	CHD-C1D	2.70	1.43	1.38
8	W	102	BCL	C3D-C2D	2.70	1.46	1.39
8	A	101	BCL	C4B-NB	-2.70	1.34	1.37
8	2	101	BCL	C1B-NB	-2.69	1.34	1.37
8	8	102	BCL	OBD-CAD	2.69	1.27	1.22
8	K	102	BCL	C1D-ND	-2.69	1.34	1.37
8	7	101	BCL	C1B-NB	-2.68	1.34	1.37
8	T	101	BCL	C1B-NB	-2.68	1.34	1.37
8	A	102	BCL	OBD-CAD	2.68	1.27	1.22
8	A	101	BCL	C1B-NB	-2.67	1.34	1.37
8	6	102	BCL	C1D-ND	-2.67	1.34	1.37
8	0	102	BCL	C1D-ND	-2.67	1.34	1.37
10	J	101	U4Z	CAQ-CAR	-2.67	1.40	1.46
8	V	101	BCL	C4B-NB	-2.67	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	0	103	U4Z	CAH-CAD	2.66	1.39	1.34
8	8	102	BCL	C3D-C2D	2.66	1.46	1.39
8	O	101	BCL	CHD-C1D	2.66	1.43	1.38
8	U	102	BCL	C1D-ND	-2.66	1.34	1.37
8	0	101	BCL	CHD-C1D	2.65	1.43	1.38
8	6	101	BCL	CHD-C1D	2.65	1.43	1.38
10	3	102	U4Z	CAQ-CAR	-2.65	1.40	1.46
8	8	101	BCL	CHD-C1D	2.65	1.43	1.38
8	L	702	BCL	MG-NA	-2.65	2.00	2.06
8	K	102	BCL	CHD-C4C	2.64	1.46	1.39
8	E	101	BCL	CHD-C1D	2.64	1.43	1.38
8	2	102	BCL	C1D-ND	-2.63	1.34	1.37
8	7	101	BCL	C1D-ND	-2.63	1.34	1.37
8	3	101	BCL	CHD-C1D	2.63	1.43	1.38
8	M	701	BCL	C4B-NB	-2.63	1.34	1.37
10	D	101	U4Z	CBN-CBL	-2.62	1.40	1.46
8	3	103	BCL	MG-NA	-2.62	2.00	2.06
8	U	101	BCL	C4B-NB	-2.62	1.34	1.37
8	E	102	BCL	CHD-C4C	2.61	1.46	1.39
8	2	102	BCL	CHC-C4B	2.61	1.45	1.39
8	V	101	BCL	CHD-C4C	2.60	1.46	1.39
8	R	102	BCL	C1B-NB	-2.60	1.34	1.37
8	3	103	BCL	C1B-NB	-2.60	1.34	1.37
8	W	101	BCL	CHD-C1D	2.60	1.43	1.38
8	7	101	BCL	CHD-C4C	2.60	1.46	1.39
8	1	101	BCL	CHD-C4C	2.59	1.46	1.39
8	O	102	BCL	CHB-C1B	2.59	1.45	1.39
8	Q	101	BCL	CHD-C1D	2.59	1.43	1.38
8	I	101	BCL	CHD-C1D	2.58	1.43	1.38
8	O	102	BCL	CHD-C4C	2.58	1.46	1.39
8	U	102	BCL	CHD-C4C	2.57	1.46	1.39
8	A	102	BCL	CHD-C4C	2.56	1.46	1.39
8	3	101	BCL	MG-NA	-2.56	2.00	2.06
8	Q	102	BCL	CHD-C4C	2.56	1.46	1.39
8	0	102	BCL	CHB-C4A	-2.56	1.31	1.37
10	R	101	U4Z	CBN-CBL	-2.55	1.40	1.46
10	R	101	U4Z	CAH-CAD	2.55	1.38	1.34
8	S	102	BCL	CHD-C4C	2.55	1.46	1.39
10	D	101	U4Z	CBF-CBH	-2.55	1.40	1.46
8	F	101	BCL	C1B-NB	-2.54	1.34	1.37
8	R	102	BCL	CHD-C4C	2.54	1.46	1.39
10	J	101	U4Z	CBN-CBL	-2.54	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	102	BCL	OBD-CAD	2.54	1.26	1.22
8	W	102	BCL	C1D-ND	-2.53	1.34	1.37
8	L	702	BCL	CHD-C4C	2.53	1.46	1.39
8	W	101	BCL	MG-NA	-2.53	2.00	2.06
8	Q	102	BCL	MG-NA	-2.53	2.00	2.06
8	W	101	BCL	C3C-C4C	-2.53	1.48	1.51
8	B	101	BCL	MG-NC	-2.52	2.00	2.06
10	J	101	U4Z	CBF-CBH	-2.52	1.40	1.46
8	G	101	BCL	CHD-C1D	2.52	1.43	1.38
8	2	102	BCL	CHB-C1B	2.52	1.45	1.39
8	5	101	BCL	C1B-NB	-2.52	1.34	1.37
8	0	102	BCL	CHD-C4C	2.52	1.46	1.39
8	P	101	BCL	MG-NA	-2.51	2.00	2.06
8	W	102	BCL	CHD-C4C	2.51	1.46	1.39
8	E	102	BCL	MG-NA	-2.51	2.00	2.06
8	2	102	BCL	CHC-C1C	-2.50	1.31	1.37
8	O	101	BCL	MG-NC	-2.50	2.00	2.06
10	0	103	U4Z	CBF-CBH	-2.50	1.40	1.46
8	9	101	BCL	C1B-NB	-2.50	1.34	1.37
8	4	101	BCL	CHD-C4C	2.50	1.46	1.39
10	3	102	U4Z	CBF-CBH	-2.49	1.40	1.46
8	W	101	BCL	MG-NC	-2.49	2.00	2.06
10	3	102	U4Z	CBN-CBL	-2.49	1.40	1.46
8	B	101	BCL	OBD-CAD	2.48	1.26	1.22
10	0	103	U4Z	CBN-CBL	-2.48	1.40	1.46
10	R	101	U4Z	CBF-CBH	-2.48	1.40	1.46
8	S	102	BCL	C1B-NB	-2.47	1.34	1.37
8	8	102	BCL	CHD-C4C	2.47	1.46	1.39
8	M	701	BCL	MG-NA	-2.47	2.00	2.06
8	I	102	BCL	CHD-C4C	2.46	1.46	1.39
8	T	101	BCL	CHD-C4C	2.46	1.46	1.39
8	G	102	BCL	C1D-ND	-2.45	1.34	1.37
8	D	102	BCL	C1B-NB	-2.44	1.34	1.37
8	L	703	BCL	C4B-NB	-2.44	1.34	1.37
8	G	102	BCL	CHD-C4C	2.44	1.46	1.39
8	4	101	BCL	CHC-C4B	2.44	1.44	1.39
8	U	102	BCL	MG-NA	-2.43	2.00	2.06
8	D	102	BCL	CHD-C4C	2.43	1.46	1.39
8	2	101	BCL	MG-NA	-2.43	2.00	2.06
8	9	101	BCL	C3C-C4C	-2.43	1.48	1.51
8	S	101	BCL	MG-NA	-2.43	2.00	2.06
8	2	102	BCL	CHD-C4C	2.42	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	6	102	BCL	CHC-C1C	-2.42	1.31	1.37
8	K	102	BCL	MG-NA	-2.42	2.00	2.06
8	4	101	BCL	C1B-C2B	2.42	1.48	1.43
8	D	102	BCL	MG-NA	-2.42	2.00	2.06
8	N	101	BCL	CHD-C4C	2.42	1.46	1.39
8	O	101	BCL	MG-NA	-2.42	2.00	2.06
8	E	101	BCL	CHC-C1C	-2.42	1.31	1.37
10	D	101	U4Z	CAH-CAD	2.42	1.38	1.34
8	3	101	BCL	MG-NC	-2.41	2.00	2.06
8	V	101	BCL	C1B-C2B	2.41	1.48	1.43
8	U	102	BCL	CHC-C1C	-2.41	1.31	1.37
8	U	101	BCL	MG-NA	-2.40	2.00	2.06
8	R	102	BCL	MG-NA	-2.40	2.00	2.06
8	K	102	BCL	OBD-CAD	2.40	1.26	1.22
8	U	101	BCL	MG-NC	-2.40	2.00	2.06
8	J	102	BCL	CHD-C4C	2.39	1.45	1.39
8	I	102	BCL	C1B-NB	-2.39	1.34	1.37
8	Q	102	BCL	OBD-CAD	2.39	1.26	1.22
8	6	102	BCL	CHD-C4C	2.39	1.45	1.39
8	0	101	BCL	MG-NA	-2.39	2.00	2.06
8	W	102	BCL	CHB-C4A	-2.38	1.31	1.37
8	P	101	BCL	CHD-C4C	2.38	1.45	1.39
8	F	101	BCL	CHD-C4C	2.38	1.45	1.39
8	L	703	BCL	CHD-C4C	2.38	1.45	1.39
8	0	102	BCL	OBD-CAD	2.38	1.26	1.22
8	9	101	BCL	CHD-C4C	2.38	1.45	1.39
8	H	101	BCL	C1B-NB	-2.37	1.34	1.37
8	2	101	BCL	CHC-C1C	-2.37	1.31	1.37
8	Q	102	BCL	CHB-C4A	-2.37	1.31	1.37
8	5	101	BCL	CHD-C4C	2.36	1.45	1.39
8	3	103	BCL	CHD-C4C	2.36	1.45	1.39
8	V	101	BCL	MG-NC	-2.36	2.00	2.06
8	H	101	BCL	C3C-C4C	-2.36	1.48	1.51
8	V	101	BCL	C1B-NB	-2.36	1.34	1.37
8	E	102	BCL	C1D-C2D	2.35	1.50	1.45
8	S	101	BCL	MG-NC	-2.34	2.00	2.06
8	K	101	BCL	CHC-C1C	-2.34	1.31	1.37
8	4	101	BCL	C3C-C4C	-2.34	1.48	1.51
8	0	102	BCL	C1D-C2D	2.34	1.50	1.45
8	F	101	BCL	C3C-C4C	-2.33	1.48	1.51
8	P	101	BCL	CHC-C1C	-2.33	1.31	1.37
8	2	101	BCL	CHD-C4C	2.33	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	703	BCL	C1D-C2D	2.33	1.49	1.45
8	9	101	BCL	MG-NA	-2.32	2.00	2.06
8	I	101	BCL	MG-NC	-2.32	2.00	2.06
8	A	101	BCL	MG-NC	-2.32	2.00	2.06
8	N	101	BCL	C1B-NB	-2.32	1.34	1.37
8	S	101	BCL	CHD-C4C	2.32	1.45	1.39
8	5	101	BCL	MG-NA	-2.32	2.00	2.06
8	7	101	BCL	MG-NC	-2.32	2.00	2.06
8	4	101	BCL	MG-NC	-2.31	2.00	2.06
8	I	102	BCL	C1B-C2B	2.31	1.48	1.43
8	K	102	BCL	C1D-C2D	2.31	1.49	1.45
8	T	101	BCL	MG-NC	-2.31	2.00	2.06
8	U	102	BCL	MG-NC	-2.31	2.00	2.06
8	S	102	BCL	MG-NA	-2.31	2.00	2.06
8	G	102	BCL	CHB-C4A	-2.30	1.31	1.37
8	T	101	BCL	MG-NA	-2.30	2.00	2.06
8	E	102	BCL	MG-NC	-2.29	2.00	2.06
8	L	703	BCL	MG-NC	-2.29	2.00	2.06
8	6	102	BCL	OBD-CAD	2.29	1.26	1.22
8	H	101	BCL	CHD-C4C	2.28	1.45	1.39
8	M	701	BCL	C1D-C2D	2.28	1.49	1.45
8	Q	101	BCL	MG-NA	-2.28	2.00	2.06
8	8	101	BCL	C3C-C4C	-2.28	1.48	1.51
8	A	102	BCL	MG-NA	-2.28	2.00	2.06
8	4	101	BCL	CHC-C1C	-2.27	1.32	1.37
8	S	102	BCL	CAA-C2A	-2.27	1.50	1.54
8	I	101	BCL	MG-NA	-2.26	2.00	2.06
8	U	102	BCL	C1D-C2D	2.26	1.49	1.45
8	A	101	BCL	MG-NA	-2.26	2.00	2.06
8	4	101	BCL	MG-NA	-2.26	2.00	2.06
8	4	101	BCL	CHB-C4A	-2.26	1.32	1.37
8	K	102	BCL	MG-NC	-2.26	2.00	2.06
8	B	101	BCL	CAA-C2A	-2.26	1.50	1.54
8	6	101	BCL	MG-NC	-2.26	2.00	2.06
8	S	102	BCL	C1D-C2D	2.26	1.49	1.45
8	G	101	BCL	MG-NA	-2.26	2.00	2.06
8	W	102	BCL	CHC-C1C	-2.25	1.32	1.37
8	O	102	BCL	C1D-C2D	2.25	1.49	1.45
8	1	101	BCL	MG-NA	-2.25	2.00	2.06
8	7	101	BCL	C3C-C4C	-2.25	1.48	1.51
8	J	102	BCL	MG-NA	-2.24	2.00	2.06
8	Q	102	BCL	MG-NC	-2.24	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	101	BCL	C1D-C2D	2.24	1.49	1.45
8	G	102	BCL	OBD-CAD	2.24	1.26	1.22
8	3	101	BCL	CAA-C2A	-2.23	1.50	1.54
8	M	701	BCL	CHD-C4C	2.23	1.45	1.39
8	8	101	BCL	CHC-C1C	-2.23	1.32	1.37
8	1	101	BCL	MG-NC	-2.22	2.01	2.06
8	2	102	BCL	C1D-C2D	2.22	1.49	1.45
8	W	102	BCL	MG-NC	-2.21	2.01	2.06
8	G	101	BCL	CHC-C1C	-2.21	1.32	1.37
8	G	102	BCL	MG-NC	-2.21	2.01	2.06
8	D	102	BCL	C3C-C4C	-2.21	1.48	1.51
8	I	102	BCL	CHB-C4A	-2.21	1.32	1.37
8	O	102	BCL	CHB-C4A	-2.21	1.32	1.37
8	0	101	BCL	MG-NC	-2.21	2.01	2.06
8	B	101	BCL	C3A-C2A	-2.21	1.48	1.54
8	8	102	BCL	MG-NC	-2.20	2.01	2.06
8	L	702	BCL	CHB-C4A	-2.20	1.32	1.37
8	G	102	BCL	C1D-C2D	2.20	1.49	1.45
8	N	101	BCL	MG-NA	-2.20	2.01	2.06
8	L	702	BCL	MG-NC	-2.20	2.01	2.06
8	K	101	BCL	CHB-C4A	-2.20	1.32	1.37
8	E	102	BCL	CHB-C4A	-2.20	1.32	1.37
8	S	102	BCL	CHB-C4A	-2.19	1.32	1.37
8	L	703	BCL	CHB-C4A	-2.19	1.32	1.37
8	K	101	BCL	CHD-C4C	2.19	1.45	1.39
8	O	102	BCL	MG-NC	-2.19	2.01	2.06
8	6	101	BCL	CHC-C1C	-2.19	1.32	1.37
8	G	102	BCL	MG-NA	-2.19	2.01	2.06
8	8	101	BCL	MG-NA	-2.18	2.01	2.06
8	8	101	BCL	MG-NC	-2.18	2.01	2.06
8	I	102	BCL	MG-NA	-2.18	2.01	2.06
8	7	101	BCL	C1D-C2D	2.18	1.49	1.45
8	F	101	BCL	MG-NA	-2.18	2.01	2.06
8	A	101	BCL	CHD-C4C	2.18	1.45	1.39
10	D	101	U4Z	CAI-CAH	-2.18	1.46	1.51
8	0	101	BCL	CHD-C4C	2.17	1.45	1.39
8	Q	102	BCL	C1D-C2D	2.17	1.49	1.45
8	8	102	BCL	CHB-C4A	-2.17	1.32	1.37
8	W	101	BCL	CHC-C1C	-2.17	1.32	1.37
8	4	101	BCL	C1D-C2D	2.17	1.49	1.45
8	7	101	BCL	CHB-C4A	-2.17	1.32	1.37
8	O	101	BCL	C3C-C4C	-2.17	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	102	BCL	MG-NA	-2.16	2.01	2.06
8	S	102	BCL	C3A-C2A	-2.16	1.48	1.54
8	P	101	BCL	C3C-C4C	-2.16	1.48	1.51
8	3	101	BCL	CHC-C1C	-2.16	1.32	1.37
20	C	501	HEC	C3B-C2B	-2.16	1.33	1.41
8	H	101	BCL	CHC-C1C	-2.16	1.32	1.37
8	A	102	BCL	CHC-C1C	-2.16	1.32	1.37
8	U	101	BCL	CHD-C4C	2.15	1.45	1.39
8	W	101	BCL	CHD-C4C	2.15	1.45	1.39
8	W	102	BCL	C1D-C2D	2.15	1.49	1.45
8	0	102	BCL	C1B-C2B	2.15	1.48	1.43
8	E	101	BCL	C1B-C2B	2.15	1.48	1.43
8	I	102	BCL	CHC-C1C	-2.15	1.32	1.37
8	5	101	BCL	C3C-C4C	-2.15	1.48	1.51
8	6	102	BCL	C1D-C2D	2.15	1.49	1.45
10	3	102	U4Z	CBJ-CBH	2.15	1.40	1.35
8	6	101	BCL	MG-NA	-2.15	2.01	2.06
8	K	102	BCL	C3A-C2A	-2.14	1.48	1.54
8	8	102	BCL	C1D-C2D	2.14	1.49	1.45
8	H	101	BCL	C1B-C2B	2.14	1.48	1.43
16	T	102	LMT	O1'-C1'	2.14	1.43	1.40
8	B	101	BCL	CHB-C4A	-2.14	1.32	1.37
11	L	704	BPH	C4D-ND	-2.14	1.35	1.38
8	2	102	BCL	C1B-C2B	2.14	1.48	1.43
8	T	101	BCL	CHC-C1C	-2.14	1.32	1.37
8	O	101	BCL	CHD-C4C	2.14	1.45	1.39
8	1	101	BCL	CHB-C4A	-2.14	1.32	1.37
8	0	102	BCL	C3C-C4C	-2.13	1.48	1.51
10	J	101	U4Z	CAI-CAH	-2.13	1.47	1.51
8	G	102	BCL	C3C-C4C	-2.13	1.48	1.51
8	6	101	BCL	C1B-C2B	2.13	1.48	1.43
8	I	102	BCL	MG-NC	-2.13	2.01	2.06
8	N	101	BCL	C1B-C2B	2.13	1.48	1.43
10	3	102	U4Z	CAV-CAR	2.13	1.40	1.35
8	P	101	BCL	C1B-C2B	2.13	1.48	1.43
8	I	101	BCL	CHC-C1C	-2.13	1.32	1.37
8	1	101	BCL	C1D-C2D	2.13	1.49	1.45
8	E	101	BCL	MG-NC	-2.12	2.01	2.06
8	Q	101	BCL	CHD-C4C	2.12	1.45	1.39
8	V	101	BCL	C1D-C2D	2.12	1.49	1.45
8	3	103	BCL	C1D-C2D	2.12	1.49	1.45
8	Q	102	BCL	CHC-C1C	-2.12	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	101	BCL	MG-NC	-2.12	2.01	2.06
8	3	101	BCL	CHD-C4C	2.12	1.45	1.39
11	L	701	BPH	C3A-C2A	-2.11	1.52	1.54
8	7	101	BCL	MG-NA	-2.11	2.01	2.06
8	2	102	BCL	CHB-C4A	-2.11	1.32	1.37
20	C	503	HEC	C3B-C2B	-2.11	1.34	1.41
8	0	101	BCL	CHB-C4A	-2.11	1.32	1.37
8	F	101	BCL	MG-NC	-2.11	2.01	2.06
8	J	102	BCL	C3C-C4C	-2.11	1.48	1.51
8	G	101	BCL	CHD-C4C	2.11	1.45	1.39
8	S	101	BCL	CHC-C1C	-2.11	1.32	1.37
8	I	102	BCL	C3A-C2A	-2.10	1.48	1.54
8	I	101	BCL	CHD-C4C	2.10	1.45	1.39
8	S	102	BCL	C3C-C4C	-2.10	1.48	1.51
8	G	101	BCL	MG-NC	-2.10	2.01	2.06
8	U	102	BCL	CHC-C4B	2.10	1.44	1.39
8	N	101	BCL	C1D-C2D	2.10	1.49	1.45
8	2	101	BCL	CHB-C4A	-2.09	1.32	1.37
8	6	102	BCL	MG-NA	-2.09	2.01	2.06
8	3	103	BCL	C1B-C2B	2.09	1.48	1.43
8	0	102	BCL	MG-NC	-2.09	2.01	2.06
8	S	102	BCL	MG-NC	-2.09	2.01	2.06
8	F	101	BCL	C1B-C2B	2.09	1.48	1.43
8	R	102	BCL	C1D-C2D	2.09	1.49	1.45
8	G	102	BCL	CHC-C1C	-2.09	1.32	1.37
8	A	102	BCL	CHB-C4A	-2.09	1.32	1.37
8	M	701	BCL	MG-NC	-2.09	2.01	2.06
8	3	103	BCL	CHC-C1C	-2.09	1.32	1.37
8	A	102	BCL	MG-NC	-2.08	2.01	2.06
8	T	101	BCL	C3C-C4C	-2.08	1.49	1.51
8	T	101	BCL	CHB-C4A	-2.08	1.32	1.37
8	8	101	BCL	CHB-C4A	-2.08	1.32	1.37
8	K	102	BCL	CHC-C1C	-2.08	1.32	1.37
8	W	102	BCL	MG-NA	-2.08	2.01	2.06
8	O	101	BCL	CHC-C1C	-2.08	1.32	1.37
8	O	102	BCL	CHC-C1C	-2.08	1.32	1.37
10	3	102	U4Z	CAI-CAH	-2.08	1.47	1.51
8	V	101	BCL	MG-NA	-2.08	2.01	2.06
10	0	103	U4Z	CAI-CAH	-2.08	1.47	1.51
8	S	102	BCL	C1B-C2B	2.08	1.48	1.43
8	3	101	BCL	C1B-C2B	2.07	1.48	1.43
8	K	102	BCL	CBD-CAD	-2.07	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	101	BCL	C1D-C2D	2.07	1.49	1.45
8	L	703	BCL	MG-NA	-2.07	2.01	2.06
8	A	102	BCL	C1D-C2D	2.07	1.49	1.45
8	R	102	BCL	MG-NC	-2.07	2.01	2.06
8	I	102	BCL	C1D-C2D	2.07	1.49	1.45
8	A	101	BCL	C1B-C2B	2.07	1.48	1.43
10	3	102	U4Z	CBI-CBL	2.07	1.40	1.35
8	H	101	BCL	C4D-CHA	2.06	1.45	1.38
8	T	101	BCL	C1B-C2B	2.06	1.48	1.43
8	U	101	BCL	C1B-C2B	2.06	1.48	1.43
8	5	101	BCL	CHB-C4A	-2.06	1.32	1.37
8	D	102	BCL	MG-NC	-2.06	2.01	2.06
8	U	101	BCL	CHB-C4A	-2.06	1.32	1.37
8	6	101	BCL	CHD-C4C	2.06	1.45	1.39
8	P	101	BCL	CHB-C4A	-2.05	1.32	1.37
8	0	102	BCL	CHC-C1C	-2.05	1.32	1.37
8	G	101	BCL	CHB-C4A	-2.05	1.32	1.37
8	E	101	BCL	CHD-C4C	2.05	1.44	1.39
8	I	101	BCL	CHB-C4A	-2.05	1.32	1.37
10	R	101	U4Z	CAI-CAH	-2.04	1.47	1.51
8	9	101	BCL	CHC-C1C	-2.04	1.32	1.37
8	M	701	BCL	C1B-C2B	2.04	1.47	1.43
8	S	102	BCL	CHC-C1C	-2.04	1.32	1.37
8	S	101	BCL	CHB-C4A	-2.04	1.32	1.37
8	K	101	BCL	MG-NA	-2.04	2.01	2.06
8	2	101	BCL	MG-NC	-2.04	2.01	2.06
8	3	103	BCL	C3C-C4C	-2.04	1.49	1.51
20	C	501	HEC	CMC-C2C	2.04	1.54	1.50
8	F	101	BCL	CHC-C1C	-2.04	1.32	1.37
8	J	102	BCL	C1D-C2D	2.03	1.49	1.45
8	A	101	BCL	CHC-C1C	-2.03	1.32	1.37
10	R	101	U4Z	CBJ-CBH	2.03	1.40	1.35
8	K	102	BCL	CHB-C4A	-2.03	1.32	1.37
8	U	101	BCL	CHC-C1C	-2.03	1.32	1.37
8	E	101	BCL	C2C-C3C	-2.03	1.49	1.54
8	E	102	BCL	C3A-C2A	-2.03	1.49	1.54
8	F	101	BCL	CHB-C4A	-2.03	1.32	1.37
20	C	504	HEC	CMC-C2C	2.03	1.54	1.50
8	R	102	BCL	C3C-C4C	-2.03	1.49	1.51
8	8	102	BCL	MG-NA	-2.02	2.01	2.06
8	9	101	BCL	MG-NC	-2.02	2.01	2.06
8	Q	101	BCL	C1B-C2B	2.02	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	8	102	BCL	CHC-C1C	-2.01	1.32	1.37
8	9	101	BCL	C1B-C2B	2.01	1.47	1.43
8	J	102	BCL	CHB-C4A	-2.01	1.32	1.37
8	D	102	BCL	C1B-C2B	2.01	1.47	1.43
8	V	101	BCL	CHB-C4A	-2.01	1.32	1.37
8	N	101	BCL	MG-NC	-2.01	2.01	2.06
8	0	102	BCL	CBD-CAD	-2.01	1.47	1.56
8	A	101	BCL	CHB-C4A	-2.01	1.32	1.37
8	0	102	BCL	MG-NA	-2.01	2.01	2.06
8	D	102	BCL	CHC-C1C	-2.01	1.32	1.37
10	J	101	U4Z	CBI-CBL	2.01	1.40	1.35
8	2	102	BCL	C4D-CHA	2.01	1.45	1.38
8	2	102	BCL	MG-NC	-2.01	2.01	2.06
8	O	101	BCL	CHB-C4A	-2.00	1.32	1.37
8	Q	101	BCL	CHC-C1C	-2.00	1.32	1.37
8	W	101	BCL	CHB-C4A	-2.00	1.32	1.37
8	W	101	BCL	C2C-C3C	-2.00	1.49	1.54

All (1302) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	102	BCL	C2B-C1B-NB	11.07	121.80	110.33
20	C	503	HEC	CBB-CAB-C3B	-9.08	109.28	127.43
8	U	102	BCL	C4A-NA-C1A	8.83	110.71	106.68
8	E	102	BCL	CMD-C2D-C1D	8.21	139.19	124.73
20	C	501	HEC	CBB-CAB-C3B	-8.21	111.03	127.43
8	8	102	BCL	CMD-C2D-C1D	8.14	139.07	124.73
8	6	102	BCL	CMD-C2D-C1D	8.02	138.86	124.73
8	4	101	BCL	CMD-C2D-C1D	8.01	138.84	124.73
20	C	502	HEC	CBC-CAC-C3C	-8.01	111.42	127.43
8	W	102	BCL	CMD-C2D-C1D	8.01	138.83	124.73
8	G	102	BCL	CMD-C2D-C1D	7.97	138.76	124.73
8	2	102	BCL	CMD-C2D-C1D	7.93	138.69	124.73
8	S	102	BCL	CMD-C2D-C1D	7.89	138.62	124.73
8	B	101	BCL	CMD-C2D-C1D	7.87	138.59	124.73
8	O	102	BCL	CMD-C2D-C1D	7.87	138.59	124.73
8	0	102	BCL	CMD-C2D-C1D	7.87	138.58	124.73
8	K	102	BCL	CMD-C2D-C1D	7.78	138.43	124.73
20	C	501	HEC	CBC-CAC-C3C	-7.76	111.92	127.43
20	C	504	HEC	CBB-CAB-C3B	-7.74	111.96	127.43
8	2	102	BCL	C2B-C1B-NB	7.72	118.33	110.33
20	C	502	HEC	CBB-CAB-C3B	-7.71	112.03	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	703	BCL	CMD-C2D-C1D	7.70	138.28	124.73
8	I	102	BCL	CMD-C2D-C1D	7.69	138.28	124.73
8	U	102	BCL	CMD-C2D-C1D	7.67	138.23	124.73
8	7	101	BCL	CMD-C2D-C1D	7.54	138.00	124.73
8	L	703	BCL	C2B-C1B-NB	7.51	118.12	110.33
8	M	701	BCL	CMD-C2D-C1D	7.47	137.89	124.73
8	Q	102	BCL	CMD-C2D-C1D	7.43	137.81	124.73
8	T	101	BCL	CMD-C2D-C1D	7.41	137.78	124.73
20	C	504	HEC	CBC-CAC-C3C	-7.37	112.71	127.43
8	1	101	BCL	O2D-CGD-CBD	7.27	123.95	111.23
8	N	101	BCL	CMD-C2D-C1D	7.26	137.52	124.73
8	W	102	BCL	C2B-C1B-NB	7.20	117.80	110.33
8	0	101	BCL	C2B-C1B-NB	7.10	117.69	110.33
8	V	101	BCL	CMD-C2D-C1D	7.05	137.14	124.73
8	O	102	BCL	C2B-C1B-NB	7.01	117.60	110.33
8	E	102	BCL	C2B-C1B-NB	7.01	117.59	110.33
8	D	102	BCL	CMD-C2D-C1D	6.99	137.04	124.73
8	1	101	BCL	CMD-C2D-C1D	6.99	137.03	124.73
8	F	101	BCL	CMD-C2D-C1D	6.99	137.03	124.73
8	I	101	BCL	C2B-C1B-NB	6.97	117.56	110.33
8	K	101	BCL	C2B-C1B-NB	6.97	117.55	110.33
8	H	101	BCL	CMD-C2D-C1D	6.96	136.99	124.73
8	G	101	BCL	C2B-C1B-NB	6.96	117.54	110.33
8	R	102	BCL	CMD-C2D-C1D	6.96	136.98	124.73
8	A	101	BCL	C2B-C1B-NB	6.95	117.53	110.33
8	L	702	BCL	C2B-C1B-NB	6.93	117.52	110.33
8	3	101	BCL	C2B-C1B-NB	6.91	117.49	110.33
8	Q	102	BCL	C2B-C1B-NB	6.89	117.47	110.33
8	3	103	BCL	CMD-C2D-C1D	6.89	136.85	124.73
8	A	102	BCL	CMD-C2D-C1D	6.88	136.84	124.73
8	7	101	BCL	C2B-C1B-NB	6.87	117.45	110.33
8	J	102	BCL	CMD-C2D-C1D	6.87	136.83	124.73
8	R	102	BCL	C2B-C1B-NB	6.87	117.45	110.33
8	9	101	BCL	CMD-C2D-C1D	6.84	136.78	124.73
8	1	101	BCL	C2B-C1B-NB	6.78	117.36	110.33
8	5	101	BCL	CMD-C2D-C1D	6.78	136.67	124.73
8	O	101	BCL	C2B-C1B-NB	6.74	117.31	110.33
8	2	101	BCL	C2B-C1B-NB	6.72	117.29	110.33
8	P	101	BCL	CMD-C2D-C1D	6.72	136.56	124.73
8	8	101	BCL	C2B-C1B-NB	6.68	117.25	110.33
20	C	503	HEC	CBC-CAC-C3C	-6.66	114.12	127.43
8	M	701	BCL	C2B-C1B-NB	6.64	117.21	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	102	BCL	C2B-C1B-NB	6.63	117.20	110.33
8	8	102	BCL	C2B-C1B-NB	6.62	117.19	110.33
8	S	101	BCL	C2B-C1B-NB	6.54	117.11	110.33
8	W	101	BCL	C2B-C1B-NB	6.53	117.10	110.33
8	U	101	BCL	C2B-C1B-NB	6.53	117.09	110.33
8	P	101	BCL	C2B-C1B-NB	6.50	117.07	110.33
8	Q	101	BCL	C2B-C1B-NB	6.49	117.06	110.33
8	A	102	BCL	C2B-C1B-NB	6.49	117.06	110.33
8	6	101	BCL	C2B-C1B-NB	6.48	117.05	110.33
8	B	101	BCL	C2B-C1B-NB	6.46	117.03	110.33
8	D	102	BCL	C2B-C1B-NB	6.45	117.02	110.33
8	5	101	BCL	C2B-C1B-NB	6.42	116.99	110.33
8	T	101	BCL	C2B-C1B-NB	6.39	116.95	110.33
8	9	101	BCL	C2B-C1B-NB	6.33	116.89	110.33
8	F	101	BCL	C2B-C1B-NB	6.32	116.88	110.33
8	3	103	BCL	C2B-C1B-NB	6.32	116.88	110.33
8	H	101	BCL	C2B-C1B-NB	6.25	116.81	110.33
8	V	101	BCL	C2B-C1B-NB	6.25	116.80	110.33
8	S	102	BCL	O2D-CGD-CBD	6.23	122.13	111.23
8	N	101	BCL	C2B-C1B-NB	6.21	116.76	110.33
8	L	702	BCL	CMD-C2D-C1D	6.20	135.64	124.73
8	M	701	BCL	O2D-CGD-CBD	6.16	122.00	111.23
8	E	101	BCL	C2B-C1B-NB	6.16	116.71	110.33
8	L	702	BCL	O2D-CGD-CBD	6.15	121.98	111.23
8	G	102	BCL	C2B-C1B-NB	6.14	116.69	110.33
8	5	101	BCL	O2D-CGD-CBD	6.05	121.80	111.23
8	J	102	BCL	O2D-CGD-CBD	6.02	121.76	111.23
8	0	102	BCL	C2B-C1B-NB	5.98	116.53	110.33
8	M	701	BCL	CHD-C1D-ND	-5.95	116.42	124.80
8	I	102	BCL	C2B-C1B-NB	5.91	116.45	110.33
8	A	102	BCL	O2D-CGD-CBD	5.87	121.49	111.23
8	B	101	BCL	CHD-C1D-ND	-5.86	116.55	124.80
8	S	102	BCL	C2B-C1B-NB	5.83	116.38	110.33
8	U	102	BCL	O2D-CGD-CBD	5.82	121.41	111.23
8	9	101	BCL	O2D-CGD-CBD	5.82	121.40	111.23
8	Q	102	BCL	CHD-C1D-ND	-5.79	116.66	124.80
8	E	102	BCL	CHD-C1D-ND	-5.77	116.68	124.80
8	K	102	BCL	C2B-C1B-NB	5.74	116.28	110.33
8	S	102	BCL	CHD-C1D-ND	-5.73	116.74	124.80
8	4	101	BCL	C2B-C1B-NB	5.71	116.25	110.33
8	8	102	BCL	O2D-CGD-CBD	5.70	121.20	111.23
8	6	102	BCL	C2B-C1B-NB	5.69	116.23	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	102	BCL	O2D-CGD-CBD	5.68	121.16	111.23
8	K	102	BCL	CHD-C1D-ND	-5.67	116.83	124.80
8	7	101	BCL	CHD-C1D-ND	-5.66	116.84	124.80
8	0	102	BCL	O2D-CGD-CBD	5.64	121.09	111.23
8	G	102	BCL	C3D-C2D-C1D	-5.63	98.15	105.83
8	N	101	BCL	O2D-CGD-CBD	5.62	121.05	111.23
8	H	101	BCL	CHD-C1D-ND	-5.60	116.93	124.80
8	6	102	BCL	C3D-C2D-C1D	-5.58	98.21	105.83
8	R	102	BCL	O2D-CGD-CBD	5.58	120.99	111.23
8	3	103	BCL	CHD-C1D-ND	-5.58	116.95	124.80
8	0	102	BCL	CHD-C1D-ND	-5.57	116.96	124.80
8	O	102	BCL	O2D-CGD-CBD	5.56	120.95	111.23
8	U	102	BCL	CHD-C1D-ND	-5.56	116.98	124.80
8	8	102	BCL	C3D-C2D-C1D	-5.55	98.25	105.83
8	D	102	BCL	CHD-C1D-ND	-5.55	116.99	124.80
8	E	102	BCL	C3D-C2D-C1D	-5.52	98.30	105.83
8	L	703	BCL	CHD-C1D-ND	-5.51	117.04	124.80
8	R	102	BCL	CHD-C1D-ND	-5.50	117.06	124.80
8	1	101	BCL	CHD-C1D-ND	-5.49	117.08	124.80
8	8	102	BCL	CHD-C1D-ND	-5.49	117.08	124.80
8	D	102	BCL	O2D-CGD-CBD	5.46	120.77	111.23
8	Q	102	BCL	C3D-C2D-C1D	-5.45	98.39	105.83
8	O	102	BCL	CHD-C1D-ND	-5.45	117.14	124.80
8	W	102	BCL	C3D-C2D-C1D	-5.45	98.40	105.83
8	F	101	BCL	O2D-CGD-CBD	5.45	120.75	111.23
8	W	102	BCL	O2D-CGD-CBD	5.44	120.74	111.23
8	T	101	BCL	CHD-C1D-ND	-5.44	117.15	124.80
8	T	101	BCL	O2D-CGD-CBD	5.42	120.71	111.23
8	4	101	BCL	C3D-C2D-C1D	-5.39	98.48	105.83
8	I	102	BCL	CHD-C1D-ND	-5.39	117.22	124.80
8	3	103	BCL	O2D-CGD-CBD	5.38	120.64	111.23
8	I	102	BCL	C3D-C2D-C1D	-5.36	98.51	105.83
8	4	101	BCL	CHD-C1D-ND	-5.36	117.26	124.80
8	I	102	BCL	O2D-CGD-CBD	5.34	120.57	111.23
8	7	101	BCL	O2D-CGD-CBD	5.33	120.56	111.23
8	0	102	BCL	C3D-C2D-C1D	-5.33	98.56	105.83
8	W	101	BCL	O2D-CGD-CBD	5.33	120.55	111.23
8	W	102	BCL	CHD-C1D-ND	-5.33	117.30	124.80
8	6	102	BCL	CHD-C1D-ND	-5.31	117.33	124.80
8	H	101	BCL	O2D-CGD-CBD	5.30	120.50	111.23
8	L	703	BCL	C3D-C2D-C1D	-5.29	98.61	105.83
8	S	102	BCL	C3D-C2D-C1D	-5.29	98.61	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	102	BCL	CHD-C1D-ND	-5.29	117.35	124.80
8	P	101	BCL	CHD-C1D-ND	-5.29	117.36	124.80
9	I	103	PGV	O01-C1-C2	5.28	122.91	111.48
8	O	102	BCL	C3D-C2D-C1D	-5.26	98.66	105.83
8	2	102	BCL	CHD-C1D-ND	-5.26	117.41	124.80
8	V	101	BCL	CHD-C1D-ND	-5.24	117.43	124.80
8	A	102	BCL	CHD-C1D-ND	-5.23	117.44	124.80
8	B	101	BCL	C3D-C2D-C1D	-5.22	98.71	105.83
8	F	101	BCL	CHD-C1D-ND	-5.22	117.46	124.80
8	N	101	BCL	CHD-C1D-ND	-5.21	117.47	124.80
8	T	101	BCL	C3D-C2D-C1D	-5.20	98.73	105.83
8	H	101	BCL	C3C-C4C-CHD	-5.20	112.43	123.39
8	9	101	BCL	CHD-C1D-ND	-5.18	117.51	124.80
8	2	102	BCL	C3D-C2D-C1D	-5.17	98.77	105.83
8	5	101	BCL	CHD-C1D-ND	-5.17	117.52	124.80
8	L	702	BCL	CHD-C1D-ND	-5.17	117.53	124.80
8	U	102	BCL	C3D-C2D-C1D	-5.15	98.80	105.83
8	P	101	BCL	O2D-CGD-CBD	5.15	120.23	111.23
8	V	101	BCL	O2D-CGD-CBD	5.15	120.23	111.23
8	K	102	BCL	C3D-C2D-C1D	-5.13	98.83	105.83
8	2	102	BCL	O2D-CGD-CBD	5.13	120.19	111.23
8	F	101	BCL	C3D-C2D-C1D	-5.12	98.84	105.83
8	J	102	BCL	CHD-C1D-ND	-5.12	117.59	124.80
8	M	701	BCL	C3D-C2D-C1D	-5.12	98.84	105.83
8	D	102	BCL	C3D-C2D-C1D	-5.09	98.89	105.83
8	9	101	BCL	C3D-C2D-C1D	-5.08	98.90	105.83
8	H	101	BCL	C3D-C2D-C1D	-5.05	98.93	105.83
8	3	103	BCL	C3D-C2D-C1D	-5.03	98.97	105.83
8	N	101	BCL	C3D-C2D-C1D	-5.02	98.99	105.83
8	7	101	BCL	C3D-C2D-C1D	-5.01	98.99	105.83
8	G	101	BCL	C3C-C4C-CHD	-5.01	112.83	123.39
8	A	101	BCL	O2D-CGD-CBD	5.00	119.98	111.23
8	4	101	BCL	O2D-CGD-CBD	5.00	119.97	111.23
8	Q	101	BCL	C3C-C4C-CHD	-5.00	112.86	123.39
8	I	101	BCL	CMD-C2D-C1D	4.99	133.51	124.73
8	P	101	BCL	C3D-C2D-C1D	-4.99	99.02	105.83
8	K	102	BCL	O2D-CGD-CBD	4.98	119.93	111.23
8	B	101	BCL	O2D-CGD-CBD	4.98	119.93	111.23
8	J	102	BCL	C3D-C2D-C1D	-4.97	99.05	105.83
8	A	101	BCL	C2D-C1D-ND	4.96	115.04	110.13
8	O	101	BCL	C3C-C4C-CHD	-4.95	112.96	123.39
8	8	101	BCL	C3C-C4C-CHD	-4.95	112.96	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	CMD-C2D-C1D	4.94	133.43	124.73
8	G	101	BCL	CMD-C2D-C1D	4.94	133.42	124.73
8	Q	101	BCL	C2D-C1D-ND	4.94	115.01	110.13
15	M	708	PEF	O2-C10-C11	4.94	119.89	111.09
8	A	102	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
8	6	102	BCL	O2D-CGD-CBD	4.93	119.84	111.23
8	V	101	BCL	C3D-C2D-C1D	-4.93	99.11	105.83
8	W	101	BCL	CMD-C2D-C1D	4.92	133.40	124.73
8	A	101	BCL	C1D-ND-C4D	-4.91	102.87	106.31
8	3	101	BCL	CMD-C2D-C1D	4.91	133.37	124.73
8	A	101	BCL	C3D-C2D-C1D	-4.90	99.14	105.83
8	0	101	BCL	C3C-C4C-CHD	-4.85	113.17	123.39
8	0	101	BCL	CMD-C2D-C1D	4.84	133.26	124.73
8	6	101	BCL	C3C-C4C-CHD	-4.84	113.19	123.39
8	U	101	BCL	CMD-C2D-C1D	4.84	133.25	124.73
8	Q	101	BCL	C3D-C2D-C1D	-4.84	99.23	105.83
8	2	101	BCL	CMD-C2D-C1D	4.83	133.24	124.73
8	1	101	BCL	C3D-C2D-C1D	-4.83	99.24	105.83
8	3	103	BCL	C3C-C4C-CHD	-4.83	113.20	123.39
8	3	101	BCL	C3C-C4C-CHD	-4.82	113.22	123.39
8	O	101	BCL	C3D-C2D-C1D	-4.82	99.26	105.83
8	R	102	BCL	C3D-C2D-C1D	-4.81	99.27	105.83
8	O	101	BCL	C2D-C1D-ND	4.79	114.87	110.13
8	A	101	BCL	C3C-C4C-CHD	-4.79	113.29	123.39
8	L	702	BCL	O2D-CGD-O1D	-4.79	114.53	123.85
8	I	101	BCL	C3C-C4C-CHD	-4.78	113.30	123.39
9	0	105	PGV	O01-C1-C2	4.78	121.83	111.48
8	5	101	BCL	C3D-C2D-C1D	-4.78	99.31	105.83
8	3	101	BCL	O2D-CGD-CBD	4.78	119.58	111.23
8	J	102	BCL	C3C-C4C-CHD	-4.78	113.32	123.39
8	S	101	BCL	CMD-C2D-C1D	4.77	133.13	124.73
8	Q	101	BCL	CMD-C2D-C1D	4.77	133.12	124.73
8	L	702	BCL	C3D-C2D-C1D	-4.76	99.33	105.83
8	6	101	BCL	C1D-ND-C4D	-4.76	102.97	106.31
8	6	101	BCL	C2D-C1D-ND	4.76	114.84	110.13
8	3	101	BCL	C1D-ND-C4D	-4.76	102.97	106.31
8	9	101	BCL	C3C-C4C-CHD	-4.72	113.44	123.39
8	E	102	BCL	O2D-CGD-CBD	4.72	119.48	111.23
8	3	101	BCL	C2D-C1D-ND	4.72	114.80	110.13
8	U	101	BCL	O2D-CGD-CBD	4.72	119.48	111.23
8	0	101	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
8	Q	101	BCL	C1D-ND-C4D	-4.70	103.01	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	101	BCL	C3C-C4C-CHD	-4.70	113.48	123.39
8	U	101	BCL	C3C-C4C-CHD	-4.70	113.48	123.39
8	E	101	BCL	O2D-CGD-CBD	4.67	119.40	111.23
8	S	101	BCL	C3C-C4C-CHD	-4.67	113.54	123.39
8	I	101	BCL	C3D-C2D-C1D	-4.67	99.45	105.83
8	K	101	BCL	C3C-C4C-CHD	-4.67	113.54	123.39
8	D	102	BCL	C3C-C4C-CHD	-4.67	113.54	123.39
8	3	101	BCL	C3D-C2D-C1D	-4.67	99.46	105.83
8	G	101	BCL	C2D-C1D-ND	4.67	114.75	110.13
9	6	103	PGV	O01-C1-C2	4.66	121.57	111.48
8	M	701	BCL	C4A-NA-C1A	4.66	108.81	106.68
8	K	101	BCL	C3D-C2D-C1D	-4.66	99.47	105.83
8	E	101	BCL	CMD-C2D-C1D	4.66	132.93	124.73
8	F	101	BCL	C3C-C4C-CHD	-4.66	113.57	123.39
9	8	103	PGV	O01-C1-C2	4.65	121.55	111.48
8	I	101	BCL	C2D-C1D-ND	4.65	114.73	110.13
8	S	101	BCL	C3D-C2D-C1D	-4.64	99.49	105.83
8	G	101	BCL	C3D-C2D-C1D	-4.64	99.50	105.83
8	2	102	BCL	C4A-NA-C1A	4.64	108.80	106.68
8	E	101	BCL	C3D-C2D-C1D	-4.63	99.51	105.83
8	0	101	BCL	O2D-CGD-CBD	4.61	119.29	111.23
8	W	101	BCL	C3D-C2D-C1D	-4.60	99.55	105.83
8	Q	101	BCL	O2D-CGD-CBD	4.59	119.25	111.23
8	8	101	BCL	O2D-CGD-CBD	4.59	119.25	111.23
18	P	102	CDL	OB6-CB5-C51	4.59	121.40	111.48
9	0	104	PGV	O01-C1-C2	4.58	121.40	111.48
8	S	101	BCL	C2D-C1D-ND	4.56	114.64	110.13
8	M	701	BCL	C3C-C4C-CHD	-4.56	113.78	123.39
8	7	101	BCL	C1D-ND-C4D	-4.55	103.12	106.31
9	O	103	PGV	O01-C1-C2	4.55	121.33	111.48
8	K	101	BCL	C2D-C1D-ND	4.53	114.61	110.13
8	5	101	BCL	C3C-C4C-CHD	-4.52	113.86	123.39
8	6	102	BCL	C3B-C4B-NB	4.52	115.72	109.76
8	O	101	BCL	CMD-C2D-C1D	4.51	132.68	124.73
8	N	101	BCL	C3C-C4C-CHD	-4.51	113.88	123.39
8	Q	102	BCL	O2D-CGD-CBD	4.50	119.10	111.23
8	6	101	BCL	O2D-CGD-CBD	4.50	119.09	111.23
8	D	102	BCL	C1D-ND-C4D	-4.50	103.16	106.31
8	G	102	BCL	C3B-C4B-NB	4.49	115.69	109.76
8	7	101	BCL	C3C-C4C-CHD	-4.49	113.92	123.39
8	0	101	BCL	C2D-C1D-ND	4.49	114.57	110.13
8	8	101	BCL	C2D-C1D-ND	4.49	114.57	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	506	PGV	O01-C1-C2	4.49	121.19	111.48
8	G	102	BCL	C3C-C4C-CHD	-4.48	113.95	123.39
8	6	101	BCL	C3D-C2D-C1D	-4.48	99.72	105.83
8	U	101	BCL	C3D-C2D-C1D	-4.47	99.73	105.83
8	4	101	BCL	C3B-C4B-NB	4.47	115.66	109.76
9	E	103	PGV	O01-C1-C2	4.46	121.13	111.48
8	K	101	BCL	CMD-C2D-C1D	4.46	132.58	124.73
8	M	701	BCL	C1D-ND-C4D	-4.46	103.18	106.31
8	E	101	BCL	C2D-C1D-ND	4.46	114.54	110.13
8	I	101	BCL	O2D-CGD-CBD	4.45	119.01	111.23
8	W	101	BCL	C2D-C1D-ND	4.45	114.53	110.13
8	6	102	BCL	C3C-C4C-CHD	-4.44	114.03	123.39
8	O	101	BCL	C1D-ND-C4D	-4.43	103.20	106.31
8	2	101	BCL	CHD-C1D-ND	-4.43	118.57	124.80
8	A	101	BCL	CHD-C1D-ND	-4.43	118.57	124.80
8	T	101	BCL	C3C-C4C-CHD	-4.42	114.06	123.39
8	U	101	BCL	C2D-C1D-ND	4.41	114.49	110.13
8	G	101	BCL	C1D-ND-C4D	-4.41	103.22	106.31
8	R	102	BCL	C1D-ND-C4D	-4.41	103.22	106.31
8	W	101	BCL	CHD-C1D-ND	-4.41	118.60	124.80
8	S	101	BCL	C1D-ND-C4D	-4.41	103.22	106.31
8	P	101	BCL	C3C-C4C-CHD	-4.40	114.11	123.39
8	4	101	BCL	C3C-C4C-CHD	-4.40	114.12	123.39
8	3	103	BCL	C1D-ND-C4D	-4.40	103.23	106.31
8	G	101	BCL	O2D-CGD-CBD	4.39	118.91	111.23
8	S	101	BCL	CHD-C1D-ND	-4.39	118.62	124.80
8	D	102	BCL	C2D-C1D-ND	4.38	114.46	110.13
8	F	101	BCL	C2D-C1D-ND	4.38	114.46	110.13
8	I	101	BCL	C1D-ND-C4D	-4.37	103.25	106.31
8	E	102	BCL	C1D-ND-C4D	-4.37	103.25	106.31
11	M	702	BPH	C4D-CHA-CBD	-4.37	106.36	108.45
8	2	101	BCL	C3D-C2D-C1D	-4.36	99.87	105.83
8	H	101	BCL	C4A-NA-C1A	4.36	108.67	106.68
8	I	102	BCL	C3C-C4C-CHD	-4.36	114.20	123.39
8	W	101	BCL	C3C-C4C-CHD	-4.36	114.21	123.39
8	H	101	BCL	C2D-C1D-ND	4.35	114.44	110.13
8	1	101	BCL	C3C-C4C-CHD	-4.34	114.24	123.39
8	2	102	BCL	C3C-C4C-CHD	-4.32	114.28	123.39
8	8	101	BCL	C3D-C2D-C1D	-4.32	99.94	105.83
8	B	101	BCL	CHC-C4B-NB	-4.32	117.57	124.05
9	U	103	PGV	O01-C1-C2	4.31	120.81	111.48
8	U	101	BCL	CHD-C1D-ND	-4.31	118.73	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	101	BCL	C1D-ND-C4D	-4.31	103.29	106.31
8	2	101	BCL	C1-C2-C3	-4.30	119.14	126.20
8	L	703	BCL	C2D-C1D-ND	4.29	114.37	110.13
8	3	103	BCL	C2D-C1D-ND	4.29	114.37	110.13
8	E	102	BCL	C3C-C4C-CHD	-4.29	114.35	123.39
9	U	104	PGV	O01-C1-C2	4.29	120.75	111.48
8	L	703	BCL	C3C-C4C-CHD	-4.28	114.36	123.39
8	2	101	BCL	C3C-C4C-CHD	-4.28	114.37	123.39
8	M	701	BCL	C2D-C1D-ND	4.27	114.36	110.13
8	S	102	BCL	C3C-C4C-CHD	-4.27	114.38	123.39
8	O	101	BCL	O2D-CGD-CBD	4.27	118.70	111.23
8	W	102	BCL	C1D-ND-C4D	-4.27	103.31	106.31
8	R	102	BCL	C3C-C4C-CHD	-4.26	114.41	123.39
11	L	701	BPH	C4D-CHA-CBD	-4.24	106.42	108.45
8	H	101	BCL	C1C-NC-C4C	-4.23	104.75	106.68
9	4	102	PGV	O01-C1-C2	4.22	120.61	111.48
9	S	103	PGV	O01-C1-C2	4.22	120.61	111.48
8	W	102	BCL	C2D-C1D-ND	4.22	114.30	110.13
8	T	101	BCL	C2D-C1D-ND	4.22	114.30	110.13
8	U	102	BCL	C1D-ND-C4D	-4.22	103.35	106.31
8	6	101	BCL	CMD-C2D-C1D	4.21	132.15	124.73
8	L	703	BCL	O2D-CGD-CBD	4.21	118.59	111.23
8	G	102	BCL	C1-C2-C3	-4.21	119.30	126.20
8	E	102	BCL	C2D-C1D-ND	4.20	114.28	110.13
8	9	101	BCL	C2D-C1D-ND	4.20	114.28	110.13
8	L	703	BCL	C1D-ND-C4D	-4.20	103.37	106.31
8	L	702	BCL	C3C-C4C-CHD	-4.20	114.55	123.39
8	6	102	BCL	C2D-C1D-ND	4.18	114.27	110.13
9	K	104	PGV	O01-C1-C2	4.18	120.52	111.48
8	8	102	BCL	C2D-C1D-ND	4.17	114.26	110.13
9	E	104	PGV	O01-C1-C2	4.17	120.50	111.48
8	3	101	BCL	CHD-C1D-ND	-4.17	118.94	124.80
9	h	102	PGV	O01-C1-C2	4.17	120.50	111.48
8	0	101	BCL	C1D-ND-C4D	-4.16	103.39	106.31
15	L	713	PEF	O2-C10-C11	4.16	120.49	111.48
8	U	102	BCL	C2D-C1D-ND	4.16	114.24	110.13
8	F	101	BCL	C1D-ND-C4D	-4.15	103.40	106.31
8	T	101	BCL	C1D-ND-C4D	-4.15	103.40	106.31
8	A	102	BCL	C3C-C4C-CHD	-4.15	114.64	123.39
8	9	101	BCL	C1D-ND-C4D	-4.15	103.40	106.31
8	J	102	BCL	C1D-ND-C4D	-4.14	103.41	106.31
8	O	101	BCL	CHD-C1D-ND	-4.14	118.98	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	712	PGV	O01-C1-C2	4.14	120.43	111.48
8	V	101	BCL	C3C-C4C-CHD	-4.14	114.67	123.39
11	L	704	BPH	C4D-CHA-CBD	-4.13	106.47	108.45
8	7	101	BCL	C2D-C1D-ND	4.12	114.20	110.13
8	N	101	BCL	C1D-ND-C4D	-4.11	103.43	106.31
8	N	101	BCL	C2D-C1D-ND	4.11	114.19	110.13
8	H	101	BCL	C1D-ND-C4D	-4.10	103.43	106.31
8	K	101	BCL	C1D-ND-C4D	-4.10	103.43	106.31
9	N	102	PGV	O01-C1-C2	4.10	120.35	111.48
8	G	102	BCL	C2D-C1D-ND	4.09	114.17	110.13
8	J	102	BCL	C2D-C1D-ND	4.09	114.17	110.13
8	6	102	BCL	C1C-NC-C4C	-4.08	104.82	106.68
8	8	101	BCL	C1D-ND-C4D	-4.08	103.45	106.31
8	U	102	BCL	C3B-C4B-NB	4.07	115.13	109.76
8	I	101	BCL	CHD-C1D-ND	-4.07	119.07	124.80
8	2	101	BCL	C2D-C1D-ND	4.07	114.15	110.13
8	P	101	BCL	C2D-C1D-ND	4.07	114.15	110.13
8	2	102	BCL	C3B-C4B-NB	4.07	115.13	109.76
8	8	102	BCL	C3C-C4C-CHD	-4.07	114.82	123.39
8	S	101	BCL	O2D-CGD-CBD	4.07	118.34	111.23
8	R	102	BCL	C2D-C1D-ND	4.06	114.15	110.13
8	E	101	BCL	C3B-C4B-NB	4.06	115.12	109.76
8	Q	102	BCL	C3C-C4C-CHD	-4.05	114.86	123.39
8	L	702	BCL	C1D-ND-C4D	-4.05	103.47	106.31
8	E	102	BCL	C3B-C4B-NB	4.03	115.08	109.76
8	W	101	BCL	C1D-ND-C4D	-4.03	103.48	106.31
8	Q	101	BCL	CHD-C1D-ND	-4.03	119.13	124.80
8	0	101	BCL	CHD-C1D-ND	-4.03	119.14	124.80
15	h	103	PEF	O2-C10-C11	4.02	120.17	111.48
8	6	101	BCL	C3B-C4B-NB	4.02	115.06	109.76
8	L	703	BCL	C3B-C4B-NB	3.99	115.03	109.76
8	I	102	BCL	C2D-C1D-ND	3.99	114.08	110.13
8	Q	102	BCL	C2D-C1D-ND	3.98	114.07	110.13
8	3	101	BCL	C3B-C4B-NB	3.98	115.01	109.76
8	0	102	BCL	C3C-C4C-CHD	-3.98	115.00	123.39
8	U	101	BCL	C1-C2-C3	-3.98	119.68	126.20
8	P	101	BCL	C3B-C4B-NB	3.98	115.01	109.76
8	K	101	BCL	C3B-C4B-NB	3.98	115.01	109.76
8	G	102	BCL	C1D-ND-C4D	-3.97	103.52	106.31
9	K	103	PGV	O01-C1-C2	3.97	120.07	111.48
8	O	102	BCL	C3C-C4C-CHD	-3.97	115.02	123.39
8	A	102	BCL	C3B-C4B-NB	3.97	115.00	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	701	BCL	C1-C2-C3	-3.96	119.72	126.20
9	M	705	PGV	O01-C1-C2	3.95	120.04	111.48
8	1	101	BCL	C2D-C1D-ND	3.95	114.03	110.13
8	U	102	BCL	C3C-C4C-CHD	-3.95	115.07	123.39
8	G	101	BCL	C3B-C4B-NB	3.94	114.95	109.76
8	R	102	BCL	C3B-C4B-NB	3.92	114.93	109.76
8	W	102	BCL	C3B-C4B-NB	3.92	114.93	109.76
9	L	706	PGV	O01-C1-C2	3.91	119.94	111.48
8	9	101	BCL	C1-C2-C3	-3.91	119.79	126.20
8	I	102	BCL	C1D-ND-C4D	-3.90	103.57	106.31
20	C	503	HEC	C4D-ND-C1D	3.89	112.17	105.82
8	U	102	BCL	CHC-C1C-NC	3.89	130.01	124.40
20	C	504	HEC	C4D-ND-C1D	3.89	112.16	105.82
8	1	101	BCL	C1D-ND-C4D	-3.88	103.59	106.31
8	U	102	BCL	C4-C3-C2	-3.87	113.68	123.63
8	2	102	BCL	C1C-NC-C4C	-3.87	104.91	106.68
8	K	102	BCL	C3C-C4C-CHD	-3.87	115.24	123.39
8	P	101	BCL	C1D-ND-C4D	-3.87	103.60	106.31
8	E	101	BCL	C1D-ND-C4D	-3.86	103.60	106.31
8	V	101	BCL	C1D-ND-C4D	-3.86	103.60	106.31
8	S	102	BCL	C2D-C1D-ND	3.86	113.95	110.13
8	O	102	BCL	C2D-C1D-ND	3.86	113.94	110.13
8	8	101	BCL	CMD-C2D-C1D	3.85	131.51	124.73
8	G	101	BCL	CHD-C1D-ND	-3.84	119.41	124.80
8	5	101	BCL	C1D-ND-C4D	-3.83	103.62	106.31
8	W	102	BCL	C3C-C4C-CHD	-3.83	115.31	123.39
18	P	102	CDL	OA6-CA5-C11	3.82	119.75	111.48
8	S	102	BCL	C1D-ND-C4D	-3.82	103.63	106.31
8	3	103	BCL	C3B-C4B-NB	3.82	114.79	109.76
8	L	702	BCL	C2D-C1D-ND	3.81	113.90	110.13
8	2	102	BCL	C2D-C1D-ND	3.81	113.90	110.13
8	4	101	BCL	C2D-C1D-ND	3.81	113.90	110.13
8	5	101	BCL	C2D-C1D-ND	3.81	113.90	110.13
8	8	102	BCL	C1D-ND-C4D	-3.81	103.64	106.31
8	1	101	BCL	O2D-CGD-O1D	-3.81	116.44	123.85
8	V	101	BCL	C2D-C1D-ND	3.80	113.89	110.13
8	6	102	BCL	C1D-ND-C4D	-3.80	103.65	106.31
8	Q	102	BCL	CHC-C4B-NB	-3.79	118.36	124.05
8	6	101	BCL	CHD-C1D-ND	-3.79	119.47	124.80
8	2	101	BCL	C1D-ND-C4D	-3.79	103.66	106.31
8	L	702	BCL	C3D-C4D-ND	3.79	116.14	109.99
8	K	101	BCL	CHD-C1D-ND	-3.77	119.50	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	101	BCL	C3B-C4B-NB	3.77	114.73	109.76
8	A	101	BCL	C1-C2-C3	-3.76	120.03	126.20
8	3	103	BCL	C1-C2-C3	-3.76	120.04	126.20
8	D	102	BCL	C3B-C4B-NB	3.76	114.72	109.76
8	E	101	BCL	C1C-NC-C4C	-3.76	104.97	106.68
8	1	101	BCL	C3B-C4B-NB	3.73	114.69	109.76
10	3	102	U4Z	CBB-CBG-CBI	3.73	131.15	123.52
8	H	101	BCL	C3B-C4B-NB	3.73	114.67	109.76
8	I	102	BCL	C3B-C4B-NB	3.72	114.67	109.76
8	F	101	BCL	C3B-C4B-NB	3.72	114.67	109.76
15	L	717	PEF	O2-C10-C11	3.72	119.52	111.48
8	L	703	BCL	CED-O2D-CGD	3.71	124.33	115.92
8	I	101	BCL	C3B-C4B-NB	3.70	114.64	109.76
8	U	101	BCL	C3B-C4B-NB	3.70	114.64	109.76
8	A	101	BCL	C3B-C4B-NB	3.70	114.64	109.76
8	A	102	BCL	C2D-C1D-ND	3.68	113.77	110.13
8	O	101	BCL	C4-C3-C5	3.68	121.61	115.23
8	O	102	BCL	O2D-CGD-O1D	-3.67	116.70	123.85
8	S	101	BCL	C3B-C4B-NB	3.67	114.61	109.76
10	D	101	U4Z	CBB-CBG-CBI	3.67	131.03	123.52
8	K	101	BCL	O2D-CGD-CBD	3.66	117.63	111.23
20	C	501	HEC	C4D-ND-C1D	3.65	111.78	105.82
8	N	101	BCL	C3B-C4B-NB	3.65	114.58	109.76
8	0	102	BCL	C2D-C1D-ND	3.63	113.72	110.13
8	B	101	BCL	C2A-C3A-C4A	-3.63	96.00	101.87
8	W	102	BCL	CHC-C4B-NB	-3.62	118.61	124.05
8	A	102	BCL	C1D-ND-C4D	-3.61	103.78	106.31
8	3	101	BCL	C1-C2-C3	-3.60	120.30	126.20
15	M	708	PEF	C2-O2-C10	-3.60	111.50	117.85
8	9	101	BCL	C3B-C4B-NB	3.59	114.50	109.76
8	0	102	BCL	C1-C2-C3	-3.59	120.31	126.20
8	Q	101	BCL	C1-C2-C3	-3.58	120.33	126.20
8	O	101	BCL	C3B-C4B-NB	3.58	114.48	109.76
8	G	102	BCL	CHC-C4B-NB	-3.58	118.68	124.05
8	K	102	BCL	CAA-C2A-C3A	-3.58	103.34	113.00
8	O	102	BCL	C1D-ND-C4D	-3.57	103.81	106.31
8	E	101	BCL	CHD-C1D-ND	-3.57	119.78	124.80
13	L	705	MQE	CAY-CAX-CBK	-3.56	118.78	124.89
8	R	102	BCL	C3D-C4D-ND	3.56	115.78	109.99
8	I	102	BCL	O2D-CGD-O1D	-3.56	116.93	123.85
8	V	101	BCL	C3B-C4B-NB	3.55	114.45	109.76
20	C	502	HEC	C4D-ND-C1D	3.54	111.60	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	8	101	BCL	C3B-C4B-NB	3.54	114.43	109.76
8	S	102	BCL	C4-C3-C5	3.54	121.38	115.23
8	K	102	BCL	O2D-CGD-O1D	-3.54	116.96	123.85
8	6	101	BCL	C3D-C4D-ND	3.54	115.74	109.99
8	8	102	BCL	C3B-C4B-NB	3.53	114.42	109.76
8	T	101	BCL	C3B-C4B-NB	3.53	114.42	109.76
8	7	101	BCL	C3B-C4B-NB	3.53	114.42	109.76
8	7	101	BCL	C3D-C4D-ND	3.53	115.72	109.99
8	M	701	BCL	C3D-C4D-ND	3.53	115.72	109.99
8	L	702	BCL	CHC-C4B-NB	-3.52	118.76	124.05
8	8	101	BCL	CHD-C1D-ND	-3.52	119.85	124.80
8	L	702	BCL	C1-C2-C3	-3.52	120.43	126.20
8	E	102	BCL	O2D-CGD-O1D	-3.52	117.00	123.85
8	A	102	BCL	O2D-CGD-O1D	-3.52	117.00	123.85
8	0	101	BCL	C1-C2-C3	-3.51	120.45	126.20
9	I	103	PGV	C02-O01-C1	-3.51	109.40	117.80
8	0	101	BCL	C3B-C4B-NB	3.51	114.39	109.76
8	A	101	BCL	C3D-C4D-ND	3.50	115.68	109.99
8	I	101	BCL	C1-C2-C3	-3.50	120.46	126.20
8	Q	102	BCL	C3B-C4B-NB	3.50	114.37	109.76
8	8	102	BCL	C1-C2-C3	-3.50	120.47	126.20
8	M	701	BCL	C3B-C4B-NB	3.49	114.37	109.76
8	2	102	BCL	C1D-ND-C4D	-3.49	103.86	106.31
8	9	101	BCL	O2A-CGA-CBA	3.49	122.48	111.83
8	S	102	BCL	C3B-C4B-NB	3.49	114.36	109.76
8	5	101	BCL	O2D-CGD-O1D	-3.48	117.07	123.85
8	S	101	BCL	C3D-C4D-ND	3.48	115.64	109.99
8	Q	101	BCL	C3B-C4B-NB	3.48	114.35	109.76
8	J	102	BCL	C3B-C4B-NB	3.48	114.34	109.76
8	0	102	BCL	C3B-C4B-NB	3.47	114.34	109.76
8	B	101	BCL	C3C-C4C-CHD	-3.47	116.08	123.39
9	1	102	PGV	O01-C1-C2	3.46	118.97	111.48
8	Q	102	BCL	C1D-ND-C4D	-3.46	103.89	106.31
8	M	701	BCL	CHC-C4B-NB	-3.46	118.86	124.05
8	J	102	BCL	O2D-CGD-O1D	-3.46	117.12	123.85
8	3	103	BCL	C3D-C4D-ND	3.45	115.60	109.99
8	3	101	BCL	O2D-CGD-O1D	-3.45	117.13	123.85
8	P	101	BCL	C1C-NC-C4C	-3.45	105.11	106.68
8	5	101	BCL	C3B-C4B-NB	3.44	114.30	109.76
8	W	102	BCL	C4-C3-C5	3.44	121.20	115.23
8	B	101	BCL	CAA-CBA-CGA	-3.44	103.44	113.21
8	U	101	BCL	C3D-C4D-ND	3.44	115.58	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3	101	BCL	C3D-C4D-ND	3.43	115.56	109.99
8	E	102	BCL	CHC-C4B-NB	-3.43	118.91	124.05
8	0	102	BCL	C1D-ND-C4D	-3.41	103.92	106.31
8	D	102	BCL	C3D-C4D-ND	3.40	115.52	109.99
8	L	702	BCL	O2A-CGA-CBA	3.40	122.20	111.83
10	D	101	U4Z	CAI-CAH-CAD	-3.40	118.11	122.70
8	2	101	BCL	C3B-C4B-NB	3.40	114.24	109.76
8	E	101	BCL	O2D-CGD-O1D	-3.39	117.24	123.85
10	J	101	U4Z	CAI-CAH-CAD	-3.39	118.12	122.70
8	Q	101	BCL	C3D-C4D-ND	3.39	115.50	109.99
8	3	101	BCL	C4-C3-C5	3.38	121.10	115.23
10	R	101	U4Z	CAI-CAH-CAD	-3.38	118.14	122.70
8	4	101	BCL	O2D-CGD-O1D	-3.37	117.28	123.85
10	J	101	U4Z	CBB-CBG-CBI	3.36	130.40	123.52
8	2	101	BCL	O2D-CGD-CBD	3.36	117.11	111.23
8	S	102	BCL	O2A-CGA-CBA	3.36	122.08	111.83
8	V	101	BCL	C1-C2-C3	-3.36	120.69	126.20
8	B	101	BCL	C2D-C1D-ND	3.36	113.45	110.13
8	2	101	BCL	C3D-C4D-ND	3.36	115.44	109.99
10	3	102	U4Z	CAI-CAH-CAD	-3.35	118.17	122.70
8	M	701	BCL	O2D-CGD-O1D	-3.33	117.36	123.85
8	E	101	BCL	C1-C2-C3	-3.33	120.74	126.20
9	L	711	PGV	O01-C1-C2	3.33	120.67	109.37
8	9	101	BCL	C3D-C4D-ND	3.33	115.40	109.99
8	2	101	BCL	CHC-C4B-NB	-3.33	119.06	124.05
8	8	101	BCL	C3D-C4D-ND	3.32	115.39	109.99
8	1	101	BCL	C3D-C4D-ND	3.32	115.39	109.99
8	J	102	BCL	C3D-C4D-ND	3.32	115.38	109.99
8	I	101	BCL	C3D-C4D-ND	3.32	115.38	109.99
8	O	101	BCL	C3D-C4D-ND	3.32	115.38	109.99
8	D	102	BCL	C1-C2-C3	-3.32	120.76	126.20
8	H	101	BCL	C1-C2-C3	-3.32	120.76	126.20
8	N	101	BCL	C3D-C4D-ND	3.31	115.37	109.99
8	V	101	BCL	C3D-C4D-ND	3.31	115.37	109.99
8	6	102	BCL	O2D-CGD-O1D	-3.31	117.41	123.85
8	A	102	BCL	C3D-C4D-ND	3.31	115.36	109.99
8	O	102	BCL	C3B-C4B-NB	3.31	114.12	109.76
8	7	101	BCL	C1-C2-C3	-3.30	120.79	126.20
8	4	101	BCL	C1D-ND-C4D	-3.30	104.00	106.31
8	Q	102	BCL	O2D-CGD-O1D	-3.29	117.44	123.85
10	0	103	U4Z	CBB-CBG-CBI	3.29	130.25	123.52
8	K	101	BCL	C3D-C4D-ND	3.29	115.33	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	102	BCL	C3B-C4B-NB	3.28	114.09	109.76
8	K	102	BCL	C2D-C1D-ND	3.28	113.38	110.13
8	8	102	BCL	C4-C3-C5	3.28	120.92	115.23
8	7	101	BCL	CHC-C4B-NB	-3.28	119.13	124.05
8	L	703	BCL	CHC-C4B-NB	-3.27	119.14	124.05
8	I	101	BCL	CHC-C4B-NB	-3.27	119.14	124.05
8	6	102	BCL	CHC-C4B-NB	-3.27	119.14	124.05
8	R	102	BCL	CHC-C4B-NB	-3.27	119.14	124.05
8	E	102	BCL	C3D-C4D-ND	3.27	115.30	109.99
8	B	101	BCL	O2D-CGD-O1D	-3.27	117.49	123.85
8	I	102	BCL	C1-C2-C3	-3.26	120.85	126.20
8	T	101	BCL	O2A-CGA-CBA	3.26	121.79	111.83
8	5	101	BCL	C3D-C4D-ND	3.26	115.29	109.99
8	R	102	BCL	C1-C2-C3	-3.26	120.86	126.20
8	U	102	BCL	O2D-CGD-O1D	-3.26	117.51	123.85
8	K	101	BCL	CHC-C4B-NB	-3.26	119.17	124.05
19	h	101	LHG	O7-C7-O9	-3.25	121.53	125.70
8	2	102	BCL	O2D-CGD-O1D	-3.25	117.53	123.85
8	P	101	BCL	C4A-NA-C1A	3.25	108.16	106.68
8	0	101	BCL	CHC-C4B-NB	-3.25	119.18	124.05
8	3	101	BCL	C4D-CHA-C1A	-3.24	117.37	121.24
10	0	103	U4Z	CAI-CAH-CAD	-3.24	118.33	122.70
8	O	101	BCL	C1-C2-C3	-3.24	120.89	126.20
8	G	102	BCL	C4-C3-C5	3.23	120.84	115.23
16	T	102	LMT	C1'-C2'-C3'	3.23	116.81	110.01
8	F	101	BCL	C3D-C4D-ND	3.23	115.24	109.99
10	R	101	U4Z	CBB-CBG-CBI	3.23	130.13	123.52
8	G	101	BCL	C3D-C4D-ND	3.23	115.24	109.99
9	L	712	PGV	O03-C19-C20	3.23	121.67	111.83
8	L	702	BCL	C3B-C4B-NB	3.22	114.01	109.76
8	0	101	BCL	C3D-C4D-ND	3.22	115.22	109.99
8	3	101	BCL	CHC-C4B-NB	-3.21	119.23	124.05
8	T	101	BCL	C3D-C4D-ND	3.21	115.21	109.99
8	S	101	BCL	CHC-C4B-NB	-3.21	119.24	124.05
8	M	701	BCL	C1C-NC-C4C	-3.21	105.22	106.68
8	K	102	BCL	CAA-CBA-CGA	-3.20	104.11	113.21
8	S	102	BCL	C1C-NC-C4C	-3.20	105.22	106.68
8	W	102	BCL	C4-C3-C2	-3.20	115.40	123.63
10	D	101	U4Z	CAN-CAM-CAO	-3.20	117.64	122.82
8	3	103	BCL	O2D-CGD-O1D	-3.20	117.63	123.85
8	U	102	BCL	CHB-C1B-C2B	-3.19	118.16	127.43
8	P	101	BCL	C3D-C4D-ND	3.19	115.18	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	O2D-CGD-O1D	-3.19	117.64	123.85
8	0	101	BCL	O2D-CGD-O1D	-3.19	117.64	123.85
8	P	101	BCL	CHC-C4B-NB	-3.19	119.26	124.05
8	8	101	BCL	C1-C2-C3	-3.19	120.97	126.20
8	B	101	BCL	C3B-C4B-NB	3.18	113.96	109.76
10	3	102	U4Z	CAN-CAM-CAO	-3.18	117.67	122.82
8	A	102	BCL	C4-C3-C5	3.18	120.74	115.23
8	H	101	BCL	C3D-C4D-ND	3.17	115.14	109.99
8	L	703	BCL	C3D-C4D-ND	3.17	115.14	109.99
8	1	101	BCL	CHC-C4B-NB	-3.17	119.29	124.05
8	U	102	BCL	C3D-C4D-ND	3.17	115.14	109.99
8	K	101	BCL	O2A-CGA-CBA	3.17	121.50	111.83
8	6	101	BCL	CHC-C4B-NB	-3.16	119.31	124.05
10	R	101	U4Z	CAN-CAM-CAO	-3.16	117.69	122.82
9	C	506	PGV	C02-O01-C1	-3.16	110.23	117.80
8	W	101	BCL	C3D-C4D-ND	3.16	115.12	109.99
8	O	102	BCL	C4-C3-C5	3.15	120.70	115.23
8	W	102	BCL	C3D-C4D-ND	3.15	115.11	109.99
8	U	102	BCL	CHC-C4B-NB	-3.15	119.32	124.05
8	O	102	BCL	O2A-CGA-CBA	3.15	121.44	111.83
10	D	101	U4Z	CAB-CAD-CAH	-3.15	118.34	122.64
8	S	102	BCL	C3D-C4D-ND	3.13	115.08	109.99
16	M	709	LMT	C1-O1'-C1'	-3.13	108.33	113.68
8	T	101	BCL	C4-C3-C5	3.13	120.66	115.23
10	J	101	U4Z	CAB-CAD-CAH	-3.13	118.36	122.64
8	N	101	BCL	O2A-CGA-CBA	3.12	121.35	111.83
8	I	102	BCL	C3D-C4D-ND	3.12	115.06	109.99
8	W	102	BCL	CHB-C4A-NA	3.12	128.90	124.40
8	O	101	BCL	CHC-C4B-NB	-3.11	119.38	124.05
8	L	702	BCL	CMB-C2B-C3B	3.11	135.49	125.67
8	6	101	BCL	C1-C2-C3	-3.11	121.11	126.20
8	2	102	BCL	CHC-C1C-NC	3.10	128.88	124.40
10	0	103	U4Z	CAB-CAD-CAH	-3.10	118.40	122.64
10	3	102	U4Z	CAB-CAD-CAH	-3.10	118.40	122.64
8	U	101	BCL	CHC-C4B-NB	-3.10	119.40	124.05
8	0	101	BCL	CMB-C2B-C3B	3.09	135.42	125.67
8	2	102	BCL	CHB-C4A-NA	3.09	128.86	124.40
8	S	101	BCL	O2A-CGA-CBA	3.09	121.26	111.83
8	N	101	BCL	C1-C2-C3	-3.09	121.14	126.20
8	0	101	BCL	C4-C3-C5	3.09	120.59	115.23
8	U	101	BCL	O2D-CGD-O1D	-3.09	117.84	123.85
8	0	102	BCL	C4-C3-C5	3.09	120.58	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	101	BCL	O2D-CGD-O1D	-3.08	117.84	123.85
8	Q	101	BCL	O2A-CGA-CBA	3.07	121.20	111.83
8	0	102	BCL	C3D-C4D-ND	3.06	114.97	109.99
8	A	101	BCL	CHC-C4B-NB	-3.06	119.46	124.05
8	G	101	BCL	CHC-C4B-NB	-3.06	119.46	124.05
8	N	101	BCL	O2D-CGD-O1D	-3.06	117.90	123.85
8	K	101	BCL	CBA-CAA-C2A	-3.05	104.71	113.79
8	M	701	BCL	O2A-CGA-CBA	3.05	121.14	111.83
8	A	102	BCL	O2A-CGA-CBA	3.05	121.14	111.83
8	9	101	BCL	O2D-CGD-O1D	-3.05	117.91	123.85
8	U	101	BCL	O2A-CGA-CBA	3.04	121.11	111.83
8	3	103	BCL	CHC-C4B-NB	-3.04	119.49	124.05
8	O	102	BCL	C3D-C4D-ND	3.04	114.92	109.99
8	D	102	BCL	O2D-CGD-O1D	-3.04	117.94	123.85
9	h	102	PGV	O03-C19-C20	3.03	121.08	111.83
9	N	102	PGV	O03-C19-C20	3.03	120.35	111.15
8	A	102	BCL	CHC-C4B-NB	-3.03	119.51	124.05
8	S	102	BCL	O2D-CGD-O1D	-3.02	117.96	123.85
8	3	101	BCL	CAA-CBA-CGA	-3.02	104.63	113.21
8	G	102	BCL	C3D-C4D-ND	3.02	114.89	109.99
8	2	102	BCL	CAA-CBA-CGA	-3.02	104.64	113.21
8	K	102	BCL	C3D-C4D-ND	3.01	114.89	109.99
10	J	101	U4Z	CAN-CAM-CAO	-3.01	117.94	122.82
8	W	101	BCL	O2D-CGD-O1D	-3.01	117.99	123.85
8	U	102	BCL	C4-C3-C5	3.01	120.45	115.23
10	0	103	U4Z	CAN-CAM-CAO	-3.01	117.94	122.82
8	K	102	BCL	C1D-ND-C4D	-3.00	104.20	106.31
8	K	101	BCL	C1C-NC-C4C	-3.00	105.31	106.68
8	2	101	BCL	O2A-CGA-CBA	3.00	120.98	111.83
8	G	101	BCL	O2D-CGD-O1D	-3.00	118.02	123.85
8	Q	102	BCL	C3D-C4D-ND	3.00	114.86	109.99
8	D	102	BCL	O2A-CGA-CBA	3.00	120.97	111.83
8	0	101	BCL	C4D-CHA-C1A	-2.99	117.67	121.24
8	U	102	BCL	O2A-CGA-CBA	2.99	120.96	111.83
13	L	705	MQE	CAY-CAX-CBQ	2.99	121.73	118.58
8	F	101	BCL	C1-C2-C3	-2.99	121.30	126.20
8	L	703	BCL	C4-C3-C2	-2.98	115.96	123.63
8	E	101	BCL	C3D-C4D-ND	2.98	114.83	109.99
8	O	102	BCL	C4-C3-C2	-2.98	115.99	123.63
8	3	103	BCL	C4-C3-C5	2.98	120.39	115.23
8	8	101	BCL	O2D-CGD-O1D	-2.97	118.06	123.85
8	R	102	BCL	O2D-CGD-O1D	-2.97	118.06	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	101	BCL	CMB-C2B-C3B	2.97	135.04	125.67
8	Q	101	BCL	O2D-CGD-O1D	-2.97	118.07	123.85
8	K	102	BCL	C2A-C3A-C4A	-2.97	97.07	101.87
8	5	101	BCL	C1-C2-C3	-2.97	121.34	126.20
9	E	103	PGV	O03-C19-C20	2.96	120.87	111.83
8	8	101	BCL	CMB-C2B-C3B	2.96	135.00	125.67
8	P	101	BCL	C4-C3-C5	2.96	120.36	115.23
8	4	101	BCL	C4-C3-C5	2.95	120.35	115.23
15	M	708	PEF	O3-C30-C31	2.95	120.82	111.83
8	6	102	BCL	C4-C3-C5	2.95	120.34	115.23
9	0	104	PGV	O03-C19-C20	2.94	120.80	111.83
8	U	102	BCL	CHB-C4A-NA	2.94	128.64	124.40
8	G	101	BCL	CMB-C2B-C3B	2.93	134.93	125.67
8	2	101	BCL	CED-O2D-CGD	2.93	122.56	115.92
8	4	101	BCL	C1-C2-C3	-2.92	121.41	126.20
10	0	103	U4Z	CBG-CBB-CAV	2.92	129.50	123.52
9	1	102	PGV	O03-C19-C20	2.92	120.75	111.83
11	L	701	BPH	C2B-C1B-NB	-2.92	107.32	109.43
20	C	503	HEC	C2A-C1A-NA	-2.92	107.51	110.32
8	1	101	BCL	C1-C2-C3	-2.92	121.42	126.20
8	M	701	BCL	CED-O2D-CGD	2.91	122.52	115.92
15	L	717	PEF	O3-C30-C31	2.91	120.71	111.83
8	6	102	BCL	C1-C2-C3	-2.91	121.43	126.20
8	R	102	BCL	C4-C3-C5	2.91	120.27	115.23
8	K	101	BCL	CMB-C2B-C3B	2.91	134.84	125.67
8	L	703	BCL	O2A-CGA-CBA	2.90	120.69	111.83
8	M	701	BCL	C1-O2A-CGA	2.90	123.68	116.65
8	3	101	BCL	CHB-C4A-NA	2.90	128.59	124.40
18	P	102	CDL	OB8-CB7-C71	2.90	120.68	111.83
8	K	101	BCL	CHB-C4A-NA	2.90	128.58	124.40
15	h	103	PEF	O3-C30-C31	2.90	120.67	111.83
8	8	101	BCL	C1C-NC-C4C	-2.89	105.36	106.68
8	H	101	BCL	CHC-C4B-NB	-2.89	119.72	124.05
8	E	102	BCL	CHC-C1C-NC	2.89	128.57	124.40
8	2	101	BCL	CMB-C2B-C3B	2.88	134.75	125.67
8	S	101	BCL	CMB-C2B-C3B	2.88	134.74	125.67
8	T	101	BCL	O2D-CGD-O1D	-2.87	118.25	123.85
15	L	713	PEF	C2-O2-C10	-2.87	110.92	117.80
8	L	703	BCL	C1-O2A-CGA	2.87	123.61	116.65
20	C	504	HEC	C2A-C1A-NA	-2.87	107.55	110.32
8	L	703	BCL	CHC-C1C-NC	2.87	128.54	124.40
8	B	101	BCL	C3D-C4D-ND	2.86	114.64	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	101	BCL	C1C-NC-C4C	-2.86	105.37	106.68
9	U	104	PGV	O03-C19-C20	2.86	120.56	111.83
8	A	101	BCL	O2A-CGA-CBA	2.86	120.56	111.83
8	8	102	BCL	CHB-C4A-NA	2.86	128.53	124.40
8	H	101	BCL	O2D-CGD-O1D	-2.86	118.28	123.85
8	I	102	BCL	O2A-CGA-CBA	2.86	120.55	111.83
8	3	101	BCL	C4A-NA-C1A	2.86	107.98	106.68
8	W	101	BCL	CMB-C2B-C3B	2.85	134.67	125.67
8	W	101	BCL	CHC-C4B-NB	-2.85	119.77	124.05
8	H	101	BCL	CHC-C1C-NC	2.85	128.51	124.40
8	A	101	BCL	CHB-C4A-NA	2.85	128.51	124.40
8	G	101	BCL	CHB-C4A-NA	2.85	128.51	124.40
8	I	101	BCL	O2D-CGD-O1D	-2.85	118.30	123.85
8	3	101	BCL	CMB-C2B-C3B	2.85	134.65	125.67
8	S	101	BCL	C4D-CHA-C1A	-2.85	117.85	121.24
8	8	102	BCL	C3D-C4D-ND	2.84	114.60	109.99
8	O	102	BCL	C4A-NA-C1A	2.84	107.97	106.68
8	N	101	BCL	CHC-C4B-NB	-2.84	119.79	124.05
9	8	103	PGV	O03-C19-C20	2.84	120.48	111.83
8	L	703	BCL	CHB-C4A-NA	2.84	128.49	124.40
8	O	101	BCL	CMB-C2B-C3B	2.83	134.61	125.67
8	U	101	BCL	C4-C3-C5	2.83	120.14	115.23
8	Q	102	BCL	CMB-C2B-C3B	2.83	134.60	125.67
8	7	101	BCL	C4-C3-C5	2.83	120.14	115.23
8	Q	101	BCL	C1C-NC-C4C	-2.83	105.39	106.68
8	W	102	BCL	O2A-CGA-CBA	2.83	120.45	111.83
9	U	103	PGV	O03-C19-C20	2.82	120.45	111.83
8	B	101	BCL	CHB-C1B-NB	-2.82	119.81	124.05
8	U	102	BCL	CBB-CAB-C3B	-2.82	114.46	120.40
8	6	102	BCL	C3D-C4D-ND	2.81	114.56	109.99
10	D	101	U4Z	CBO-CBL-CBI	-2.81	118.26	122.82
8	4	101	BCL	C3D-C4D-ND	2.81	114.56	109.99
8	G	102	BCL	O2A-CGA-CBA	2.81	120.41	111.83
8	D	102	BCL	CHC-C4B-NB	-2.81	119.83	124.05
8	A	101	BCL	CMB-C2B-C3B	2.81	134.53	125.67
8	F	101	BCL	O2D-CGD-O1D	-2.81	118.38	123.85
8	2	102	BCL	C3D-C4D-ND	2.81	114.55	109.99
8	V	101	BCL	C4-C3-C5	2.81	120.10	115.23
15	L	713	PEF	O3-C30-C31	2.81	120.39	111.83
8	U	101	BCL	CMB-C2B-C3B	2.81	134.52	125.67
9	8	103	PGV	C02-O01-C1	-2.80	111.10	117.80
9	S	103	PGV	O03-C19-C20	2.80	120.37	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	8	101	BCL	CHC-C4B-NB	-2.80	119.85	124.05
8	9	101	BCL	CHC-C4B-NB	-2.80	119.85	124.05
8	I	101	BCL	O2A-CGA-CBA	2.80	120.36	111.83
8	G	101	BCL	C4D-CHA-C1A	-2.79	117.91	121.24
8	F	101	BCL	O2A-CGA-CBA	2.79	120.35	111.83
8	O	101	BCL	O2D-CGD-O1D	-2.79	118.42	123.85
8	F	101	BCL	CHC-C4B-NB	-2.79	119.86	124.05
8	L	703	BCL	CMB-C2B-C3B	2.79	134.46	125.67
8	7	101	BCL	O2D-CGD-O1D	-2.79	118.42	123.85
8	U	102	BCL	CMB-C2B-C3B	2.79	134.46	125.67
8	U	102	BCL	CHB-C1B-NB	-2.78	119.87	124.05
8	8	101	BCL	O2A-CGA-CBA	2.78	120.32	111.83
8	L	702	BCL	C1-O2A-CGA	2.78	123.38	116.65
9	6	103	PGV	O03-C19-C20	2.78	120.31	111.83
8	2	101	BCL	C1C-NC-C4C	-2.78	105.41	106.68
8	6	101	BCL	O2D-CGD-O1D	-2.77	118.45	123.85
8	Q	101	BCL	CMB-C2B-C3B	2.77	134.42	125.67
9	E	104	PGV	O03-C19-C20	2.77	120.29	111.83
8	J	102	BCL	CHC-C4B-NB	-2.77	119.89	124.05
8	V	101	BCL	O2D-CGD-O1D	-2.77	118.45	123.85
8	J	102	BCL	C4-C3-C5	2.77	120.04	115.23
10	0	103	U4Z	CBO-CBL-CBI	-2.77	118.33	122.82
10	J	101	U4Z	CBG-CBB-CAV	2.77	129.18	123.52
8	4	101	BCL	O2A-CGA-CBA	2.77	120.28	111.83
8	B	101	BCL	CMB-C2B-C3B	2.77	134.40	125.67
10	3	102	U4Z	CBG-CBB-CAV	2.76	129.17	123.52
11	M	702	BPH	C2B-C1B-NB	-2.76	107.44	109.43
8	3	103	BCL	O2A-CGA-CBA	2.76	120.25	111.83
8	T	101	BCL	C1-C2-C3	-2.76	121.68	126.20
11	L	701	BPH	C1-C2-C3	-2.75	121.69	126.20
8	0	102	BCL	O2D-CGD-O1D	-2.75	118.49	123.85
15	h	103	PEF	C2-O2-C10	-2.75	111.22	117.80
9	O	103	PGV	O03-C19-C20	2.75	120.21	111.83
9	L	711	PGV	O03-C19-C20	2.75	120.21	111.83
8	H	101	BCL	C4-C3-C5	2.74	119.99	115.23
8	P	101	BCL	O2A-CGA-CBA	2.74	120.19	111.83
8	P	101	BCL	C1-C2-C3	-2.74	121.71	126.20
9	K	104	PGV	O03-C19-C20	2.74	120.18	111.83
10	3	102	U4Z	CBO-CBL-CBI	-2.74	118.38	122.82
8	0	101	BCL	CHB-C4A-NA	2.73	128.35	124.40
8	V	101	BCL	CHC-C1C-NC	2.73	128.35	124.40
8	B	101	BCL	C1D-ND-C4D	-2.73	104.39	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	102	BCL	CMB-C2B-C3B	2.73	134.28	125.67
8	G	101	BCL	CBA-CAA-C2A	-2.73	105.68	113.79
8	Q	101	BCL	CHB-C4A-NA	2.73	128.34	124.40
8	2	102	BCL	O2A-CGA-CBA	2.73	120.15	111.83
9	L	706	PGV	O03-C19-C20	2.73	120.15	111.83
8	V	101	BCL	CHB-C4A-NA	2.73	128.33	124.40
18	P	102	CDL	OA8-CA7-C31	2.72	120.14	111.83
8	G	102	BCL	C1D-CHD-C4C	-2.72	120.05	126.62
8	D	102	BCL	C6-C5-C3	-2.72	106.84	113.47
9	1	102	PGV	C02-O01-C1	-2.72	111.28	117.80
8	4	101	BCL	CAA-CBA-CGA	-2.72	105.48	113.21
8	8	102	BCL	C4A-NA-C1A	2.72	107.92	106.68
8	G	101	BCL	C1C-NC-C4C	-2.72	105.44	106.68
10	R	101	U4Z	CBG-CBB-CAV	2.71	129.07	123.52
8	U	102	BCL	C3B-C2B-C1B	-2.71	97.74	106.40
8	8	101	BCL	CHB-C4A-NA	2.71	128.31	124.40
8	G	102	BCL	O1D-CGD-CBD	-2.71	119.18	124.52
8	O	101	BCL	CHB-C4A-NA	2.70	128.30	124.40
8	6	101	BCL	CHB-C4A-NA	2.70	128.30	124.40
10	R	101	U4Z	CBO-CBL-CBI	-2.70	118.45	122.82
8	5	101	BCL	CHC-C4B-NB	-2.70	120.01	124.05
16	1	104	LMT	C1B-O1B-C4'	-2.69	111.60	117.98
10	J	101	U4Z	CBO-CBL-CBI	-2.69	118.46	122.82
10	0	103	U4Z	CBK-CBH-CBJ	-2.69	118.46	122.82
8	J	102	BCL	O2A-CGA-CBA	2.69	120.03	111.83
8	K	102	BCL	O2A-CGA-CBA	2.68	120.02	111.83
8	U	101	BCL	CHB-C4A-NA	2.68	128.27	124.40
8	H	101	BCL	O2A-CGA-CBA	2.68	120.01	111.83
8	H	101	BCL	C1D-CHD-C4C	-2.68	120.16	126.62
8	L	702	BCL	C6-C5-C3	-2.68	106.95	113.47
8	S	101	BCL	CHB-C4A-NA	2.68	128.26	124.40
8	6	101	BCL	CMB-C2B-C3B	2.67	134.11	125.67
8	I	102	BCL	CAA-CBA-CGA	-2.67	105.63	113.21
8	U	101	BCL	C4D-CHA-C1A	-2.67	118.06	121.24
8	8	101	BCL	C1D-CHD-C4C	-2.67	120.19	126.62
8	L	702	BCL	C4-C3-C5	2.67	119.85	115.23
8	E	102	BCL	O2A-CGA-CBA	2.66	119.95	111.83
8	0	102	BCL	CED-O2D-CGD	2.66	121.95	115.92
10	3	102	U4Z	CBN-CBL-CBI	2.66	123.19	119.01
10	D	101	U4Z	CBN-CBL-CBI	2.66	123.19	119.01
8	B	101	BCL	CAA-C2A-C3A	-2.66	105.82	113.00
9	I	103	PGV	O03-C19-C20	2.66	119.94	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	102	U4Z	CAU-CAR-CAV	-2.65	118.52	122.82
8	A	101	BCL	C4D-CHA-C1A	-2.65	118.08	121.24
8	5	101	BCL	O2A-CGA-CBA	2.65	119.92	111.83
8	W	102	BCL	CAA-CBA-CGA	-2.65	105.68	113.21
8	Q	102	BCL	CHC-C1C-NC	2.65	128.22	124.40
8	V	101	BCL	O2A-CGA-CBA	2.65	119.90	111.83
8	E	101	BCL	C1D-CHD-C4C	-2.64	120.24	126.62
8	W	101	BCL	C4D-CHA-C1A	-2.64	118.09	121.24
8	5	101	BCL	C4-C3-C5	2.64	119.81	115.23
8	2	101	BCL	O2A-CGA-O1A	-2.64	117.03	123.63
9	E	104	PGV	C02-O01-C1	-2.64	111.48	117.80
8	W	101	BCL	C1D-CHD-C4C	-2.64	120.26	126.62
8	0	102	BCL	O2A-CGA-CBA	2.64	119.87	111.83
8	I	101	BCL	CHB-C4A-NA	2.63	128.20	124.40
8	E	101	BCL	CMB-C2B-C3B	2.63	133.98	125.67
8	O	101	BCL	C1D-CHD-C4C	-2.63	120.27	126.62
8	6	101	BCL	O2A-CGA-CBA	2.63	119.84	111.83
10	0	103	U4Z	CAU-CAR-CAV	-2.62	118.57	122.82
8	E	101	BCL	C4D-CHA-C1A	-2.62	118.12	121.24
8	O	101	BCL	C4D-CHA-C1A	-2.62	118.12	121.24
8	W	102	BCL	O2D-CGD-O1D	-2.62	118.75	123.85
8	4	101	BCL	C4A-NA-C1A	2.62	107.87	106.68
8	L	702	BCL	CHB-C1B-C2B	-2.62	119.83	127.43
10	R	101	U4Z	CBK-CBH-CBJ	-2.62	118.58	122.82
8	8	101	BCL	C4-C3-C5	2.62	119.77	115.23
8	Q	102	BCL	C4-C3-C5	2.61	119.77	115.23
8	6	102	BCL	C1D-CHD-C4C	-2.61	120.32	126.62
8	K	102	BCL	CHC-C4B-NB	-2.61	120.13	124.05
10	3	102	U4Z	CAQ-CAR-CAV	2.60	123.11	119.01
8	6	101	BCL	C1C-NC-C4C	-2.60	105.49	106.68
8	K	101	BCL	C1-C2-C3	-2.60	121.93	126.20
8	P	101	BCL	CHB-C4A-NA	2.60	128.16	124.40
8	0	102	BCL	CHC-C1C-NC	2.60	128.15	124.40
8	O	102	BCL	CHB-C4A-NA	2.60	128.15	124.40
8	9	101	BCL	CHB-C4A-NA	2.60	128.15	124.40
8	7	101	BCL	O2A-CGA-CBA	2.59	119.74	111.83
8	E	101	BCL	C4-C3-C5	2.59	119.73	115.23
8	6	101	BCL	C1D-CHD-C4C	-2.59	120.37	126.62
8	I	102	BCL	CHC-C1C-NC	2.59	128.14	124.40
9	C	506	PGV	O01-C1-O02	-2.59	117.65	123.70
10	0	103	U4Z	CAQ-CAR-CAV	2.59	123.08	119.01
8	R	102	BCL	O2A-CGA-CBA	2.59	119.72	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	102	BCL	C1D-CHD-C4C	-2.58	120.39	126.62
8	I	101	BCL	C4D-CHA-C1A	-2.58	118.16	121.24
9	0	104	PGV	C02-O01-C1	-2.58	111.62	117.80
8	5	101	BCL	C1C-NC-C4C	-2.58	105.50	106.68
8	L	703	BCL	C4D-CHA-C1A	-2.57	118.18	121.24
9	N	102	PGV	C02-O01-C1	-2.57	111.64	117.80
8	G	101	BCL	C1D-CHD-C4C	-2.57	120.42	126.62
10	3	102	U4Z	CBK-CBH-CBJ	-2.57	118.65	122.82
8	2	102	BCL	CHB-C1B-NB	-2.57	120.19	124.05
8	0	102	BCL	C1C-NC-C4C	-2.57	105.51	106.68
8	K	101	BCL	C1D-CHD-C4C	-2.57	120.43	126.62
10	J	101	U4Z	CAU-CAR-CAV	-2.57	118.66	122.82
8	3	101	BCL	CBA-CAA-C2A	-2.57	106.16	113.79
8	N	101	BCL	C4-C3-C5	2.56	119.68	115.23
9	4	102	PGV	C02-O01-C1	-2.56	111.66	117.80
9	C	506	PGV	O03-C19-C20	2.56	119.64	111.83
9	K	103	PGV	O03-C19-C20	2.56	119.64	111.83
8	W	101	BCL	CHB-C4A-NA	2.56	128.09	124.40
8	R	102	BCL	C6-C5-C3	-2.55	107.25	113.47
8	B	101	BCL	O2A-CGA-CBA	2.55	119.61	111.83
8	W	101	BCL	C1C-NC-C4C	-2.55	105.52	106.68
8	E	101	BCL	CHC-C4B-NB	-2.55	120.23	124.05
8	T	101	BCL	CHC-C4B-NB	-2.55	120.23	124.05
8	I	101	BCL	C1D-CHD-C4C	-2.54	120.49	126.62
8	1	101	BCL	CMB-C2B-C3B	2.54	133.69	125.67
10	D	101	U4Z	CBK-CBH-CBJ	-2.54	118.70	122.82
8	G	102	BCL	CMB-C2B-C3B	2.54	133.68	125.67
16	T	102	LMT	O5'-C5'-C6'	2.54	112.73	106.44
8	J	102	BCL	C1-O2A-CGA	2.53	122.79	116.65
8	S	102	BCL	C1D-CHD-C4C	-2.53	120.51	126.62
20	C	502	HEC	C2A-C1A-NA	-2.53	107.88	110.32
8	E	102	BCL	C4-C3-C5	2.53	119.62	115.23
8	S	101	BCL	CED-O2D-CGD	2.53	121.66	115.92
8	L	702	BCL	C1D-CHD-C4C	-2.53	120.52	126.62
8	W	101	BCL	C6-C5-C3	-2.53	107.31	113.47
8	1	101	BCL	C4-C3-C5	2.53	119.61	115.23
8	U	102	BCL	O2A-CGA-O1A	-2.52	117.31	123.63
9	0	105	PGV	O03-C19-C20	2.52	119.53	111.83
10	0	103	U4Z	CBN-CBL-CBI	2.52	122.98	119.01
8	6	102	BCL	CHB-C1B-NB	-2.52	120.26	124.05
8	Q	101	BCL	C4D-CHA-C1A	-2.52	118.24	121.24
8	8	101	BCL	C4D-CHA-C1A	-2.52	118.24	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	101	BCL	CMB-C2B-C3B	2.52	133.61	125.67
10	R	101	U4Z	CAU-CAR-CAV	-2.51	118.74	122.82
8	8	102	BCL	CAA-CBA-CGA	-2.51	106.08	113.21
8	6	101	BCL	C4-C3-C5	2.51	119.59	115.23
8	8	102	BCL	O2D-CGD-O1D	-2.51	118.96	123.85
8	1	101	BCL	O2A-CGA-CBA	2.51	119.49	111.83
8	L	702	BCL	CHC-C1C-NC	2.51	128.02	124.40
8	I	102	BCL	C1D-CHD-C4C	-2.51	120.57	126.62
8	K	102	BCL	C1-O2A-CGA	2.51	122.72	116.65
8	Q	101	BCL	CHC-C4B-NB	-2.51	120.29	124.05
8	3	101	BCL	O2A-CGA-CBA	2.50	119.47	111.83
8	N	101	BCL	CHB-C4A-NA	2.50	128.01	124.40
8	R	102	BCL	CMB-C2B-C3B	2.50	133.56	125.67
9	L	712	PGV	C02-O01-C1	-2.50	111.81	117.80
8	O	102	BCL	CMB-C2B-C1B	2.50	129.23	125.42
10	J	101	U4Z	CBK-CBH-CBJ	-2.50	118.77	122.82
8	D	102	BCL	CHC-C1C-NC	2.50	128.00	124.40
8	1	101	BCL	O1D-CGD-CBD	-2.49	119.61	124.52
8	O	102	BCL	CHC-C4B-NB	-2.49	120.31	124.05
8	4	101	BCL	CHC-C1C-NC	2.49	127.99	124.40
8	4	101	BCL	C1D-CHD-C4C	-2.49	120.62	126.62
10	J	101	U4Z	CBE-CBA-CAW	-2.49	124.19	127.69
8	U	101	BCL	C1D-CHD-C4C	-2.48	120.64	126.62
8	U	101	BCL	C6-C7-C8	-2.48	107.73	115.97
8	K	102	BCL	C6-C7-C8	-2.48	107.73	115.97
8	2	101	BCL	C4-C3-C5	2.48	119.53	115.23
8	S	102	BCL	CHC-C1C-NC	2.47	127.97	124.40
8	2	102	BCL	C1D-CHD-C4C	-2.47	120.65	126.62
8	2	102	BCL	CMB-C2B-C3B	2.47	133.47	125.67
8	1	101	BCL	CHC-C1C-NC	2.47	127.97	124.40
8	A	102	BCL	C1-C2-C3	-2.47	122.16	126.20
8	6	101	BCL	C4D-CHA-C1A	-2.47	118.30	121.24
8	M	701	BCL	CMB-C2B-C3B	2.47	133.45	125.67
8	0	101	BCL	C1D-CHD-C4C	-2.47	120.67	126.62
8	L	702	BCL	C2A-C3A-C4A	-2.46	97.89	101.87
10	D	101	U4Z	CAU-CAR-CAV	-2.46	118.83	122.82
8	D	102	BCL	C4A-NA-C1A	2.46	107.80	106.68
8	8	102	BCL	O2A-CGA-CBA	2.46	119.34	111.83
8	2	101	BCL	CHB-C4A-NA	2.46	127.95	124.40
8	0	102	BCL	C1D-CHD-C4C	-2.46	120.69	126.62
10	R	101	U4Z	CBN-CBL-CBI	2.46	122.87	119.01
8	O	102	BCL	CHC-C1C-NC	2.46	127.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3	101	BCL	C1C-NC-C4C	-2.45	105.56	106.68
8	8	102	BCL	CHC-C1C-NC	2.45	127.94	124.40
8	Q	101	BCL	C1D-CHD-C4C	-2.45	120.71	126.62
8	6	102	BCL	C1-O2A-CGA	2.45	122.58	116.65
8	3	101	BCL	C1D-CHD-C4C	-2.44	120.72	126.62
8	A	102	BCL	CMB-C2B-C3B	2.44	133.37	125.67
8	E	102	BCL	C1-C2-C3	-2.44	122.20	126.20
10	J	101	U4Z	CBN-CBL-CBI	2.44	122.84	119.01
8	3	103	BCL	CHC-C1C-NC	2.43	127.91	124.40
8	1	101	BCL	CHB-C1B-C2B	-2.43	120.36	127.43
8	S	101	BCL	O2D-CGD-O1D	-2.43	119.11	123.85
10	D	101	U4Z	CBG-CBB-CAV	2.43	128.50	123.52
10	R	101	U4Z	CAQ-CAR-CAV	2.43	122.83	119.01
8	H	101	BCL	C6-C5-C3	-2.43	107.55	113.47
11	L	704	BPH	C2B-C1B-NB	-2.43	107.68	109.43
9	U	104	PGV	C02-O01-C1	-2.43	111.99	117.80
8	I	102	BCL	CHB-C4A-NA	2.42	127.90	124.40
8	E	102	BCL	CHB-C1B-C2B	-2.42	120.39	127.43
8	L	703	BCL	CHB-C1B-C2B	-2.42	120.39	127.43
9	4	102	PGV	O03-C19-C20	2.42	119.21	111.83
8	0	101	BCL	CHB-C1B-C2B	-2.42	120.42	127.43
8	G	101	BCL	O2A-CGA-CBA	2.41	119.19	111.83
8	J	102	BCL	CMB-C2B-C3B	2.41	133.27	125.67
8	I	101	BCL	C4-C3-C5	2.41	119.41	115.23
8	Q	102	BCL	O2A-CGA-CBA	2.41	119.17	111.83
8	M	701	BCL	CHB-C4A-NA	2.40	127.87	124.40
10	R	101	U4Z	CBF-CBH-CBJ	2.40	122.79	119.01
8	6	102	BCL	CHB-C4A-NA	2.40	127.86	124.40
10	3	102	U4Z	CBF-CBH-CBJ	2.40	122.78	119.01
8	O	102	BCL	O2A-CGA-O1A	-2.40	117.64	123.63
8	Q	102	BCL	C1-C2-C3	-2.39	122.28	126.20
8	A	102	BCL	CHC-C1C-NC	2.39	127.85	124.40
8	M	701	BCL	CHC-C1C-NC	2.38	127.84	124.40
8	N	101	BCL	C4A-NA-C1A	2.38	107.77	106.68
9	I	103	PGV	O01-C1-O02	-2.38	118.14	123.70
8	G	102	BCL	CED-O2D-CGD	2.38	121.32	115.92
8	S	102	BCL	CED-O2D-CGD	2.38	121.31	115.92
8	W	102	BCL	C1D-CHD-C4C	-2.38	120.88	126.62
8	0	101	BCL	CAA-CBA-CGA	-2.38	106.45	113.21
10	J	101	U4Z	CAQ-CAR-CAV	2.38	122.75	119.01
8	1	101	BCL	CHB-C4A-NA	2.38	127.83	124.40
8	G	101	BCL	C1-C2-C3	-2.37	122.31	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1	102	PGV	O14-P-O13	2.37	120.08	110.83
10	0	103	U4Z	CBF-CBH-CBJ	2.37	122.74	119.01
8	8	102	BCL	O1D-CGD-CBD	-2.37	119.84	124.52
8	E	101	BCL	CHB-C4A-NA	2.37	127.82	124.40
8	D	102	BCL	C1D-CHD-C4C	-2.37	120.91	126.62
8	0	102	BCL	CAA-CBA-CGA	-2.36	106.49	113.21
8	2	101	BCL	CHB-C1B-C2B	-2.36	120.56	127.43
8	4	101	BCL	CHB-C1B-NB	-2.36	120.50	124.05
8	K	102	BCL	C1D-CHD-C4C	-2.36	120.93	126.62
8	5	101	BCL	CHB-C4A-NA	2.36	127.81	124.40
8	Q	102	BCL	C1-O2A-CGA	2.36	122.36	116.65
8	D	102	BCL	CMB-C2B-C3B	2.36	133.10	125.67
8	F	101	BCL	CMB-C2B-C3B	2.35	133.09	125.67
8	0	102	BCL	CMB-C2B-C1B	2.35	129.00	125.42
9	O	103	PGV	C02-O01-C1	-2.35	112.17	117.80
9	M	705	PGV	O03-C19-C20	2.35	119.00	111.83
8	6	102	BCL	CHC-C1C-NC	2.35	127.79	124.40
8	A	101	BCL	C1D-CHD-C4C	-2.35	120.96	126.62
8	S	101	BCL	O2A-CGA-O1A	-2.35	117.76	123.63
8	3	101	BCL	C2A-C1A-CHA	-2.35	119.80	123.87
10	0	103	U4Z	CAN-CAM-CAL	2.34	121.67	118.09
10	3	102	U4Z	CAE-CAI-CAH	2.34	118.23	114.06
8	P	101	BCL	CMB-C2B-C3B	2.34	133.05	125.67
10	J	101	U4Z	CAN-CAM-CAL	2.34	121.66	118.09
8	L	703	BCL	CBA-CAA-C2A	-2.34	106.83	113.79
8	G	101	BCL	CED-O2D-CGD	2.34	121.22	115.92
8	2	101	BCL	CHC-C1C-NC	2.34	127.77	124.40
8	S	102	BCL	O1D-CGD-CBD	-2.34	119.91	124.52
8	S	102	BCL	CHC-C4B-NB	-2.33	120.55	124.05
8	A	102	BCL	CHB-C4A-NA	2.33	127.77	124.40
8	T	101	BCL	CHB-C4A-NA	2.33	127.76	124.40
9	h	102	PGV	O14-P-O13	2.33	119.92	110.83
13	M	704	MQE	CAY-CAX-CBK	-2.33	120.89	124.89
8	R	102	BCL	CHB-C4A-NA	2.33	127.76	124.40
8	H	101	BCL	CMB-C2B-C3B	2.33	133.00	125.67
8	7	101	BCL	CHB-C1B-C2B	-2.33	120.68	127.43
20	C	501	HEC	C2A-C1A-NA	-2.32	108.08	110.32
8	9	101	BCL	C1D-CHD-C4C	-2.32	121.03	126.62
9	h	102	PGV	C02-O01-C1	-2.32	112.25	117.80
8	S	102	BCL	O2A-CGA-O1A	-2.32	117.83	123.63
8	5	101	BCL	C1D-CHD-C4C	-2.31	121.04	126.62
8	9	101	BCL	C4-C3-C5	2.31	119.23	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	101	BCL	C1D-CHD-C4C	-2.31	121.06	126.62
8	8	102	BCL	C1C-NC-C4C	-2.31	105.63	106.68
8	2	102	BCL	CHC-C4B-NB	-2.30	120.59	124.05
8	E	102	BCL	C1D-CHD-C4C	-2.30	121.07	126.62
8	4	101	BCL	C1C-NC-C4C	-2.30	105.63	106.68
8	5	101	BCL	CMB-C2B-C3B	2.30	132.92	125.67
8	L	703	BCL	C4-C3-C5	2.30	119.22	115.23
8	8	102	BCL	CHC-C4B-NB	-2.29	120.61	124.05
8	E	102	BCL	C1-O2A-CGA	2.29	122.19	116.65
8	I	101	BCL	C1C-NC-C4C	-2.29	105.64	106.68
8	B	101	BCL	C1D-CHD-C4C	-2.29	121.11	126.62
8	G	101	BCL	C2A-C1A-CHA	-2.28	119.91	123.87
8	E	101	BCL	O2A-CGA-CBA	2.28	118.79	111.83
8	2	101	BCL	C1D-CHD-C4C	-2.28	121.12	126.62
10	0	103	U4Z	CAE-CAI-CAH	2.28	118.12	114.06
8	3	103	BCL	CMB-C2B-C3B	2.28	132.85	125.67
8	O	102	BCL	C1C-NC-C4C	-2.28	105.64	106.68
8	4	101	BCL	CHB-C4A-NA	2.28	127.69	124.40
8	S	101	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
8	W	102	BCL	CED-O2D-CGD	2.27	121.07	115.92
8	3	103	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
8	I	101	BCL	O2A-CGA-O1A	-2.27	117.95	123.63
10	3	102	U4Z	CAK-CAH-CAD	2.27	126.96	124.48
8	8	102	BCL	C1D-CHD-C4C	-2.27	121.15	126.62
8	I	102	BCL	C1C-NC-C4C	-2.26	105.65	106.68
8	U	102	BCL	C4D-CHA-C1A	-2.26	118.54	121.24
8	E	102	BCL	CMD-C2D-C3D	-2.26	122.50	127.69
15	L	713	PEF	O2-C10-O4	-2.26	118.42	123.70
8	J	102	BCL	C1D-CHD-C4C	-2.26	121.17	126.62
8	T	101	BCL	O2A-CGA-O1A	-2.26	117.98	123.63
8	P	101	BCL	C1D-CHD-C4C	-2.26	121.18	126.62
8	R	102	BCL	CHC-C1C-NC	2.25	127.65	124.40
8	3	101	BCL	CHC-C1C-NC	2.25	127.65	124.40
8	T	101	BCL	CMB-C2B-C3B	2.25	132.78	125.67
10	R	101	U4Z	CAN-CAM-CAL	2.25	121.53	118.09
8	4	101	BCL	CHC-C4B-C3B	-2.25	122.77	131.72
8	F	101	BCL	C4-C3-C5	2.25	119.14	115.23
8	S	101	BCL	CHC-C1C-NC	2.25	127.65	124.40
9	8	103	PGV	O01-C1-O02	-2.25	118.44	123.70
10	J	101	U4Z	CAE-CAI-CAH	2.25	118.07	114.06
8	8	101	BCL	CHB-C1B-C2B	-2.25	120.90	127.43
8	2	102	BCL	CMD-C2D-C3D	-2.25	122.53	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	BCL	C1D-CHD-C4C	-2.25	121.20	126.62
18	P	102	CDL	OA6-CA5-OA7	-2.25	118.45	123.70
8	Q	101	BCL	C4-C3-C5	2.24	119.12	115.23
8	F	101	BCL	CHC-C1C-NC	2.24	127.64	124.40
8	V	101	BCL	C1D-CHD-C4C	-2.24	121.21	126.62
8	L	703	BCL	O2D-CGD-O1D	-2.24	119.48	123.85
8	D	102	BCL	C4-C3-C5	2.24	119.12	115.23
8	I	102	BCL	CAA-C2A-C3A	-2.24	106.94	113.00
8	G	101	BCL	CHB-C1B-C2B	-2.24	120.92	127.43
8	I	101	BCL	CED-O2D-CGD	2.24	121.00	115.92
8	0	102	BCL	CHB-C4A-NA	2.24	127.63	124.40
10	J	101	U4Z	CBF-CBH-CBJ	2.24	122.53	119.01
8	2	102	BCL	C1-O2A-CGA	2.24	122.07	116.65
8	K	101	BCL	CHB-C1B-C2B	-2.24	120.93	127.43
8	A	102	BCL	C1D-CHD-C4C	-2.24	121.23	126.62
8	W	102	BCL	CMB-C2B-C3B	2.23	132.71	125.67
10	J	101	U4Z	CAK-CAH-CAD	2.23	126.92	124.48
8	7	101	BCL	CHB-C4A-NA	2.23	127.62	124.40
8	O	101	BCL	C1C-NC-C4C	-2.23	105.66	106.68
8	I	101	BCL	CHB-C1B-C2B	-2.23	120.95	127.43
8	E	102	BCL	CHB-C4A-NA	2.23	127.62	124.40
9	L	712	PGV	O03-C19-O04	-2.23	118.05	123.63
10	R	101	U4Z	CAE-CAI-CAH	2.23	118.02	114.06
8	3	103	BCL	C6-C5-C3	-2.22	108.05	113.47
8	M	701	BCL	C1D-CHD-C4C	-2.22	121.27	126.62
8	W	102	BCL	CHB-C1B-C2B	-2.22	120.98	127.43
8	T	101	BCL	C1D-CHD-C4C	-2.22	121.27	126.62
8	5	101	BCL	CHB-C1B-C2B	-2.22	120.99	127.43
8	K	101	BCL	CED-O2D-CGD	2.22	120.94	115.92
10	3	102	U4Z	CAN-CAM-CAL	2.21	121.47	118.09
8	D	102	BCL	CHB-C4A-NA	2.21	127.58	124.40
8	3	103	BCL	C1C-NC-C4C	-2.21	105.67	106.68
8	U	101	BCL	CHC-C1C-NC	2.21	127.58	124.40
8	6	102	BCL	O2A-CGA-CBA	2.20	118.56	111.83
8	G	102	BCL	CHC-C1C-NC	2.20	127.58	124.40
9	S	103	PGV	O01-C1-O02	-2.20	118.56	123.70
8	W	102	BCL	CHC-C1C-NC	2.20	127.58	124.40
10	D	101	U4Z	CAQ-CAR-CAV	2.20	122.47	119.01
8	2	102	BCL	C1-C2-C3	-2.20	122.60	126.20
8	S	102	BCL	C6-C5-C3	-2.20	108.12	113.47
8	J	102	BCL	CHC-C1C-NC	2.19	127.56	124.40
8	J	102	BCL	CHB-C4A-NA	2.19	127.56	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	101	BCL	CHB-C1B-C2B	-2.19	121.08	127.43
8	2	102	BCL	C4-C3-C5	2.19	119.02	115.23
8	8	102	BCL	CMD-C2D-C3D	-2.19	122.68	127.69
8	8	102	BCL	CHB-C1B-C2B	-2.19	121.08	127.43
8	9	101	BCL	CED-O2D-CGD	2.18	120.87	115.92
8	9	101	BCL	CMB-C2B-C3B	2.18	132.56	125.67
8	R	102	BCL	CHB-C1B-C2B	-2.18	121.09	127.43
8	4	101	BCL	CMD-C2D-C3D	-2.18	122.68	127.69
8	2	102	BCL	CAA-C2A-C1A	2.18	119.13	111.97
8	2	102	BCL	C3B-C2B-C1B	-2.18	99.43	106.40
8	B	101	BCL	CMD-C2D-C3D	-2.18	122.69	127.69
8	S	101	BCL	CHB-C1B-C2B	-2.18	121.11	127.43
8	J	102	BCL	CHB-C1B-C2B	-2.18	121.11	127.43
8	9	101	BCL	C1C-NC-C4C	-2.17	105.69	106.68
8	A	101	BCL	CHC-C1C-NC	2.17	127.53	124.40
9	4	102	PGV	O01-C1-O02	-2.17	118.63	123.70
9	U	103	PGV	C02-O01-C1	-2.17	112.61	117.80
8	O	102	BCL	C1D-CHD-C4C	-2.17	121.40	126.62
9	0	105	PGV	C02-O01-C1	-2.16	112.61	117.80
9	E	103	PGV	C02-O01-C1	-2.16	112.62	117.80
8	G	101	BCL	C6-C7-C8	-2.16	108.77	115.97
8	K	102	BCL	CMD-C2D-C3D	-2.16	122.74	127.69
8	B	101	BCL	CHD-C1D-C2D	2.16	129.97	125.49
20	C	504	HEC	CMC-C2C-C1C	-2.15	122.14	125.42
8	G	102	BCL	O2D-CGD-O1D	-2.15	119.66	123.85
8	N	101	BCL	CMB-C2B-C3B	2.15	132.46	125.67
8	9	101	BCL	O2A-CGA-O1A	-2.15	118.24	123.63
8	O	102	BCL	CMD-C2D-C3D	-2.15	122.75	127.69
16	T	102	LMT	O1B-C4'-C3'	2.15	112.69	107.23
8	O	101	BCL	CHB-C1B-C2B	-2.15	121.19	127.43
8	W	102	BCL	C1-O2A-CGA	2.15	121.85	116.65
9	0	105	PGV	O01-C1-O02	-2.15	118.69	123.70
8	E	101	BCL	CHC-C1C-NC	2.15	127.50	124.40
8	W	102	BCL	CMD-C2D-C3D	-2.15	122.77	127.69
16	M	709	LMT	O1'-C1'-C2'	2.15	111.53	108.27
8	A	101	BCL	C4-C3-C5	2.14	118.95	115.23
8	2	101	BCL	O2D-CGD-O1D	-2.14	119.67	123.85
8	A	101	BCL	C1C-NC-C4C	-2.14	105.70	106.68
8	O	102	BCL	CHB-C1B-C2B	-2.14	121.20	127.43
9	S	103	PGV	C02-O01-C1	-2.14	112.67	117.80
8	H	101	BCL	CHB-C1B-C2B	-2.14	121.21	127.43
8	S	102	BCL	CMD-C2D-C3D	-2.14	122.78	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	0	104	PGV	O01-C1-O02	-2.14	118.70	123.70
9	h	102	PGV	O03-C19-O04	-2.14	118.27	123.63
8	8	101	BCL	CHC-C1C-NC	2.14	127.49	124.40
8	7	101	BCL	CHC-C1C-NC	2.14	127.49	124.40
14	M	707	BGL	C1'-O2-C2	-2.14	109.27	114.02
8	Q	102	BCL	CHB-C1B-C2B	-2.14	121.22	127.43
8	F	101	BCL	CED-O2D-CGD	2.14	120.77	115.92
8	W	101	BCL	CHC-C1C-NC	2.14	127.48	124.40
16	H	102	LMT	C1B-O1B-C4'	-2.13	112.92	117.98
8	T	101	BCL	C1C-NC-C4C	-2.13	105.71	106.68
10	D	101	U4Z	CBF-CBH-CBJ	2.13	122.36	119.01
8	U	102	BCL	C1D-CHD-C4C	-2.13	121.49	126.62
8	S	102	BCL	CAA-C2A-C3A	-2.12	107.26	113.00
9	U	103	PGV	O01-C1-O02	-2.12	118.74	123.70
8	A	102	BCL	CHB-C1B-C2B	-2.12	121.26	127.43
9	U	104	PGV	O01-C1-O02	-2.12	118.75	123.70
8	G	101	BCL	C4-C3-C5	2.12	118.91	115.23
8	A	102	BCL	C2A-C1A-CHA	-2.12	120.19	123.87
8	B	101	BCL	C1-C2-C3	-2.12	122.73	126.20
8	G	101	BCL	C6-C5-C3	-2.12	108.31	113.47
8	K	101	BCL	O2D-CGD-O1D	-2.11	119.73	123.85
14	L	715	BGL	O5-C5-C4	2.11	113.51	109.70
8	A	102	BCL	C1C-NC-C4C	-2.11	105.72	106.68
8	V	101	BCL	C2A-C1A-CHA	-2.11	120.20	123.87
8	G	102	BCL	C4-C3-C2	-2.11	118.21	123.63
8	3	101	BCL	CHB-C1B-C2B	-2.11	121.30	127.43
8	9	101	BCL	CHC-C1C-NC	2.11	127.44	124.40
8	5	101	BCL	C6-C5-C3	-2.11	108.34	113.47
8	0	102	BCL	CMD-C2D-C3D	-2.10	122.86	127.69
8	O	102	BCL	CAA-C2A-C1A	2.10	118.86	111.97
8	4	101	BCL	CMB-C2B-C1B	2.10	128.62	125.42
8	1	101	BCL	C1D-CHD-C4C	-2.10	121.56	126.62
8	7	101	BCL	C1D-CHD-C4C	-2.10	121.56	126.62
8	4	101	BCL	C6-C5-C3	-2.10	108.36	113.47
8	M	701	BCL	CHB-C1B-C2B	-2.09	121.35	127.43
8	U	102	BCL	C5-C3-C2	2.09	125.87	121.17
8	O	101	BCL	CED-O2D-CGD	2.09	120.66	115.92
8	R	102	BCL	C1D-CHD-C4C	-2.09	121.57	126.62
8	E	101	BCL	CHB-C1B-NB	-2.09	120.91	124.05
8	L	703	BCL	C1D-CHD-C4C	-2.09	121.58	126.62
8	I	102	BCL	C4-C3-C5	2.09	118.86	115.23
8	U	101	BCL	C2A-C1A-CHA	-2.09	120.24	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	104	PGV	O01-C1-O02	-2.09	118.82	123.70
8	G	101	BCL	CHC-C1C-NC	2.08	127.41	124.40
8	7	101	BCL	CAC-C3C-C4C	-2.08	107.96	112.58
8	5	101	BCL	CHC-C1C-NC	2.08	127.41	124.40
8	0	102	BCL	O1D-CGD-CBD	-2.08	120.41	124.52
8	U	102	BCL	CED-O2D-CGD	2.08	120.64	115.92
9	K	103	PGV	O01-C1-O02	-2.08	118.84	123.70
8	A	101	BCL	C2A-C1A-CHA	-2.08	120.26	123.87
8	J	102	BCL	C1C-NC-C4C	-2.08	105.73	106.68
8	6	102	BCL	CMD-C2D-C3D	-2.07	122.93	127.69
8	5	101	BCL	C1-O2A-CGA	2.07	121.67	116.65
11	M	702	BPH	CMC-C2C-C1C	-2.07	110.15	114.61
8	2	102	BCL	CHB-C1B-C2B	-2.07	121.41	127.43
8	0	101	BCL	C6-C5-C3	-2.07	108.42	113.47
8	9	101	BCL	C4A-NA-C1A	2.07	107.62	106.68
8	D	102	BCL	CHB-C1B-C2B	-2.06	121.43	127.43
8	U	101	BCL	CED-O2D-CGD	2.06	120.59	115.92
8	P	101	BCL	CED-O2D-CGD	2.06	120.59	115.92
8	U	102	BCL	CMD-C2D-C3D	-2.06	122.96	127.69
8	K	102	BCL	CHD-C1D-C2D	2.06	129.78	125.49
8	0	101	BCL	CED-O2D-CGD	2.06	120.59	115.92
8	5	101	BCL	C16-C15-C13	-2.06	109.12	115.97
8	K	101	BCL	C4D-CHA-C1A	-2.06	118.79	121.24
8	U	102	BCL	C1C-NC-C4C	-2.06	105.74	106.68
8	0	101	BCL	C11-C10-C8	-2.06	109.13	115.97
8	S	101	BCL	C1-O2A-CGA	2.05	121.62	116.65
8	K	102	BCL	CHC-C1C-NC	2.05	127.36	124.40
8	U	101	BCL	CHB-C1B-C2B	-2.05	121.47	127.43
8	0	101	BCL	O2A-CGA-CBA	2.05	118.08	111.83
8	7	101	BCL	C2A-C1A-CHA	-2.05	120.31	123.87
18	P	102	CDL	CA4-OA6-CA5	-2.05	112.89	117.80
8	G	101	BCL	C4A-NA-C1A	2.05	107.61	106.68
8	D	102	BCL	O2A-CGA-O1A	-2.05	118.50	123.63
8	D	102	BCL	CED-O2D-CGD	2.05	120.56	115.92
8	W	101	BCL	CHB-C1B-C2B	-2.05	121.49	127.43
8	6	101	BCL	CHC-C1C-NC	2.04	127.35	124.40
8	0	102	BCL	CHB-C1B-NB	-2.04	120.98	124.05
8	7	101	BCL	CMD-C2D-C3D	-2.04	123.01	127.69
9	6	103	PGV	O01-C1-O02	-2.04	118.93	123.70
8	0	101	BCL	CHC-C1C-NC	2.04	127.35	124.40
8	Q	101	BCL	CED-O2D-CGD	2.04	120.54	115.92
8	Q	102	BCL	C1C-NC-C4C	-2.04	105.75	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	103	PGV	C03-C02-C01	-2.04	107.03	111.78
8	K	102	BCL	CHB-C1B-NB	-2.04	120.99	124.05
8	V	101	BCL	CMB-C2B-C1B	2.04	128.52	125.42
8	7	101	BCL	CBA-CAA-C2A	-2.03	107.74	113.79
8	W	102	BCL	O1D-CGD-CBD	-2.03	120.51	124.52
9	6	103	PGV	C02-O01-C1	-2.03	112.94	117.80
10	R	101	U4Z	CAB-CAD-CAH	-2.03	119.86	122.64
8	8	101	BCL	CED-O2D-CGD	2.03	120.51	115.92
8	6	101	BCL	CHB-C1B-C2B	-2.02	121.56	127.43
8	K	101	BCL	C11-C12-C13	-2.02	109.26	115.97
8	E	102	BCL	CAA-CBA-CGA	-2.02	107.48	113.21
8	6	101	BCL	CED-O2D-CGD	2.02	120.49	115.92
8	8	102	BCL	CED-O2D-CGD	2.01	120.49	115.92
10	D	101	U4Z	CAE-CAI-CAH	2.01	117.64	114.06
16	M	709	LMT	C3B-C4B-C5B	2.01	113.88	110.23
8	F	101	BCL	CHB-C1B-C2B	-2.01	121.59	127.43
8	G	102	BCL	CMD-C2D-C3D	-2.01	123.09	127.69
9	K	103	PGV	C02-O01-C1	-2.01	112.99	117.80
8	P	101	BCL	CHB-C1B-C2B	-2.01	121.60	127.43
8	W	102	BCL	C1C-NC-C4C	-2.00	105.77	106.68
8	S	102	BCL	CHB-C4A-NA	2.00	127.29	124.40

There are no chirality outliers.

All (1272) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	W	101	BCL	C1A-C2A-CAA-CBA
8	W	101	BCL	C4C-C3C-CAC-CBC
8	W	102	BCL	C2-C1-O2A-CGA
8	W	102	BCL	C2C-C3C-CAC-CBC
8	U	102	BCL	C2C-C3C-CAC-CBC
8	U	102	BCL	C2-C3-C5-C6
8	U	102	BCL	C4-C3-C5-C6
8	S	102	BCL	C4C-C3C-CAC-CBC
8	S	102	BCL	CHA-CBD-CGD-O1D
8	S	102	BCL	CHA-CBD-CGD-O2D
8	S	102	BCL	C11-C10-C8-C9
8	S	102	BCL	C11-C12-C13-C15
8	Q	102	BCL	C1A-C2A-CAA-CBA
8	Q	102	BCL	C2C-C3C-CAC-CBC
8	O	102	BCL	C2C-C3C-CAC-CBC
8	O	102	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	O	102	BCL	C2-C3-C5-C6
8	O	102	BCL	C4-C3-C5-C6
8	K	101	BCL	C4C-C3C-CAC-CBC
8	K	102	BCL	C1A-C2A-CAA-CBA
8	K	102	BCL	C2C-C3C-CAC-CBC
8	K	102	BCL	C4C-C3C-CAC-CBC
8	I	102	BCL	C2C-C3C-CAC-CBC
8	I	102	BCL	C4C-C3C-CAC-CBC
8	G	102	BCL	C1A-C2A-CAA-CBA
8	G	102	BCL	C2C-C3C-CAC-CBC
8	G	102	BCL	C4C-C3C-CAC-CBC
8	G	102	BCL	CHA-CBD-CGD-O2D
8	E	101	BCL	C1A-C2A-CAA-CBA
8	E	101	BCL	C2-C3-C5-C6
8	E	101	BCL	C4-C3-C5-C6
8	E	102	BCL	C4-C3-C5-C6
8	0	102	BCL	C2C-C3C-CAC-CBC
8	0	102	BCL	C4C-C3C-CAC-CBC
8	0	102	BCL	CHA-CBD-CGD-O1D
8	0	102	BCL	CHA-CBD-CGD-O2D
8	8	101	BCL	C11-C12-C13-C14
8	8	102	BCL	C2C-C3C-CAC-CBC
8	6	102	BCL	C2C-C3C-CAC-CBC
8	6	102	BCL	C4C-C3C-CAC-CBC
8	6	102	BCL	CBD-CGD-O2D-CED
8	4	101	BCL	C4C-C3C-CAC-CBC
8	4	101	BCL	C6-C7-C8-C9
8	2	102	BCL	C2C-C3C-CAC-CBC
8	2	102	BCL	C4C-C3C-CAC-CBC
8	2	102	BCL	CBD-CGD-O2D-CED
8	L	702	BCL	C1A-C2A-CAA-CBA
8	L	703	BCL	C1A-C2A-CAA-CBA
8	H	101	BCL	C2C-C3C-CAC-CBC
8	H	101	BCL	C4C-C3C-CAC-CBC
8	J	102	BCL	C4C-C3C-CAC-CBC
8	T	101	BCL	C2C-C3C-CAC-CBC
8	T	101	BCL	C4C-C3C-CAC-CBC
8	V	101	BCL	C1A-C2A-CAA-CBA
8	V	101	BCL	C3A-C2A-CAA-CBA
8	1	101	BCL	C1A-C2A-CAA-CBA
8	3	103	BCL	C1A-C2A-CAA-CBA
8	5	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
8	D	102	BCL	C1A-C2A-CAA-CBA
8	D	102	BCL	C2C-C3C-CAC-CBC
8	D	102	BCL	C4C-C3C-CAC-CBC
8	F	101	BCL	C1A-C2A-CAA-CBA
8	F	101	BCL	C3A-C2A-CAA-CBA
8	F	101	BCL	C4C-C3C-CAC-CBC
9	U	103	PGV	C03-O11-P-O12
9	U	103	PGV	C03-O11-P-O14
9	U	104	PGV	C03-O11-P-O13
9	U	104	PGV	C04-O12-P-O13
9	U	104	PGV	O01-C02-C03-O11
9	S	103	PGV	C04-O12-P-O11
9	O	103	PGV	C03-O11-P-O12
9	O	103	PGV	C04-O12-P-O11
9	K	103	PGV	C03-O11-P-O12
9	K	103	PGV	C04-O12-P-O11
9	K	103	PGV	O01-C02-C03-O11
9	K	104	PGV	C03-O11-P-O12
9	K	104	PGV	C03-O11-P-O14
9	K	104	PGV	C04-O12-P-O11
9	K	104	PGV	C04-O12-P-O14
9	K	104	PGV	C2-C1-O01-C02
9	I	103	PGV	C04-O12-P-O11
9	I	103	PGV	C04-O12-P-O14
9	E	103	PGV	C03-O11-P-O13
9	E	103	PGV	C04-O12-P-O13
9	E	104	PGV	C04-O12-P-O11
9	E	104	PGV	C04-O12-P-O13
9	0	104	PGV	C03-O11-P-O12
9	0	104	PGV	C03-O11-P-O13
9	0	104	PGV	C04-O12-P-O11
9	0	104	PGV	C04-O12-P-O13
9	6	103	PGV	C2-C1-O01-C02
9	4	102	PGV	C03-O11-P-O12
9	4	102	PGV	C04-O12-P-O13
9	4	102	PGV	O01-C02-C03-O11
9	M	705	PGV	C04-C05-C06-O06
9	L	706	PGV	C04-O12-P-O13
9	L	711	PGV	C04-O12-P-O11
9	L	711	PGV	C04-O12-P-O14
9	L	712	PGV	C03-O11-P-O12
9	L	712	PGV	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
9	h	102	PGV	C03-O11-P-O12
9	C	506	PGV	C03-O11-P-O12
9	C	506	PGV	C03-O11-P-O13
9	C	506	PGV	C03-O11-P-O14
9	C	506	PGV	O03-C01-C02-O01
10	J	101	U4Z	CAH-CAD-CAJ-CAL
11	M	702	BPH	C4C-C3C-CAC-CBC
11	M	702	BPH	C2C-C3C-CAC-CBC
11	L	701	BPH	C1-C2-C3-C5
11	L	704	BPH	O2A-C1-C2-C3
13	L	705	MQE	CBQ-CAX-CAY-CBL
15	M	708	PEF	C1-O3P-P-O1P
15	M	708	PEF	C1-O3P-P-O4P
15	M	708	PEF	C4-O4P-P-O1P
15	M	708	PEF	C4-O4P-P-O2P
15	M	708	PEF	C4-O4P-P-O3P
15	L	713	PEF	C11-C10-O2-C2
15	L	713	PEF	O4-C10-O2-C2
15	L	713	PEF	C4-O4P-P-O2P
15	L	717	PEF	C1-O3P-P-O1P
15	h	103	PEF	C1-O3P-P-O1P
15	h	103	PEF	C1-O3P-P-O2P
15	h	103	PEF	C1-O3P-P-O4P
15	h	103	PEF	C4-O4P-P-O3P
18	P	102	CDL	CA2-OA2-PA1-OA4
18	P	102	CDL	CA2-OA2-PA1-OA5
18	P	102	CDL	CB2-OB2-PB2-OB3
18	P	102	CDL	CB3-OB5-PB2-OB2
18	P	102	CDL	CB3-OB5-PB2-OB3
18	P	102	CDL	CB3-OB5-PB2-OB4
18	P	102	CDL	C51-CB5-OB6-CB4
19	h	101	LHG	C4-C5-C6-O8
19	h	101	LHG	O7-C5-C6-O8
19	h	101	LHG	C6-C5-O7-C7
19	h	101	LHG	O9-C7-O7-C5
20	C	501	HEC	C2B-C3B-CAB-CBB
20	C	501	HEC	C4B-C3B-CAB-CBB
20	C	501	HEC	C2C-C3C-CAC-CBC
20	C	501	HEC	C4C-C3C-CAC-CBC
20	C	502	HEC	C2B-C3B-CAB-CBB
20	C	502	HEC	C4B-C3B-CAB-CBB
20	C	502	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	C	503	HEC	C2B-C3B-CAB-CBB
20	C	503	HEC	C2C-C3C-CAC-CBC
20	C	503	HEC	C4C-C3C-CAC-CBC
20	C	504	HEC	C2B-C3B-CAB-CBB
20	C	504	HEC	C4B-C3B-CAB-CBB
20	C	504	HEC	C2C-C3C-CAC-CBC
8	K	102	BCL	O1D-CGD-O2D-CED
15	M	708	PEF	C11-C10-O2-C2
8	W	102	BCL	CBD-CGD-O2D-CED
8	U	102	BCL	CBD-CGD-O2D-CED
8	Q	102	BCL	CBD-CGD-O2D-CED
8	K	102	BCL	CBD-CGD-O2D-CED
8	I	102	BCL	CBD-CGD-O2D-CED
8	E	102	BCL	CBD-CGD-O2D-CED
8	4	101	BCL	CBD-CGD-O2D-CED
8	6	101	BCL	O1A-CGA-O2A-C1
8	2	102	BCL	O1D-CGD-O2D-CED
15	M	708	PEF	O4-C10-O2-C2
8	S	102	BCL	O1A-CGA-O2A-C1
9	K	104	PGV	O02-C1-O01-C02
9	6	103	PGV	O02-C1-O01-C02
18	P	102	CDL	OB7-CB5-OB6-CB4
8	W	102	BCL	C3-C5-C6-C7
8	U	101	BCL	C3-C5-C6-C7
8	E	102	BCL	C3-C5-C6-C7
8	B	101	BCL	C3-C5-C6-C7
8	0	102	BCL	C3-C5-C6-C7
8	6	101	BCL	C3-C5-C6-C7
8	6	102	BCL	C3-C5-C6-C7
8	R	102	BCL	C3-C5-C6-C7
8	V	101	BCL	C3-C5-C6-C7
8	5	101	BCL	C3-C5-C6-C7
8	S	101	BCL	CBA-CGA-O2A-C1
9	1	102	PGV	C20-C19-O03-C01
8	G	101	BCL	CBD-CGD-O2D-CED
8	B	101	BCL	CBD-CGD-O2D-CED
8	8	102	BCL	CBD-CGD-O2D-CED
8	1	101	BCL	CBD-CGD-O2D-CED
8	O	102	BCL	O1D-CGD-O2D-CED
8	E	102	BCL	O1D-CGD-O2D-CED
8	6	102	BCL	O1D-CGD-O2D-CED
8	W	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	G	102	BCL	C4-C3-C5-C6
8	0	102	BCL	C4-C3-C5-C6
8	6	102	BCL	C4-C3-C5-C6
8	4	101	BCL	C4-C3-C5-C6
8	L	703	BCL	C4-C3-C5-C6
8	G	102	BCL	C2-C3-C5-C6
8	E	102	BCL	C2-C3-C5-C6
8	0	102	BCL	C2-C3-C5-C6
8	6	102	BCL	C2-C3-C5-C6
8	4	101	BCL	C2-C3-C5-C6
8	L	703	BCL	C2-C3-C5-C6
16	H	102	LMT	C3'-C4'-O1B-C1B
8	U	102	BCL	O1D-CGD-O2D-CED
8	A	102	BCL	C2A-CAA-CBA-CGA
8	Q	101	BCL	O1A-CGA-O2A-C1
8	U	102	BCL	C3-C5-C6-C7
8	O	102	BCL	C3-C5-C6-C7
8	I	101	BCL	C3-C5-C6-C7
8	G	101	BCL	C3-C5-C6-C7
8	G	102	BCL	C3-C5-C6-C7
8	2	102	BCL	C3-C5-C6-C7
8	T	101	BCL	C3-C5-C6-C7
8	1	101	BCL	C3-C5-C6-C7
8	S	102	BCL	CBA-CGA-O2A-C1
8	Q	101	BCL	CBA-CGA-O2A-C1
8	0	101	BCL	CBA-CGA-O2A-C1
8	6	101	BCL	CBA-CGA-O2A-C1
8	2	101	BCL	CBA-CGA-O2A-C1
16	M	709	LMT	C3'-C4'-O1B-C1B
8	W	101	BCL	O1A-CGA-O2A-C1
8	S	101	BCL	O1A-CGA-O2A-C1
8	Q	102	BCL	O1D-CGD-O2D-CED
8	3	103	BCL	C3-C5-C6-C7
18	P	102	CDL	O1-C1-CB2-OB2
8	W	102	BCL	O1D-CGD-O2D-CED
8	I	102	BCL	O1D-CGD-O2D-CED
8	I	102	BCL	CBA-CGA-O2A-C1
8	A	101	BCL	CBA-CGA-O2A-C1
11	L	701	BPH	CBA-CGA-O2A-C1
9	1	102	PGV	O04-C19-O03-C01
8	H	101	BCL	C15-C16-C17-C18
8	E	101	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	3	101	BCL	CBD-CGD-O2D-CED
8	0	101	BCL	O1A-CGA-O2A-C1
8	8	102	BCL	C3-C5-C6-C7
11	L	701	BPH	CBD-CGD-O2D-CED
8	W	101	BCL	CBA-CGA-O2A-C1
8	V	101	BCL	C4-C3-C5-C6
13	M	704	MQE	CBA-CAU-CAZ-CBZ
8	V	101	BCL	C2-C3-C5-C6
13	M	704	MQE	CBA-CAU-CAZ-CBI
8	2	101	BCL	O1A-CGA-O2A-C1
13	M	704	MQE	CAR-CAE-CAL-CBF
8	M	701	BCL	CBD-CGD-O2D-CED
8	4	101	BCL	O1D-CGD-O2D-CED
8	A	101	BCL	O1A-CGA-O2A-C1
11	L	701	BPH	O1A-CGA-O2A-C1
16	M	709	LMT	O5'-C1'-O1'-C1
8	U	102	BCL	CBA-CGA-O2A-C1
8	8	101	BCL	CBA-CGA-O2A-C1
8	O	101	BCL	CBD-CGD-O2D-CED
8	L	702	BCL	CBD-CGD-O2D-CED
8	5	101	BCL	CBD-CGD-O2D-CED
8	A	102	BCL	CBD-CGD-O2D-CED
8	I	102	BCL	O1A-CGA-O2A-C1
8	G	102	BCL	CBD-CGD-O2D-CED
8	A	101	BCL	CBD-CGD-O2D-CED
11	M	702	BPH	CBD-CGD-O2D-CED
9	O	103	PGV	C2-C1-O01-C02
9	C	506	PGV	C2-C1-O01-C02
8	Q	102	BCL	C3-C5-C6-C7
8	U	102	BCL	O1A-CGA-O2A-C1
8	O	102	BCL	O1A-CGA-O2A-C1
8	8	101	BCL	O1A-CGA-O2A-C1
8	W	102	BCL	CBA-CGA-O2A-C1
8	O	101	BCL	CBA-CGA-O2A-C1
8	O	102	BCL	CBA-CGA-O2A-C1
8	K	102	BCL	CBA-CGA-O2A-C1
8	8	102	BCL	CBA-CGA-O2A-C1
8	2	102	BCL	CBA-CGA-O2A-C1
8	V	101	BCL	CBD-CGD-O2D-CED
8	8	102	BCL	O1D-CGD-O2D-CED
8	O	101	BCL	O1A-CGA-O2A-C1
11	M	702	BPH	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	W	102	BCL	C2-C3-C5-C6
11	M	702	BPH	C2-C3-C5-C6
11	L	704	BPH	CBD-CGD-O2D-CED
8	U	102	BCL	C11-C10-C8-C9
8	S	102	BCL	C14-C13-C15-C16
8	Q	101	BCL	C11-C12-C13-C14
8	Q	102	BCL	C11-C10-C8-C9
8	K	101	BCL	C6-C7-C8-C9
8	K	101	BCL	C11-C10-C8-C9
8	G	101	BCL	C11-C10-C8-C9
8	E	101	BCL	C11-C10-C8-C9
8	E	101	BCL	C11-C12-C13-C14
8	E	102	BCL	C6-C7-C8-C9
8	E	102	BCL	C11-C12-C13-C14
8	0	102	BCL	C6-C7-C8-C9
8	2	102	BCL	C11-C12-C13-C14
8	2	102	BCL	C14-C13-C15-C16
8	1	101	BCL	C6-C7-C8-C9
8	3	103	BCL	C6-C7-C8-C9
8	3	103	BCL	C11-C12-C13-C14
8	F	101	BCL	C11-C10-C8-C9
11	M	702	BPH	C11-C10-C8-C9
11	M	702	BPH	C11-C12-C13-C14
11	M	702	BPH	C14-C13-C15-C16
16	M	709	LMT	C4'-C5'-C6'-O6'
16	M	709	LMT	C2'-C1'-O1'-C1
9	C	506	PGV	O12-C04-C05-O05
8	2	102	BCL	O1A-CGA-O2A-C1
16	M	709	LMT	O5'-C5'-C6'-O6'
8	G	101	BCL	O1D-CGD-O2D-CED
8	W	102	BCL	O1A-CGA-O2A-C1
8	K	102	BCL	C3-C5-C6-C7
8	3	101	BCL	C3-C5-C6-C7
16	T	102	LMT	C3'-C4'-O1B-C1B
9	0	104	PGV	O01-C02-C03-O11
8	4	101	BCL	CBA-CGA-O2A-C1
8	H	101	BCL	C8-C10-C11-C12
9	K	103	PGV	C19-C20-C21-C22
8	1	101	BCL	O1D-CGD-O2D-CED
9	h	102	PGV	C26-C27-C28-C29
8	1	101	BCL	C10-C11-C12-C13
8	4	101	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	B	101	BCL	O1D-CGD-O2D-CED
8	J	102	BCL	CBD-CGD-O2D-CED
8	Q	102	BCL	C6-C7-C8-C10
8	2	102	BCL	C11-C10-C8-C7
14	L	715	BGL	O2-C1'-C2'-C3'
8	U	101	BCL	C4-C3-C5-C6
9	O	103	PGV	O02-C1-O01-C02
9	C	506	PGV	O02-C1-O01-C02
8	D	102	BCL	C3-C5-C6-C7
8	W	101	BCL	C5-C6-C7-C8
8	M	701	BCL	C15-C16-C17-C18
16	T	102	LMT	C5'-C4'-O1B-C1B
9	I	103	PGV	C19-C20-C21-C22
8	K	102	BCL	O1A-CGA-O2A-C1
8	4	101	BCL	O1A-CGA-O2A-C1
8	Q	101	BCL	C8-C10-C11-C12
8	E	101	BCL	C10-C11-C12-C13
8	B	101	BCL	C5-C6-C7-C8
8	P	101	BCL	C8-C10-C11-C12
8	7	101	BCL	C5-C6-C7-C8
8	F	101	BCL	C15-C16-C17-C18
8	K	102	BCL	C2A-CAA-CBA-CGA
8	J	102	BCL	C2A-CAA-CBA-CGA
8	U	101	BCL	C10-C11-C12-C13
8	I	101	BCL	C15-C16-C17-C18
8	8	101	BCL	C13-C15-C16-C17
8	6	102	BCL	C13-C15-C16-C17
8	2	102	BCL	C13-C15-C16-C17
8	N	101	BCL	C10-C11-C12-C13
8	A	101	BCL	C10-C11-C12-C13
8	A	102	BCL	C13-C15-C16-C17
8	D	102	BCL	C15-C16-C17-C18
8	F	101	BCL	C8-C10-C11-C12
11	M	702	BPH	C13-C15-C16-C17
9	4	102	PGV	C19-C20-C21-C22
9	C	506	PGV	C1-C2-C3-C4
8	I	101	BCL	CBD-CGD-O2D-CED
8	S	102	BCL	C10-C11-C12-C13
8	K	102	BCL	C15-C16-C17-C18
8	I	102	BCL	C10-C11-C12-C13
8	E	101	BCL	C8-C10-C11-C12
8	E	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	6	101	BCL	C10-C11-C12-C13
8	L	703	BCL	C15-C16-C17-C18
8	1	101	BCL	C5-C6-C7-C8
8	3	101	BCL	C13-C15-C16-C17
8	3	101	BCL	C15-C16-C17-C18
8	F	101	BCL	C5-C6-C7-C8
16	1	104	LMT	C5'-C4'-O1B-C1B
8	G	101	BCL	C8-C10-C11-C12
8	E	102	BCL	C15-C16-C17-C18
8	H	101	BCL	C5-C6-C7-C8
8	Q	102	BCL	C13-C15-C16-C17
8	G	102	BCL	C8-C10-C11-C12
8	0	102	BCL	C15-C16-C17-C18
8	8	102	BCL	C5-C6-C7-C8
8	8	102	BCL	O1A-CGA-O2A-C1
8	W	101	BCL	C15-C16-C17-C18
8	P	101	BCL	C13-C15-C16-C17
8	5	101	BCL	C13-C15-C16-C17
8	I	101	BCL	CBA-CGA-O2A-C1
8	G	102	BCL	CBA-CGA-O2A-C1
8	O	101	BCL	C3-C5-C6-C7
15	h	103	PEF	C35-C36-C37-C38
8	E	101	BCL	C2A-CAA-CBA-CGA
8	9	101	BCL	C2A-CAA-CBA-CGA
11	L	701	BPH	C2A-CAA-CBA-CGA
8	3	103	BCL	CBA-CGA-O2A-C1
18	P	102	CDL	C71-CB7-OB8-CB6
8	U	101	BCL	C13-C15-C16-C17
8	G	101	BCL	C5-C6-C7-C8
8	E	102	BCL	C5-C6-C7-C8
8	6	102	BCL	C8-C10-C11-C12
8	2	101	BCL	C5-C6-C7-C8
8	2	101	BCL	C10-C11-C12-C13
8	M	701	BCL	C10-C11-C12-C13
8	M	701	BCL	C13-C15-C16-C17
8	5	101	BCL	C10-C11-C12-C13
11	L	704	BPH	C10-C11-C12-C13
8	9	101	BCL	CBD-CGD-O2D-CED
8	W	101	BCL	C8-C10-C11-C12
8	N	101	BCL	C8-C10-C11-C12
16	1	104	LMT	C3'-C4'-O1B-C1B
8	3	101	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
8	Q	102	BCL	C10-C11-C12-C13
8	0	101	BCL	C10-C11-C12-C13
8	6	101	BCL	C13-C15-C16-C17
11	L	701	BPH	O1D-CGD-O2D-CED
8	2	101	BCL	C3-C5-C6-C7
9	1	102	PGV	C2-C1-O01-C02
8	Q	102	BCL	C11-C12-C13-C14
8	D	102	BCL	C14-C13-C15-C16
8	E	101	BCL	O1D-CGD-O2D-CED
9	I	103	PGV	O12-C04-C05-O05
9	0	105	PGV	O12-C04-C05-O05
8	J	102	BCL	CBA-CGA-O2A-C1
8	8	102	BCL	C16-C17-C18-C19
8	A	101	BCL	C16-C17-C18-C20
8	0	101	BCL	C15-C16-C17-C18
8	U	102	BCL	C5-C6-C7-C8
8	G	102	BCL	C10-C11-C12-C13
8	I	101	BCL	O1A-CGA-O2A-C1
8	W	101	BCL	C2A-CAA-CBA-CGA
8	2	101	BCL	C2A-CAA-CBA-CGA
8	3	103	BCL	C2A-CAA-CBA-CGA
16	M	709	LMT	C5'-C4'-O1B-C1B
8	U	102	BCL	C15-C16-C17-C18
8	I	102	BCL	C8-C10-C11-C12
8	E	102	BCL	C10-C11-C12-C13
8	P	101	BCL	C5-C6-C7-C8
8	5	101	BCL	C5-C6-C7-C8
9	K	104	PGV	C04-C05-C06-O06
9	L	706	PGV	C04-C05-C06-O06
18	P	102	CDL	CB6-CB4-OB6-CB5
8	G	102	BCL	C16-C17-C18-C20
8	B	101	BCL	C16-C17-C18-C20
8	H	101	BCL	C16-C17-C18-C19
8	N	101	BCL	C16-C17-C18-C19
16	D	104	LMT	O5'-C1'-O1'-C1
8	U	101	BCL	C2-C3-C5-C6
8	G	101	BCL	CBA-CGA-O2A-C1
8	I	101	BCL	C16-C17-C18-C19
8	8	102	BCL	C16-C17-C18-C20
8	L	702	BCL	C16-C17-C18-C19
8	3	103	BCL	C16-C17-C18-C19
14	Y	103	BGL	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
9	h	102	PGV	C27-C28-C29-C30
16	D	104	LMT	C5-C6-C7-C8
8	S	101	BCL	C10-C11-C12-C13
9	1	102	PGV	O02-C1-O01-C02
9	K	104	PGV	O05-C05-C06-O06
9	M	705	PGV	O05-C05-C06-O06
9	O	103	PGV	C20-C21-C22-C23
8	M	701	BCL	O1D-CGD-O2D-CED
8	5	101	BCL	O1D-CGD-O2D-CED
9	S	103	PGV	C5-C6-C7-C8
8	Q	102	BCL	C16-C17-C18-C20
8	I	101	BCL	C16-C17-C18-C20
8	B	101	BCL	C16-C17-C18-C19
8	L	702	BCL	C16-C17-C18-C20
8	H	101	BCL	C16-C17-C18-C20
8	N	101	BCL	C16-C17-C18-C20
8	G	102	BCL	O1A-CGA-O2A-C1
9	0	105	PGV	C2-C3-C4-C5
8	O	101	BCL	C10-C11-C12-C13
18	P	102	CDL	C11-CA5-OA6-CA4
8	W	101	BCL	C6-C7-C8-C10
8	E	102	BCL	C12-C13-C15-C16
8	V	101	BCL	C11-C10-C8-C7
8	1	101	BCL	C11-C12-C13-C15
8	Q	102	BCL	C8-C10-C11-C12
8	A	102	BCL	C10-C11-C12-C13
16	H	102	LMT	O5B-C5B-C6B-O6B
9	8	103	PGV	C6-C7-C8-C9
8	J	102	BCL	O1A-CGA-O2A-C1
8	3	103	BCL	O1A-CGA-O2A-C1
8	L	702	BCL	C3-C5-C6-C7
8	S	102	BCL	C3A-C2A-CAA-CBA
8	Q	102	BCL	C3A-C2A-CAA-CBA
8	I	102	BCL	C3A-C2A-CAA-CBA
8	G	102	BCL	C3A-C2A-CAA-CBA
8	E	102	BCL	C3A-C2A-CAA-CBA
8	B	101	BCL	C3A-C2A-CAA-CBA
8	L	702	BCL	C3A-C2A-CAA-CBA
8	L	703	BCL	C3A-C2A-CAA-CBA
8	J	102	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	C3A-C2A-CAA-CBA
8	1	101	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	3	103	BCL	C3A-C2A-CAA-CBA
8	9	101	BCL	C3A-C2A-CAA-CBA
8	D	102	BCL	C3A-C2A-CAA-CBA
11	L	701	BPH	C3A-C2A-CAA-CBA
8	W	102	BCL	C5-C6-C7-C8
8	H	101	BCL	C13-C15-C16-C17
8	T	101	BCL	C15-C16-C17-C18
8	D	102	BCL	C16-C17-C18-C19
9	O	103	PGV	C29-C30-C31-C32
15	L	717	PEF	C17-C18-C19-C20
9	U	104	PGV	C20-C21-C22-C23
8	S	101	BCL	C3-C5-C6-C7
9	E	103	PGV	C1-C2-C3-C4
9	8	103	PGV	C1-C2-C3-C4
19	h	101	LHG	C33-C34-C35-C36
18	P	102	CDL	OB9-CB7-OB8-CB6
9	h	102	PGV	C24-C25-C26-C27
15	L	713	PEF	C37-C38-C39-C40
9	K	103	PGV	C29-C30-C31-C32
19	h	101	LHG	C23-C24-C25-C26
16	D	104	LMT	O5'-C5'-C6'-O6'
10	0	103	U4Z	CAH-CAD-CAJ-CAL
10	J	101	U4Z	CAB-CAD-CAJ-CAL
10	R	101	U4Z	CAH-CAD-CAJ-CAL
10	3	102	U4Z	CAB-CAD-CAJ-CAL
10	3	102	U4Z	CAH-CAD-CAJ-CAL
10	D	101	U4Z	CAB-CAD-CAJ-CAL
10	D	101	U4Z	CAH-CAD-CAJ-CAL
8	A	102	BCL	O1D-CGD-O2D-CED
8	W	102	BCL	C8-C10-C11-C12
8	0	102	BCL	C5-C6-C7-C8
8	V	101	BCL	C13-C15-C16-C17
8	V	101	BCL	C15-C16-C17-C18
9	C	506	PGV	C20-C21-C22-C23
8	O	101	BCL	O1D-CGD-O2D-CED
9	U	103	PGV	C27-C28-C29-C30
8	G	101	BCL	O1A-CGA-O2A-C1
9	I	103	PGV	C25-C26-C27-C28
18	P	102	CDL	OA7-CA5-OA6-CA4
9	8	103	PGV	C20-C21-C22-C23
14	Y	103	BGL	C4'-C5'-C6'-C7'
15	h	103	PEF	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
8	V	101	BCL	C16-C17-C18-C20
9	E	104	PGV	C27-C28-C29-C30
9	U	104	PGV	C29-C30-C31-C32
16	1	104	LMT	C3-C4-C5-C6
16	D	104	LMT	C3-C4-C5-C6
8	O	101	BCL	C8-C10-C11-C12
8	K	102	BCL	C5-C6-C7-C8
8	T	101	BCL	C13-C15-C16-C17
9	0	105	PGV	C1-C2-C3-C4
16	H	102	LMT	C5'-C4'-O1B-C1B
9	U	103	PGV	C22-C23-C24-C25
8	S	102	BCL	C5-C6-C7-C8
8	R	102	BCL	C10-C11-C12-C13
11	M	702	BPH	C10-C11-C12-C13
9	L	712	PGV	C19-C20-C21-C22
9	0	104	PGV	C20-C21-C22-C23
13	L	705	MQE	CBK-CAX-CAY-CBL
9	E	103	PGV	C28-C29-C30-C31
9	E	104	PGV	C6-C7-C8-C9
8	K	101	BCL	C10-C11-C12-C13
8	V	101	BCL	C5-C6-C7-C8
8	I	102	BCL	C2A-CAA-CBA-CGA
8	4	101	BCL	C16-C17-C18-C19
8	4	101	BCL	C16-C17-C18-C20
8	V	101	BCL	C16-C17-C18-C19
15	L	717	PEF	C15-C16-C17-C18
9	O	103	PGV	C28-C29-C30-C31
19	h	101	LHG	C32-C33-C34-C35
8	G	102	BCL	O1D-CGD-O2D-CED
8	R	102	BCL	C8-C10-C11-C12
9	0	105	PGV	C27-C28-C29-C30
9	C	506	PGV	C22-C23-C24-C25
8	6	102	BCL	C5-C6-C7-C8
9	E	103	PGV	O01-C02-C03-O11
9	L	706	PGV	C2-C1-O01-C02
8	N	101	BCL	C15-C16-C17-C18
8	A	102	BCL	C15-C16-C17-C18
8	Q	102	BCL	C16-C17-C18-C19
8	G	102	BCL	C16-C17-C18-C19
8	0	102	BCL	C13-C15-C16-C17
8	N	101	BCL	C5-C6-C7-C8
8	9	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
11	M	702	BPH	O1D-CGD-O2D-CED
15	L	713	PEF	O2-C2-C3-O3
9	L	711	PGV	C20-C19-O03-C01
9	L	712	PGV	C20-C19-O03-C01
9	L	706	PGV	C21-C22-C23-C24
8	O	102	BCL	C5-C6-C7-C8
9	I	103	PGV	C6-C7-C8-C9
14	L	708	BGL	O5-C5-C6-O6
14	L	714	BGL	O5-C5-C6-O6
8	A	101	BCL	C16-C17-C18-C19
8	8	101	BCL	C10-C11-C12-C13
8	7	101	BCL	C15-C16-C17-C18
8	B	101	BCL	C2-C3-C5-C6
18	P	102	CDL	CA2-C1-CB2-OB2
8	Q	101	BCL	C10-C11-C12-C13
8	I	101	BCL	C2A-CAA-CBA-CGA
8	V	101	BCL	O1D-CGD-O2D-CED
8	3	103	BCL	C5-C6-C7-C8
8	A	101	BCL	O1D-CGD-O2D-CED
9	C	506	PGV	C2-C3-C4-C5
9	K	103	PGV	C30-C31-C32-C33
8	S	102	BCL	C1A-C2A-CAA-CBA
8	O	102	BCL	C1A-C2A-CAA-CBA
8	I	102	BCL	C1A-C2A-CAA-CBA
8	E	102	BCL	C1A-C2A-CAA-CBA
8	B	101	BCL	C1A-C2A-CAA-CBA
8	0	102	BCL	C1A-C2A-CAA-CBA
8	J	102	BCL	C1A-C2A-CAA-CBA
8	P	101	BCL	C1A-C2A-CAA-CBA
8	9	101	BCL	C1A-C2A-CAA-CBA
8	B	101	BCL	C8-C10-C11-C12
9	0	104	PGV	C01-C02-C03-O11
9	C	506	PGV	C01-C02-C03-O11
15	L	713	PEF	O3P-C1-C2-C3
8	N	101	BCL	C3-C5-C6-C7
8	U	102	BCL	C11-C10-C8-C7
8	S	101	BCL	C11-C12-C13-C15
8	S	102	BCL	C12-C13-C15-C16
8	O	101	BCL	C11-C10-C8-C7
8	K	102	BCL	C11-C10-C8-C7
8	I	102	BCL	C6-C7-C8-C10
8	E	102	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
8	2	102	BCL	C6-C7-C8-C10
8	2	102	BCL	C12-C13-C15-C16
8	M	701	BCL	C6-C7-C8-C10
8	H	101	BCL	C11-C10-C8-C7
8	V	101	BCL	C6-C7-C8-C10
8	3	101	BCL	C12-C13-C15-C16
8	3	103	BCL	C6-C7-C8-C10
8	9	101	BCL	C6-C7-C8-C10
8	A	101	BCL	C11-C10-C8-C7
11	M	702	BPH	C11-C12-C13-C15
11	M	702	BPH	C12-C13-C15-C16
8	W	101	BCL	C2C-C3C-CAC-CBC
8	S	102	BCL	C2C-C3C-CAC-CBC
8	4	101	BCL	C2C-C3C-CAC-CBC
8	J	102	BCL	C2C-C3C-CAC-CBC
8	R	102	BCL	C2C-C3C-CAC-CBC
8	5	101	BCL	C2C-C3C-CAC-CBC
8	9	101	BCL	C2C-C3C-CAC-CBC
8	F	101	BCL	C2C-C3C-CAC-CBC
9	O	103	PGV	C5-C6-C7-C8
9	S	103	PGV	C28-C29-C30-C31
8	Q	101	BCL	C4-C3-C5-C6
11	L	701	BPH	C13-C15-C16-C17
8	K	102	BCL	C4B-C3B-CAB-OB
8	8	101	BCL	C2A-CAA-CBA-CGA
8	U	102	BCL	C11-C12-C13-C14
8	S	101	BCL	C14-C13-C15-C16
8	O	101	BCL	C11-C10-C8-C9
8	O	102	BCL	C6-C7-C8-C9
8	0	102	BCL	C11-C12-C13-C14
8	6	102	BCL	C6-C7-C8-C9
8	M	701	BCL	C6-C7-C8-C9
8	L	702	BCL	C14-C13-C15-C16
8	V	101	BCL	C11-C10-C8-C9
8	9	101	BCL	C6-C7-C8-C9
8	A	101	BCL	C11-C10-C8-C9
14	Y	103	BGL	O5-C5-C6-O6
8	J	102	BCL	O1D-CGD-O2D-CED
9	U	104	PGV	C23-C24-C25-C26
8	6	102	BCL	C15-C16-C17-C18
11	L	704	BPH	O1D-CGD-O2D-CED
8	Q	102	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	h	103	PEF	C34-C35-C36-C37
14	H	103	BGL	O5-C5-C6-O6
14	Y	101	BGL	O5-C5-C6-O6
9	U	104	PGV	C26-C27-C28-C29
16	H	102	LMT	O5'-C5'-C6'-O6'
19	h	101	LHG	C25-C26-C27-C28
8	2	102	BCL	C10-C11-C12-C13
9	E	103	PGV	C19-C20-C21-C22
8	B	101	BCL	C4-C3-C5-C6
8	U	102	BCL	C10-C11-C12-C13
8	I	102	BCL	C13-C15-C16-C17
9	6	103	PGV	C30-C31-C32-C33
16	T	102	LMT	O5'-C5'-C6'-O6'
8	U	102	BCL	C8-C10-C11-C12
9	1	102	PGV	C03-O11-P-O13
9	h	102	PGV	C03-O11-P-O13
9	L	712	PGV	C22-C23-C24-C25
8	P	101	BCL	C15-C16-C17-C18
8	S	101	BCL	O2A-C1-C2-C3
8	W	101	BCL	C13-C15-C16-C17
8	L	702	BCL	O1D-CGD-O2D-CED
9	O	103	PGV	O01-C02-C03-O11
11	L	704	BPH	C4-C3-C5-C6
8	Q	101	BCL	C2-C3-C5-C6
11	L	704	BPH	C2-C3-C5-C6
8	U	101	BCL	C16-C17-C18-C19
9	K	104	PGV	C24-C25-C26-C27
14	L	708	BGL	C4'-C5'-C6'-C7'
9	8	103	PGV	C5-C6-C7-C8
9	L	712	PGV	O04-C19-O03-C01
8	I	101	BCL	O1D-CGD-O2D-CED
8	F	101	BCL	CBA-CGA-O2A-C1
8	Q	102	BCL	C15-C16-C17-C18
8	M	701	BCL	C16-C17-C18-C19
11	M	702	BPH	C16-C17-C18-C19
8	W	101	BCL	C4-C3-C5-C6
8	K	101	BCL	C4-C3-C5-C6
8	F	101	BCL	C4-C3-C5-C6
10	D	101	U4Z	CAT-CAS-CAW-CAZ
8	0	102	BCL	CBA-CGA-O2A-C1
11	M	702	BPH	CBA-CGA-O2A-C1
15	h	103	PEF	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
16	M	709	LMT	C2-C1-O1'-C1'
8	S	101	BCL	C11-C12-C13-C14
8	K	102	BCL	C11-C10-C8-C9
8	I	102	BCL	C6-C7-C8-C9
8	G	102	BCL	C14-C13-C15-C16
8	B	101	BCL	C14-C13-C15-C16
8	2	101	BCL	C11-C12-C13-C14
8	2	102	BCL	C6-C7-C8-C9
8	H	101	BCL	C11-C10-C8-C9
8	V	101	BCL	C6-C7-C8-C9
8	3	101	BCL	C14-C13-C15-C16
8	5	101	BCL	C11-C10-C8-C9
11	M	702	BPH	C6-C7-C8-C9
9	U	103	PGV	C7-C8-C9-C10
16	T	102	LMT	C6-C7-C8-C9
8	9	101	BCL	O1D-CGD-O2D-CED
8	9	101	BCL	C5-C6-C7-C8
9	L	711	PGV	O04-C19-O03-C01
8	D	102	BCL	C16-C17-C18-C20
9	U	104	PGV	C01-C02-C03-O11
9	E	103	PGV	C01-C02-C03-O11
9	L	712	PGV	C01-C02-C03-O11
18	P	102	CDL	OB5-CB3-CB4-CB6
8	U	101	BCL	C6-C7-C8-C10
8	U	102	BCL	C11-C12-C13-C15
8	S	101	BCL	C12-C13-C15-C16
8	O	102	BCL	C6-C7-C8-C10
8	G	102	BCL	C12-C13-C15-C16
8	B	101	BCL	C12-C13-C15-C16
8	0	102	BCL	C11-C12-C13-C15
8	6	102	BCL	C6-C7-C8-C10
8	4	101	BCL	C6-C7-C8-C10
8	2	101	BCL	C11-C12-C13-C15
8	L	702	BCL	C11-C10-C8-C7
8	L	702	BCL	C12-C13-C15-C16
11	M	702	BPH	C6-C7-C8-C10
11	M	702	BPH	C11-C10-C8-C7
8	2	102	BCL	C15-C16-C17-C18
8	G	102	BCL	C13-C15-C16-C17
8	G	101	BCL	C4-C3-C5-C6
8	M	701	BCL	C3A-C2A-CAA-CBA
8	H	101	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	A	101	BCL	C4-C3-C5-C6
13	M	704	MQE	CAL-CAE-CAR-CBV
13	M	704	MQE	CAL-CAE-CAR-CBD
19	h	101	LHG	C34-C35-C36-C37
8	3	103	BCL	C16-C17-C18-C20
16	M	709	LMT	C7-C8-C9-C10
8	G	101	BCL	C10-C11-C12-C13
9	h	102	PGV	C20-C21-C22-C23
9	O	103	PGV	O03-C01-C02-C03
9	6	103	PGV	O03-C01-C02-C03
9	L	712	PGV	O03-C01-C02-C03
15	L	713	PEF	C1-C2-C3-O3
18	P	102	CDL	CA3-CA4-CA6-OA8
9	K	104	PGV	C4-C5-C6-C7
8	U	101	BCL	C16-C17-C18-C20
8	L	702	BCL	C13-C15-C16-C17
9	L	712	PGV	C27-C28-C29-C30
11	L	701	BPH	C1-C2-C3-C4
11	L	704	BPH	C1-C2-C3-C4
9	E	104	PGV	C2-C3-C4-C5
8	N	101	BCL	C4-C3-C5-C6
9	C	506	PGV	C19-C20-C21-C22
8	K	101	BCL	C2-C3-C5-C6
8	A	101	BCL	C2-C3-C5-C6
8	F	101	BCL	C2-C3-C5-C6
10	D	101	U4Z	CAT-CAS-CAW-CBA
11	M	702	BPH	C16-C17-C18-C20
9	O	103	PGV	C19-C20-C21-C22
9	h	102	PGV	O01-C02-C03-O11
15	h	103	PEF	O3P-C1-C2-O2
8	L	702	BCL	C15-C16-C17-C18
9	0	104	PGV	C26-C27-C28-C29
8	G	101	BCL	C15-C16-C17-C18
16	T	102	LMT	C11-C10-C9-C8
8	E	102	BCL	C16-C17-C18-C19
9	O	103	PGV	O03-C01-C02-O01
9	L	712	PGV	O03-C01-C02-O01
18	P	102	CDL	OA6-CA4-CA6-OA8
9	L	706	PGV	O02-C1-O01-C02
9	0	104	PGV	C1-C2-C3-C4
8	W	101	BCL	C2-C3-C5-C6
8	G	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	N	101	BCL	C2-C3-C5-C6
11	M	702	BPH	C1-C2-C3-C5
11	L	704	BPH	C1-C2-C3-C5
8	S	102	BCL	C16-C17-C18-C20
8	M	701	BCL	C16-C17-C18-C20
16	T	102	LMT	C5-C6-C7-C8
8	R	102	BCL	C11-C10-C8-C9
8	V	101	BCL	C11-C12-C13-C14
9	L	711	PGV	C24-C25-C26-C27
9	K	103	PGV	C7-C8-C9-C10
8	U	102	BCL	C4C-C3C-CAC-CBC
8	O	102	BCL	C4C-C3C-CAC-CBC
8	G	101	BCL	C4C-C3C-CAC-CBC
8	8	102	BCL	C4C-C3C-CAC-CBC
8	L	702	BCL	C4C-C3C-CAC-CBC
8	R	102	BCL	C4C-C3C-CAC-CBC
8	5	101	BCL	C4C-C3C-CAC-CBC
8	9	101	BCL	C4C-C3C-CAC-CBC
19	h	101	LHG	C27-C28-C29-C30
8	B	101	BCL	C10-C11-C12-C13
8	0	102	BCL	C8-C10-C11-C12
11	M	702	BPH	O1A-CGA-O2A-C1
9	0	104	PGV	C27-C28-C29-C30
9	8	103	PGV	C31-C32-C33-C34
8	6	102	BCL	CBA-CGA-O2A-C1
9	I	103	PGV	C27-C28-C29-C30
9	1	102	PGV	C2-C3-C4-C5
9	K	103	PGV	C01-C02-C03-O11
9	L	706	PGV	C01-C02-C03-O11
9	L	711	PGV	C01-C02-C03-O11
9	h	102	PGV	C01-C02-C03-O11
8	E	102	BCL	C13-C15-C16-C17
8	W	102	BCL	C6-C7-C8-C10
8	U	102	BCL	C6-C7-C8-C10
8	S	101	BCL	C6-C7-C8-C10
8	G	101	BCL	C11-C10-C8-C7
8	0	101	BCL	C12-C13-C15-C16
8	R	102	BCL	C11-C10-C8-C7
8	V	101	BCL	C11-C12-C13-C15
8	7	101	BCL	C11-C10-C8-C7
15	L	713	PEF	C31-C30-O3-C3
14	Y	101	BGL	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
8	0	102	BCL	O1A-CGA-O2A-C1
8	F	101	BCL	O1A-CGA-O2A-C1
8	P	101	BCL	C3-C5-C6-C7
8	J	102	BCL	C8-C10-C11-C12
8	J	102	BCL	C13-C15-C16-C17
8	H	101	BCL	C10-C11-C12-C13
9	L	706	PGV	O01-C02-C03-O11
9	L	711	PGV	O01-C02-C03-O11
9	C	506	PGV	O01-C02-C03-O11
15	L	713	PEF	O3P-C1-C2-O2
9	8	103	PGV	O03-C01-C02-C03
9	S	103	PGV	C19-C20-C21-C22
8	V	101	BCL	C8-C10-C11-C12
8	T	101	BCL	CBA-CGA-O2A-C1
8	E	101	BCL	C5-C6-C7-C8
9	L	706	PGV	O03-C01-C02-O01
8	L	703	BCL	C8-C10-C11-C12
8	O	101	BCL	C16-C17-C18-C20
15	L	717	PEF	C13-C14-C15-C16
19	h	101	LHG	C30-C31-C32-C33
9	6	103	PGV	C20-C21-C22-C23
14	M	706	BGL	C3'-C4'-C5'-C6'
9	U	103	PGV	C23-C24-C25-C26
8	6	102	BCL	O1A-CGA-O2A-C1
9	K	104	PGV	C27-C28-C29-C30
8	6	102	BCL	C16-C17-C18-C20
16	H	102	LMT	C5-C6-C7-C8
10	3	102	U4Z	CAT-CAS-CAW-CAZ
8	7	101	BCL	C3-C5-C6-C7
9	I	103	PGV	O12-C04-C05-C06
18	P	102	CDL	CB2-C1-CA2-OA2
15	L	713	PEF	O5-C30-O3-C3
14	L	714	BGL	C1'-C2'-C3'-C4'
8	7	101	BCL	C16-C17-C18-C19
9	U	104	PGV	C19-C20-C21-C22
9	I	103	PGV	C24-C25-C26-C27
8	S	102	BCL	C16-C17-C18-C19
9	0	104	PGV	C19-C20-C21-C22
8	H	101	BCL	C1A-C2A-CAA-CBA
8	1	101	BCL	C4-C3-C5-C6
8	7	101	BCL	C4-C3-C5-C6
9	8	103	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
8	Q	101	BCL	C16-C17-C18-C19
15	L	713	PEF	C18-C19-C20-C21
9	4	102	PGV	C01-C02-C03-O11
15	h	103	PEF	O3P-C1-C2-C3
8	K	101	BCL	CBD-CGD-O2D-CED
15	h	103	PEF	C38-C39-C40-C41
8	W	102	BCL	C11-C12-C13-C15
8	G	102	BCL	C11-C12-C13-C15
8	2	102	BCL	C11-C12-C13-C15
8	L	703	BCL	C12-C13-C15-C16
8	J	102	BCL	C11-C10-C8-C7
8	N	101	BCL	C12-C13-C15-C16
8	T	101	BCL	C6-C7-C8-C10
8	7	101	BCL	C12-C13-C15-C16
8	F	101	BCL	C6-C7-C8-C10
8	F	101	BCL	C11-C10-C8-C7
11	L	701	BPH	C6-C7-C8-C10
8	E	102	BCL	C16-C17-C18-C20
9	0	104	PGV	C30-C31-C32-C33
8	T	101	BCL	O1A-CGA-O2A-C1
9	K	103	PGV	C5-C6-C7-C8
8	L	703	BCL	C2C-C3C-CAC-CBC
8	P	101	BCL	C2C-C3C-CAC-CBC
9	0	105	PGV	C30-C31-C32-C33
16	D	104	LMT	O1'-C1-C2-C3
8	4	101	BCL	C5-C6-C7-C8
8	I	102	BCL	C4-C3-C5-C6
20	C	502	HEC	C4C-C3C-CAC-CBC
20	C	503	HEC	C4B-C3B-CAB-CBB
20	C	504	HEC	C4C-C3C-CAC-CBC
8	F	101	BCL	C16-C17-C18-C20
9	U	104	PGV	C24-C25-C26-C27
16	M	709	LMT	O1'-C1-C2-C3
9	L	712	PGV	O01-C02-C03-O11
8	K	102	BCL	C4B-C3B-CAB-CBB
8	U	101	BCL	C6-C7-C8-C9
8	S	101	BCL	C6-C7-C8-C9
8	Q	102	BCL	C6-C7-C8-C9
8	0	101	BCL	C14-C13-C15-C16
8	2	102	BCL	C11-C10-C8-C9
8	7	101	BCL	C11-C10-C8-C9
15	h	103	PEF	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
9	1	102	PGV	C22-C23-C24-C25
9	6	103	PGV	O03-C01-C02-O01
9	U	103	PGV	C6-C7-C8-C9
8	0	101	BCL	C13-C15-C16-C17
8	R	102	BCL	C15-C16-C17-C18
9	8	103	PGV	C4-C5-C6-C7
9	C	506	PGV	O03-C01-C02-C03
16	M	709	LMT	C6-C7-C8-C9
8	2	101	BCL	CBD-CGD-O2D-CED
8	M	701	BCL	CAD-CBD-CGD-O2D
9	0	104	PGV	C5-C6-C7-C8
8	O	102	BCL	C16-C17-C18-C19
8	S	101	BCL	C15-C16-C17-C18
8	W	102	BCL	CHA-CBD-CGD-O1D
8	W	102	BCL	CHA-CBD-CGD-O2D
8	G	102	BCL	CHA-CBD-CGD-O1D
8	M	701	BCL	CAD-CBD-CGD-O1D
8	1	101	BCL	CHA-CBD-CGD-O2D
9	U	103	PGV	C04-O12-P-O11
9	U	103	PGV	C04-O12-P-O14
9	S	103	PGV	C04-O12-P-O13
9	O	103	PGV	C03-O11-P-O13
9	O	103	PGV	C04-O12-P-O13
9	K	103	PGV	C03-O11-P-O13
9	K	103	PGV	C04-O12-P-O13
9	8	103	PGV	C04-O12-P-O13
9	6	103	PGV	C04-O12-P-O13
9	4	102	PGV	C03-O11-P-O13
9	4	102	PGV	C04-O12-P-O11
9	M	705	PGV	C03-O11-P-O13
9	M	705	PGV	C04-O12-P-O13
9	L	712	PGV	C03-O11-P-O13
9	C	506	PGV	C04-O12-P-O13
15	M	708	PEF	C1-O3P-P-O2P
15	L	713	PEF	C4-O4P-P-O1P
15	L	713	PEF	C4-O4P-P-O3P
15	L	717	PEF	C1-O3P-P-O2P
15	h	103	PEF	C4-O4P-P-O1P
8	S	101	BCL	C13-C15-C16-C17
8	T	101	BCL	C16-C17-C18-C20
8	F	101	BCL	C16-C17-C18-C19
10	J	101	U4Z	CAT-CAS-CAW-CAZ

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Mol	Chain	Res	Type	Atoms
13	L	705	MQE	CAJ-CAD-CAQ-CBU
8	H	101	BCL	C3-C5-C6-C7
9	U	104	PGV	C1-C2-C3-C4
8	Q	102	BCL	O1A-CGA-O2A-C1
9	U	104	PGV	C25-C26-C27-C28
9	0	104	PGV	C25-C26-C27-C28
14	M	706	BGL	C2'-C3'-C4'-C5'
9	L	706	PGV	O05-C05-C06-O06
8	9	101	BCL	C3-C5-C6-C7
9	h	102	PGV	C25-C26-C27-C28
9	U	103	PGV	C1-C2-C3-C4
9	E	104	PGV	C4-C5-C6-C7
9	O	103	PGV	C01-C02-C03-O11
9	S	103	PGV	C3-C4-C5-C6
9	0	105	PGV	C4-C5-C6-C7
8	F	101	BCL	C10-C11-C12-C13
8	U	102	BCL	C6-C7-C8-C9
8	G	102	BCL	C11-C10-C8-C9
8	6	102	BCL	C14-C13-C15-C16
8	L	702	BCL	C11-C10-C8-C9
8	N	101	BCL	C11-C10-C8-C9
11	L	704	BPH	C11-C10-C8-C9
9	0	104	PGV	C21-C22-C23-C24
8	K	101	BCL	C11-C12-C13-C15
8	G	102	BCL	C11-C10-C8-C7
8	0	102	BCL	C6-C7-C8-C10
8	6	101	BCL	C12-C13-C15-C16
8	6	102	BCL	C12-C13-C15-C16
15	L	717	PEF	C30-C31-C32-C33
9	C	506	PGV	O12-C04-C05-C06
18	P	102	CDL	OB5-CB3-CB4-OB6
8	O	102	BCL	C16-C17-C18-C20
8	Q	102	BCL	CBA-CGA-O2A-C1
8	R	102	BCL	O1A-CGA-O2A-C1
8	D	102	BCL	C13-C15-C16-C17
13	M	704	MQE	CAI-CAC-CAP-CBT
8	U	102	BCL	C16-C17-C18-C20
8	O	101	BCL	C16-C17-C18-C19
8	6	102	BCL	C16-C17-C18-C19
9	0	105	PGV	C23-C24-C25-C26
9	1	102	PGV	C1-C2-C3-C4
8	N	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	T	102	LMT	C4B-C5B-C6B-O6B
8	I	102	BCL	C3-C5-C6-C7
8	R	102	BCL	CBA-CGA-O2A-C1
13	L	705	MQE	CAK-CAF-CAT-CBW
8	S	101	BCL	C16-C17-C18-C20
8	2	102	BCL	C16-C17-C18-C19
13	M	704	MQE	CBM-CBJ-CBO-CCB
8	N	101	BCL	CBA-CGA-O2A-C1
8	8	102	BCL	C8-C10-C11-C12
9	L	706	PGV	C4-C5-C6-C7
9	S	103	PGV	C27-C28-C29-C30
8	0	101	BCL	C16-C17-C18-C19
8	I	102	BCL	C2-C3-C5-C6
8	7	101	BCL	C2-C3-C5-C6
8	R	102	BCL	C16-C17-C18-C20
8	W	102	BCL	C11-C12-C13-C14
8	K	101	BCL	C11-C12-C13-C14
8	L	703	BCL	C14-C13-C15-C16
8	N	101	BCL	C14-C13-C15-C16
8	F	101	BCL	C6-C7-C8-C9
8	K	101	BCL	CBA-CGA-O2A-C1
9	M	705	PGV	C5-C6-C7-C8
9	6	103	PGV	C20-C19-O03-C01
9	4	102	PGV	C20-C19-O03-C01
8	K	102	BCL	C10-C11-C12-C13
8	K	101	BCL	O1A-CGA-O2A-C1
9	L	711	PGV	C25-C26-C27-C28
8	M	701	BCL	C4-C3-C5-C6
14	M	710	BGL	C4-C5-C6-O6
13	L	705	MQE	CAJ-CAD-CAQ-CBE
13	L	705	MQE	CAK-CAF-CAT-CBG
9	0	105	PGV	O01-C02-C03-O11
9	8	103	PGV	O01-C02-C03-O11
9	6	103	PGV	O01-C02-C03-O11
8	8	101	BCL	C15-C16-C17-C18
14	C	507	BGL	C3'-C4'-C5'-C6'
8	2	101	BCL	O1D-CGD-O2D-CED
8	Q	101	BCL	C11-C10-C8-C7
8	M	701	BCL	C11-C10-C8-C7
8	D	102	BCL	C6-C7-C8-C10
8	E	101	BCL	C15-C16-C17-C18
9	4	102	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	E	101	BCL	C3A-C2A-CAA-CBA
8	8	101	BCL	C4-C3-C5-C6
13	M	704	MQE	CAU-CBA-CBN-CBM
8	R	102	BCL	C16-C17-C18-C19
8	O	102	BCL	C10-C11-C12-C13
9	4	102	PGV	C20-C21-C22-C23
11	L	704	BPH	C2-C1-O2A-CGA
9	8	103	PGV	C30-C31-C32-C33
8	1	101	BCL	C2-C3-C5-C6
10	J	101	U4Z	CAT-CAS-CAW-CBA
10	3	102	U4Z	CAT-CAS-CAW-CBA
13	M	704	MQE	CAI-CAC-CAP-CBC
8	W	101	BCL	C11-C12-C13-C14
8	Q	101	BCL	C11-C10-C8-C9
8	I	102	BCL	C11-C10-C8-C9
8	I	102	BCL	C11-C12-C13-C14
8	E	102	BCL	C11-C10-C8-C9
8	E	102	BCL	C14-C13-C15-C16
8	N	101	BCL	C11-C12-C13-C14
8	T	101	BCL	C6-C7-C8-C9
8	D	102	BCL	C6-C7-C8-C9
9	6	103	PGV	C29-C30-C31-C32
8	K	102	BCL	C2B-C3B-CAB-OBB
11	L	701	BPH	C1A-C2A-CAA-CBA
10	R	101	U4Z	CAT-CAS-CAW-CAZ
8	Q	101	BCL	C16-C17-C18-C20
9	6	103	PGV	C31-C32-C33-C34
8	N	101	BCL	C13-C15-C16-C17
8	4	101	BCL	C1A-C2A-CAA-CBA
8	M	701	BCL	C1A-C2A-CAA-CBA
9	S	103	PGV	C24-C25-C26-C27
9	O	103	PGV	C26-C27-C28-C29
8	8	101	BCL	C2-C3-C5-C6
10	R	101	U4Z	CAT-CAS-CAW-CBA
15	L	717	PEF	C19-C20-C21-C22
8	O	102	BCL	C12-C13-C15-C16
8	K	102	BCL	C6-C7-C8-C10
8	E	102	BCL	C11-C10-C8-C7
8	8	101	BCL	C11-C12-C13-C15
8	L	703	BCL	C11-C12-C13-C15
8	3	103	BCL	C11-C12-C13-C15
8	5	101	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
8	F	101	BCL	C12-C13-C15-C16
11	L	704	BPH	C11-C10-C8-C7
8	L	703	BCL	C16-C17-C18-C20
8	T	101	BCL	C16-C17-C18-C19
9	8	103	PGV	O03-C01-C02-O01
9	M	705	PGV	O03-C01-C02-O01
9	U	103	PGV	C25-C26-C27-C28
9	6	103	PGV	C21-C22-C23-C24
14	H	103	BGL	C4'-C5'-C6'-C7'
8	M	701	BCL	C2-C3-C5-C6
8	2	101	BCL	C6-C7-C8-C9
8	6	102	BCL	C10-C11-C12-C13
9	E	103	PGV	C6-C7-C8-C9
16	H	102	LMT	C2-C3-C4-C5
8	A	102	BCL	C5-C6-C7-C8
8	2	102	BCL	C8-C10-C11-C12
9	K	104	PGV	C29-C30-C31-C32
9	C	506	PGV	C4-C5-C6-C7
9	4	102	PGV	O04-C19-O03-C01
19	h	101	LHG	O10-C23-O8-C6
9	K	104	PGV	O03-C01-C02-C03
9	E	103	PGV	O03-C01-C02-C03
8	L	703	BCL	C4C-C3C-CAC-CBC
8	A	101	BCL	C8-C10-C11-C12
9	E	104	PGV	C1-C2-C3-C4
15	L	717	PEF	C14-C15-C16-C17
9	1	102	PGV	C5-C6-C7-C8
8	6	101	BCL	C4-C3-C5-C6
9	E	103	PGV	C3-C4-C5-C6
9	6	103	PGV	O04-C19-O03-C01
20	C	504	HEC	CAA-CBA-CGA-O2A
8	0	102	BCL	O1D-CGD-O2D-CED
8	Q	101	BCL	CBD-CGD-O2D-CED
19	h	101	LHG	C29-C30-C31-C32
8	S	101	BCL	C16-C17-C18-C19
9	L	706	PGV	O12-C04-C05-C06
16	T	102	LMT	O1'-C1-C2-C3
9	C	506	PGV	C25-C26-C27-C28
8	I	102	BCL	C11-C10-C8-C7
8	K	101	BCL	O1D-CGD-O2D-CED
9	L	706	PGV	O12-C04-C05-O05
8	0	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
8	8	101	BCL	C11-C10-C8-C9
8	H	101	BCL	C6-C7-C8-C9
8	J	102	BCL	C11-C10-C8-C9
8	T	101	BCL	C11-C10-C8-C9
8	3	101	BCL	C11-C10-C8-C9
8	A	102	BCL	C14-C13-C15-C16
11	L	701	BPH	C6-C7-C8-C9
8	A	101	BCL	C2A-CAA-CBA-CGA
8	F	101	BCL	C2A-CAA-CBA-CGA
8	Q	101	BCL	C2-C1-O2A-CGA
8	B	101	BCL	C2-C1-O2A-CGA
8	L	703	BCL	C2-C1-O2A-CGA
8	T	101	BCL	C2-C1-O2A-CGA
8	E	101	BCL	C3-C5-C6-C7
8	U	102	BCL	C16-C17-C18-C19
8	W	101	BCL	C3A-C2A-CAA-CBA
9	S	103	PGV	C29-C30-C31-C32
9	E	104	PGV	C20-C19-O03-C01
9	M	705	PGV	C2-C3-C4-C5
11	M	702	BPH	O2A-C1-C2-C3
20	C	504	HEC	CAA-CBA-CGA-O1A
9	O	103	PGV	C4-C5-C6-C7
8	A	102	BCL	C8-C10-C11-C12
16	D	104	LMT	C4-C5-C6-C7
14	M	707	BGL	C3'-C4'-C5'-C6'
11	L	701	BPH	C16-C17-C18-C19
9	4	102	PGV	C6-C7-C8-C9
9	S	103	PGV	C4-C5-C6-C7
9	L	706	PGV	O03-C01-C02-C03
8	J	102	BCL	C15-C16-C17-C18
8	T	101	BCL	C5-C6-C7-C8
9	L	712	PGV	C28-C29-C30-C31
14	L	708	BGL	C5'-C6'-C7'-C8'
15	h	103	PEF	C31-C32-C33-C34
19	h	101	LHG	O8-C23-C24-C25
9	C	506	PGV	C28-C29-C30-C31
8	W	101	BCL	C6-C7-C8-C9
8	W	102	BCL	C6-C7-C8-C9
8	S	102	BCL	C11-C12-C13-C14
8	G	102	BCL	C11-C12-C13-C14
8	8	101	BCL	C6-C7-C8-C9
8	6	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
8	6	101	BCL	C14-C13-C15-C16
8	7	101	BCL	C14-C13-C15-C16
8	A	101	BCL	C6-C7-C8-C9
8	L	703	BCL	C16-C17-C18-C19
9	E	103	PGV	C25-C26-C27-C28
9	h	102	PGV	C11-C12-C13-C14
19	h	101	LHG	C31-C32-C33-C34
16	M	709	LMT	O5B-C1B-O1B-C4'
8	4	101	BCL	C10-C11-C12-C13
9	8	103	PGV	C01-C02-C03-O11
16	D	104	LMT	C5'-C4'-O1B-C1B
8	L	703	BCL	C13-C15-C16-C17
9	K	104	PGV	C25-C26-C27-C28
8	W	101	BCL	C11-C12-C13-C15
8	S	102	BCL	C11-C10-C8-C7
8	I	102	BCL	C11-C12-C13-C15
8	E	102	BCL	C11-C12-C13-C15
8	0	101	BCL	C11-C10-C8-C7
8	8	101	BCL	C11-C10-C8-C7
8	2	101	BCL	C6-C7-C8-C10
8	H	101	BCL	C6-C7-C8-C10
8	T	101	BCL	C11-C10-C8-C7
8	3	101	BCL	C11-C10-C8-C7
19	h	101	LHG	C24-C25-C26-C27
10	0	103	U4Z	CAB-CAD-CAJ-CAL
10	R	101	U4Z	CAB-CAD-CAJ-CAL
8	M	701	BCL	C2-C1-O2A-CGA
8	7	101	BCL	C2-C1-O2A-CGA
9	4	102	PGV	C30-C31-C32-C33
8	0	101	BCL	C16-C17-C18-C20
9	K	103	PGV	C1-C2-C3-C4
8	S	102	BCL	CAA-CBA-CGA-O2A
8	I	102	BCL	CAA-CBA-CGA-O2A
15	L	713	PEF	C16-C17-C18-C19
8	2	102	BCL	C16-C17-C18-C20
9	M	705	PGV	O01-C1-C2-C3
15	L	717	PEF	C11-C12-C13-C14
18	P	102	CDL	O1-C1-CA2-OA2
8	7	101	BCL	C2A-CAA-CBA-CGA
15	h	103	PEF	C40-C41-C42-C43
15	L	717	PEF	O3-C30-C31-C32
8	K	101	BCL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
9	E	104	PGV	O04-C19-O03-C01
9	L	706	PGV	C2-C3-C4-C5
8	O	102	BCL	C14-C13-C15-C16
8	K	102	BCL	C6-C7-C8-C9
8	I	101	BCL	C6-C7-C8-C9
9	E	104	PGV	C3-C4-C5-C6
18	P	102	CDL	C51-C52-C53-C54
16	D	104	LMT	O5B-C1B-O1B-C4'
8	5	101	BCL	C1A-C2A-CAA-CBA
8	U	101	BCL	CAA-CBA-CGA-O2A
8	S	101	BCL	CAA-CBA-CGA-O2A
8	3	101	BCL	CAA-CBA-CGA-O2A
9	M	705	PGV	C3-C4-C5-C6
9	h	102	PGV	O03-C01-C02-O01
14	M	706	BGL	O2-C1'-C2'-C3'
16	M	709	LMT	C2B-C1B-O1B-C4'
9	1	102	PGV	O03-C19-C20-C21
16	D	104	LMT	C3'-C4'-O1B-C1B
15	h	103	PEF	O5-C30-O3-C3
8	6	101	BCL	C2-C1-O2A-CGA
8	A	101	BCL	C2-C1-O2A-CGA
8	Q	101	BCL	C11-C12-C13-C15
8	K	101	BCL	C6-C7-C8-C10
8	M	701	BCL	C11-C12-C13-C15
8	1	101	BCL	C6-C7-C8-C10
8	5	101	BCL	C12-C13-C15-C16
8	W	102	BCL	C10-C11-C12-C13
9	K	103	PGV	C6-C7-C8-C9
8	G	101	BCL	C16-C17-C18-C20
8	3	103	BCL	C10-C11-C12-C13
9	I	103	PGV	C20-C21-C22-C23
9	4	102	PGV	C23-C24-C25-C26
8	N	101	BCL	C2C-C3C-CAC-CBC
8	A	102	BCL	C2C-C3C-CAC-CBC
19	h	101	LHG	C24-C23-O8-C6
8	2	101	BCL	C13-C15-C16-C17
9	K	104	PGV	C20-C21-C22-C23
8	5	101	BCL	C3A-C2A-CAA-CBA
8	K	102	BCL	CAA-CBA-CGA-O2A
15	h	103	PEF	C32-C33-C34-C35
9	4	102	PGV	C22-C23-C24-C25
8	I	102	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	M	708	PEF	C30-C31-C32-C33
8	D	102	BCL	C5-C6-C7-C8
8	L	703	BCL	C11-C12-C13-C14
9	6	103	PGV	C22-C23-C24-C25
16	M	709	LMT	C3-C4-C5-C6
8	8	101	BCL	C8-C10-C11-C12
8	K	101	BCL	CAA-CBA-CGA-O1A
15	L	717	PEF	O5-C30-C31-C32
19	h	101	LHG	C4-C5-O7-C7
9	E	103	PGV	C26-C27-C28-C29
9	E	103	PGV	C21-C22-C23-C24
15	h	103	PEF	C12-C13-C14-C15
8	3	101	BCL	CAA-CBA-CGA-O1A
9	1	102	PGV	O04-C19-C20-C21
19	h	101	LHG	O10-C23-C24-C25
9	0	105	PGV	C21-C22-C23-C24
8	L	703	BCL	O1A-CGA-O2A-C1
20	C	501	HEC	CAA-CBA-CGA-O2A
8	S	101	BCL	CAA-CBA-CGA-O1A
9	L	712	PGV	O01-C1-C2-C3
18	P	102	CDL	CB3-CB4-CB6-OB8
9	M	705	PGV	O02-C1-C2-C3
18	P	102	CDL	CB5-C51-C52-C53
9	L	712	PGV	C24-C25-C26-C27
9	6	103	PGV	C27-C28-C29-C30
8	W	102	BCL	CAD-CBD-CGD-O2D
11	L	701	BPH	CAD-CBD-CGD-O2D
8	O	101	BCL	C2-C1-O2A-CGA
8	E	102	BCL	C2-C1-O2A-CGA
8	9	101	BCL	C2-C1-O2A-CGA
13	M	704	MQE	CAD-CAJ-CBC-CAP
8	0	102	BCL	CBD-CGD-O2D-CED
16	D	104	LMT	C2B-C1B-O1B-C4'
9	4	102	PGV	C24-C25-C26-C27
9	0	105	PGV	O03-C19-C20-C21
9	1	102	PGV	C21-C22-C23-C24
9	8	103	PGV	C27-C28-C29-C30
9	L	711	PGV	C22-C23-C24-C25

There are no ring outliers.

72 monomers are involved in 169 short contacts:

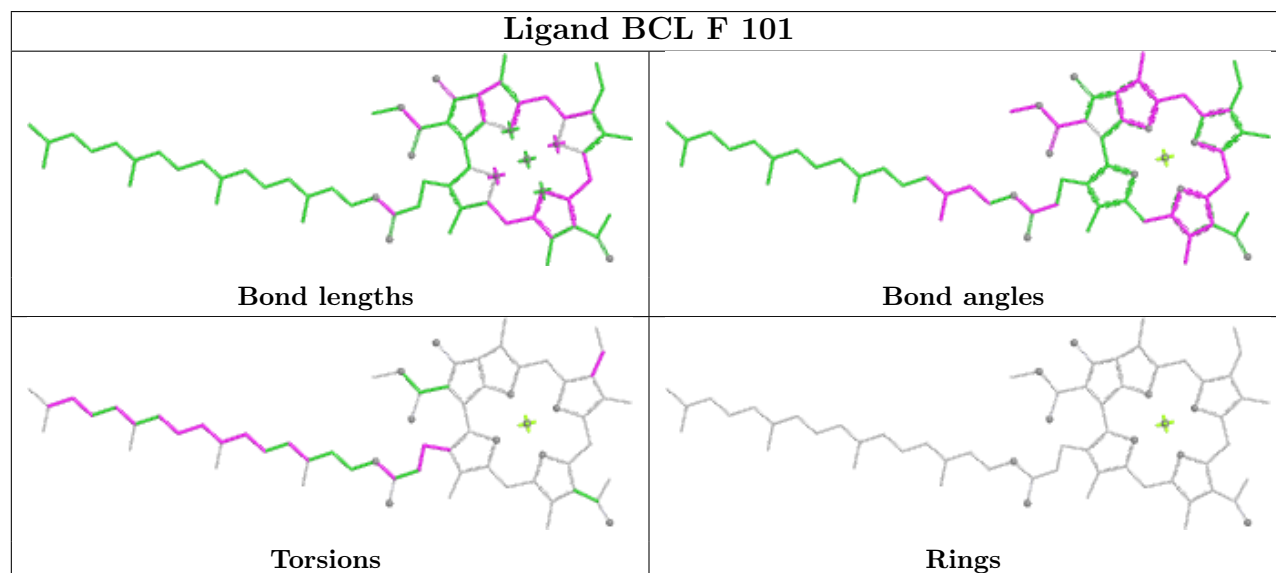
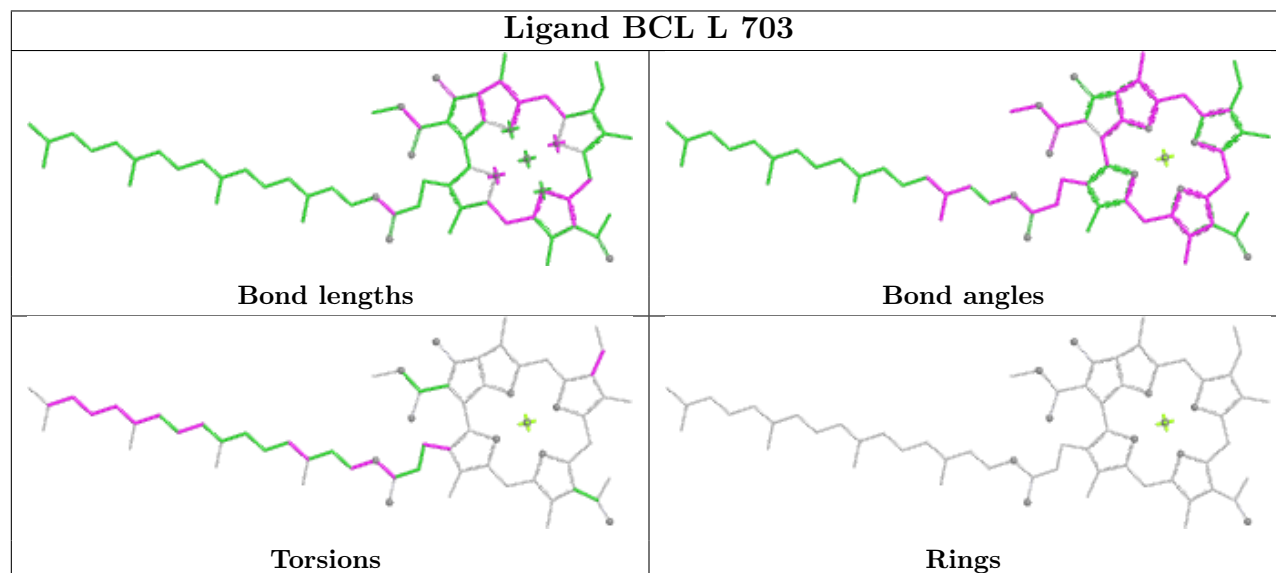
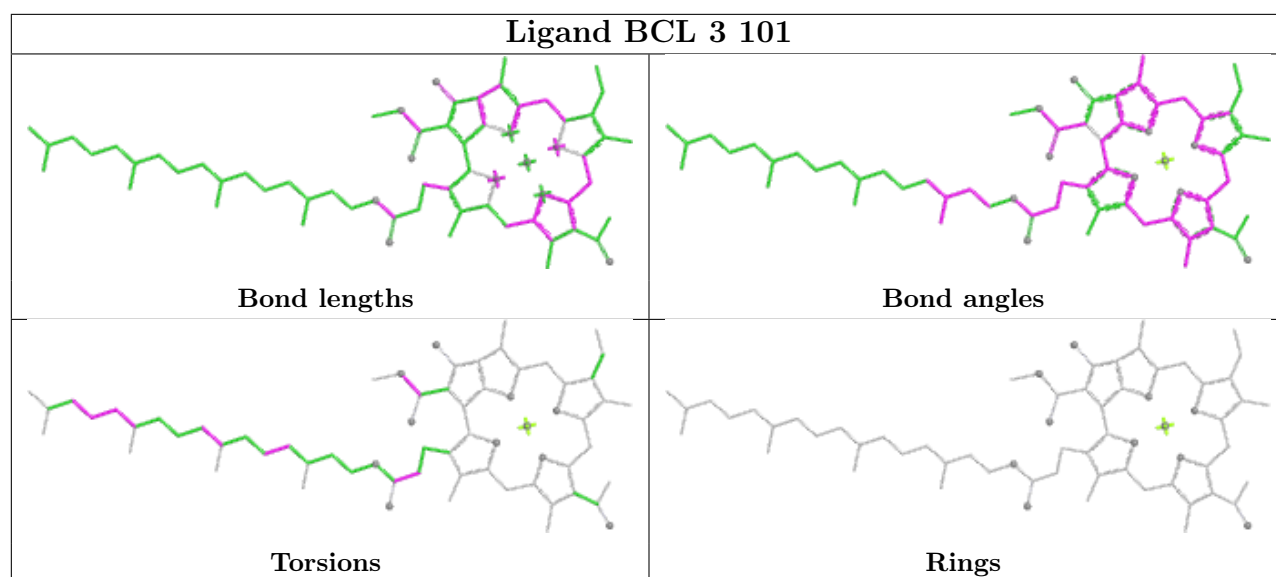
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	703	BCL	2	0
8	F	101	BCL	3	0
9	6	103	PGV	1	0
8	M	701	BCL	2	0
8	H	101	BCL	1	0
20	C	501	HEC	2	0
9	h	102	PGV	2	0
8	E	102	BCL	3	0
8	4	101	BCL	6	0
8	5	101	BCL	2	0
8	6	101	BCL	1	0
8	7	101	BCL	1	0
8	W	101	BCL	3	0
10	R	101	U4Z	1	0
9	4	102	PGV	1	0
8	G	101	BCL	1	0
8	V	101	BCL	8	0
16	H	102	LMT	2	0
8	8	101	BCL	1	0
16	D	104	LMT	3	0
8	B	101	BCL	2	0
9	I	103	PGV	3	0
19	h	101	LHG	5	0
8	L	702	BCL	6	0
8	Q	102	BCL	2	0
9	K	103	PGV	2	0
8	8	102	BCL	3	0
8	W	102	BCL	3	0
8	R	102	BCL	3	0
8	U	102	BCL	4	0
8	2	102	BCL	7	0
8	0	102	BCL	8	0
9	L	711	PGV	3	0
13	M	704	MQE	1	0
8	E	101	BCL	7	0
8	D	102	BCL	3	0
9	U	103	PGV	2	0
14	L	715	BGL	1	0
9	K	104	PGV	1	0
8	1	101	BCL	3	0
9	O	103	PGV	1	0
9	1	102	PGV	1	0
8	A	102	BCL	3	0

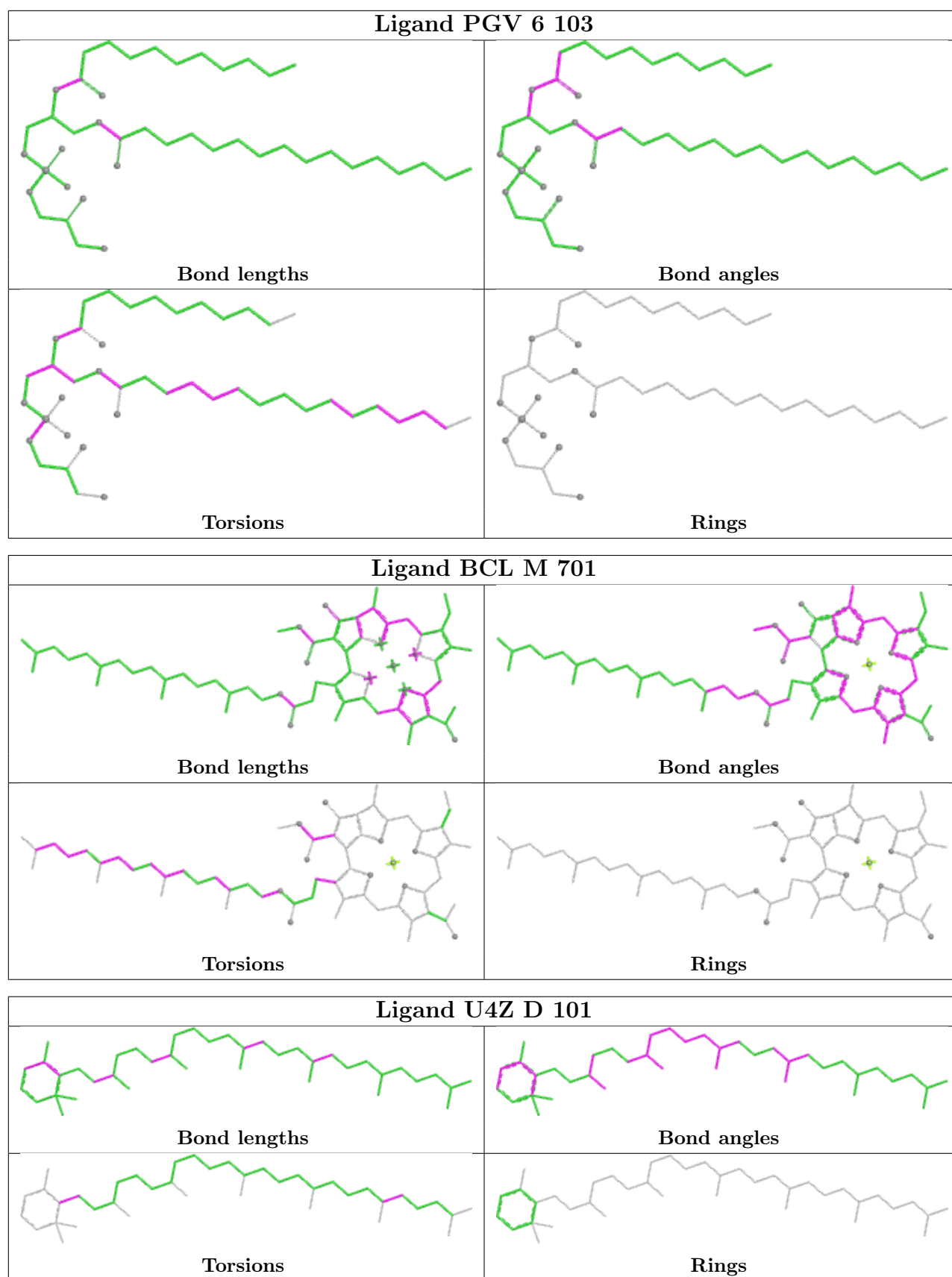
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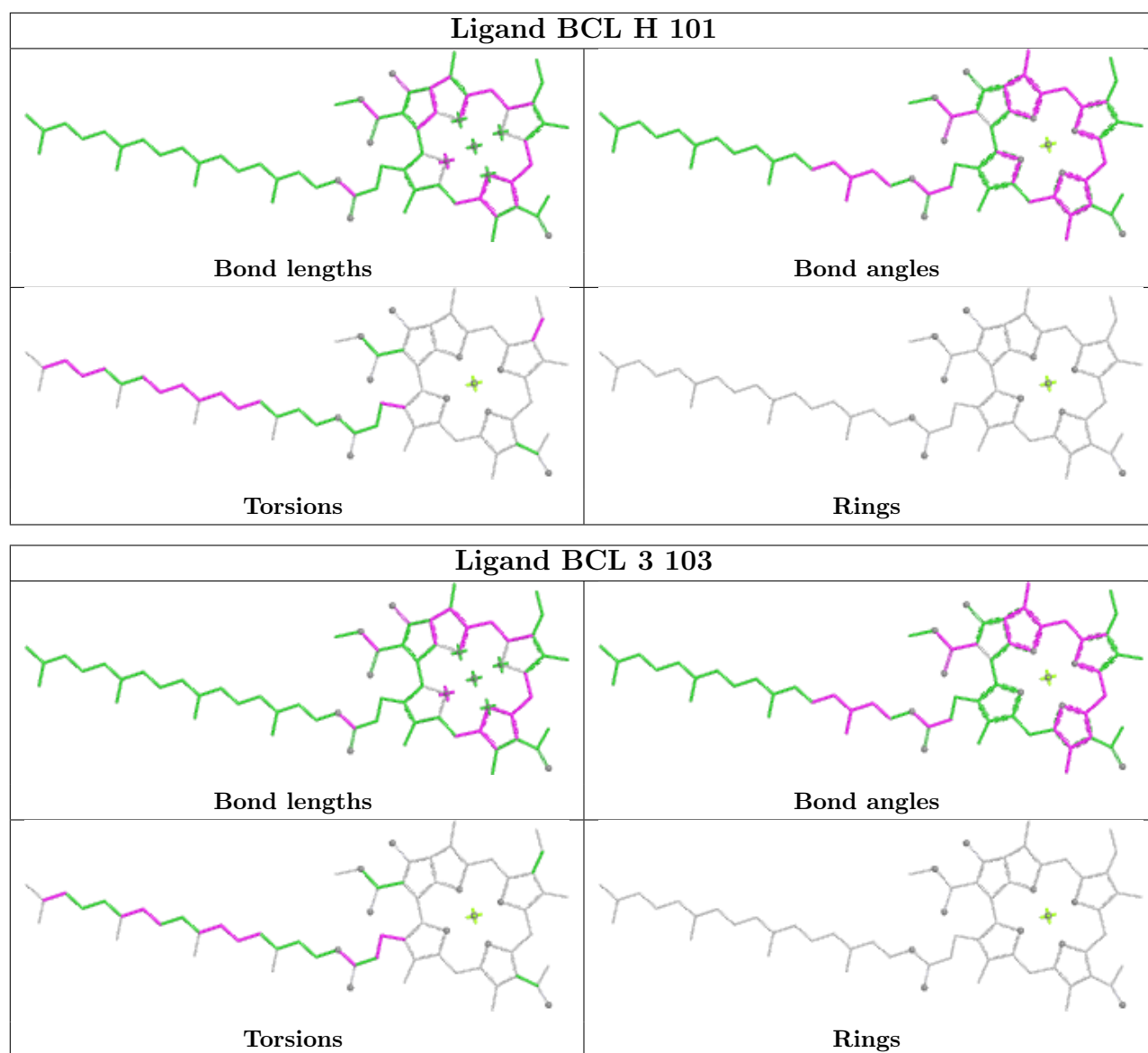
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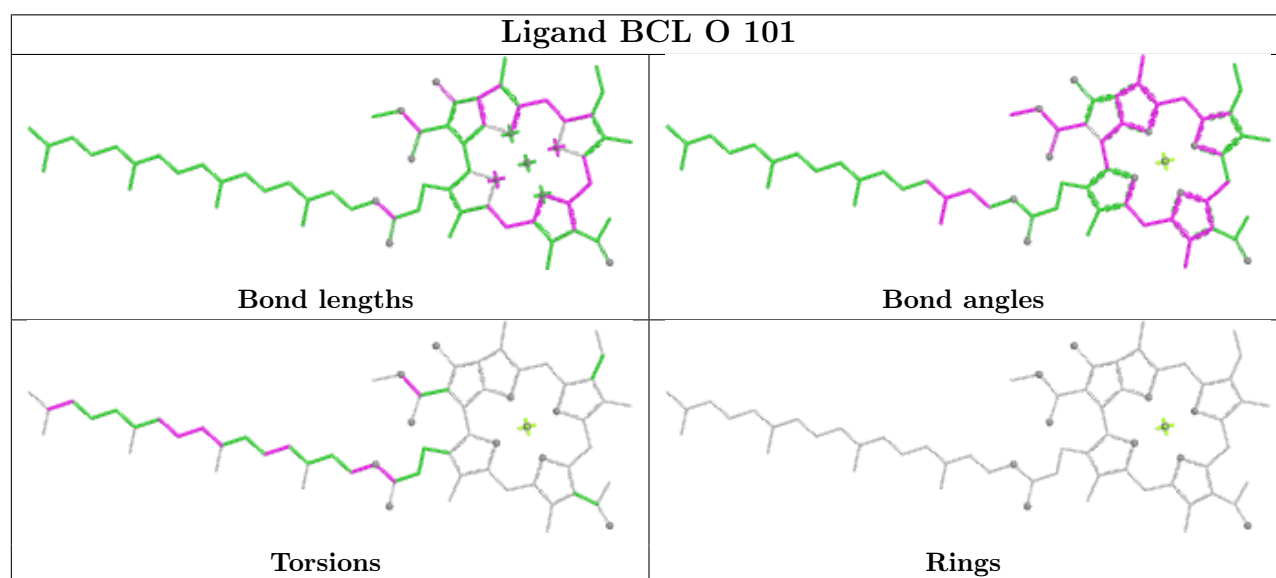
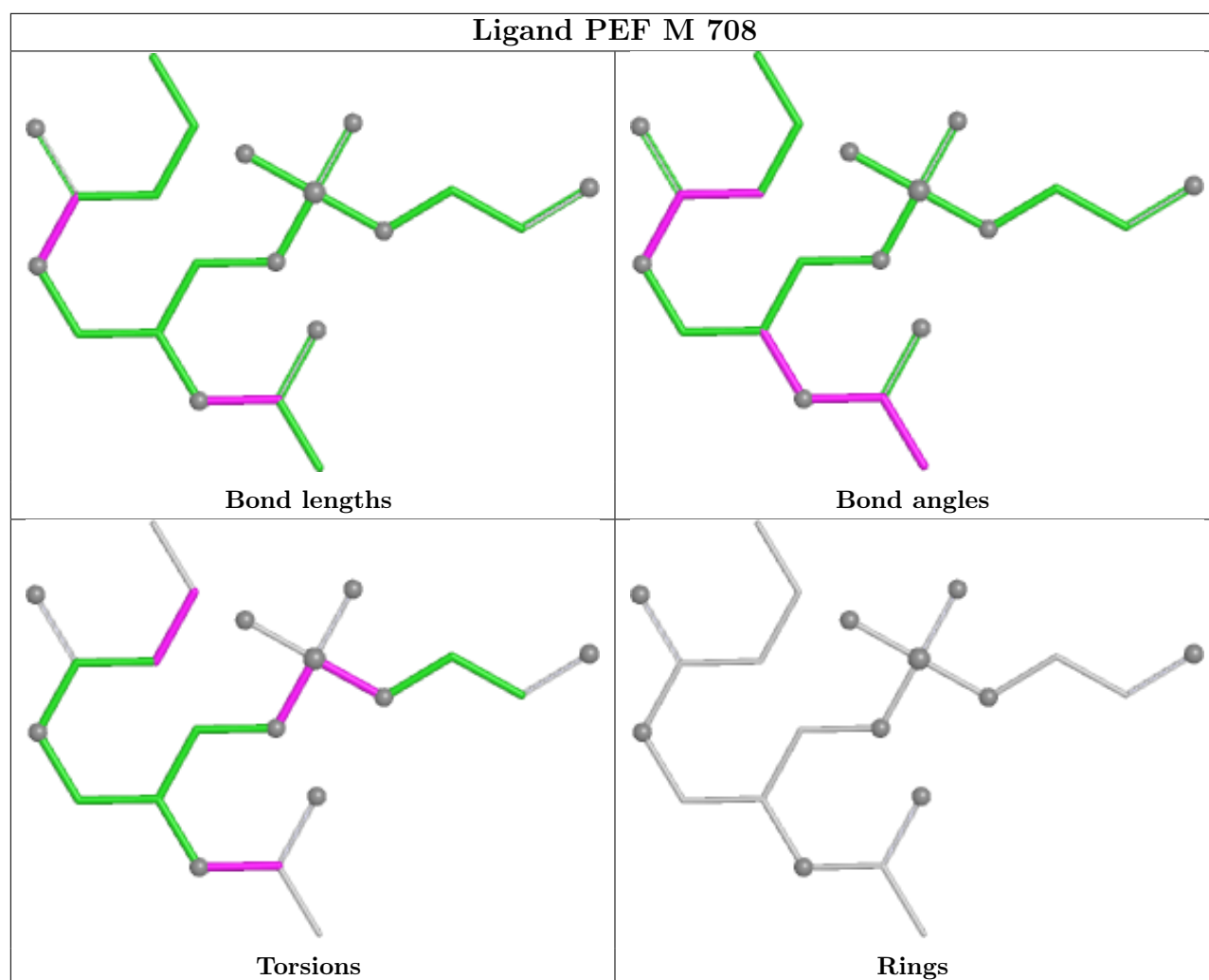
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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9	E	103	PGV	2	0
9	O	104	PGV	2	0
8	N	101	BCL	3	0
8	P	101	BCL	2	0
11	L	704	BPH	3	0
15	h	103	PEF	4	0
8	G	102	BCL	2	0
8	Q	101	BCL	2	0
8	S	102	BCL	4	0
8	O	102	BCL	4	0
15	L	713	PEF	2	0
8	U	101	BCL	3	0
8	I	101	BCL	1	0
9	C	506	PGV	1	0
11	M	702	BPH	2	0
15	L	717	PEF	2	0
8	6	102	BCL	3	0
16	M	709	LMT	2	0
14	M	710	BGL	2	0
20	C	504	HEC	3	0
8	I	102	BCL	2	0
10	3	102	U4Z	2	0
9	S	103	PGV	1	0
9	8	103	PGV	1	0
16	T	102	LMT	2	0
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18	P	102	CDL	2	0
9	M	705	PGV	5	0

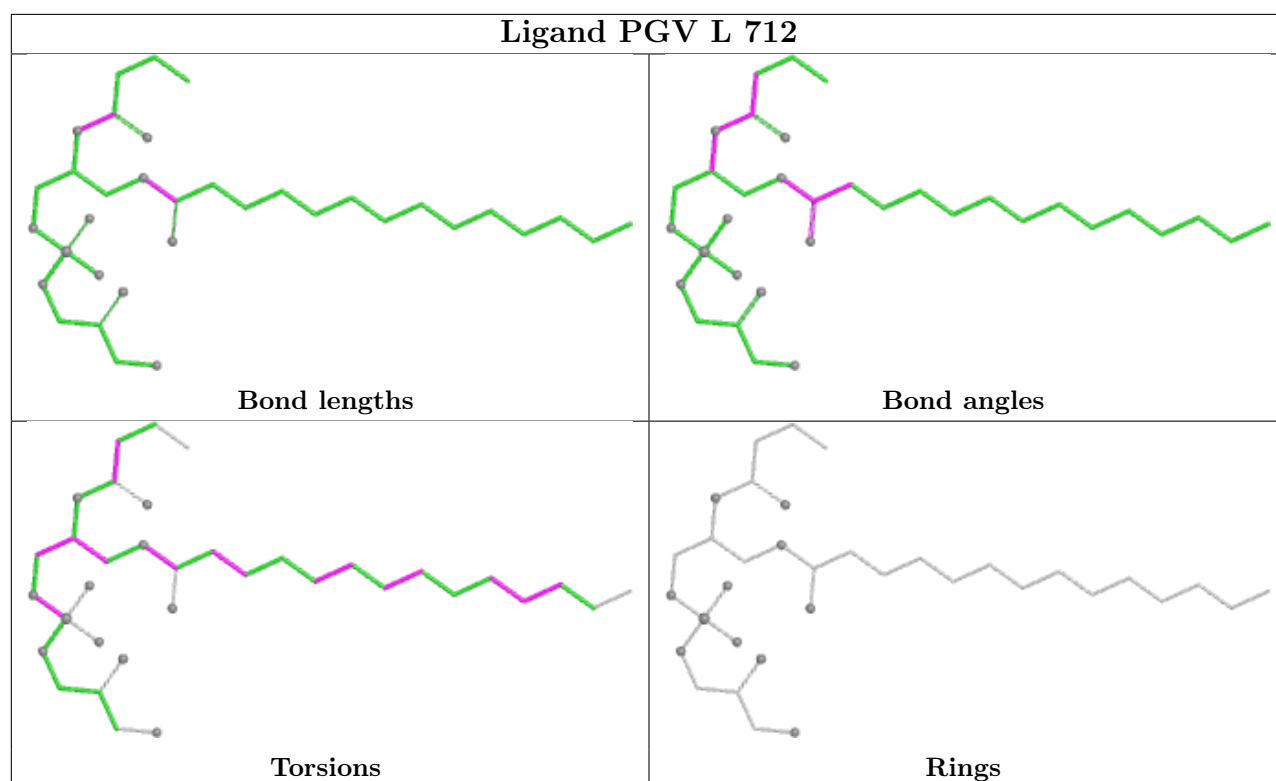
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



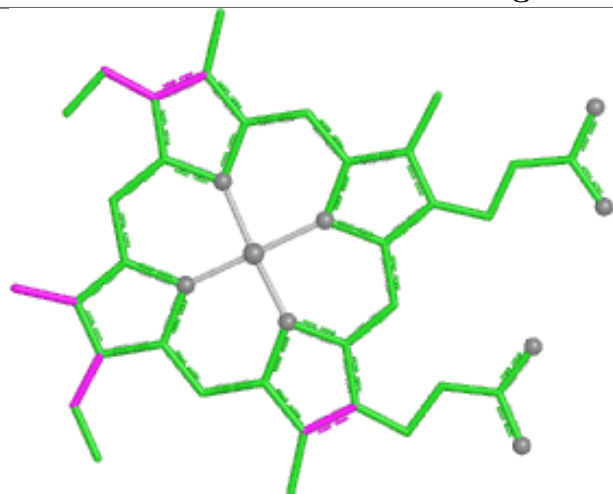




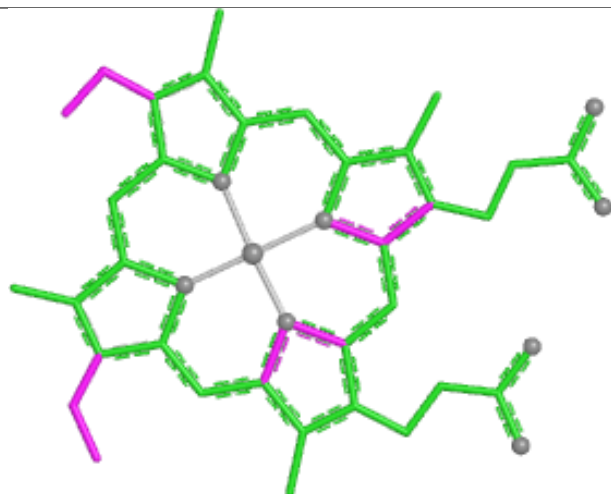




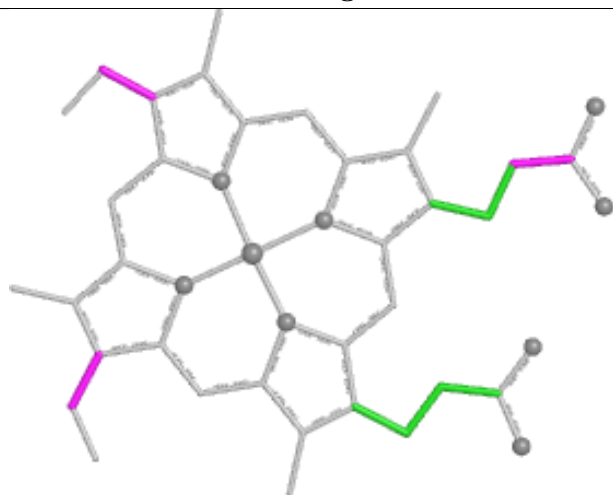
Ligand HEC C 501



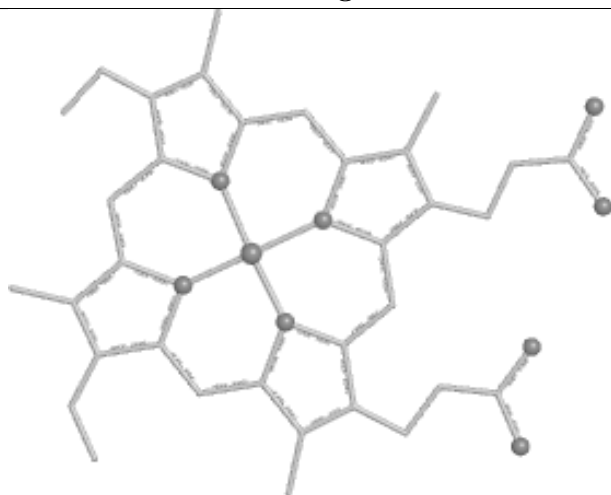
Bond lengths



Bond angles

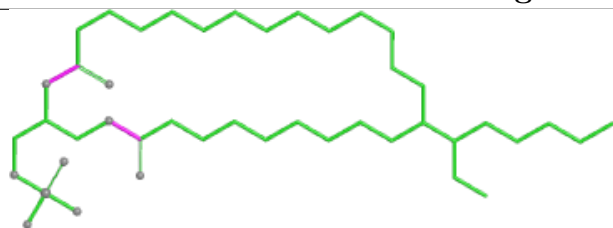


Torsions

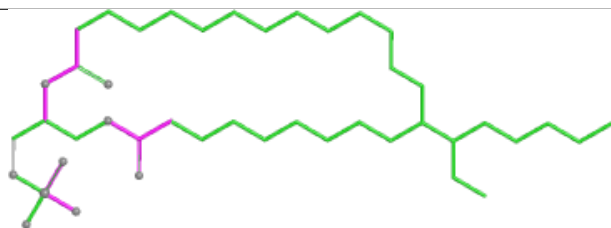


Rings

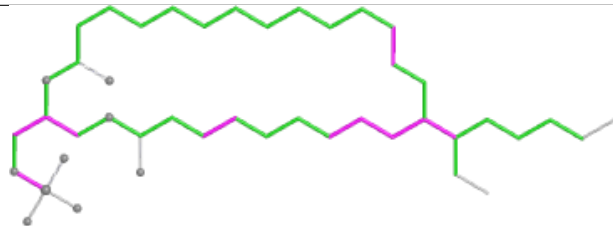
Ligand PGV h 102



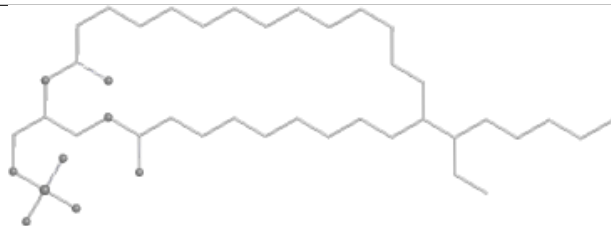
Bond lengths



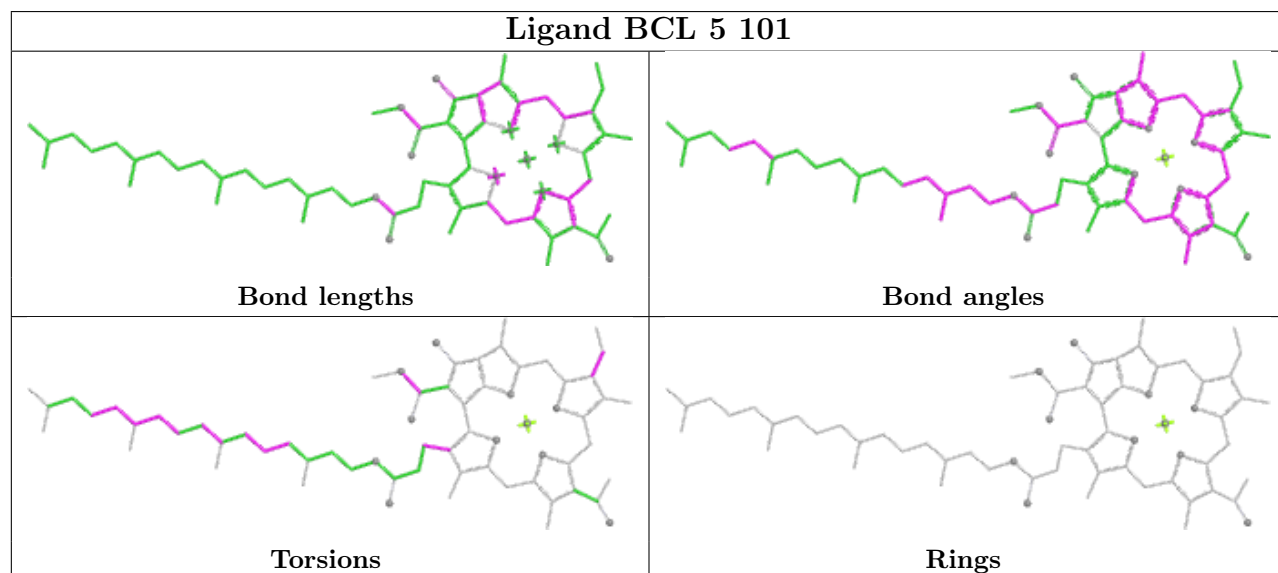
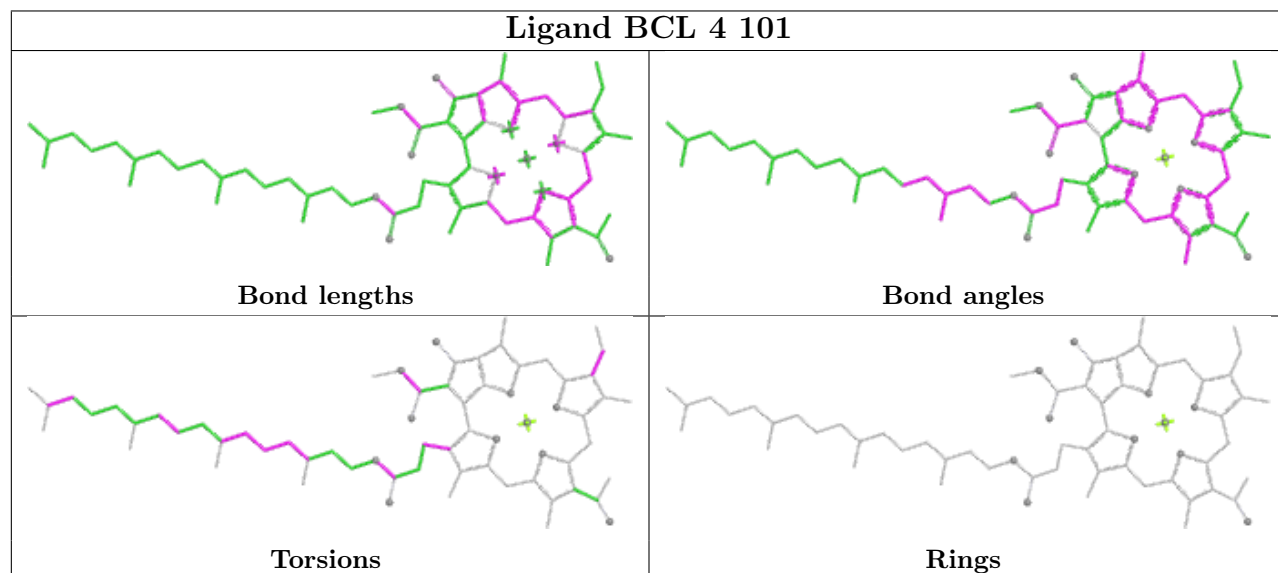
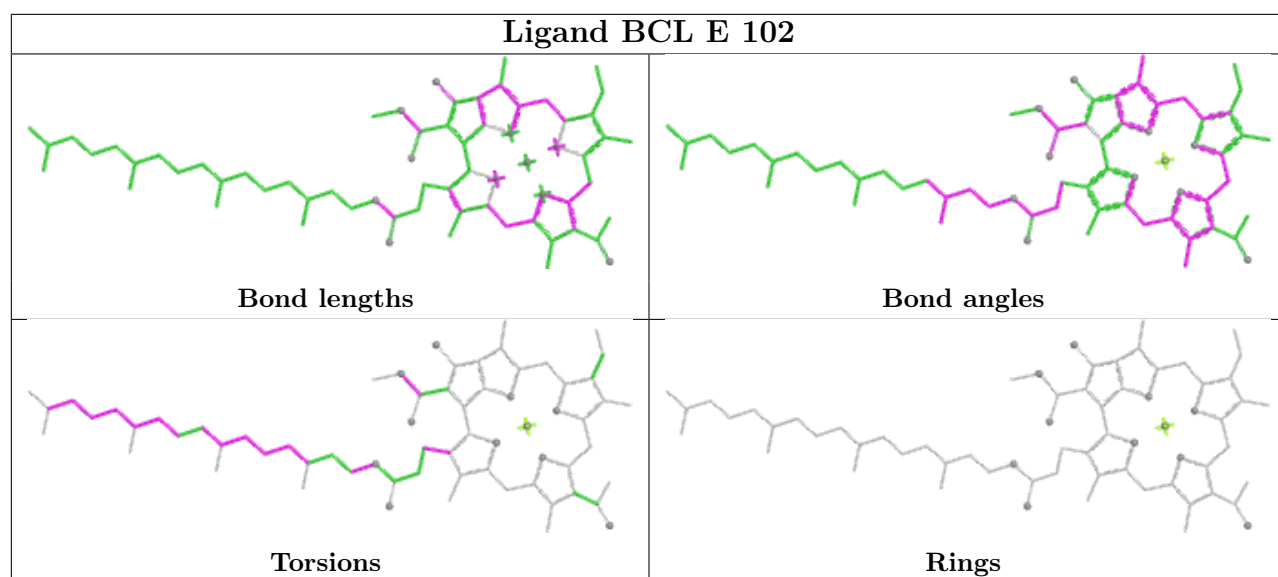
Bond angles

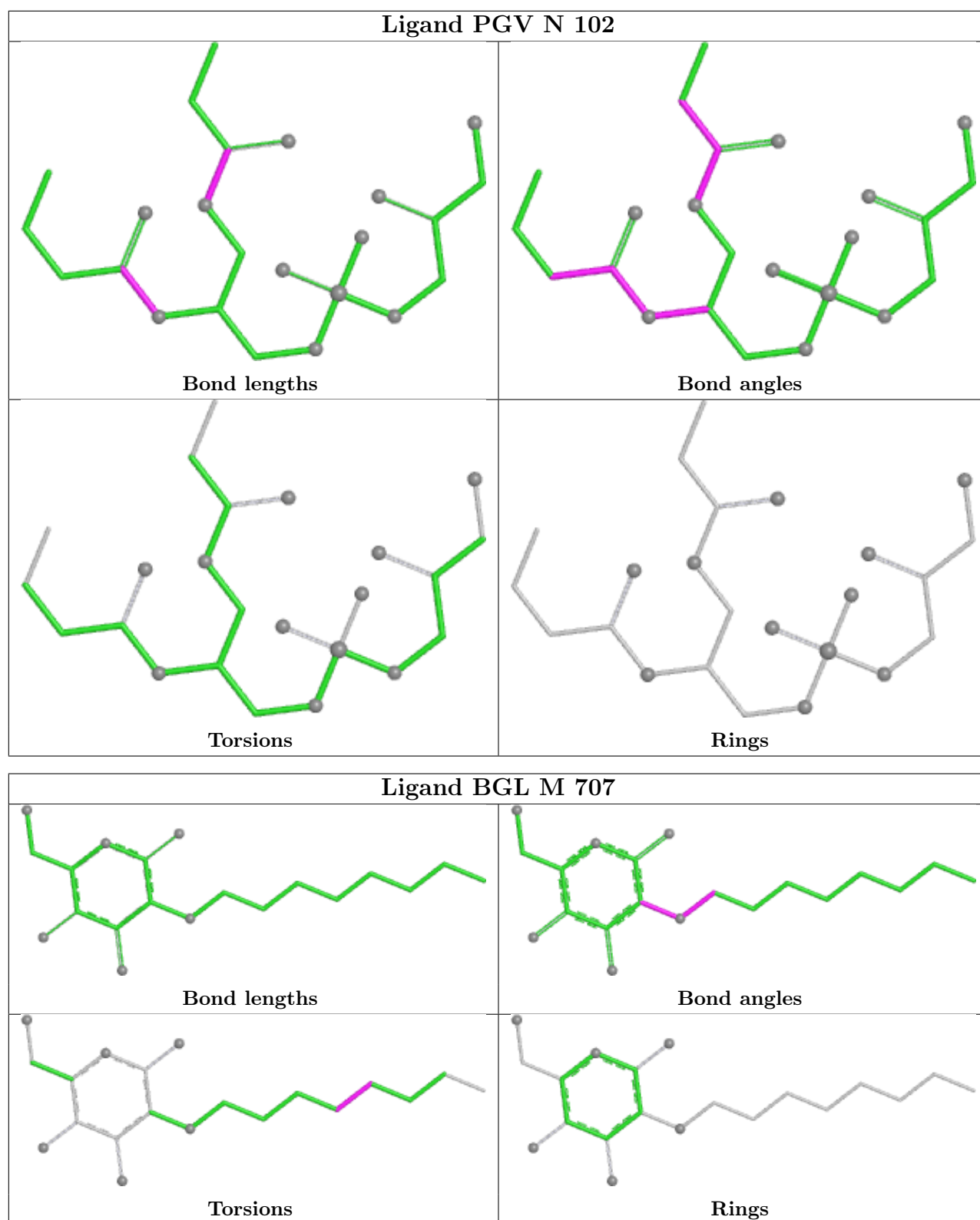


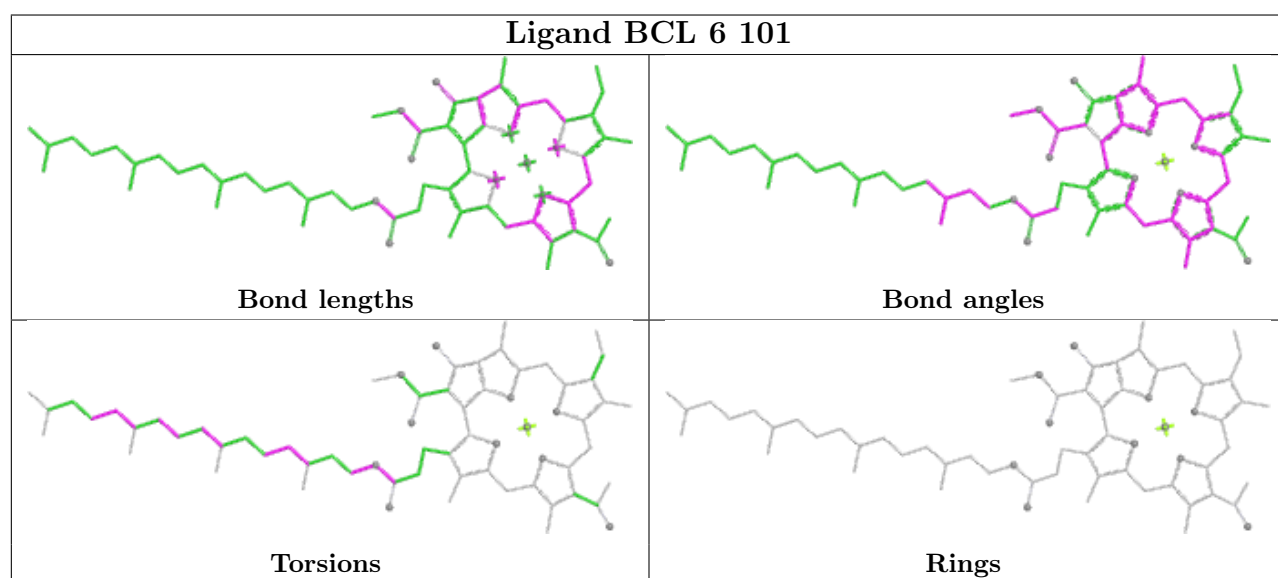
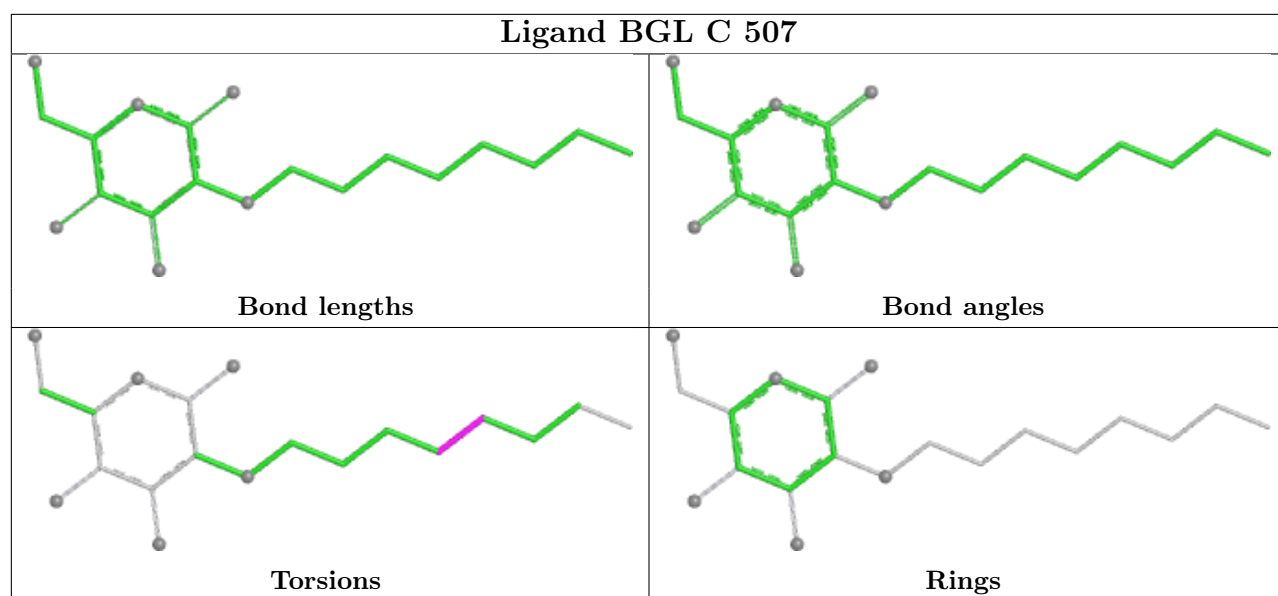
Torsions

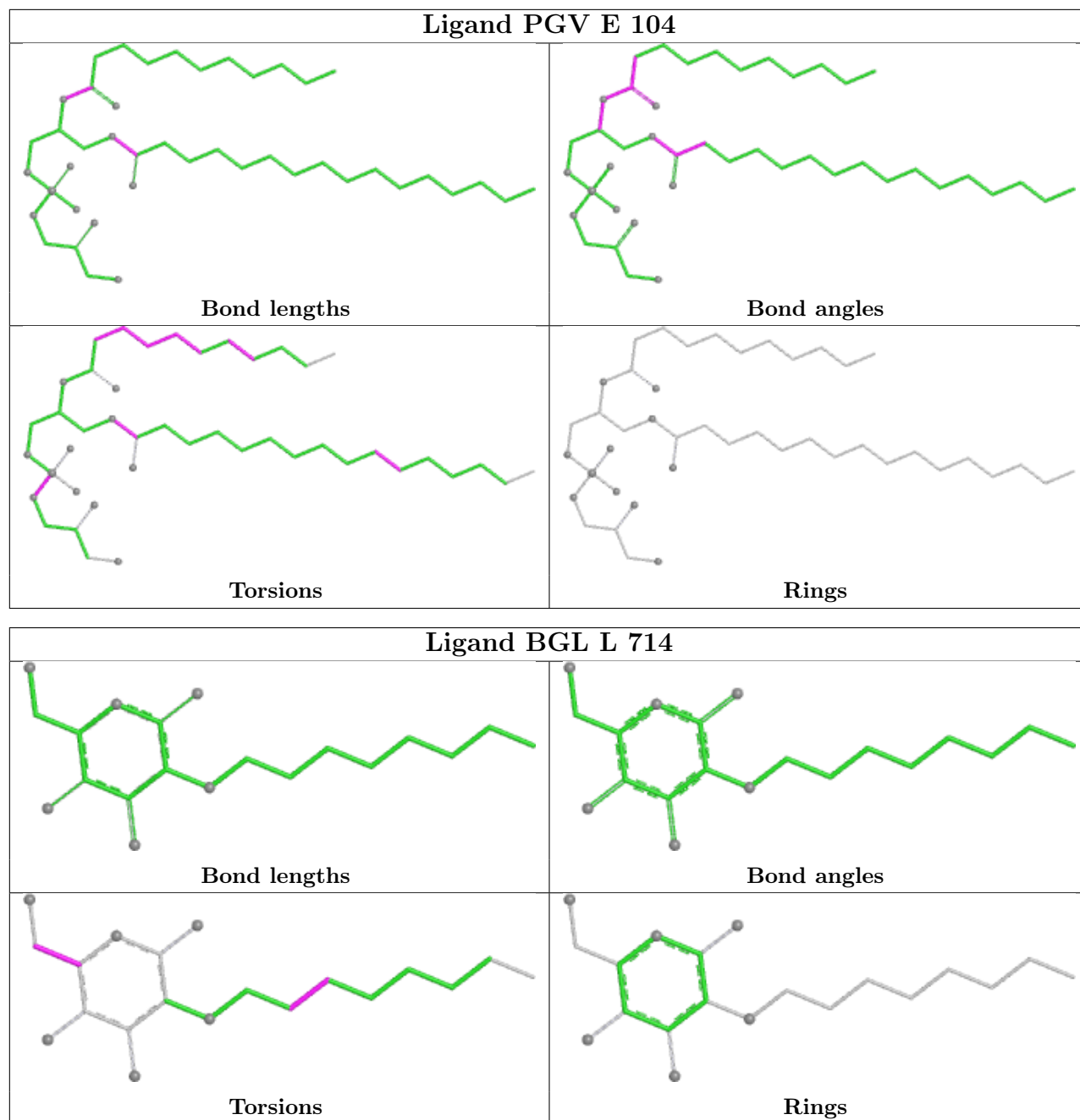


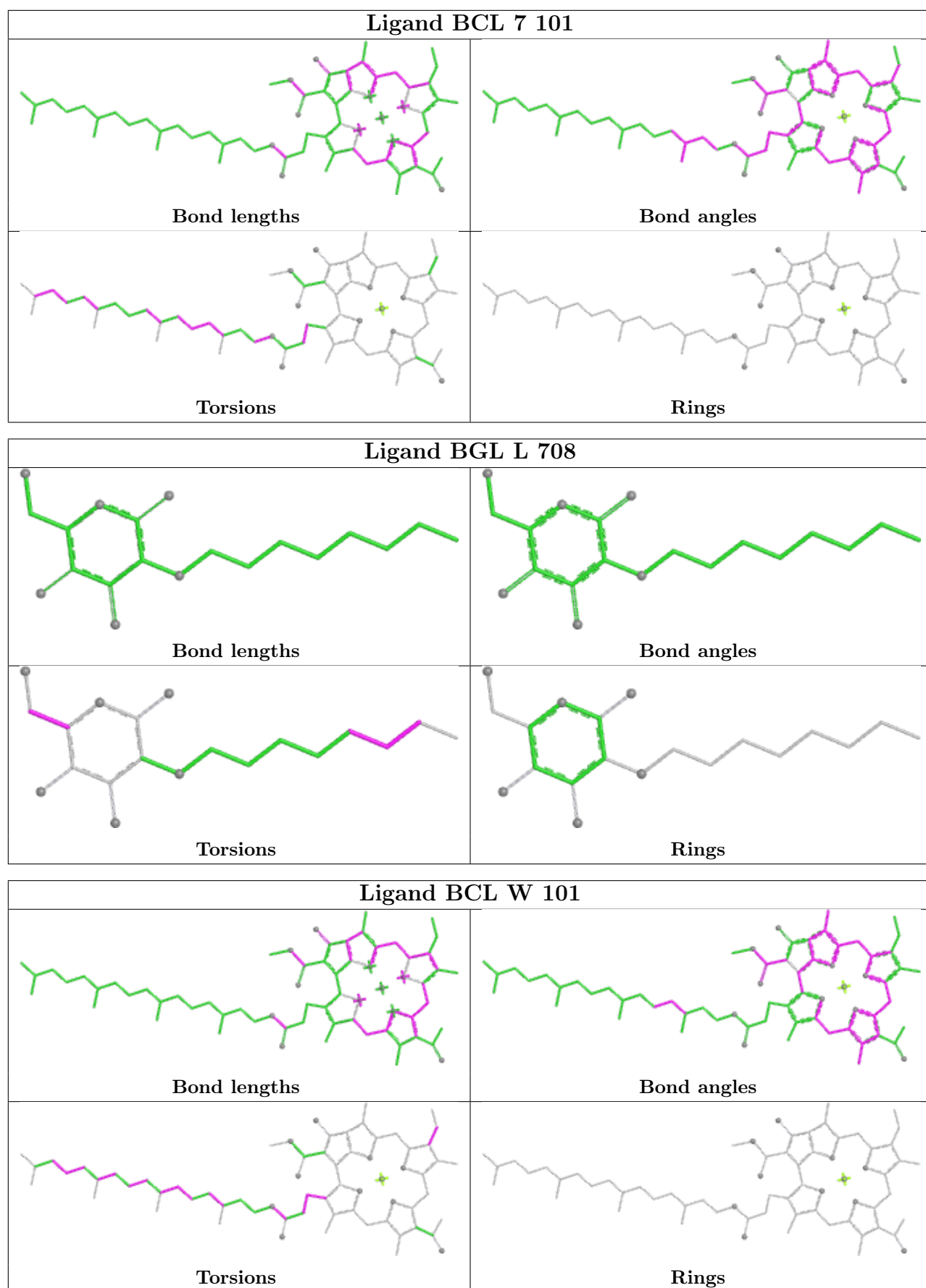
Rings

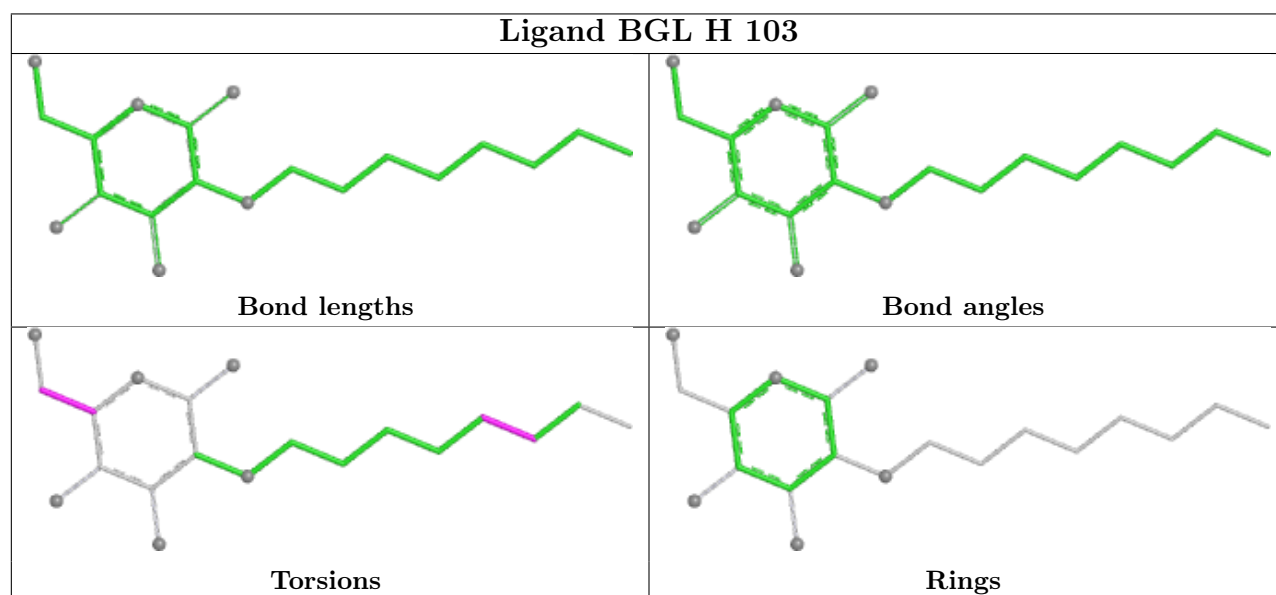
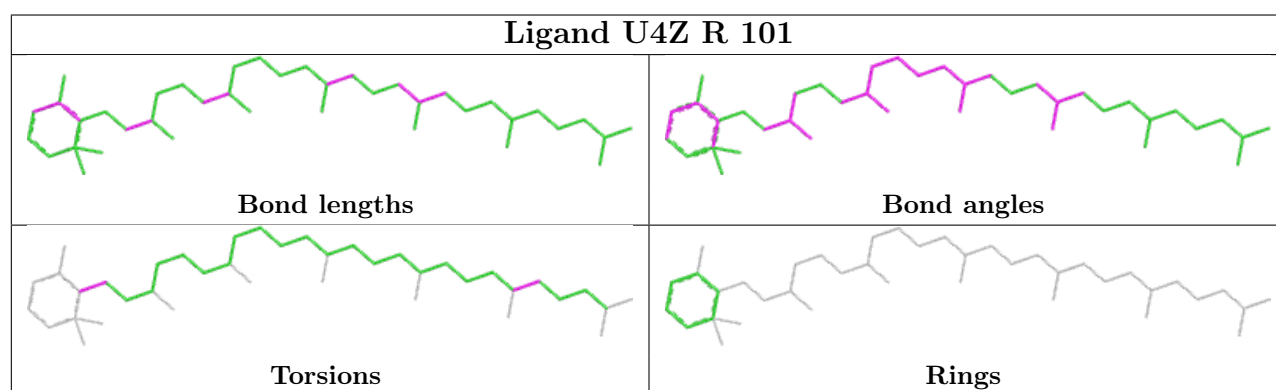
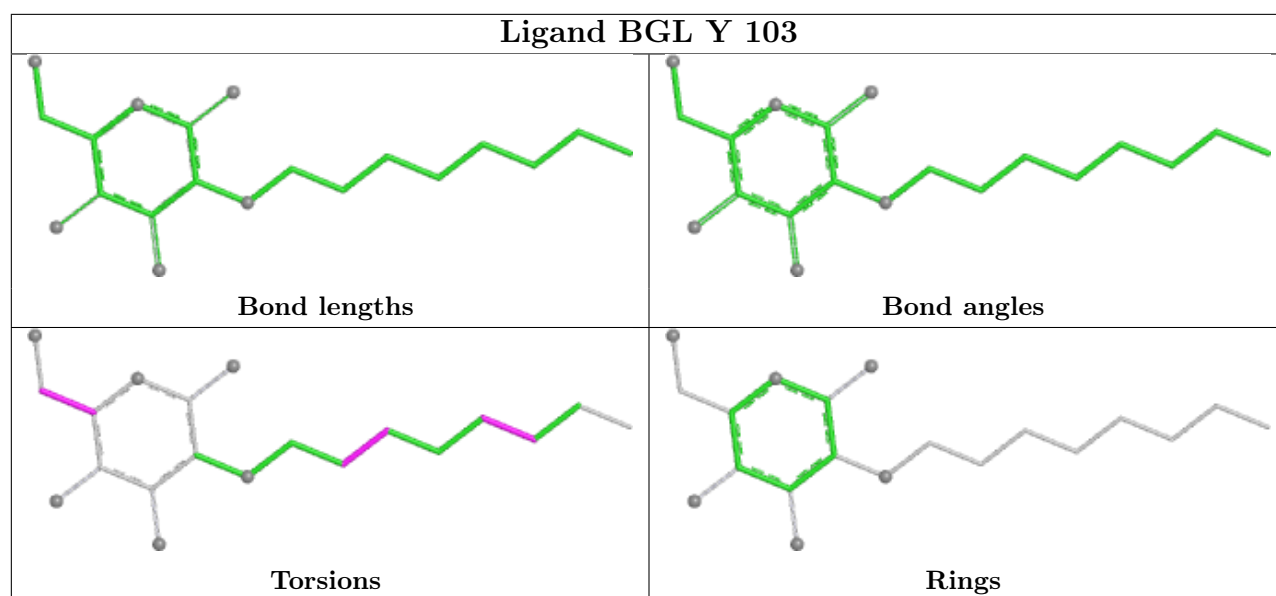


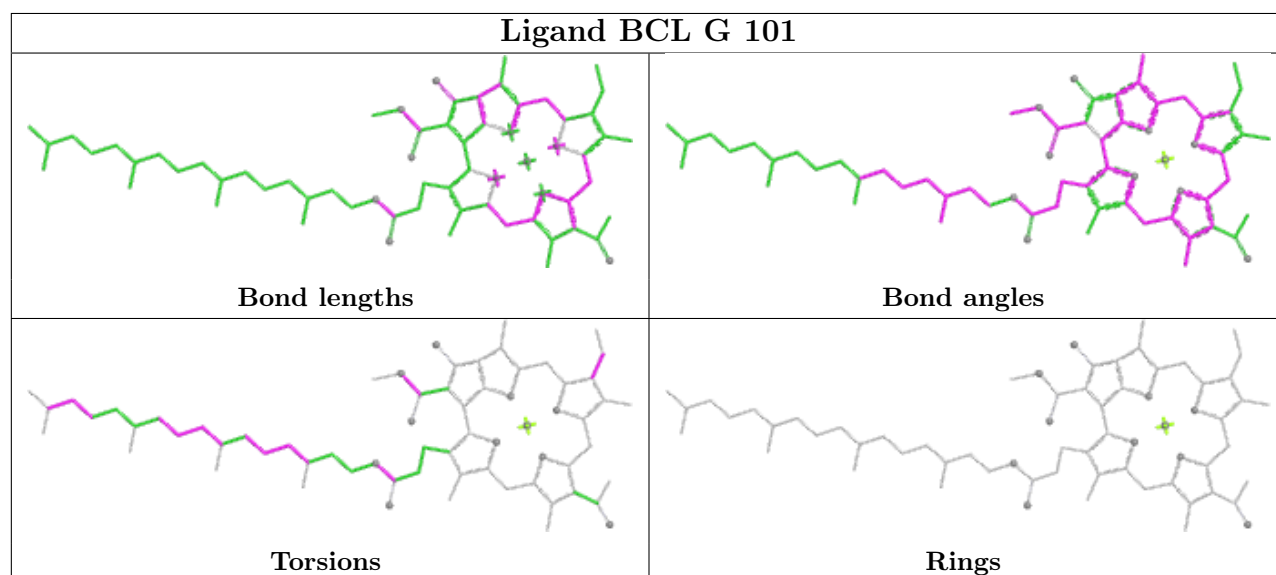
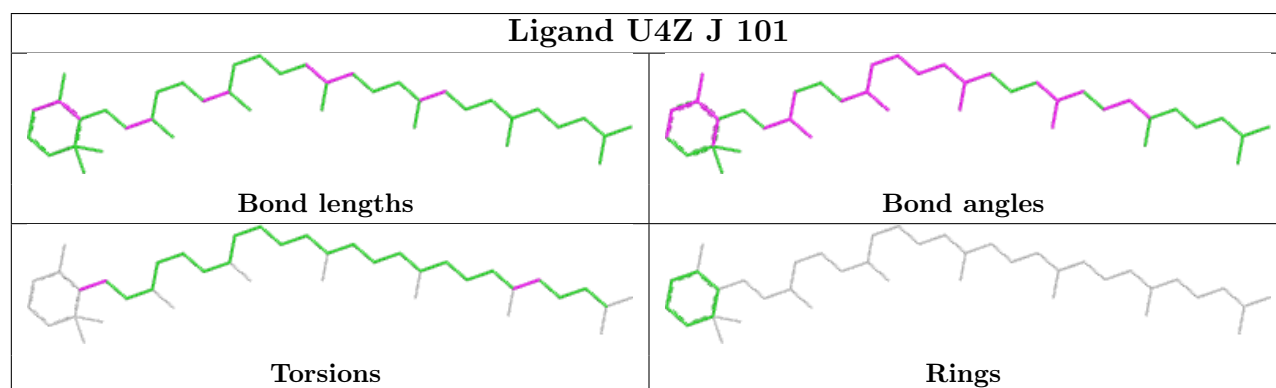
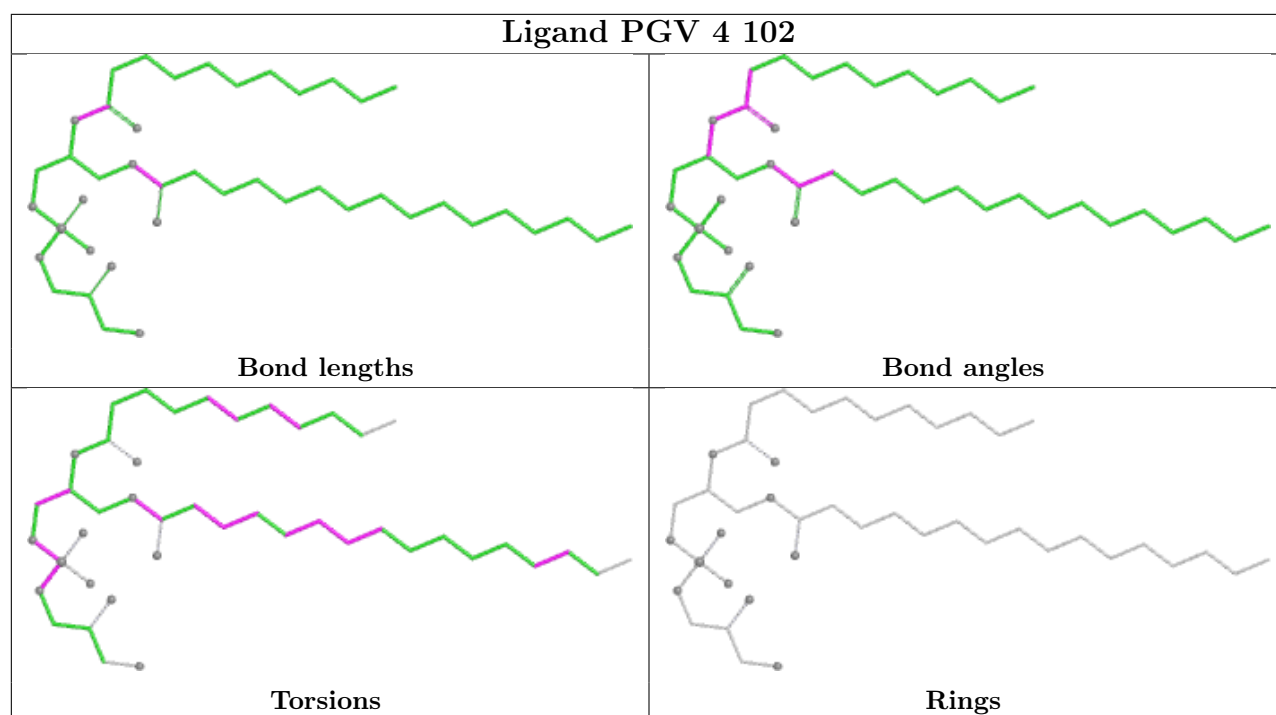




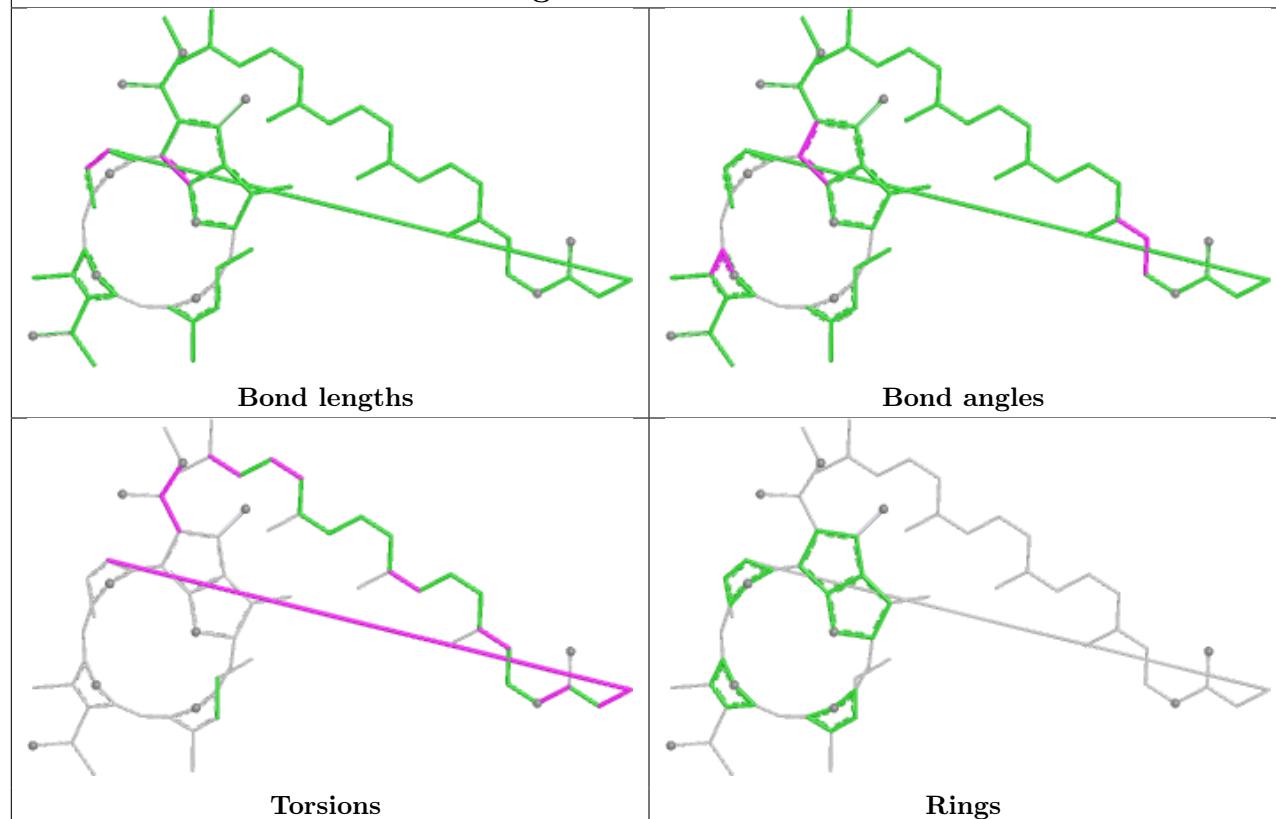




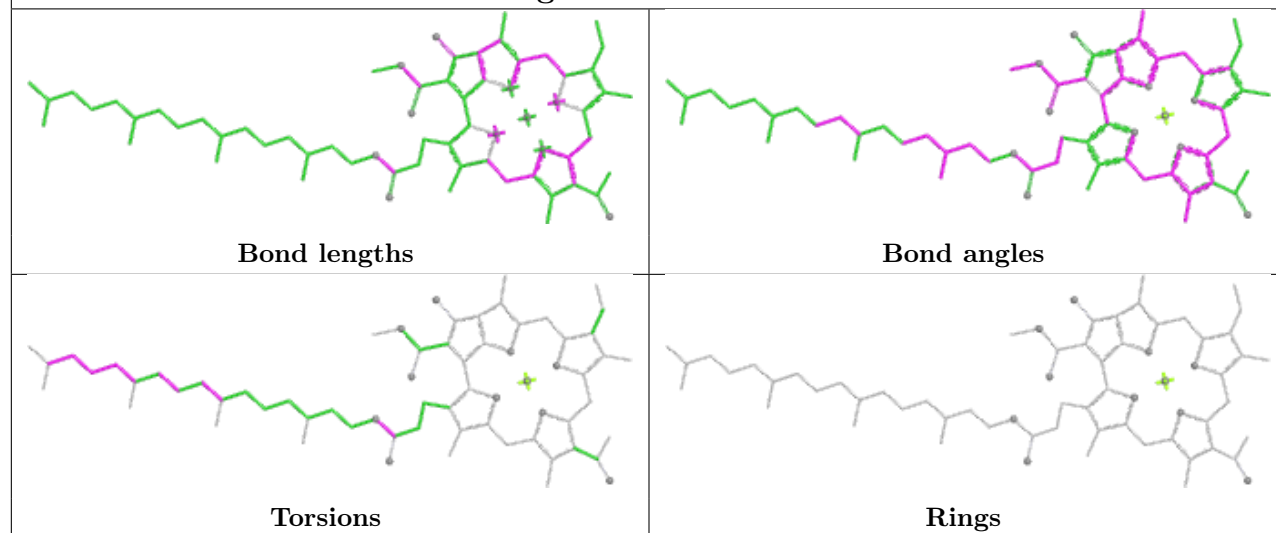


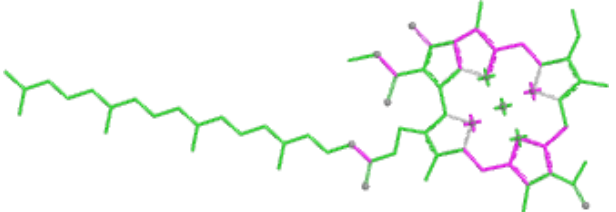
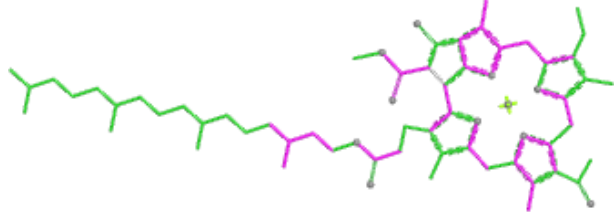
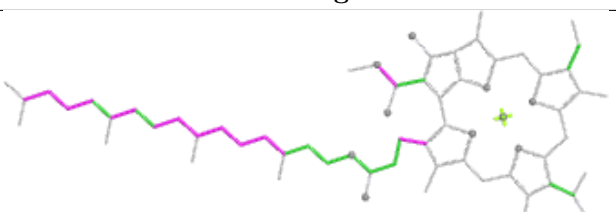
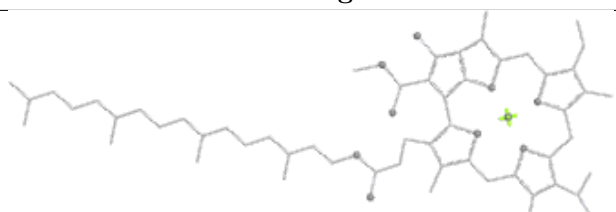
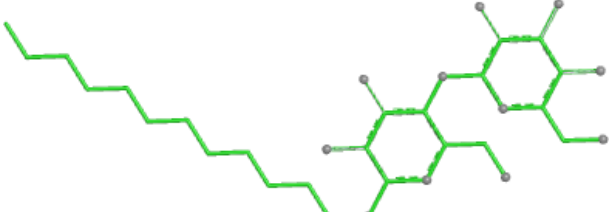
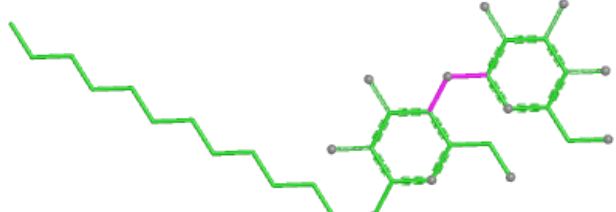
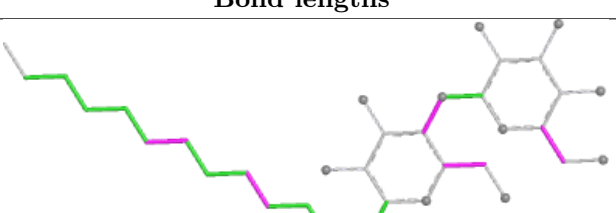
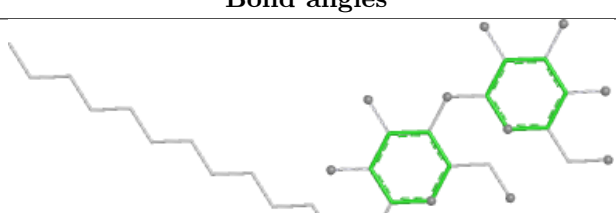
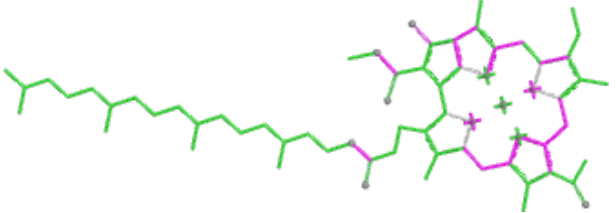
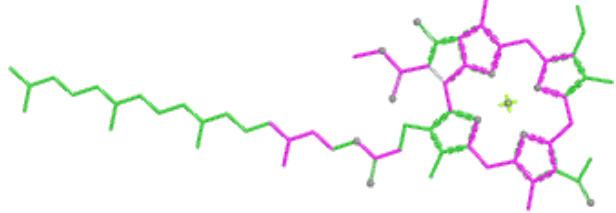
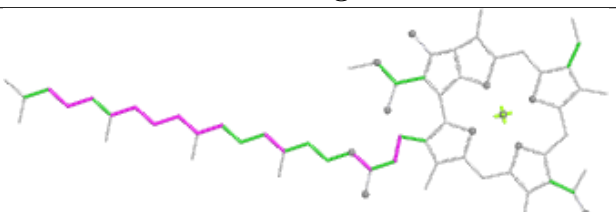
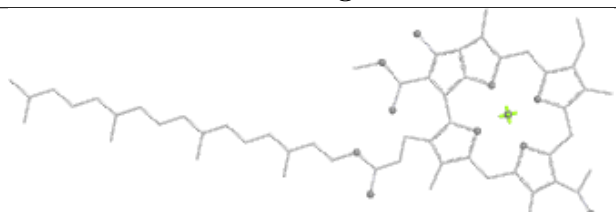


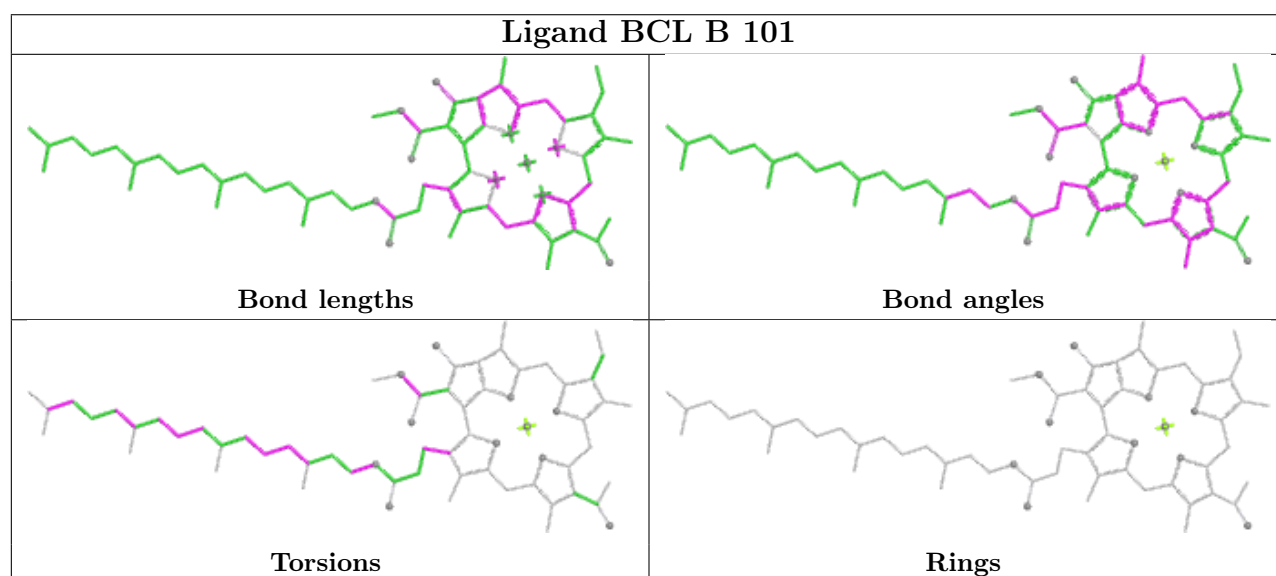
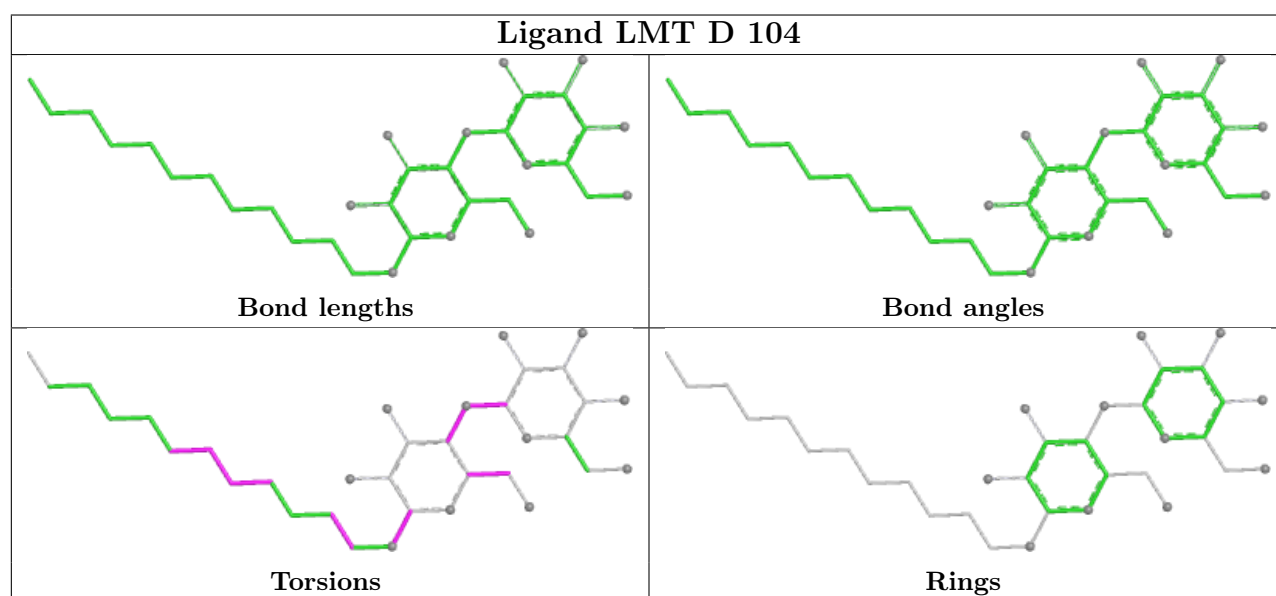
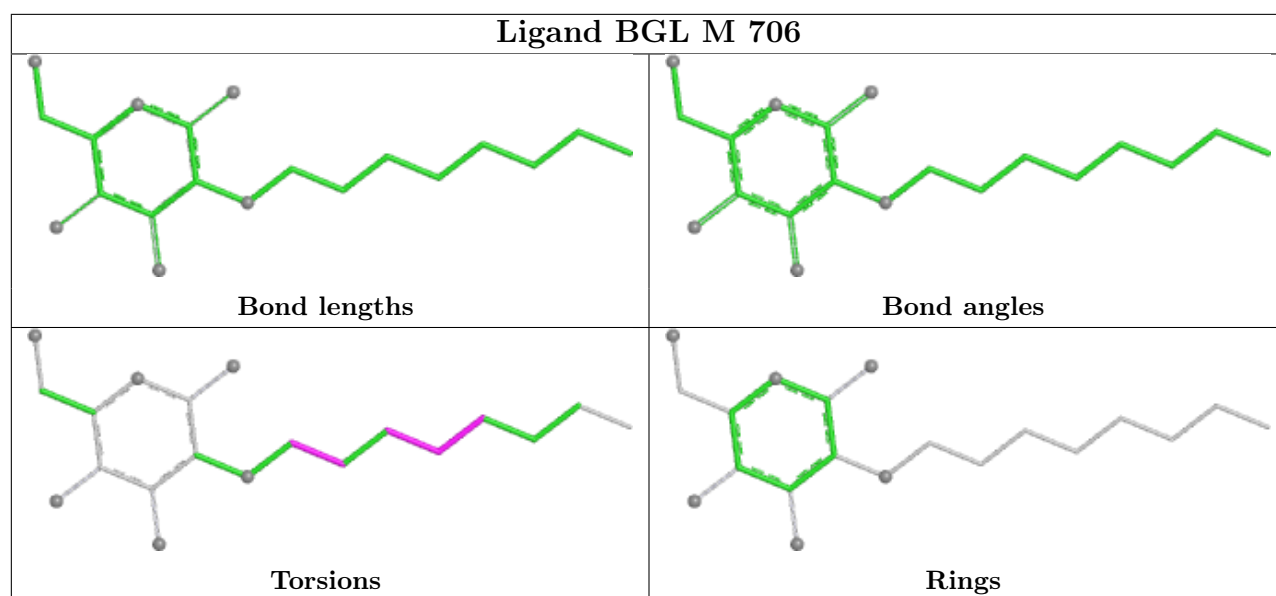
Ligand BPH L 701



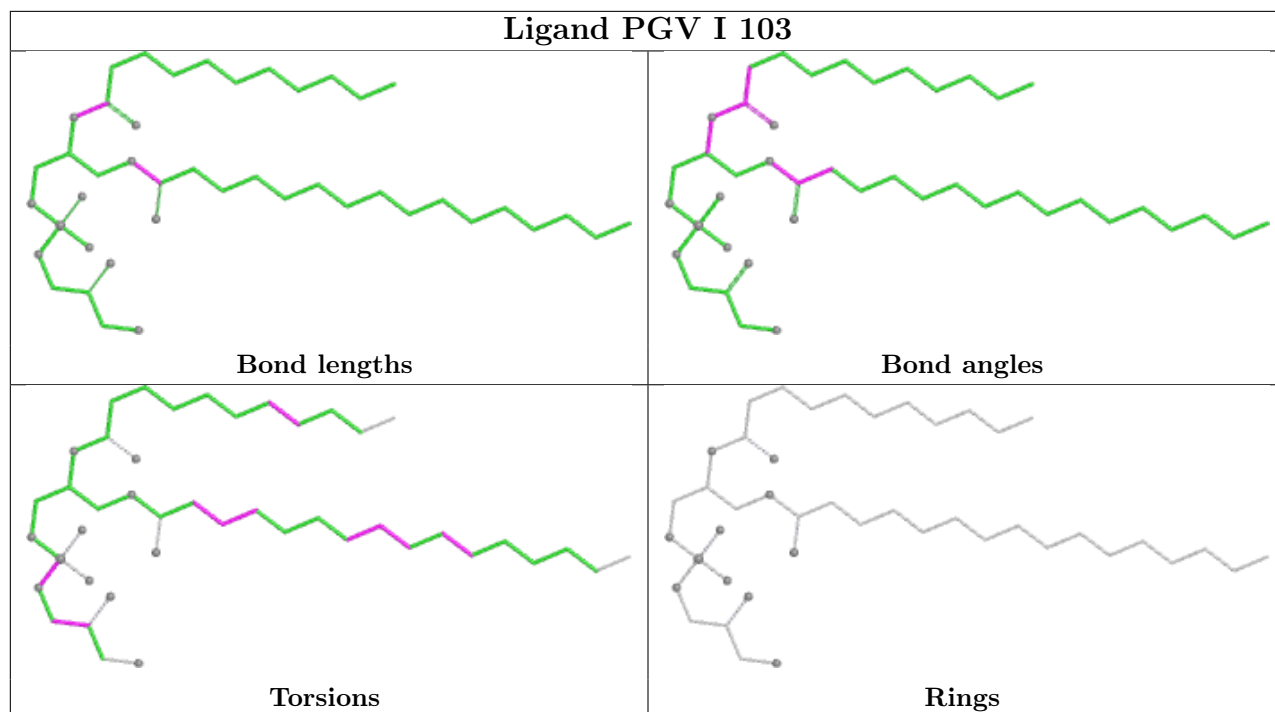
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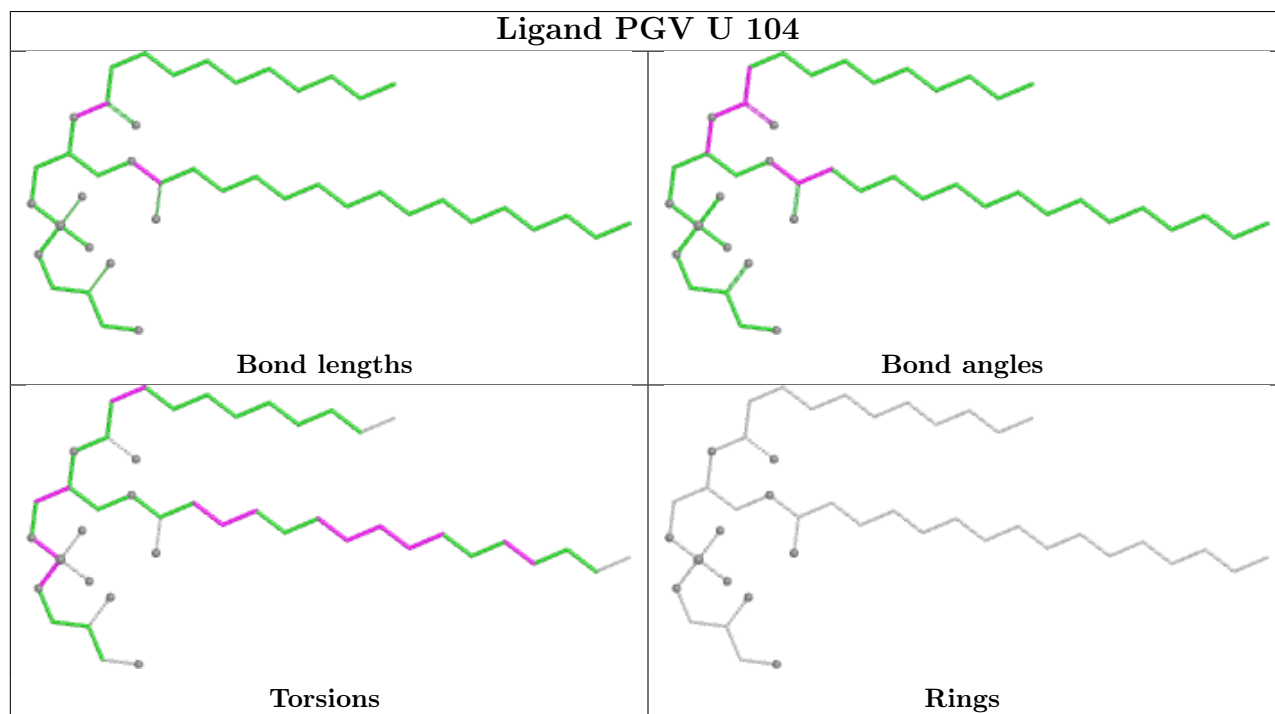
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT H 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL 8 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

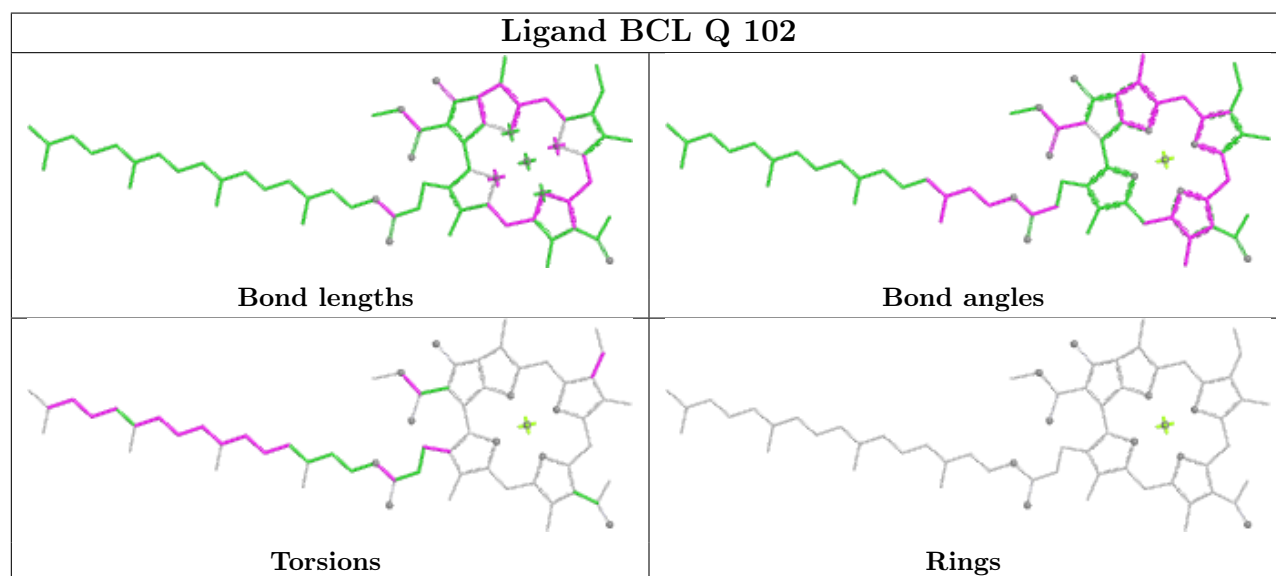
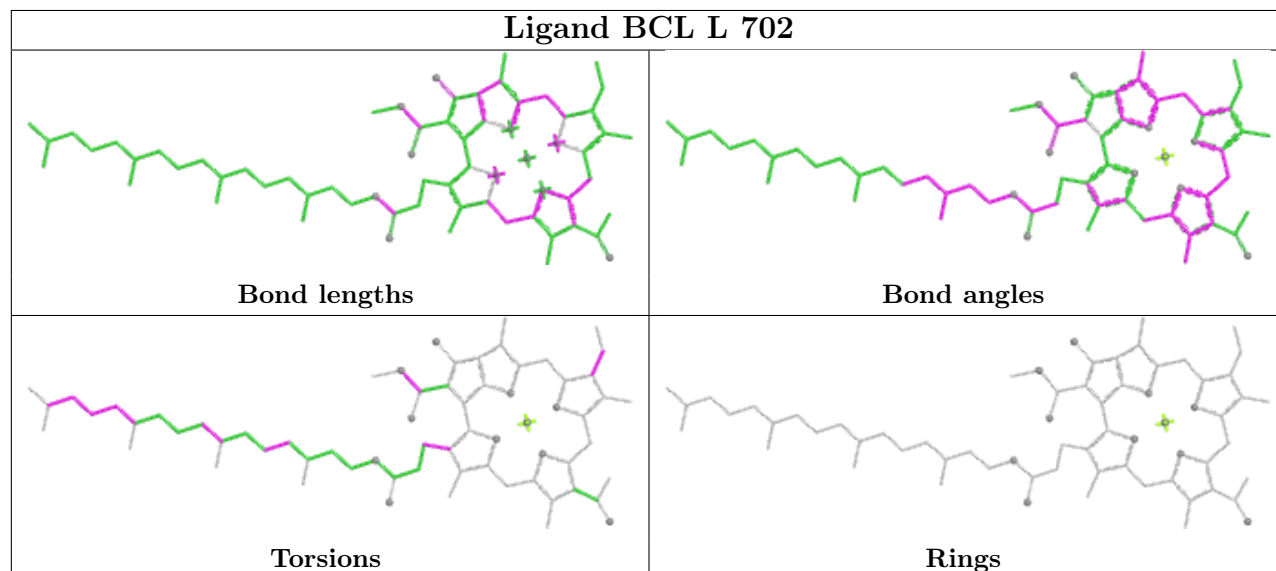
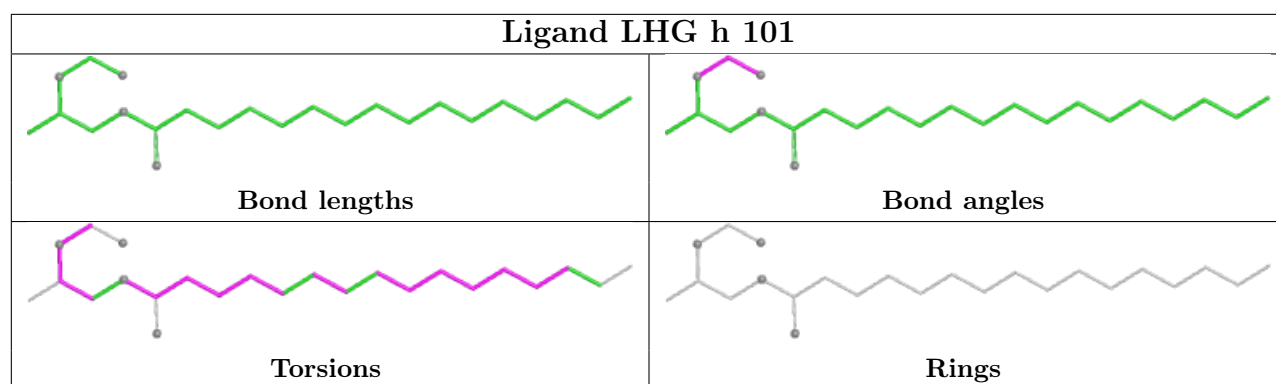


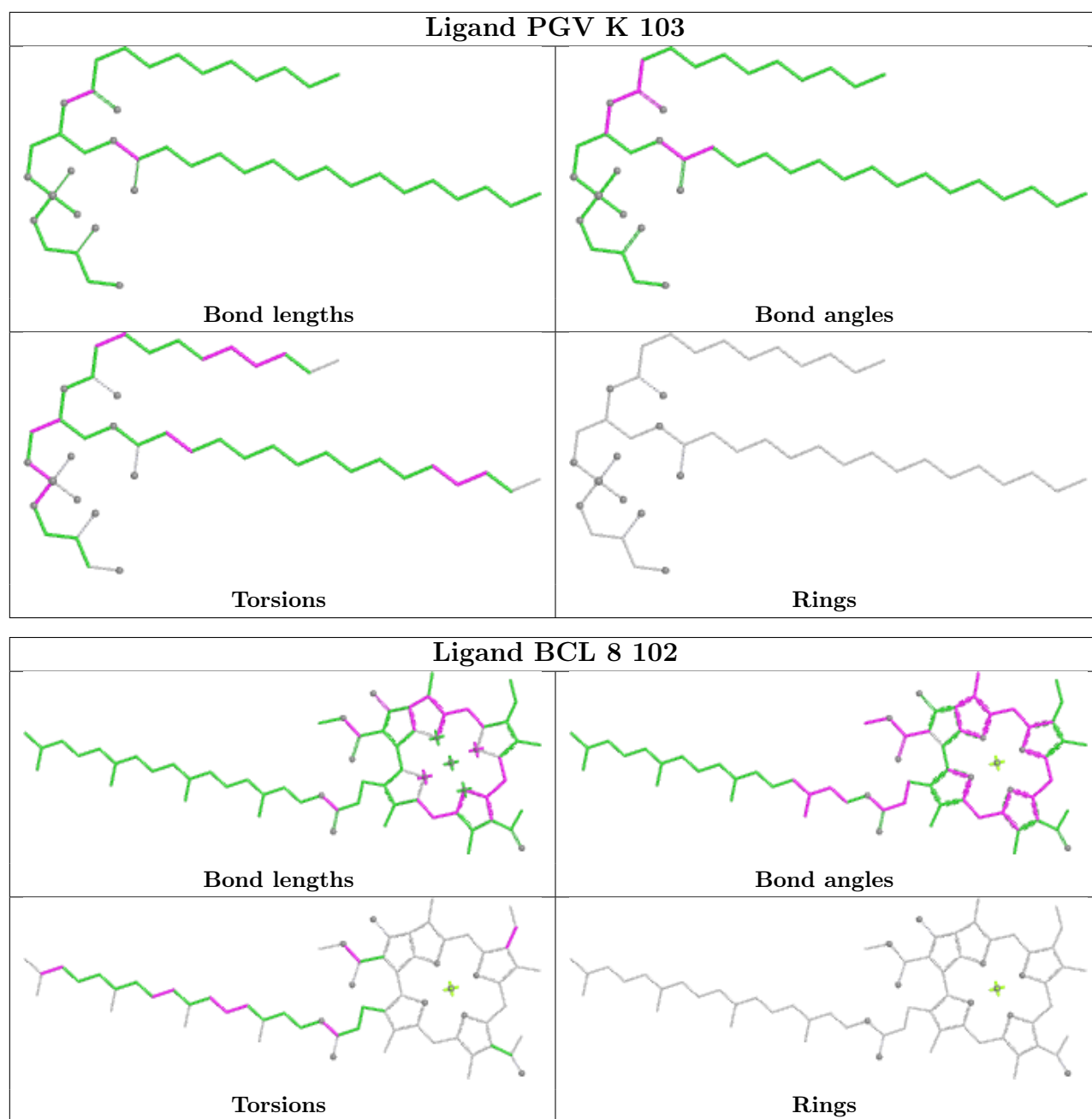
Ligand PGV I 103

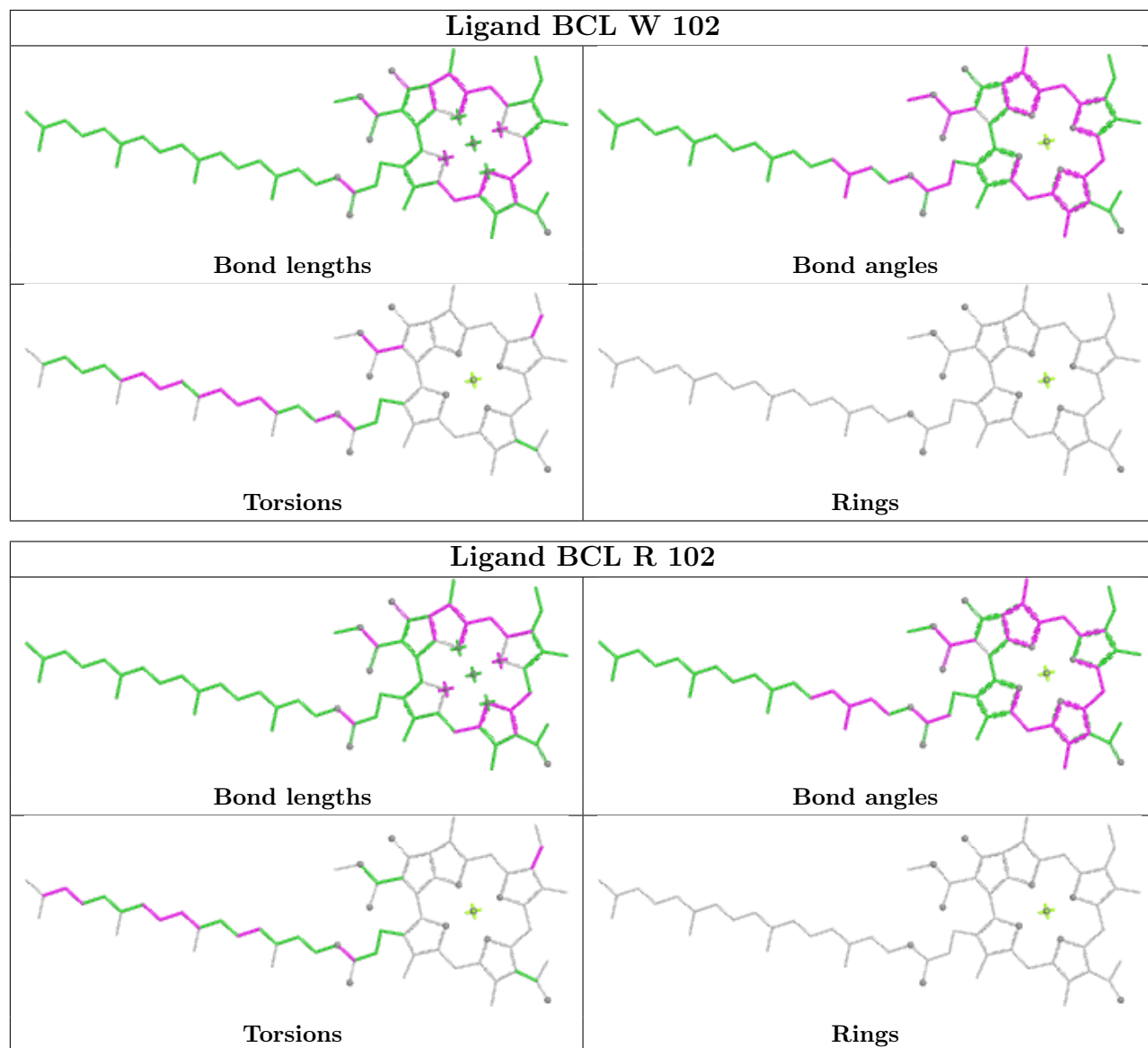


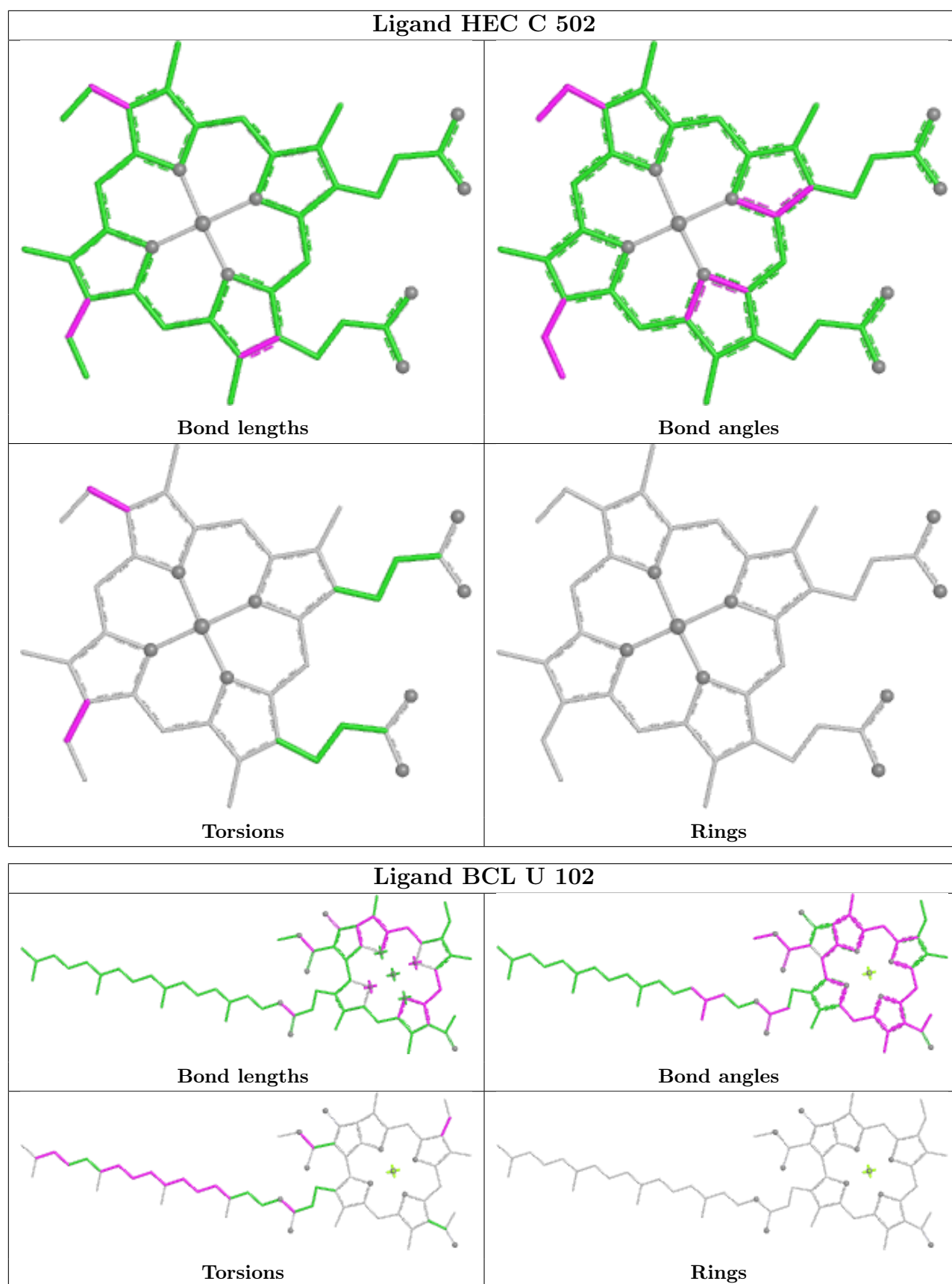
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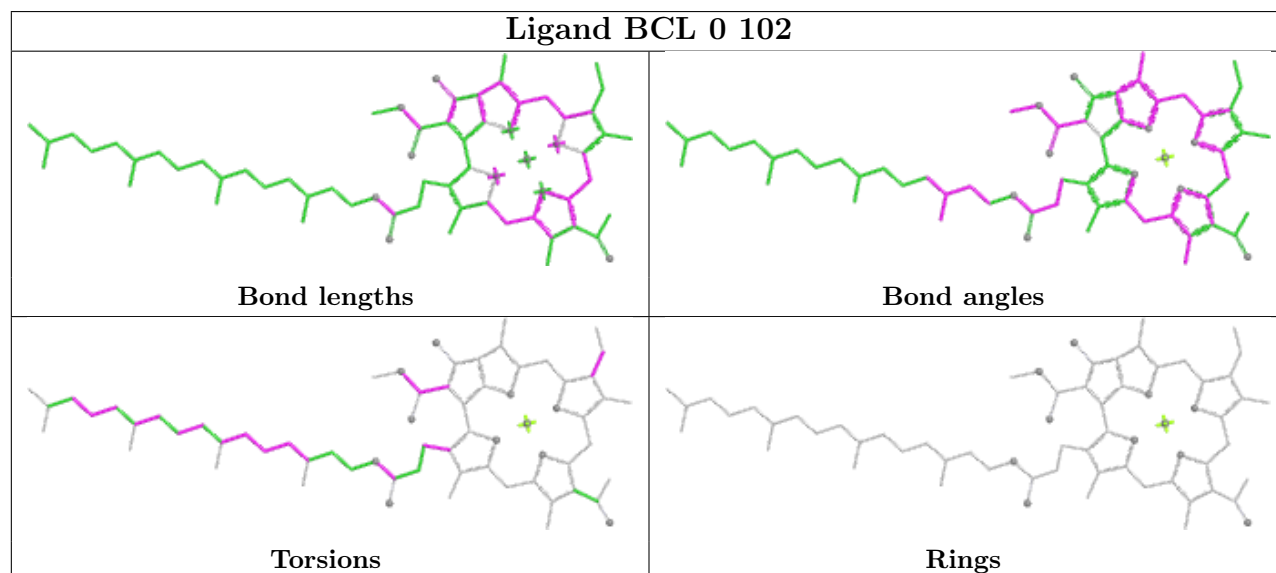
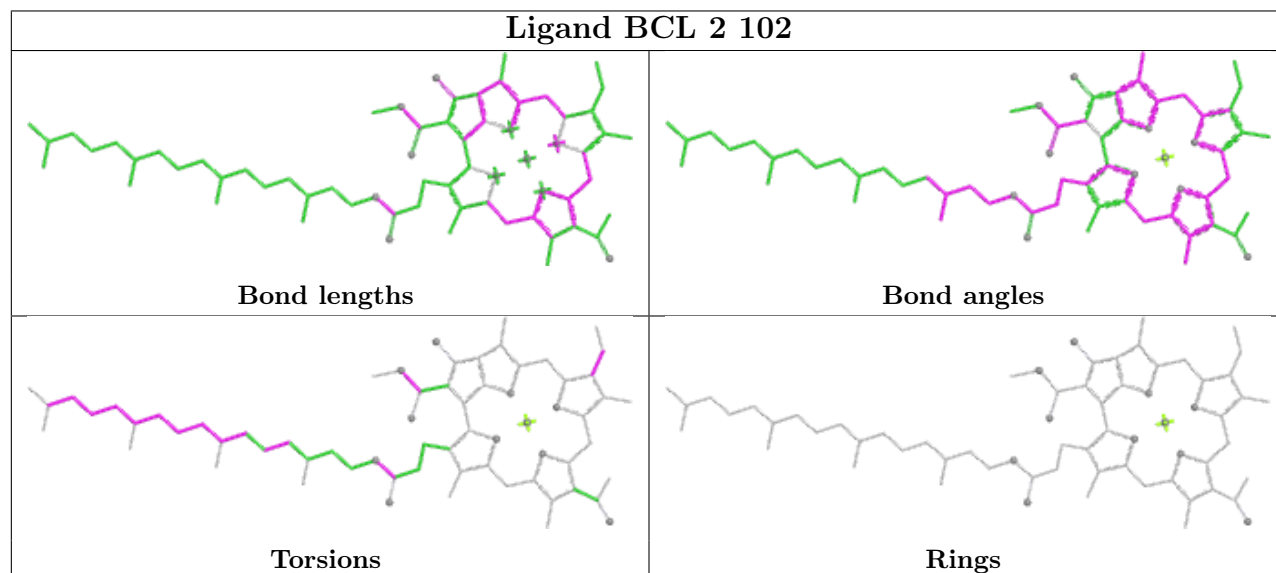
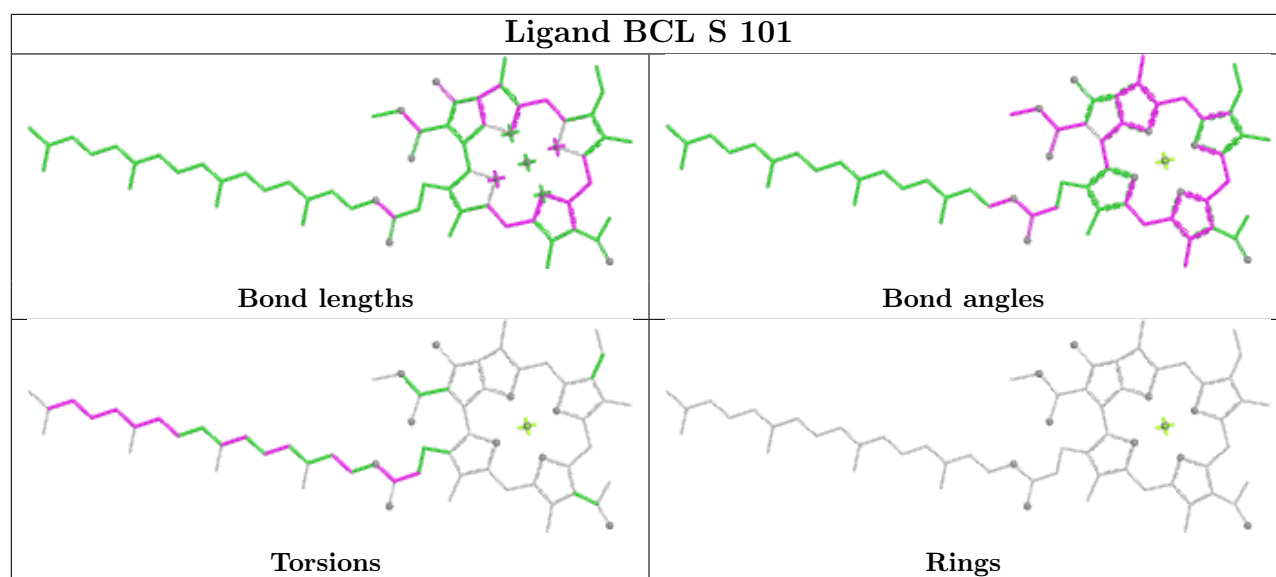


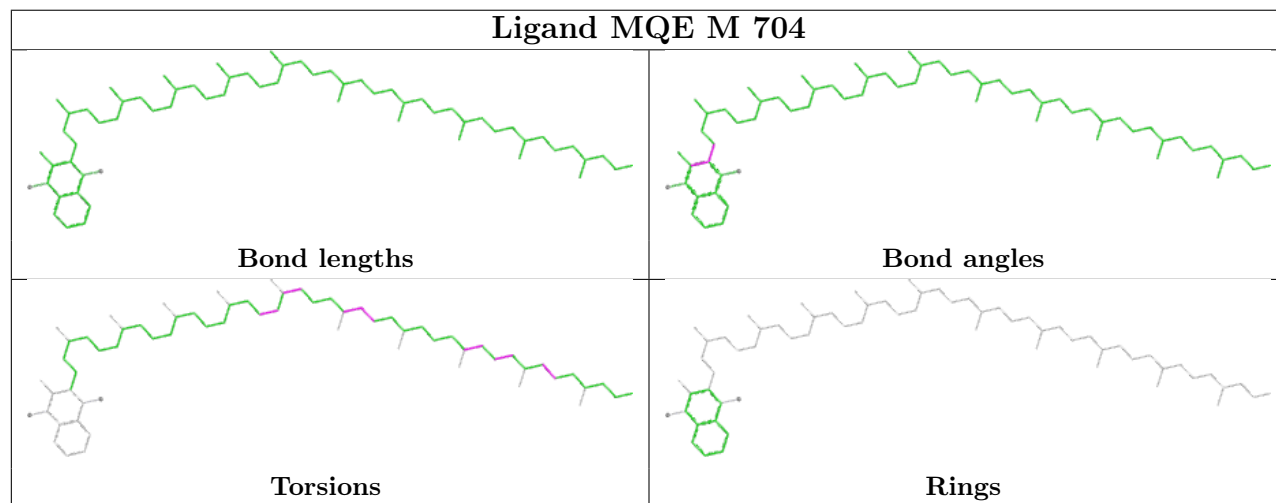
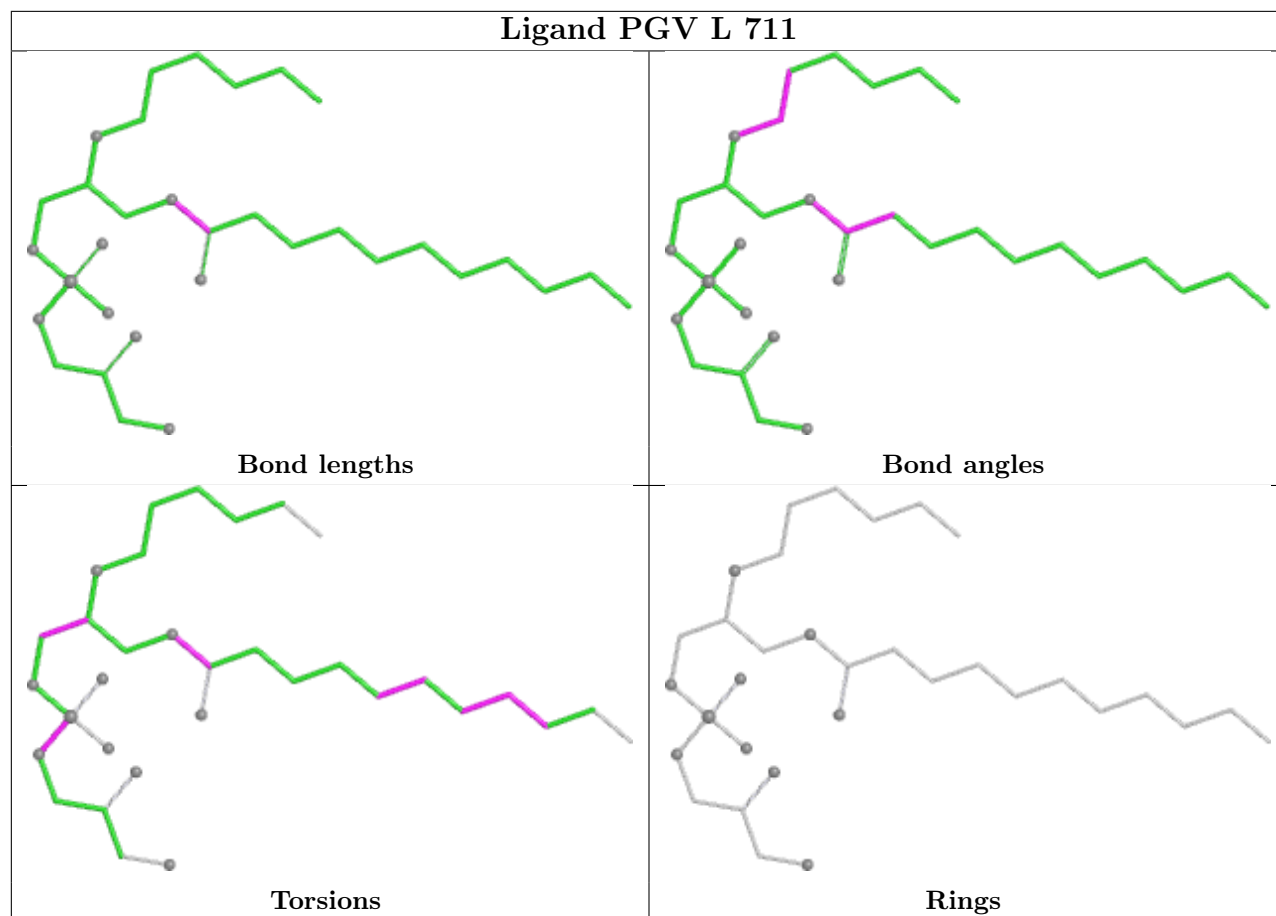


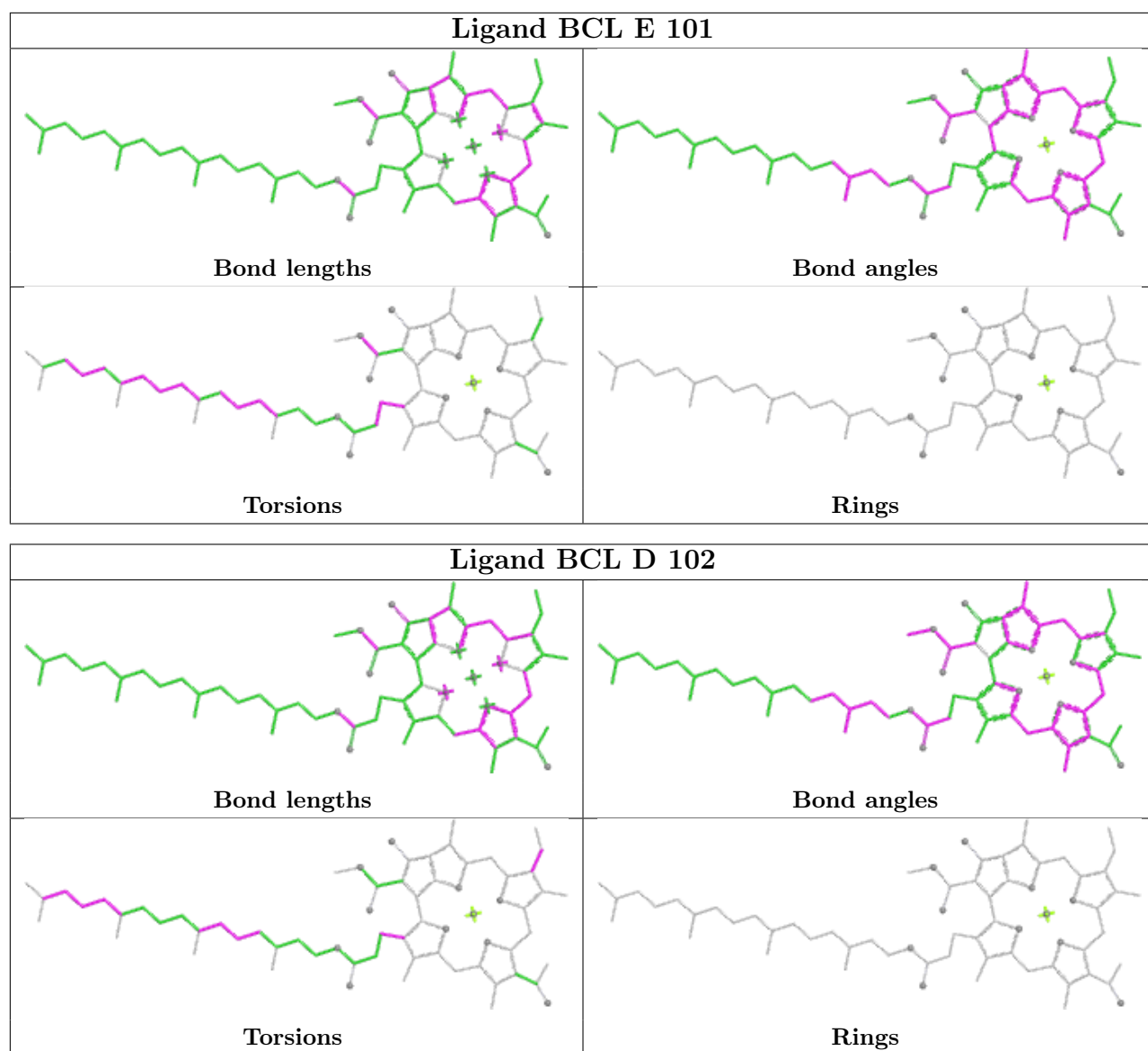


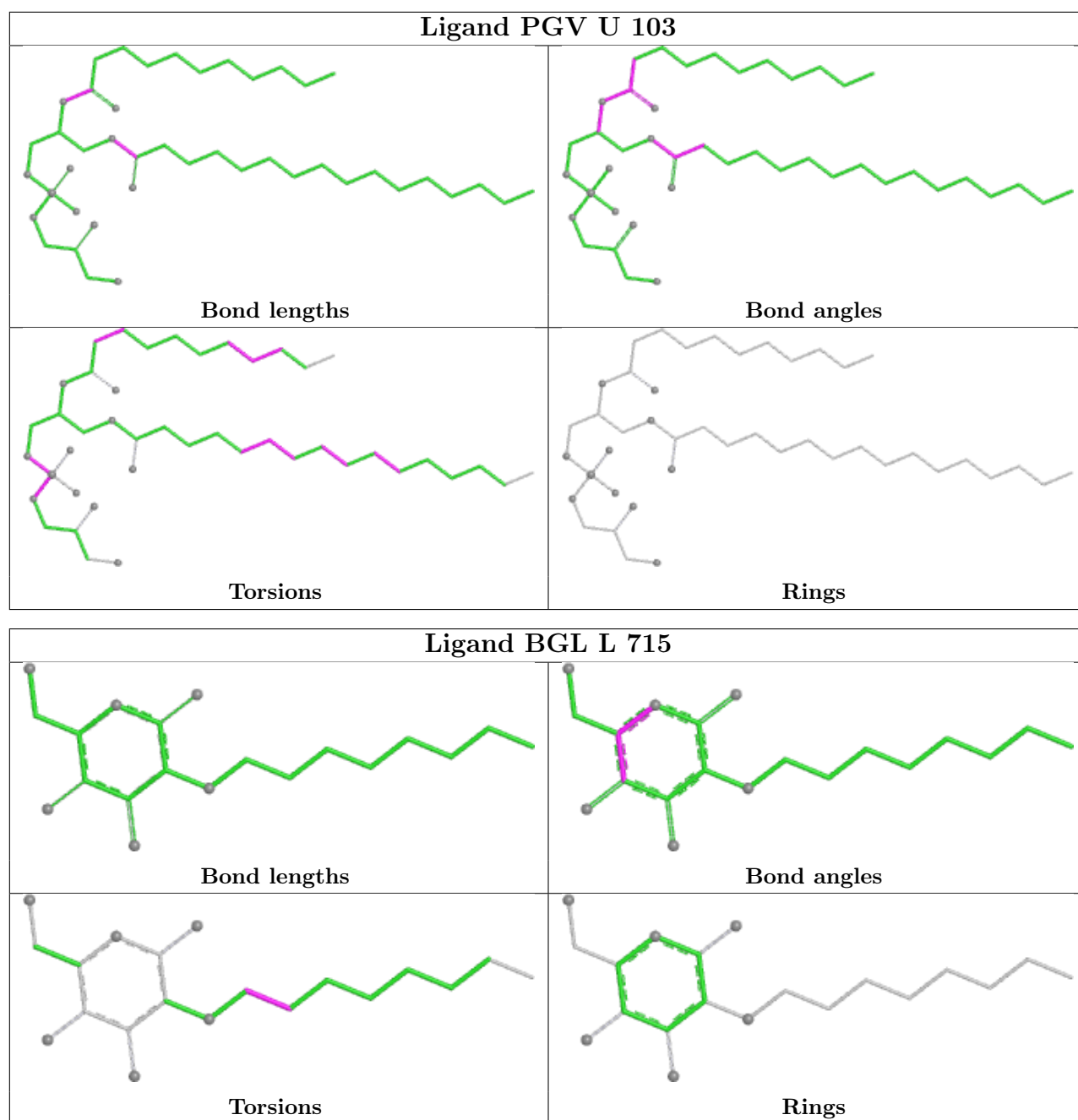


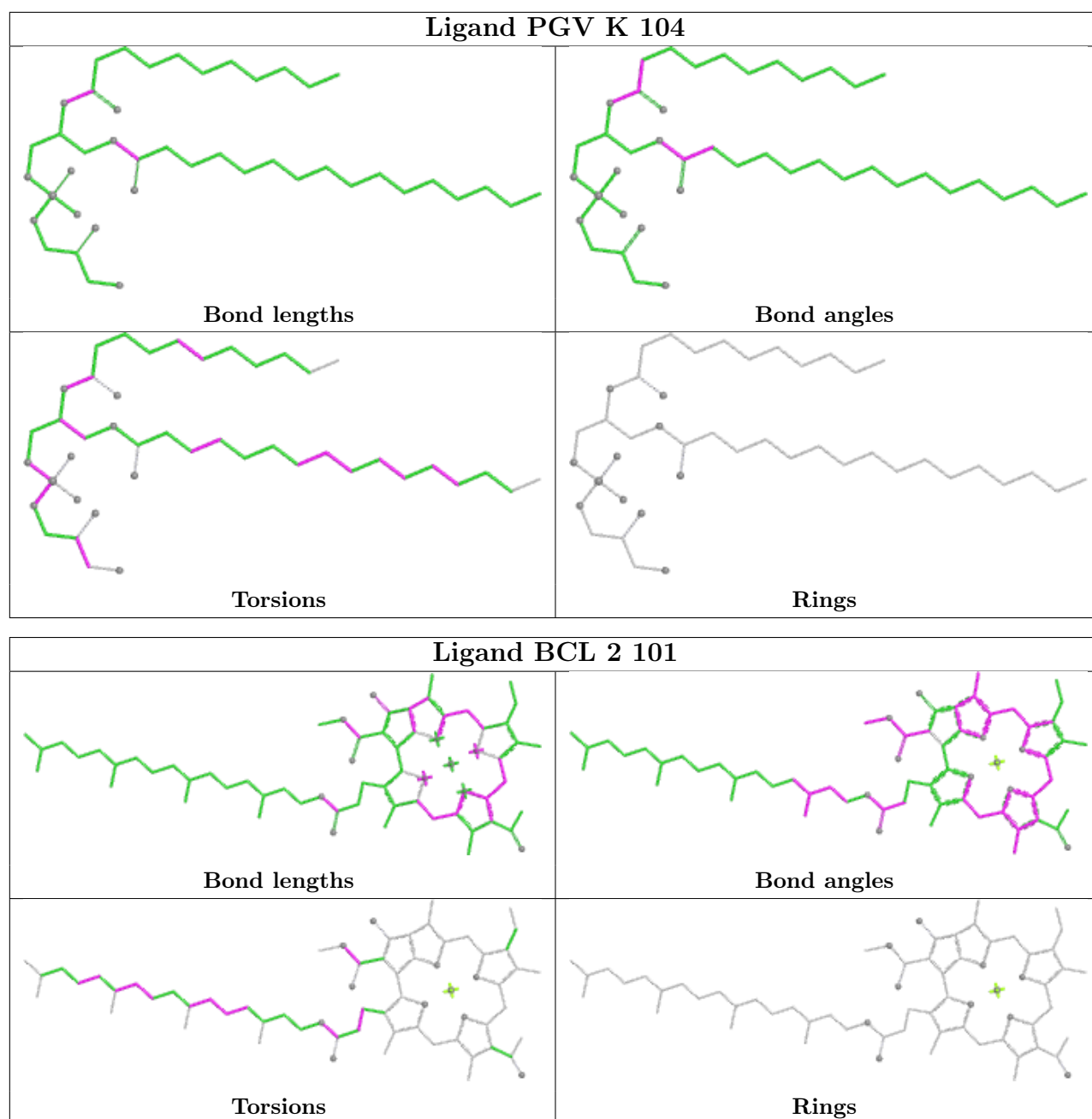


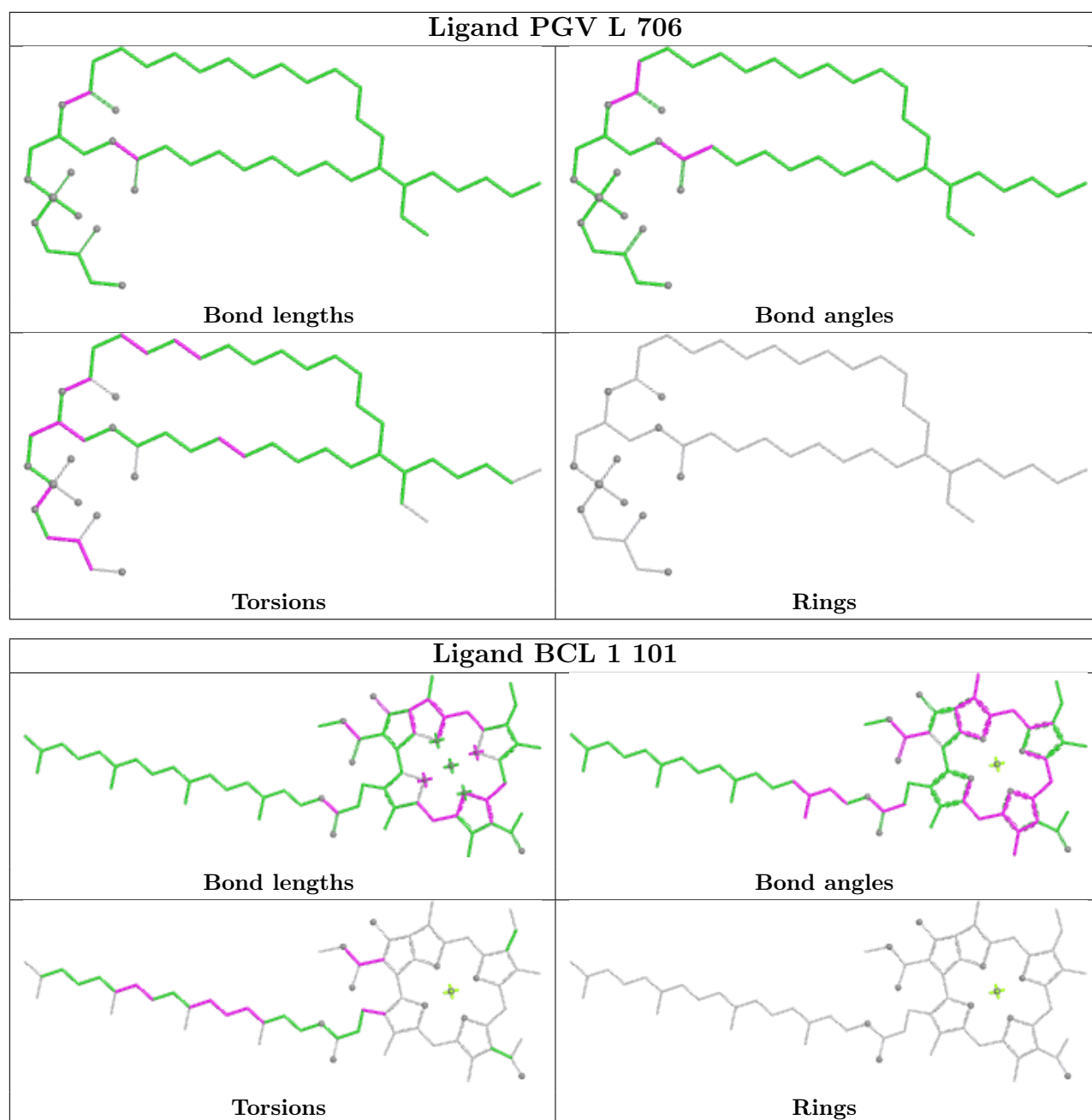


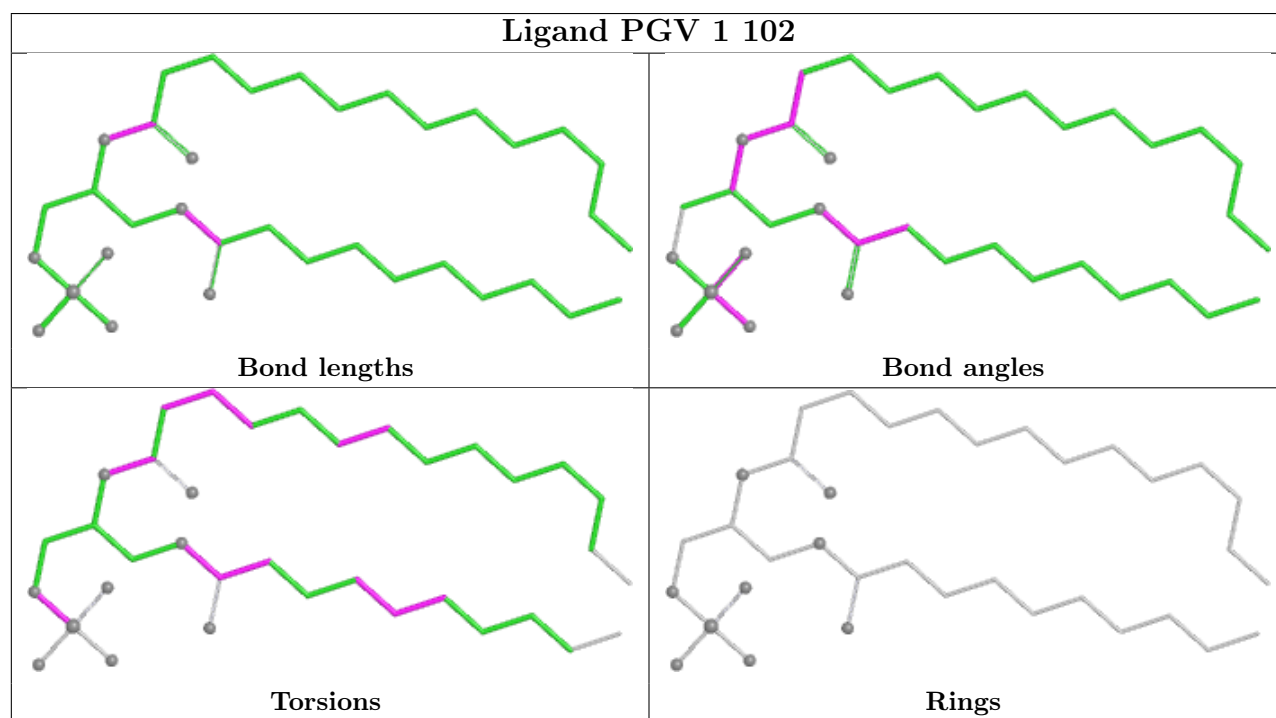
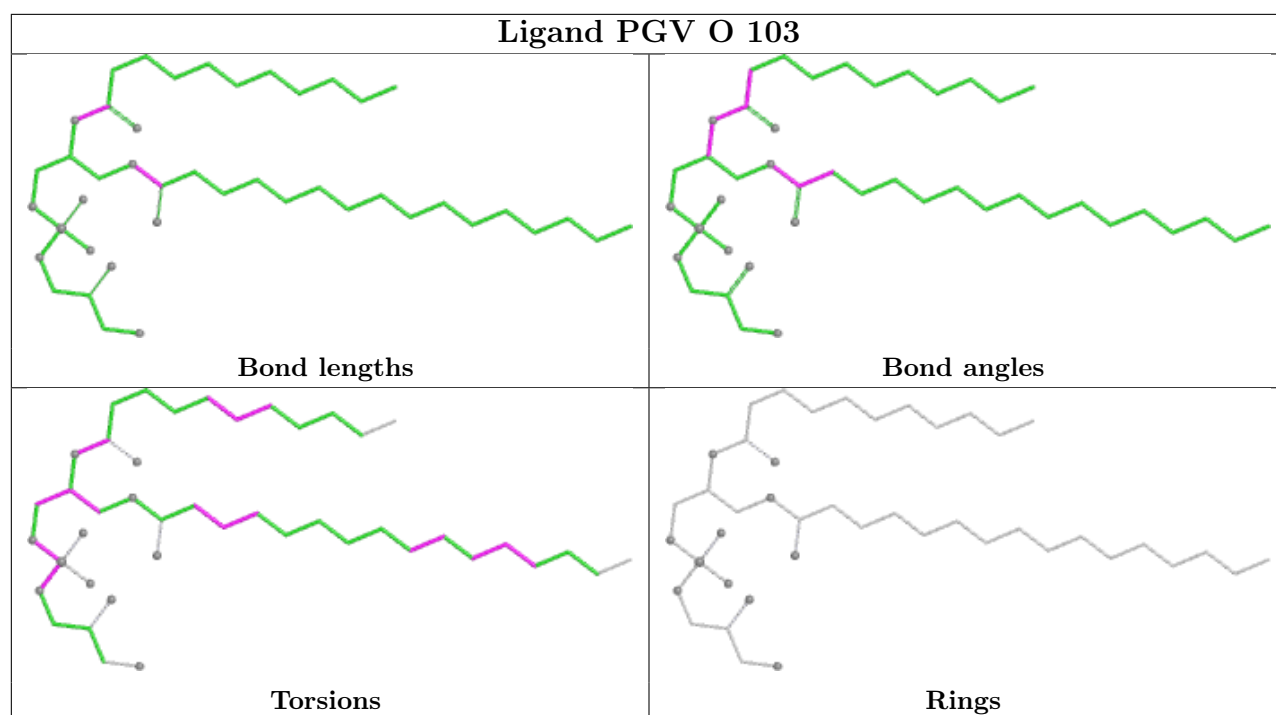


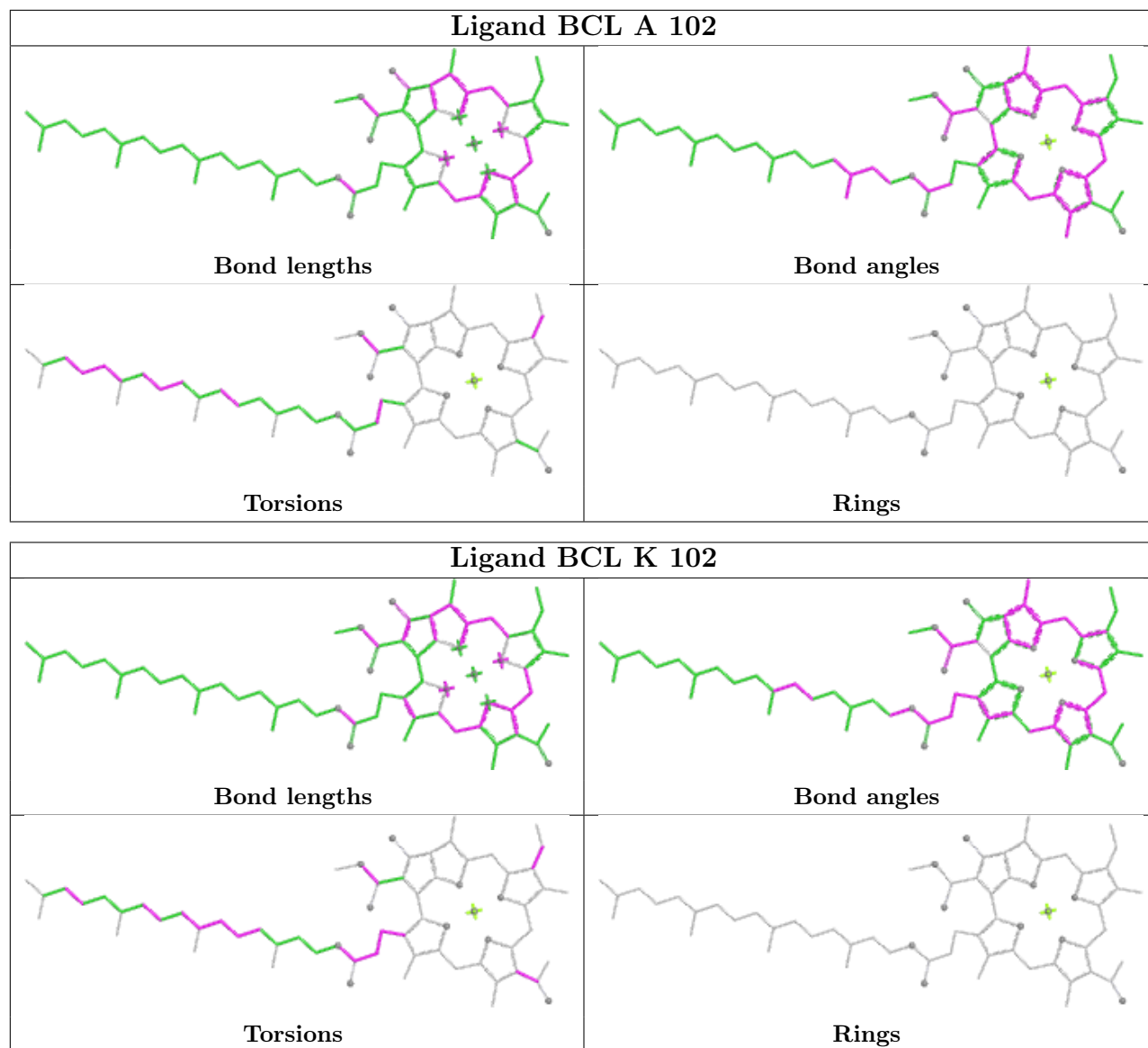


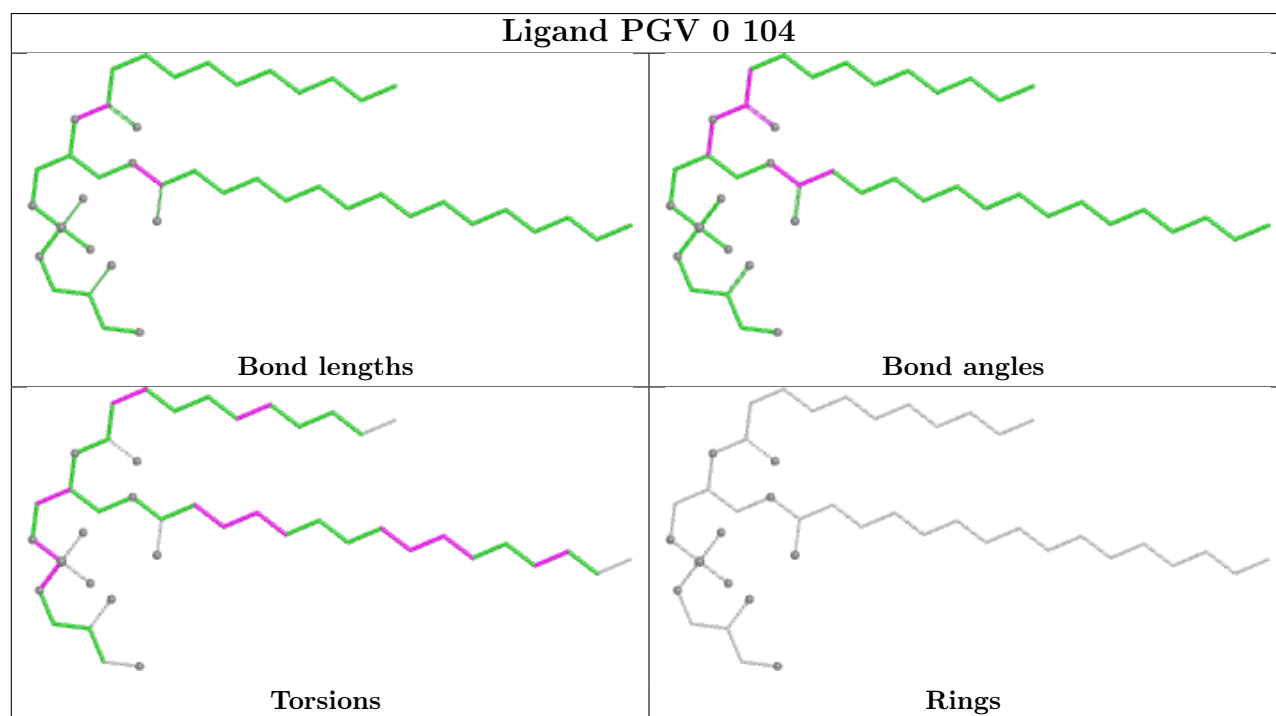
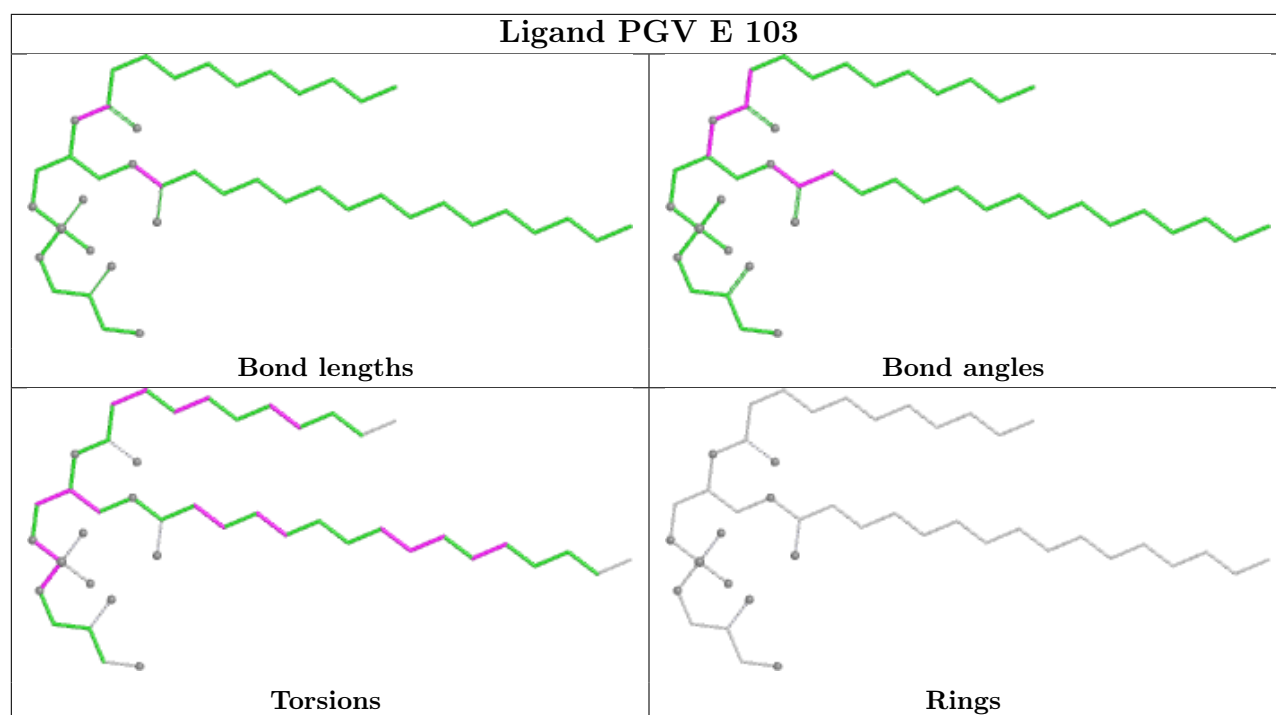


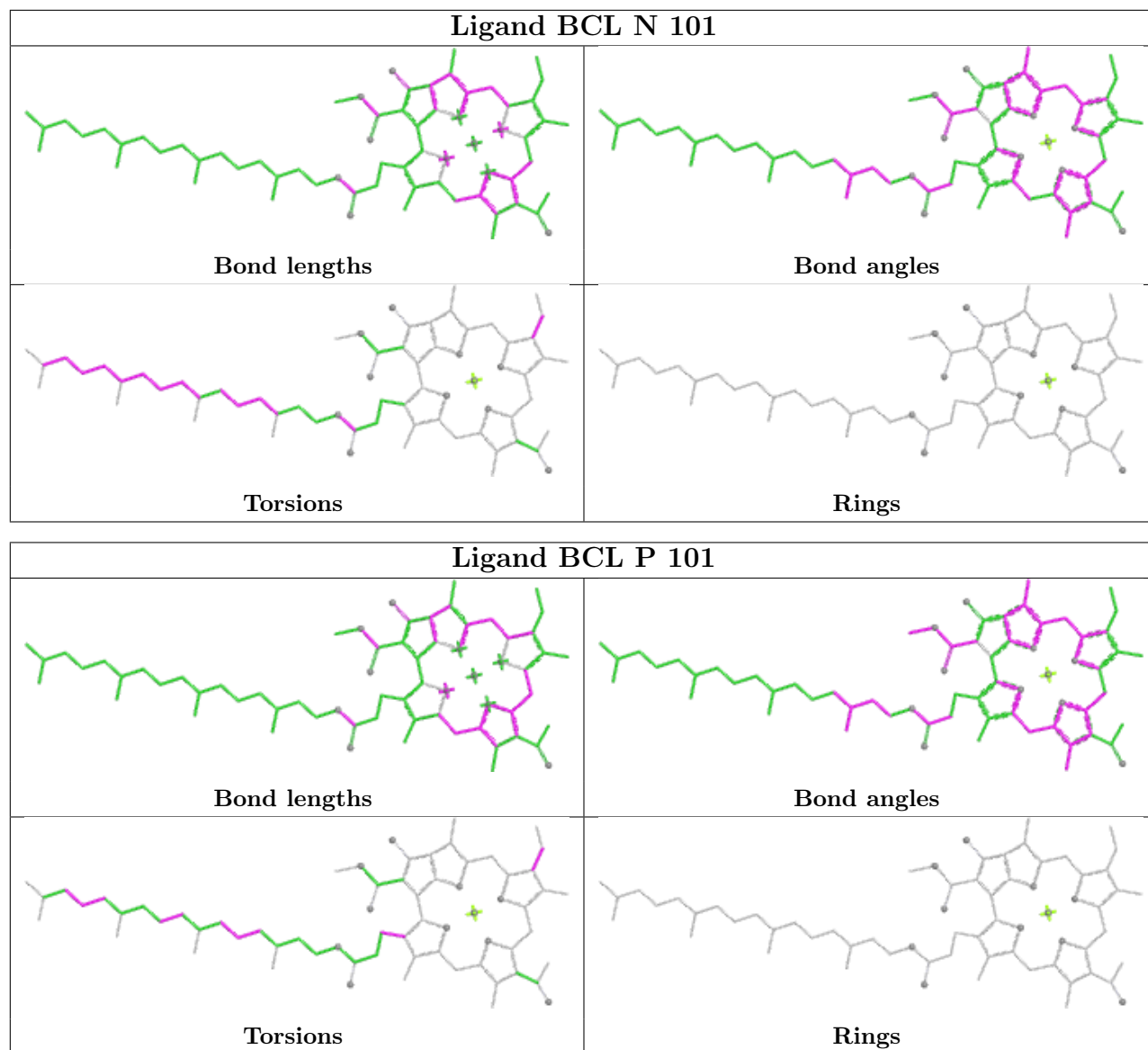


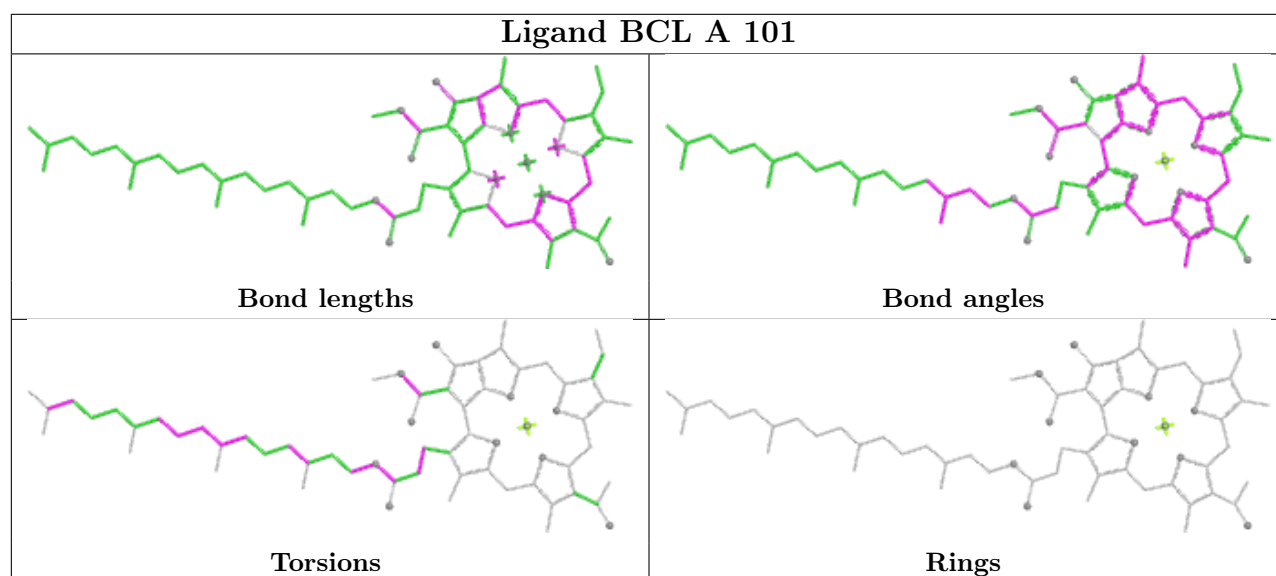
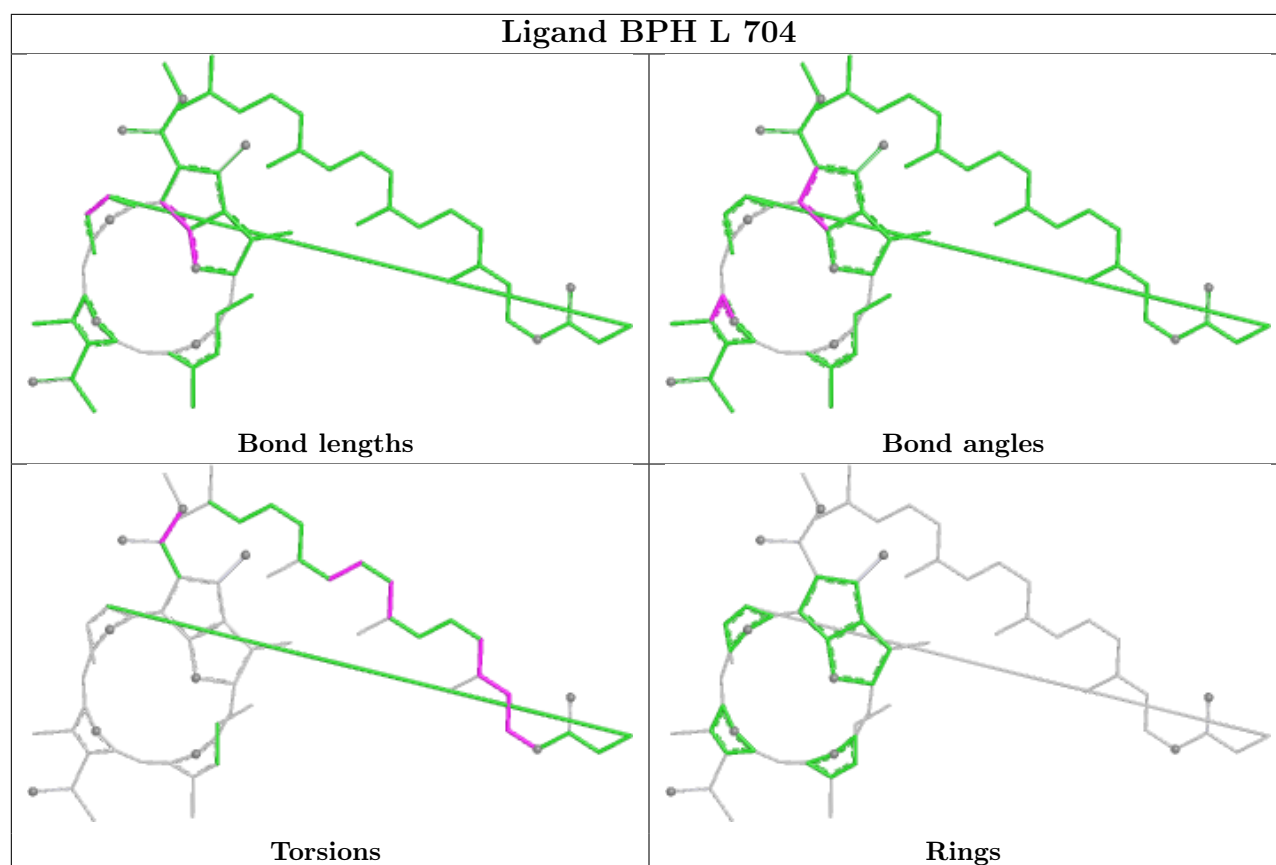




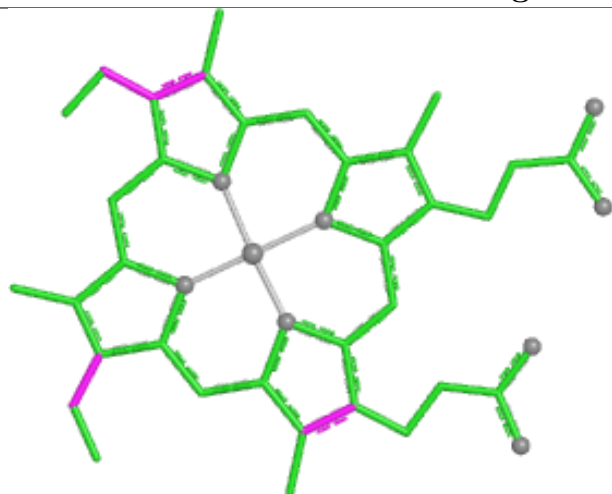




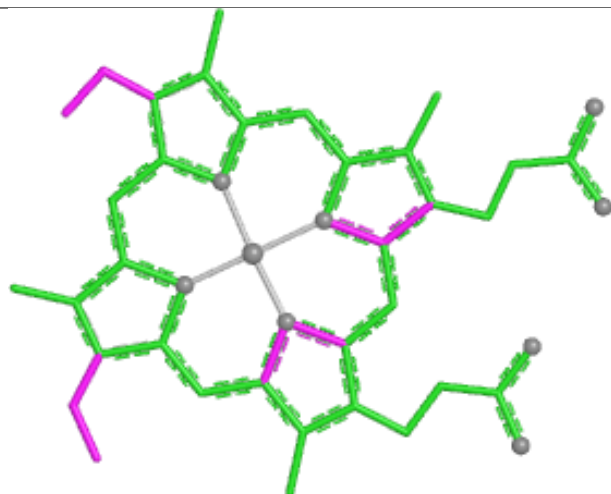




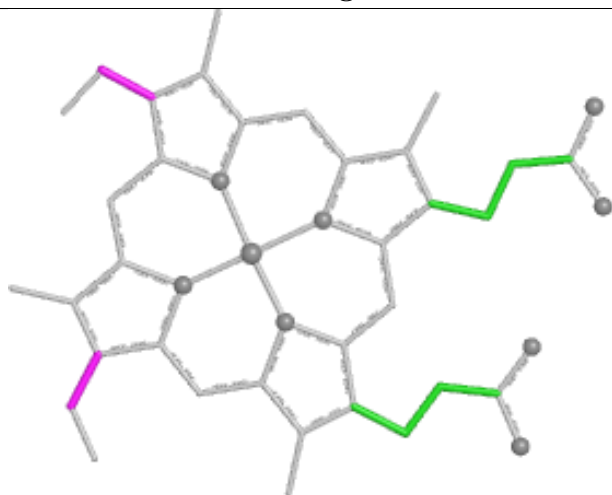
Ligand HEC C 503



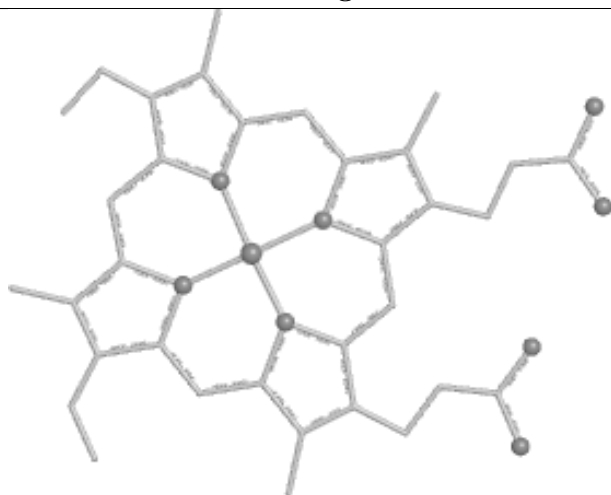
Bond lengths



Bond angles

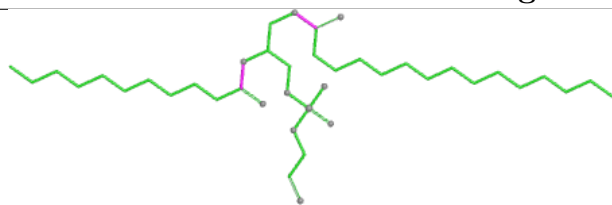


Torsions

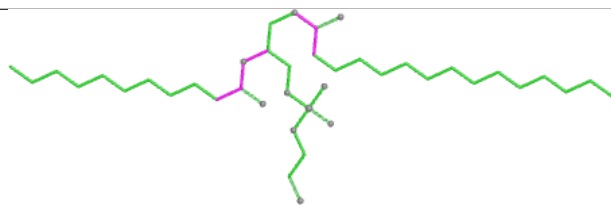


Rings

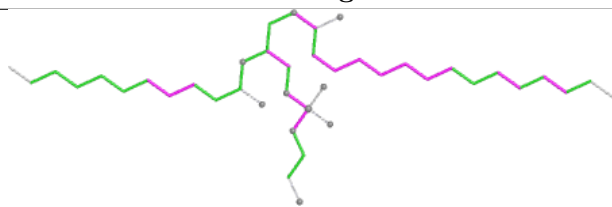
Ligand PEF h 103



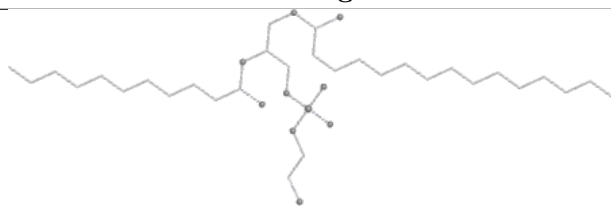
Bond lengths



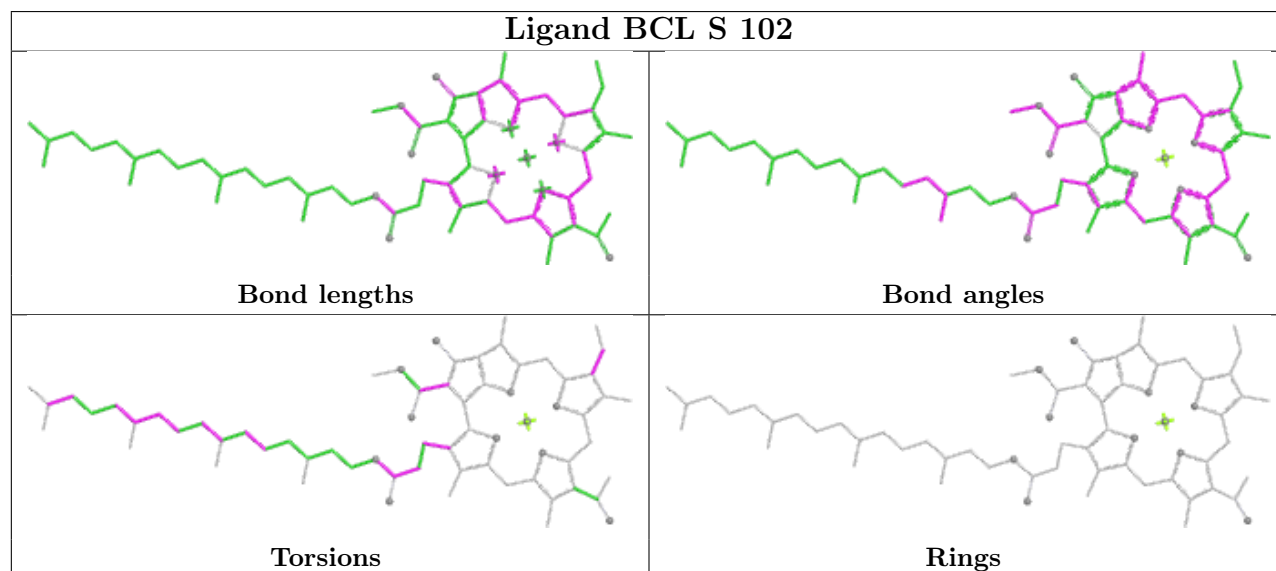
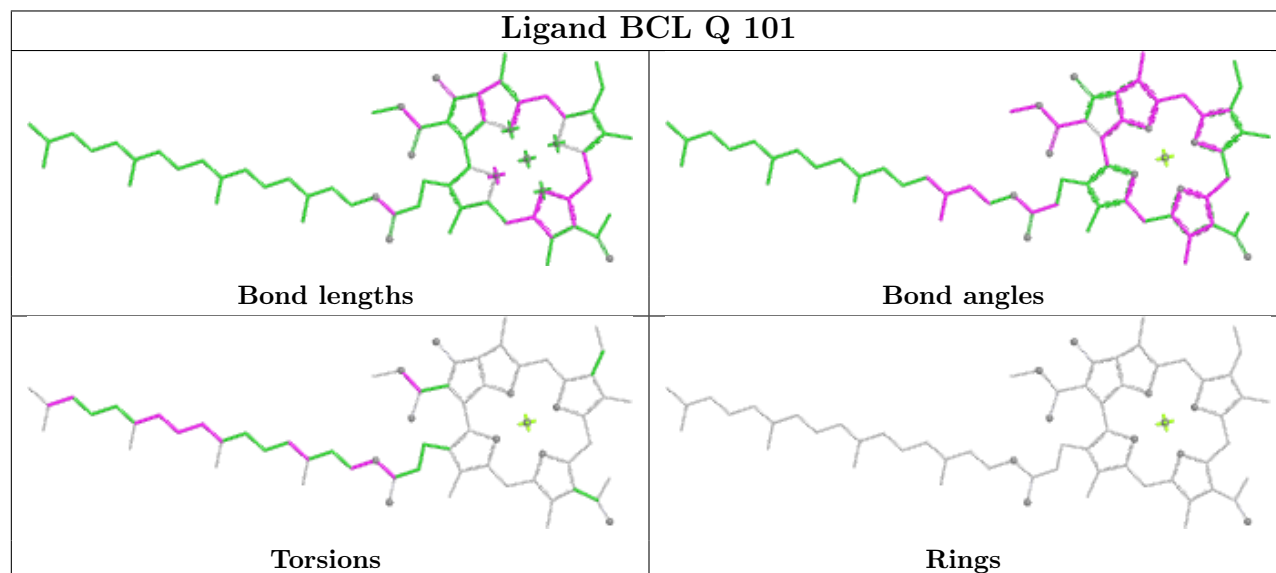
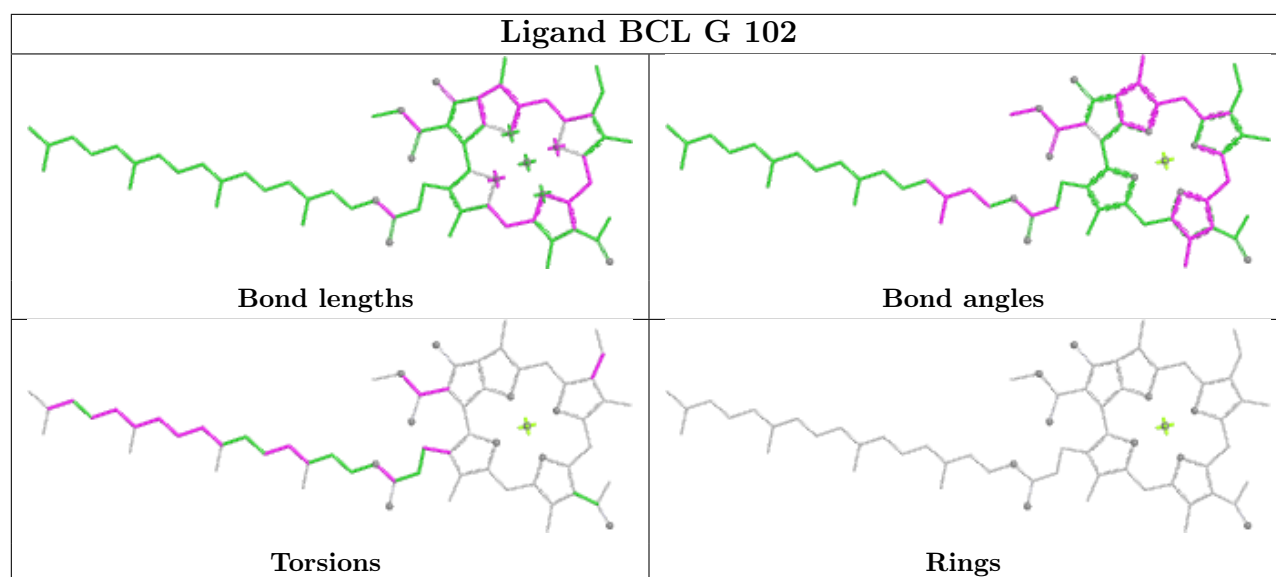
Bond angles

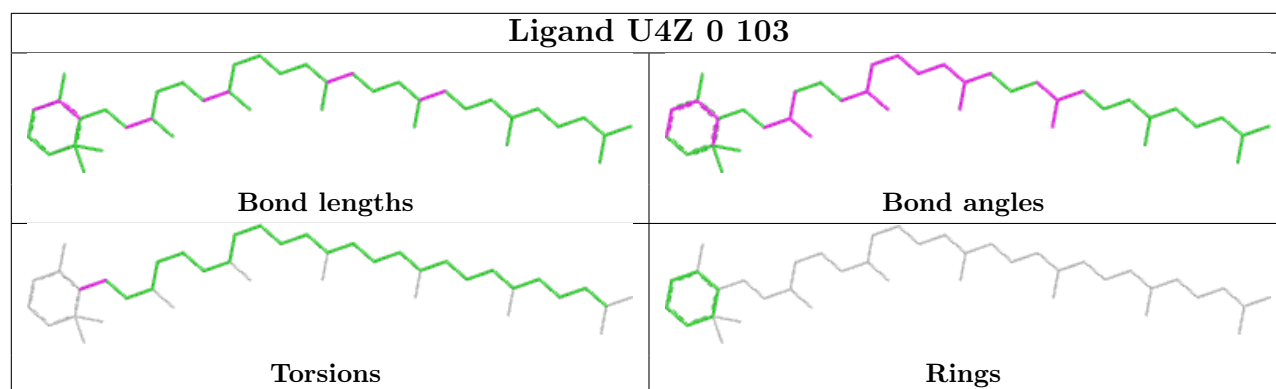
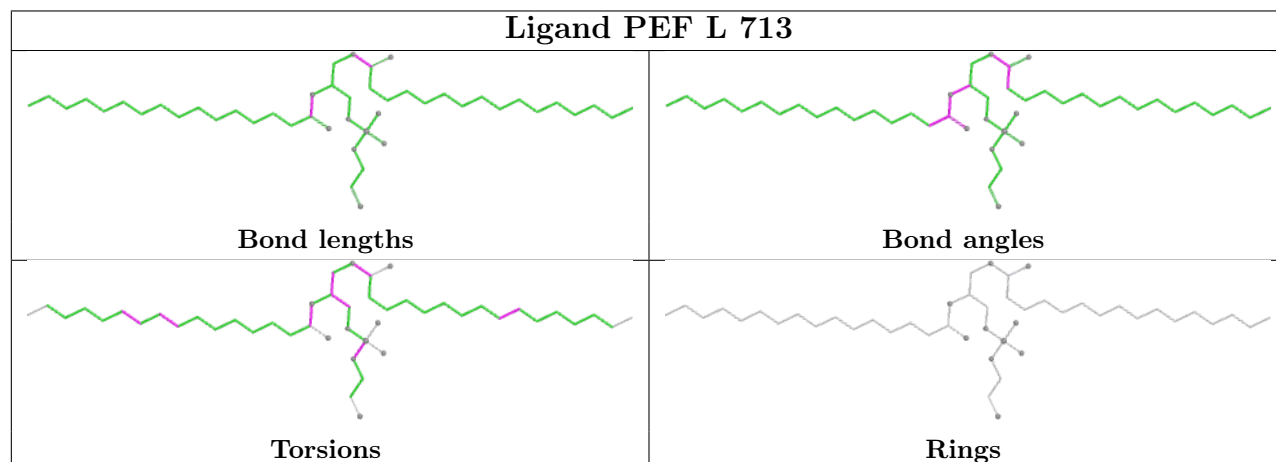
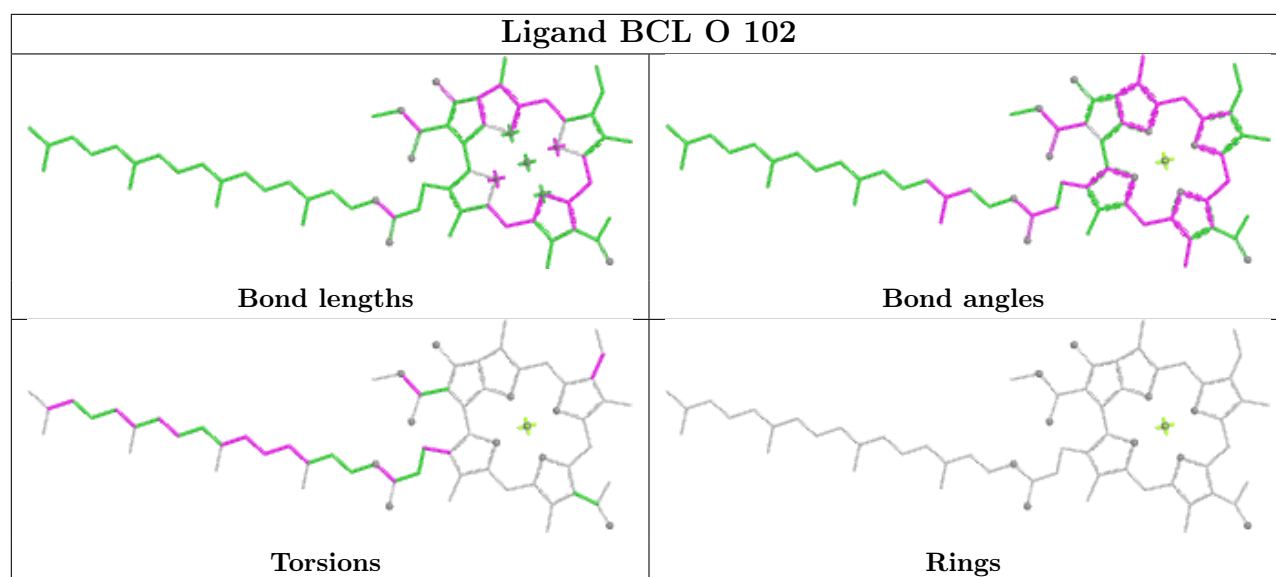


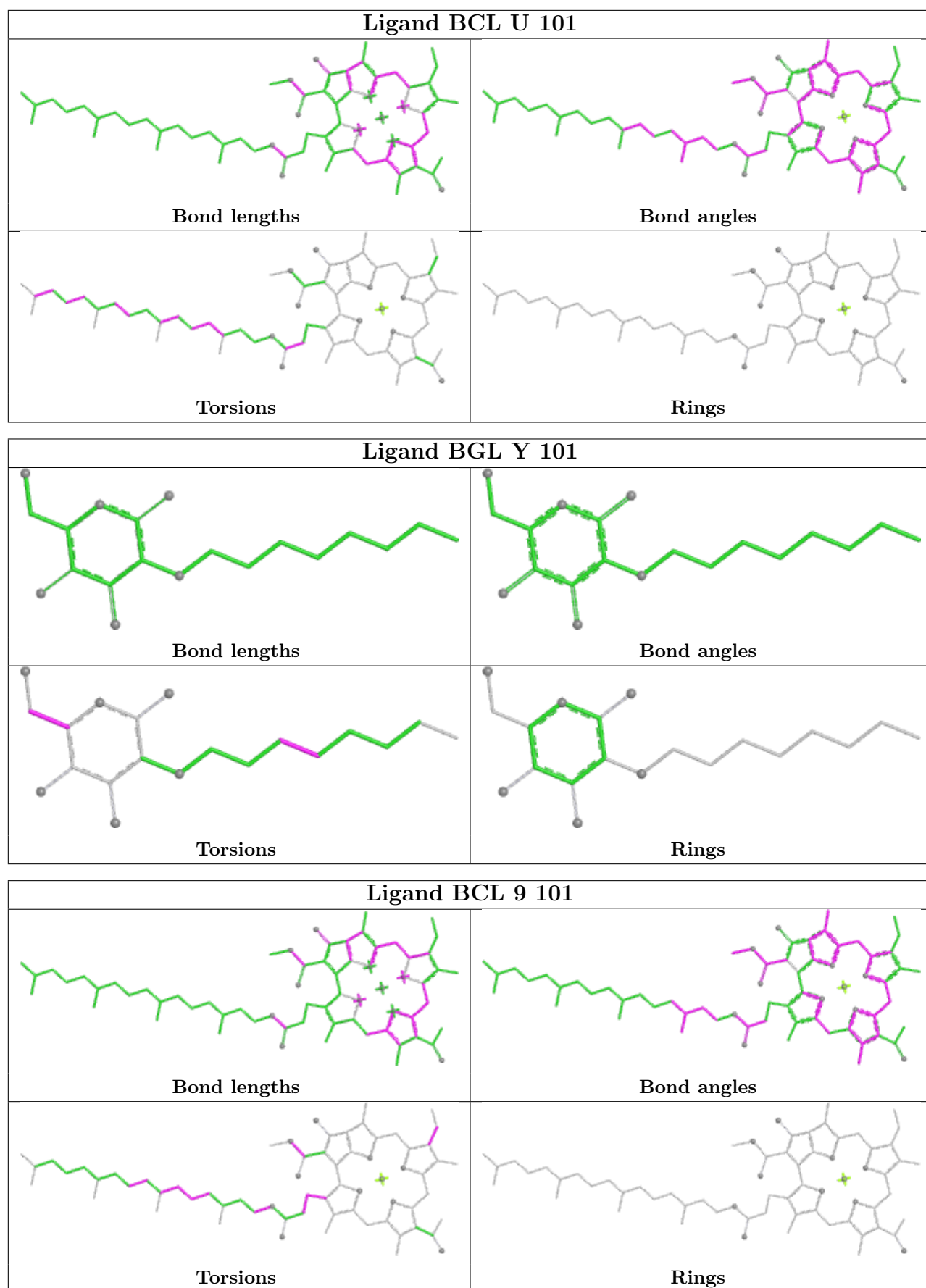
Torsions

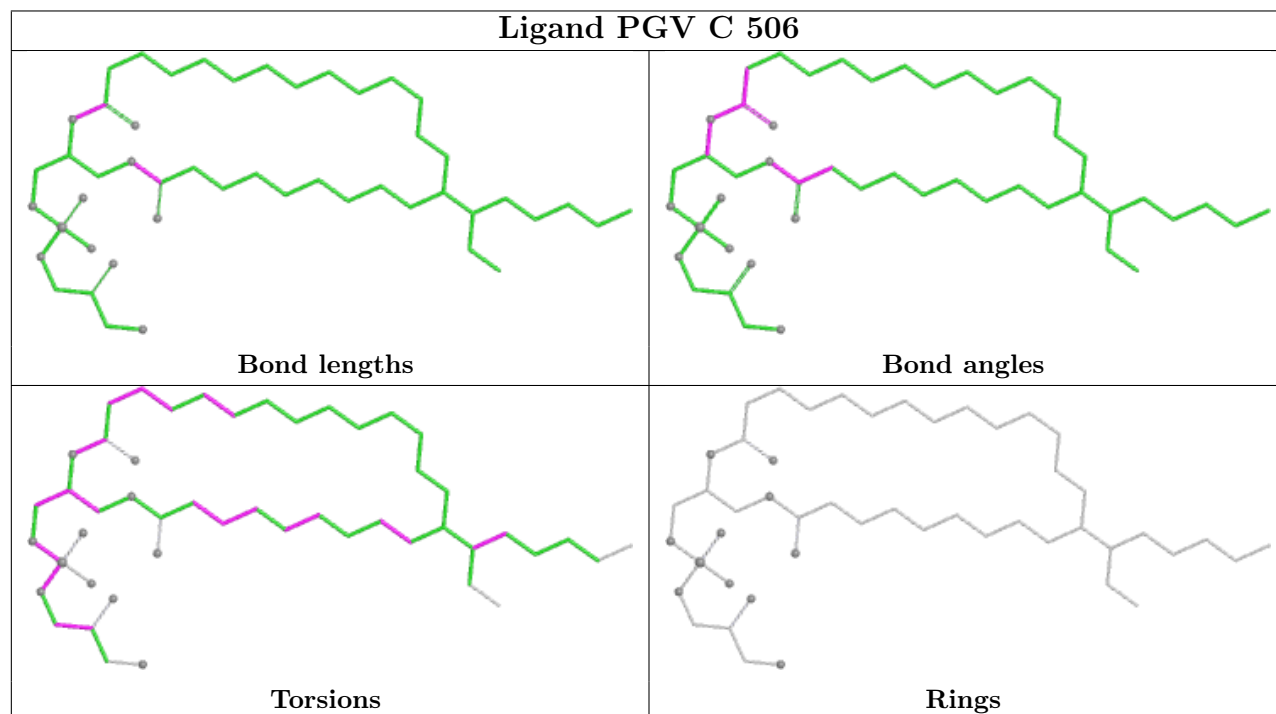
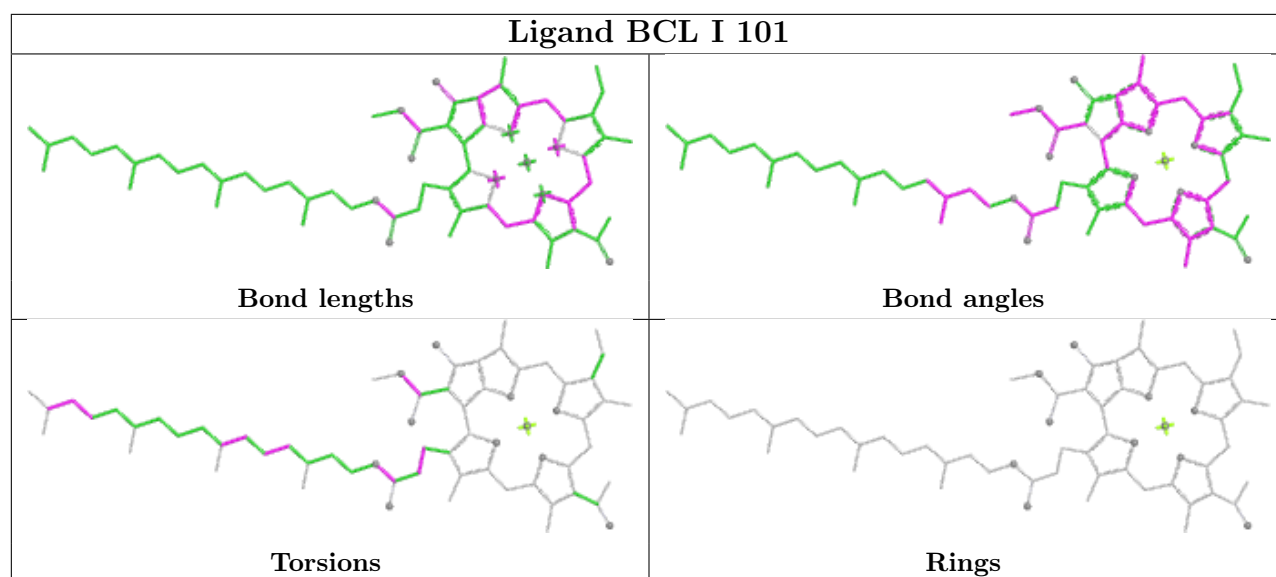


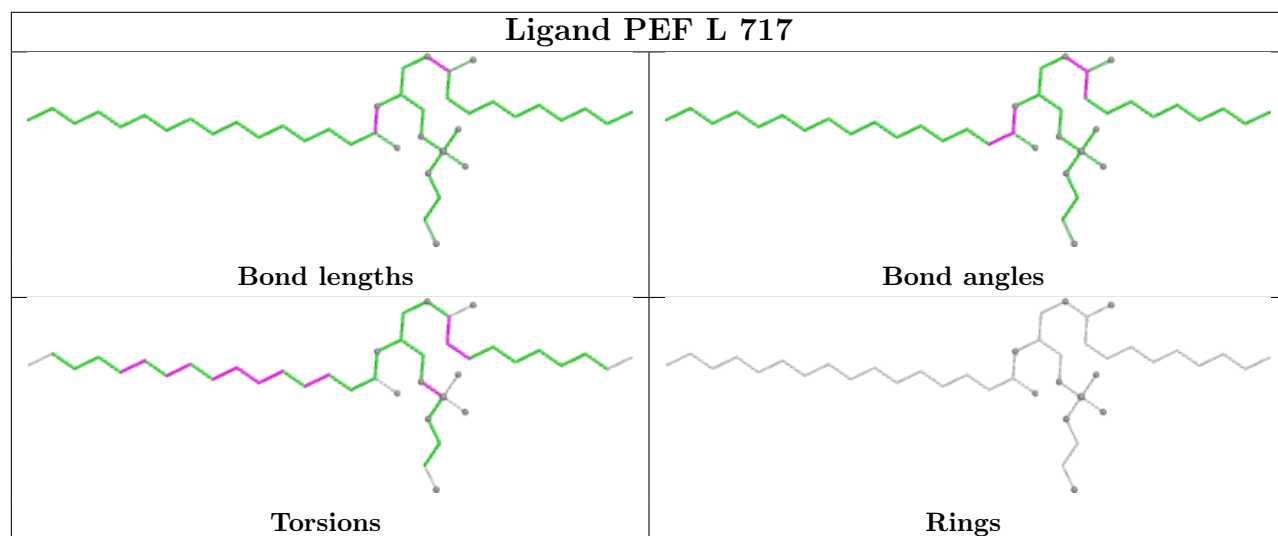
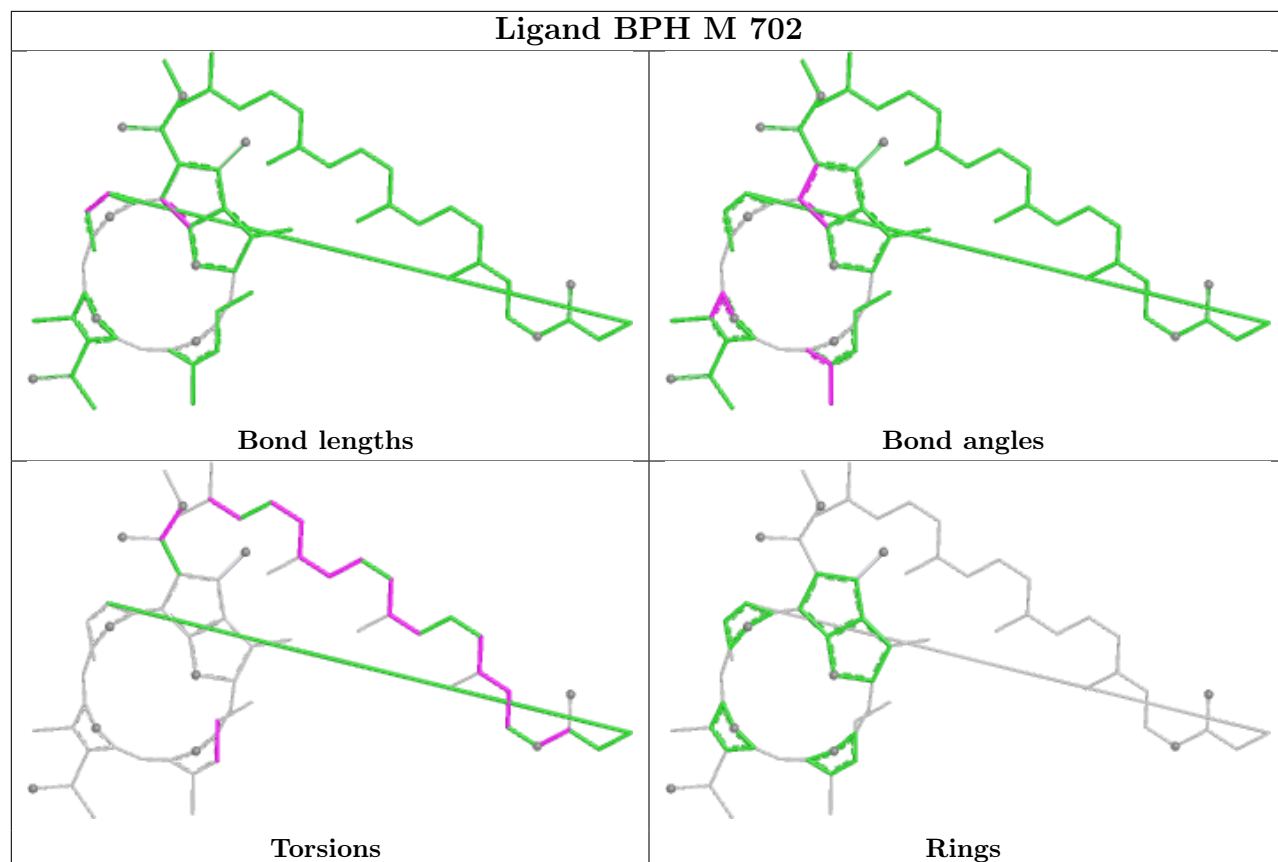
Rings

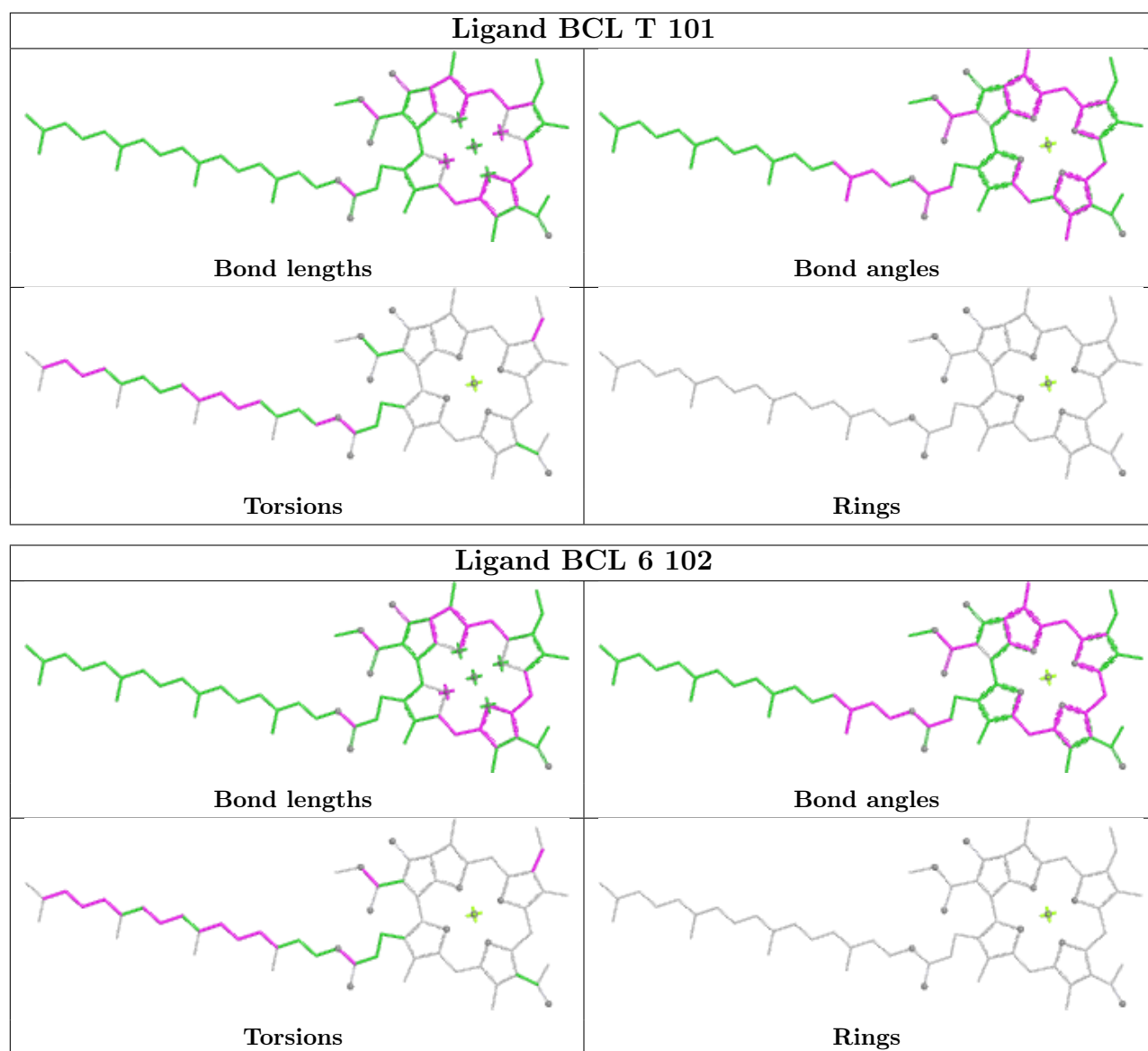


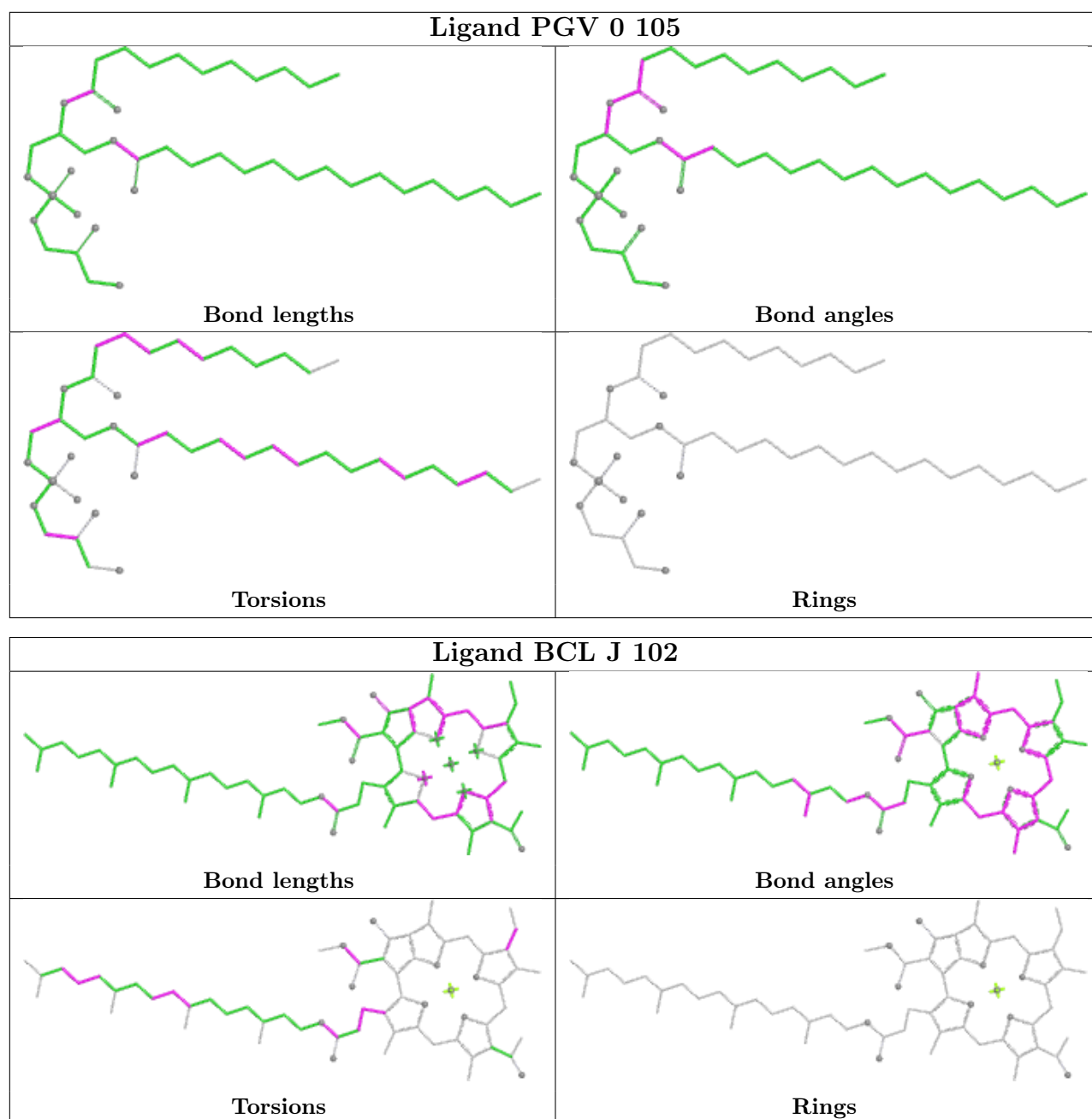


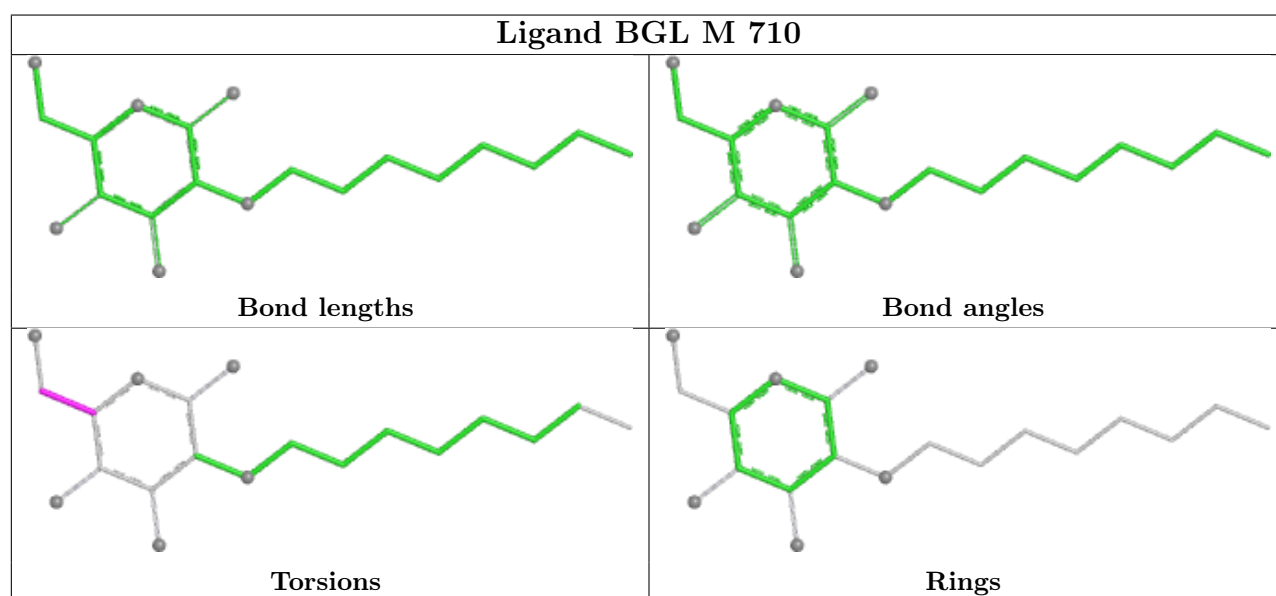
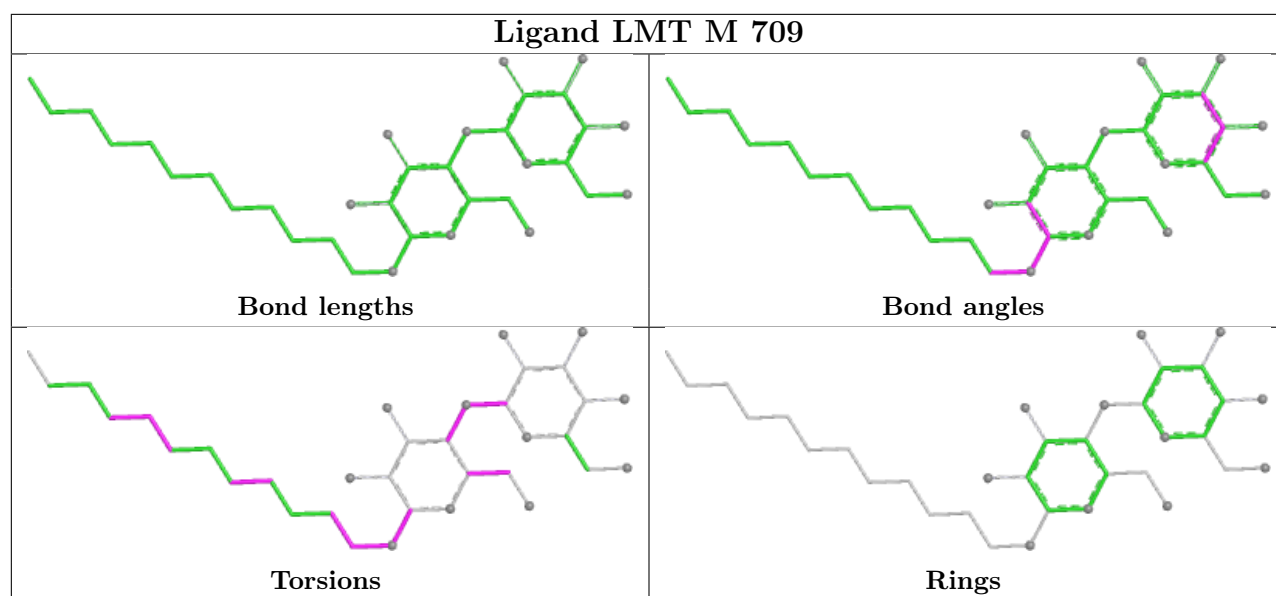


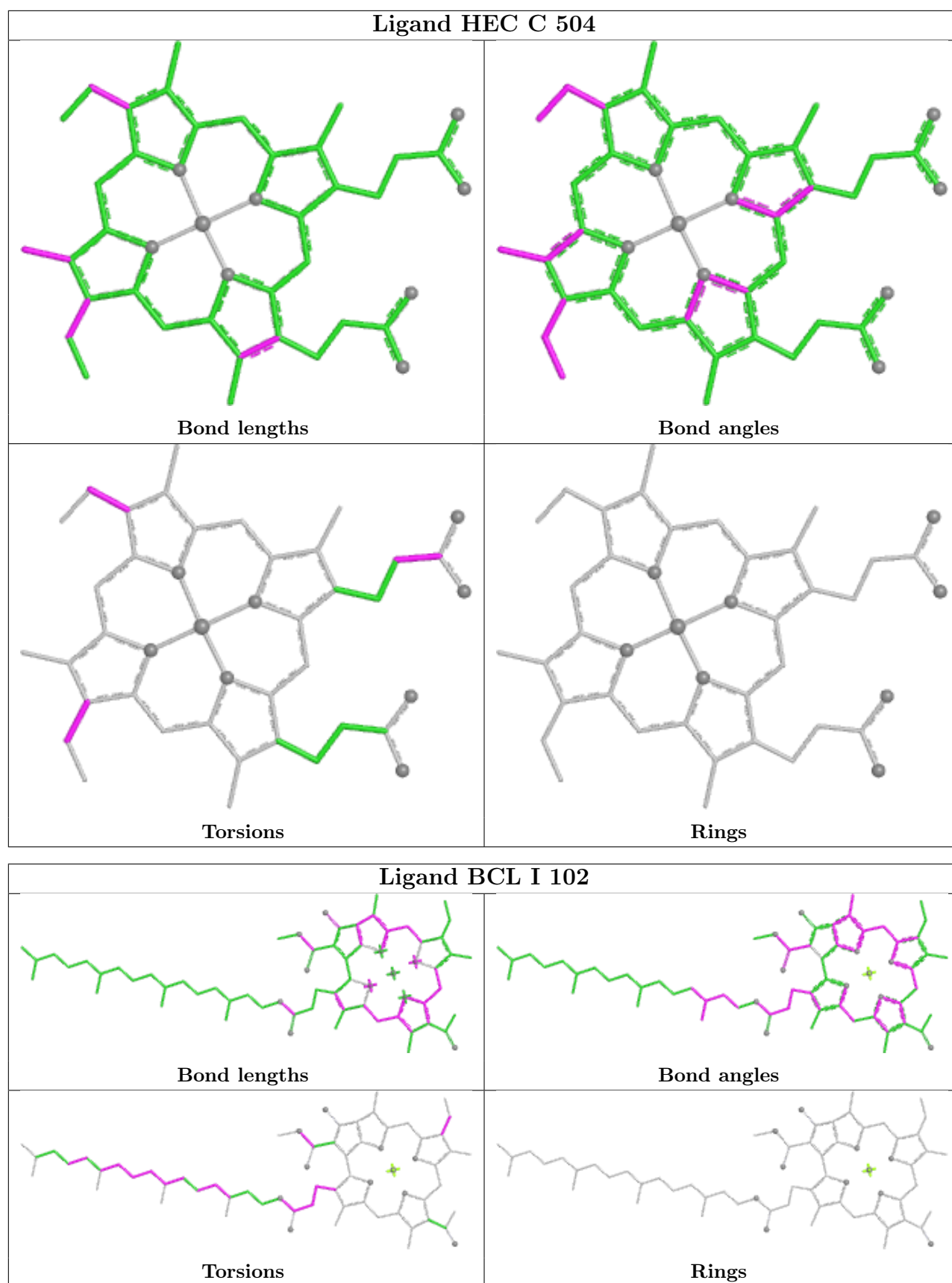


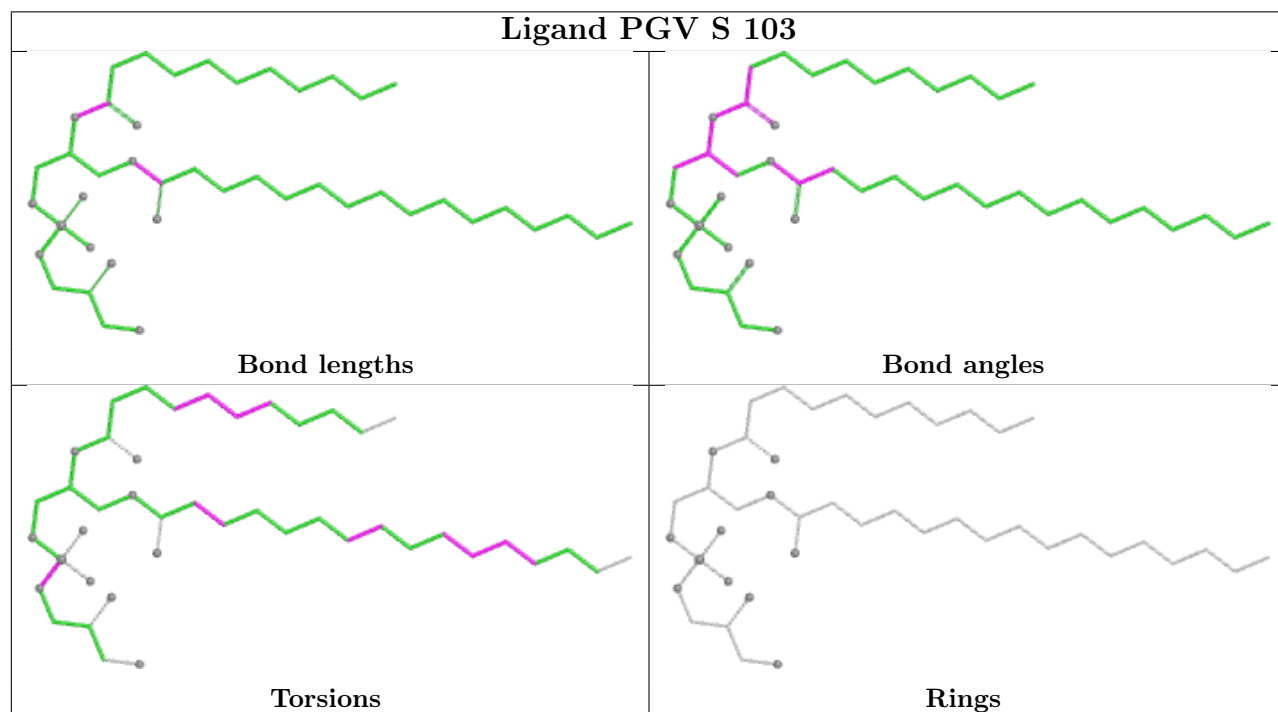
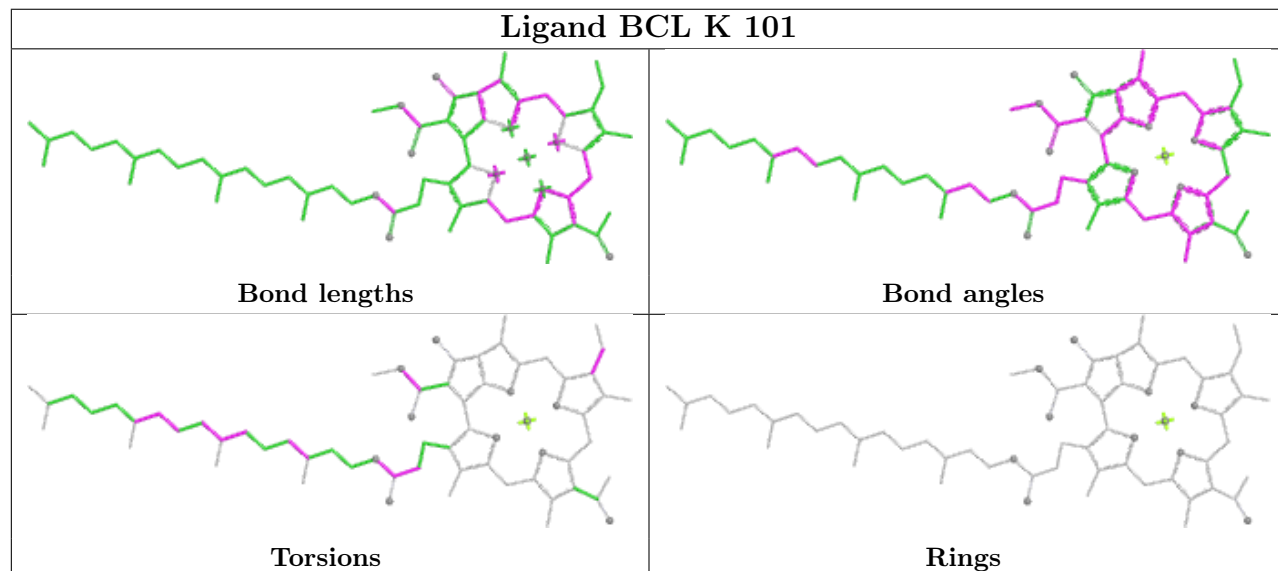
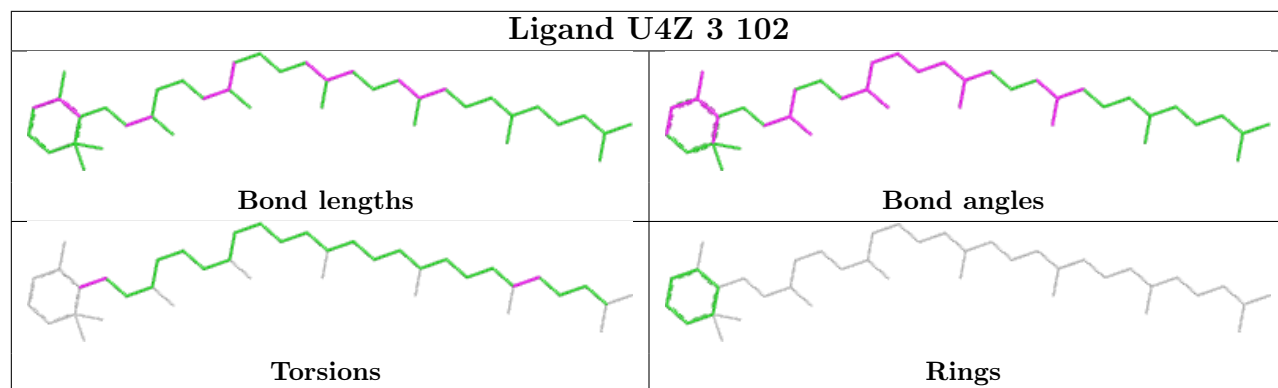


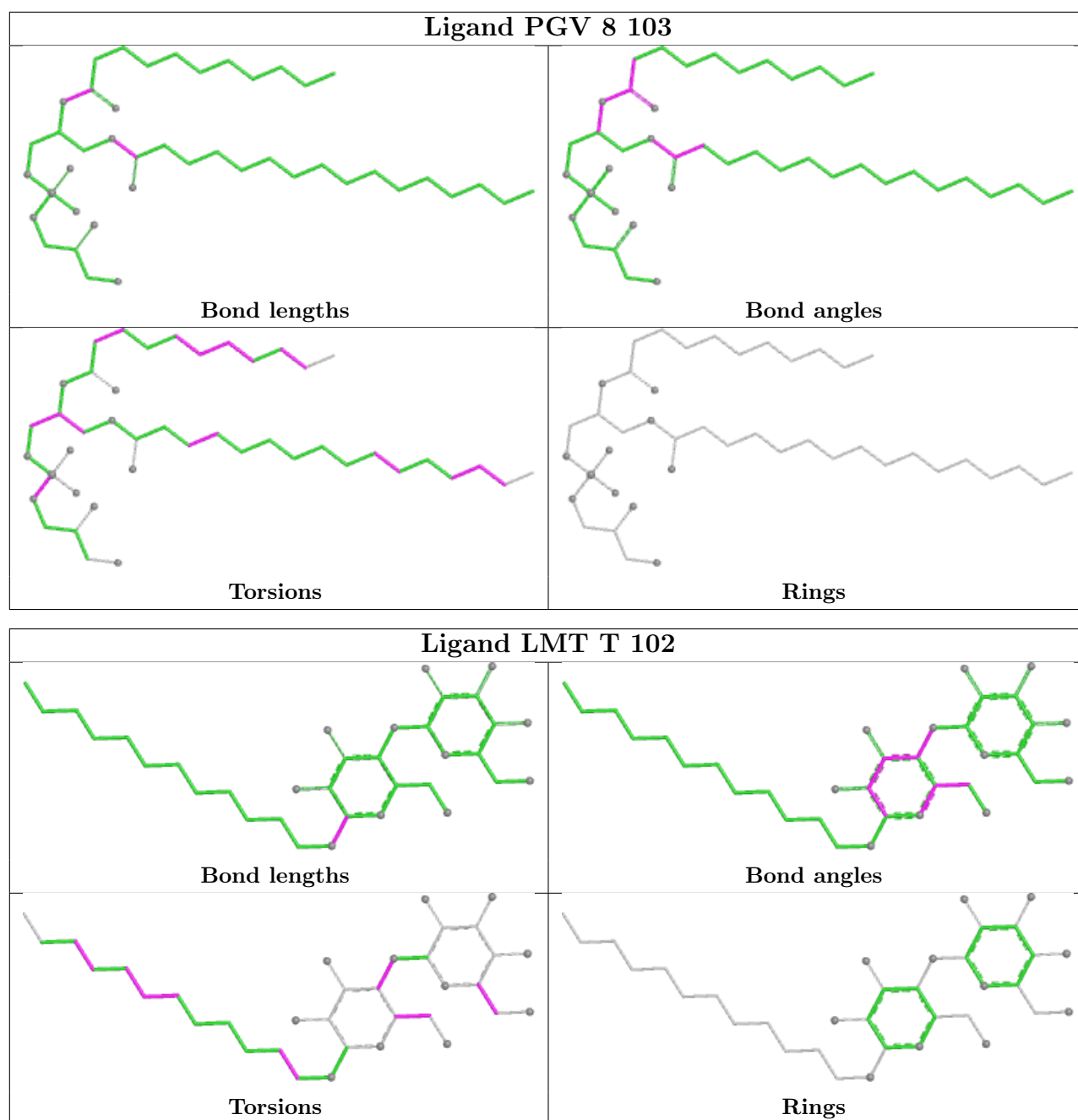


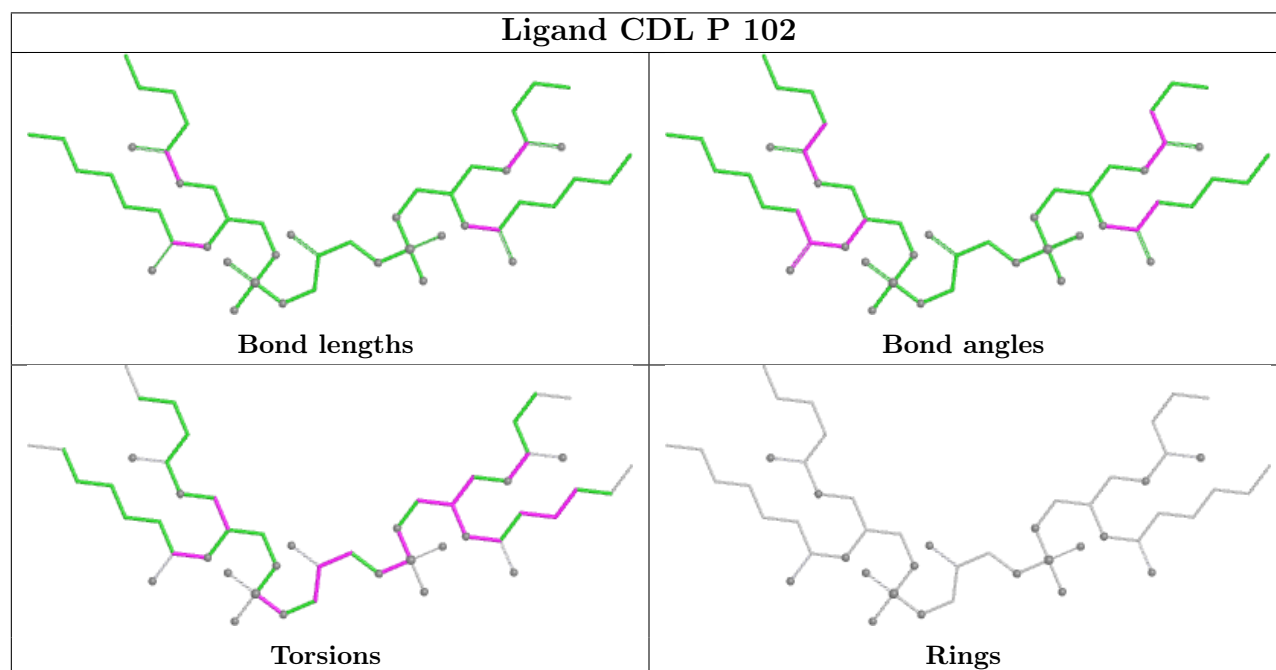
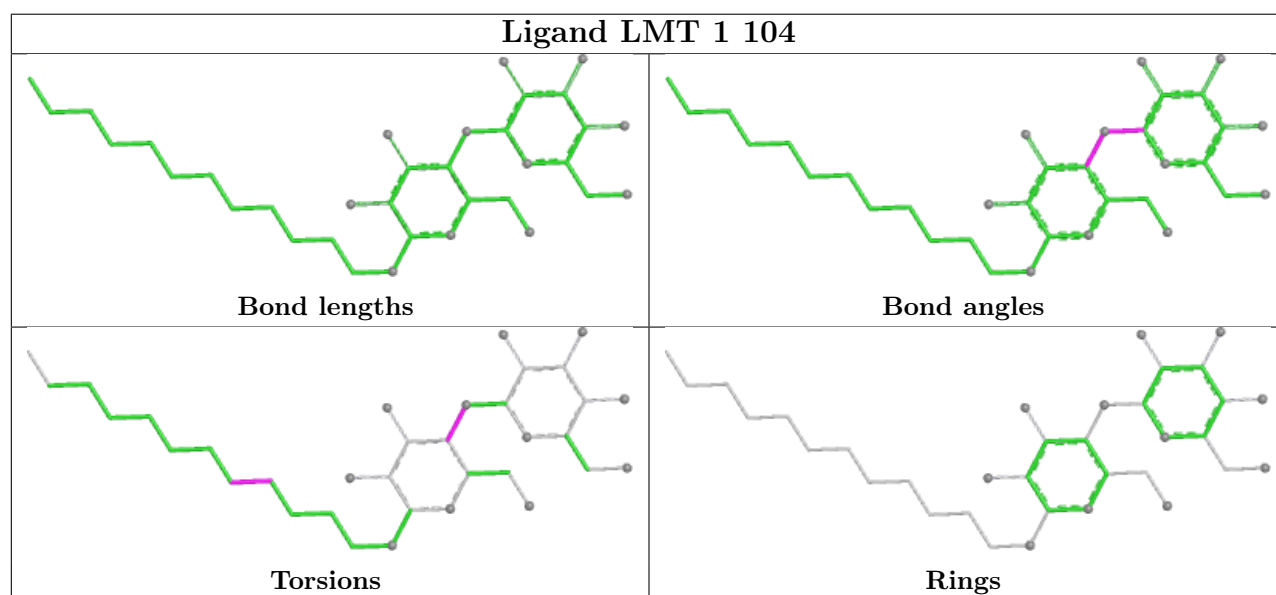
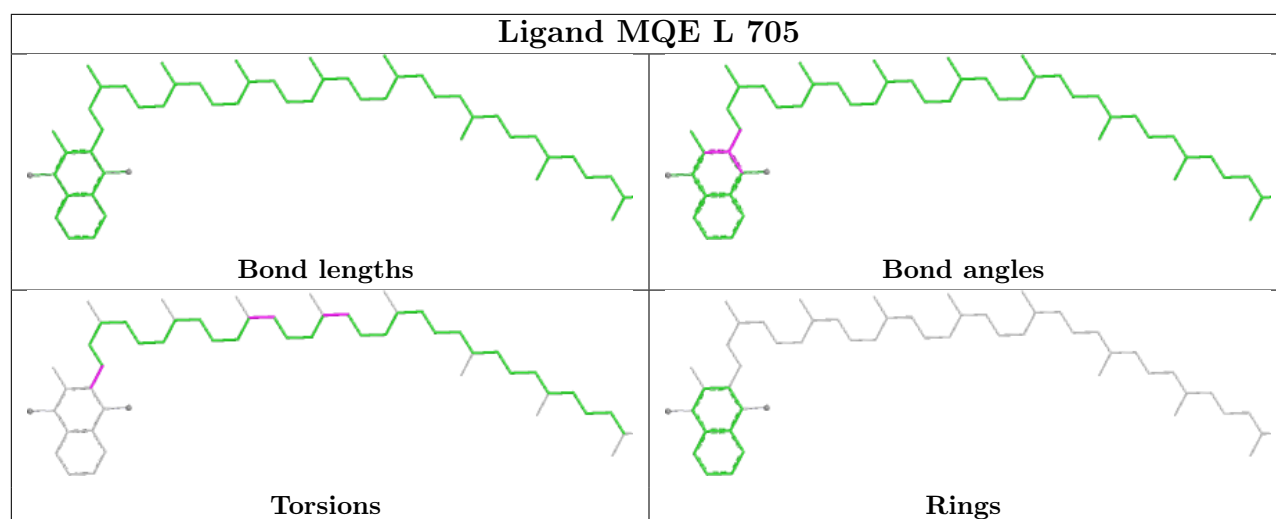


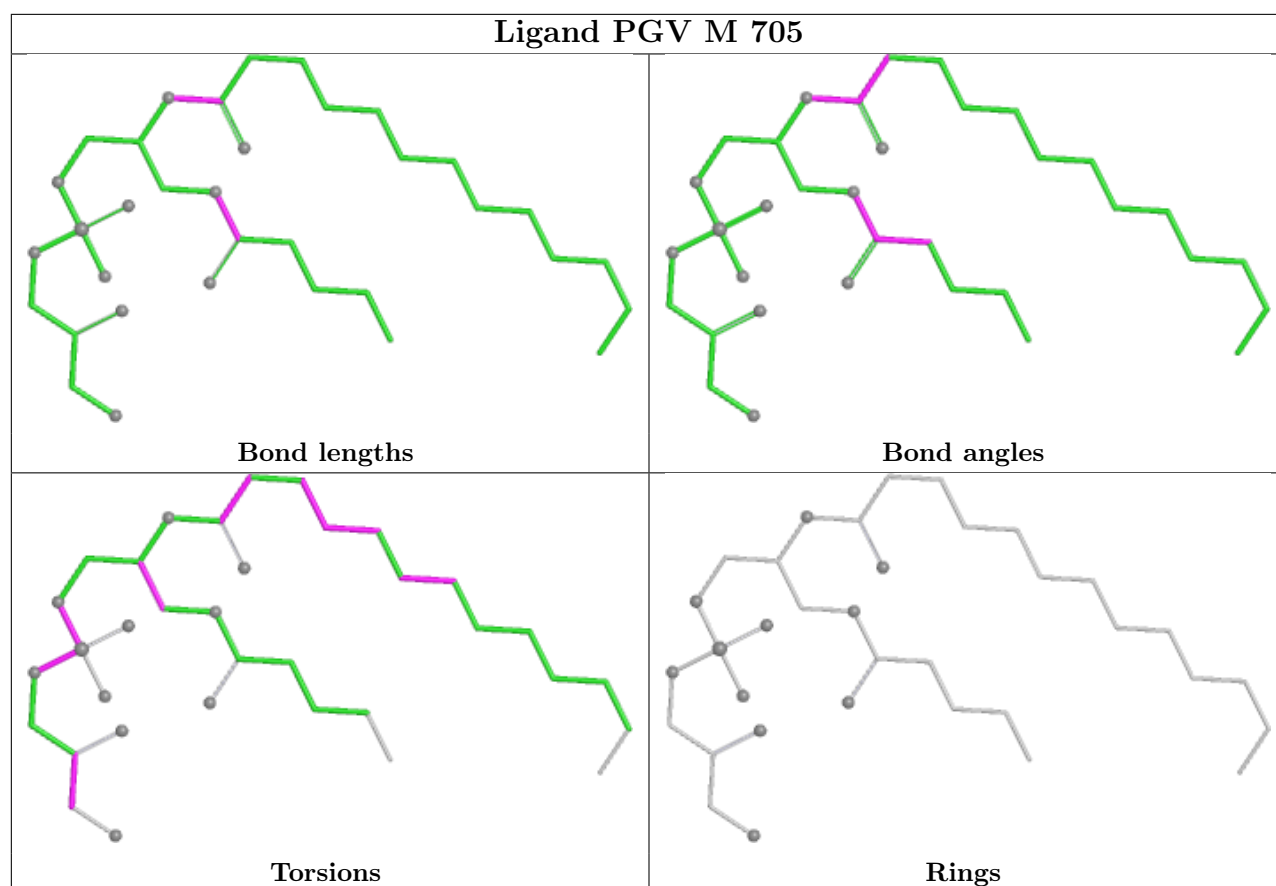












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

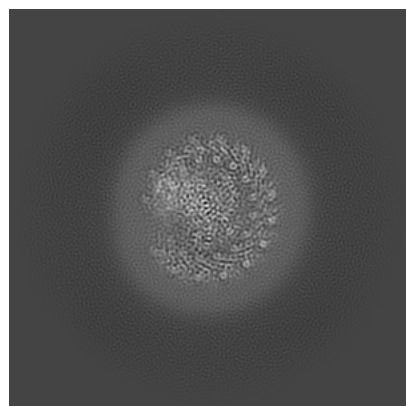
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35727. These allow visual inspection of the internal detail of the map and identification of artifacts.

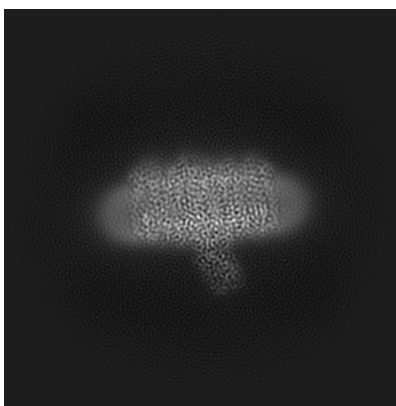
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

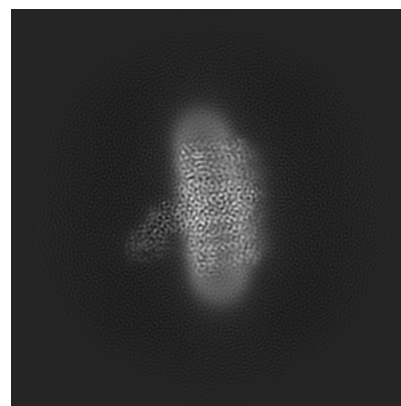
6.1.1 Primary map



X

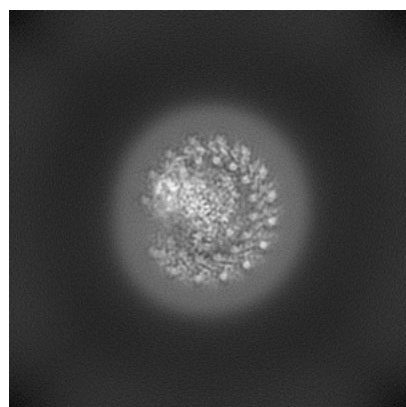


Y

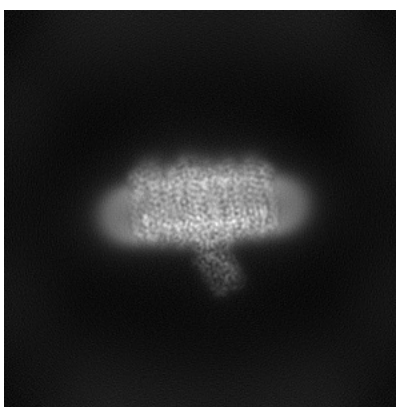


Z

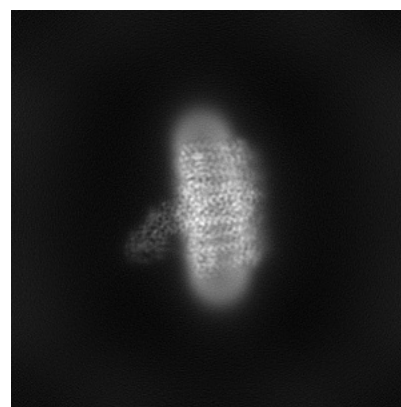
6.1.2 Raw map



X



Y

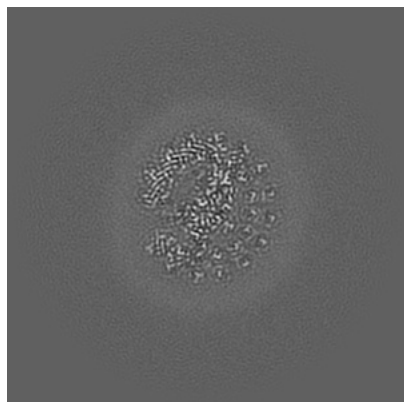


Z

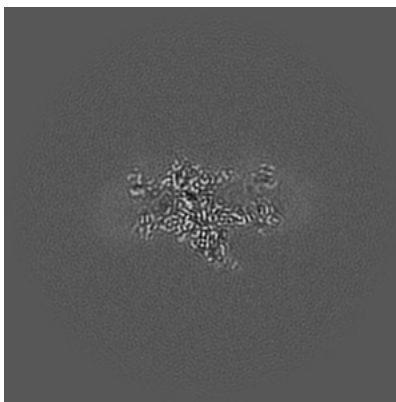
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

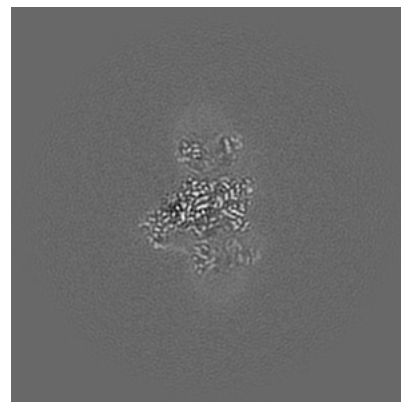
6.2.1 Primary map



X Index: 180

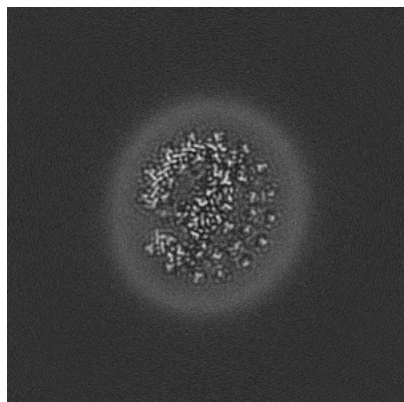


Y Index: 180

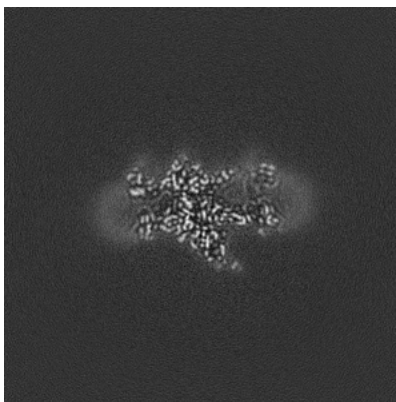


Z Index: 180

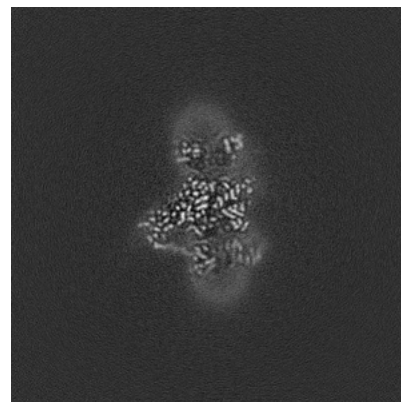
6.2.2 Raw map



X Index: 180



Y Index: 180

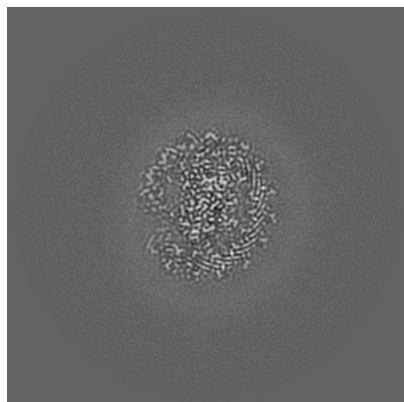


Z Index: 180

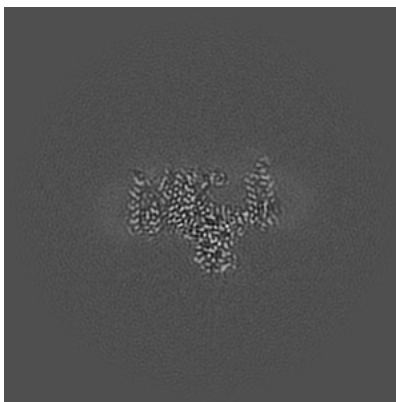
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

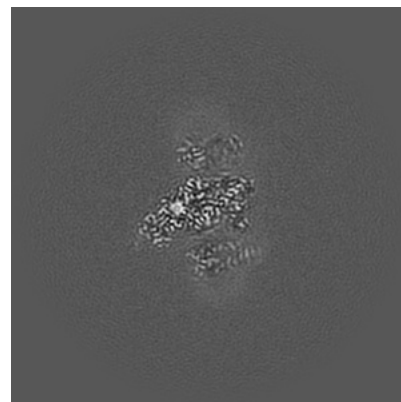
6.3.1 Primary map



X Index: 168

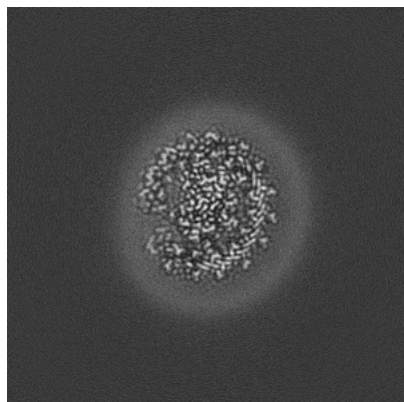


Y Index: 170

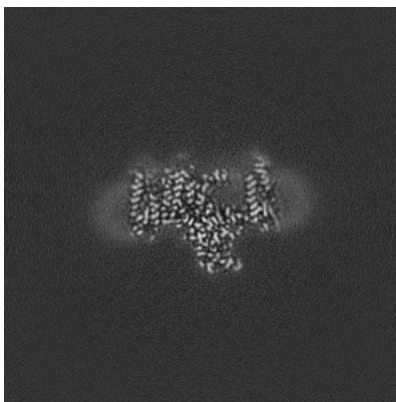


Z Index: 183

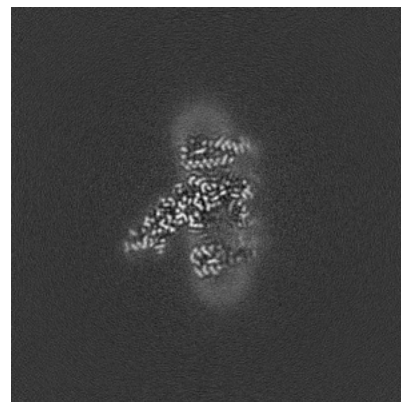
6.3.2 Raw map



X Index: 168



Y Index: 172

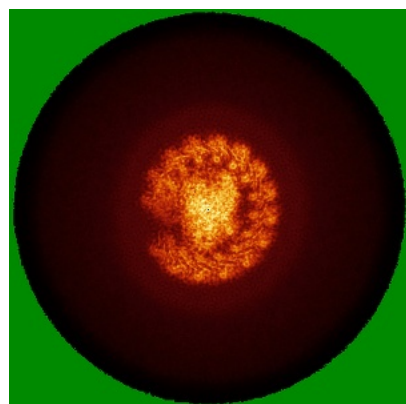


Z Index: 190

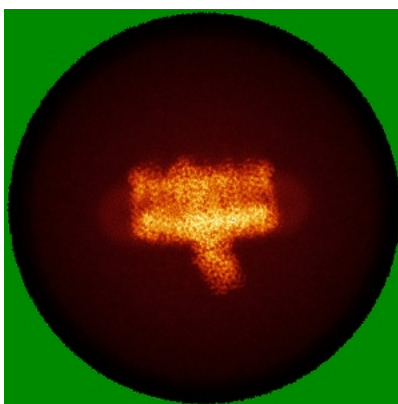
The images above show the largest variance slices of the map in three orthogonal directions.

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

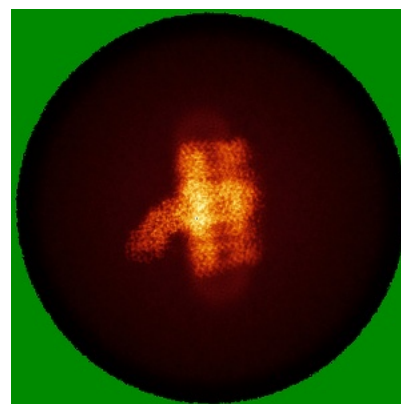
6.4.1 Primary map



X

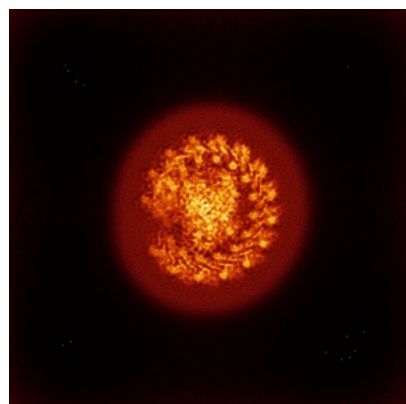


Y

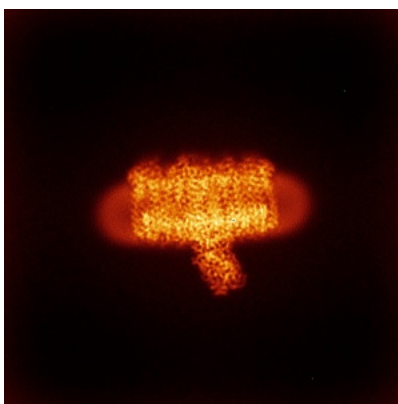


Z

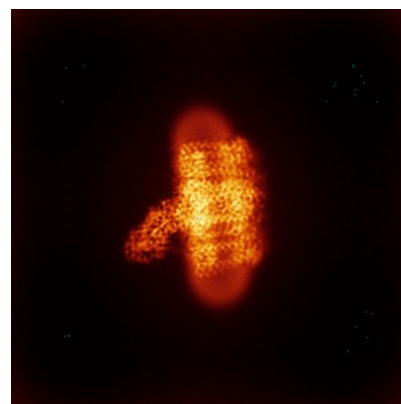
6.4.2 Raw map



X



Y

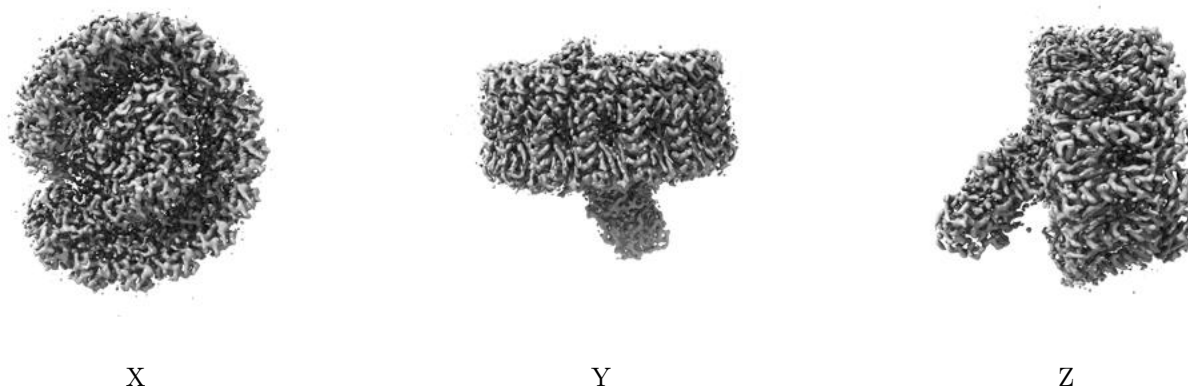


Z

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.

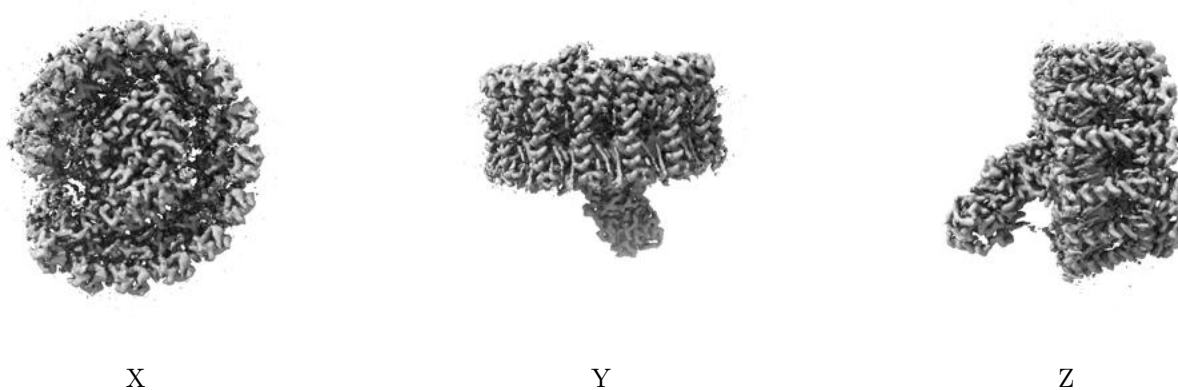
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.307. 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.

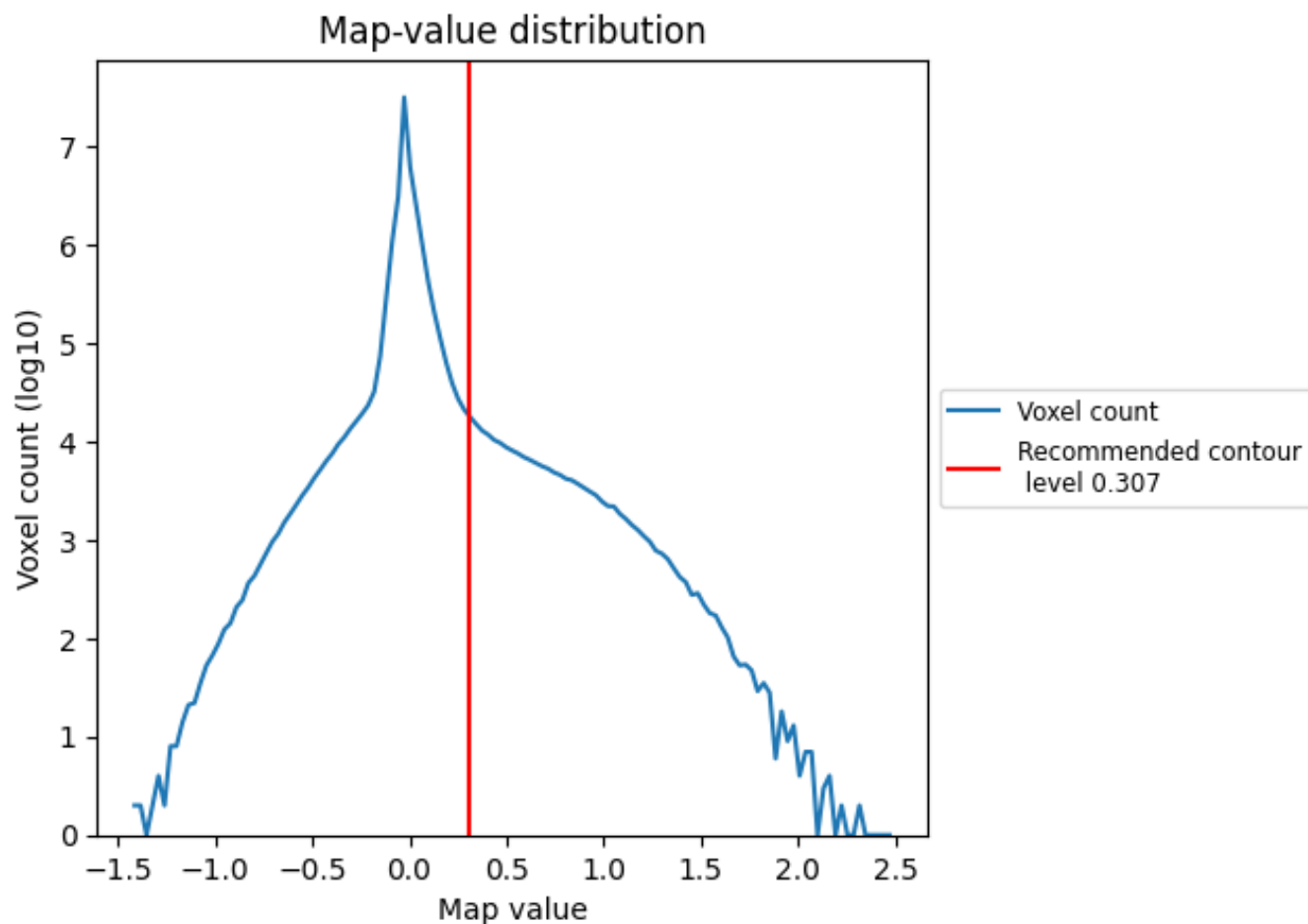
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

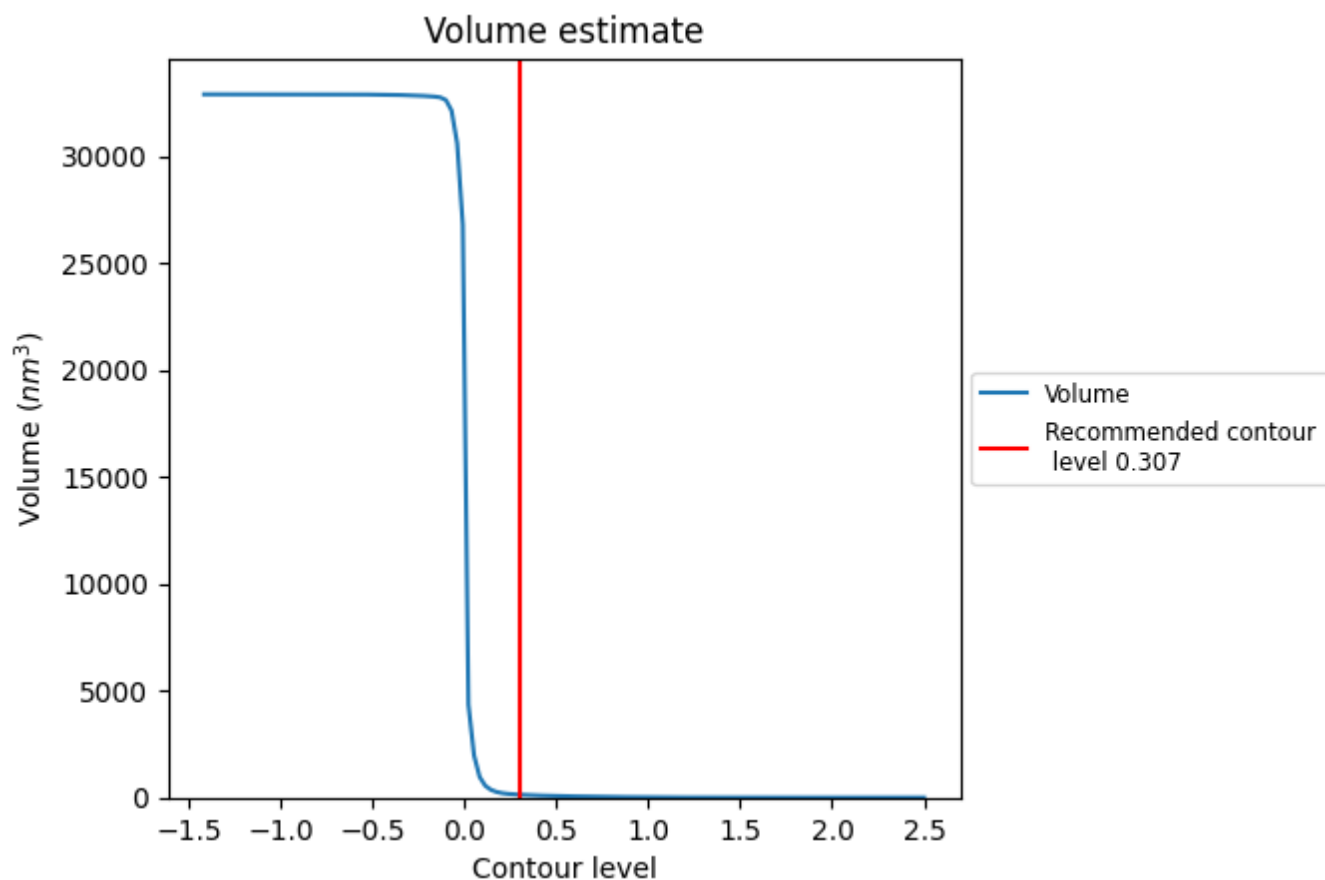
This section contains the results of statistical analysis of the map.

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.

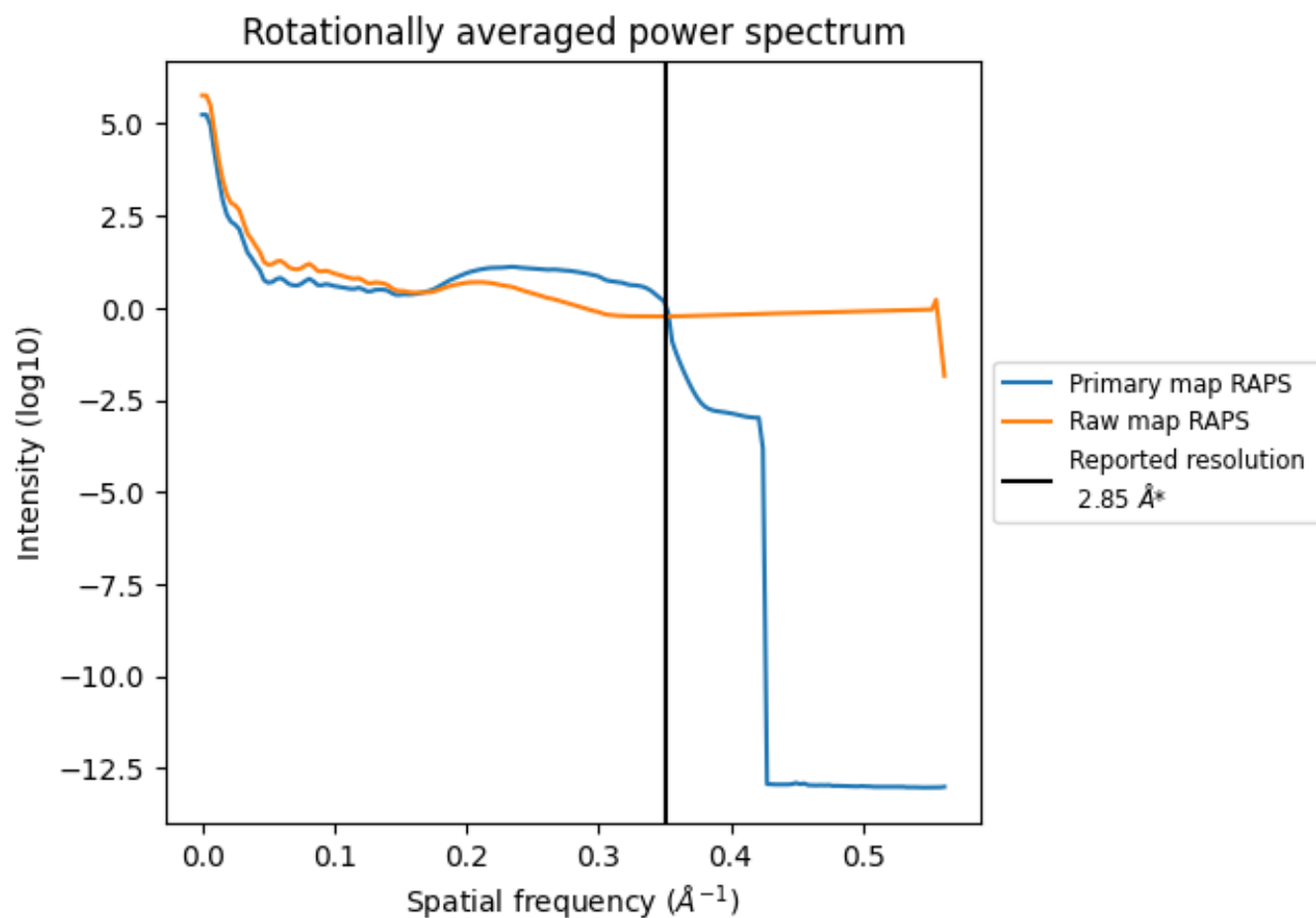
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm³; this corresponds to an approximate mass of 118 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 ⓘ

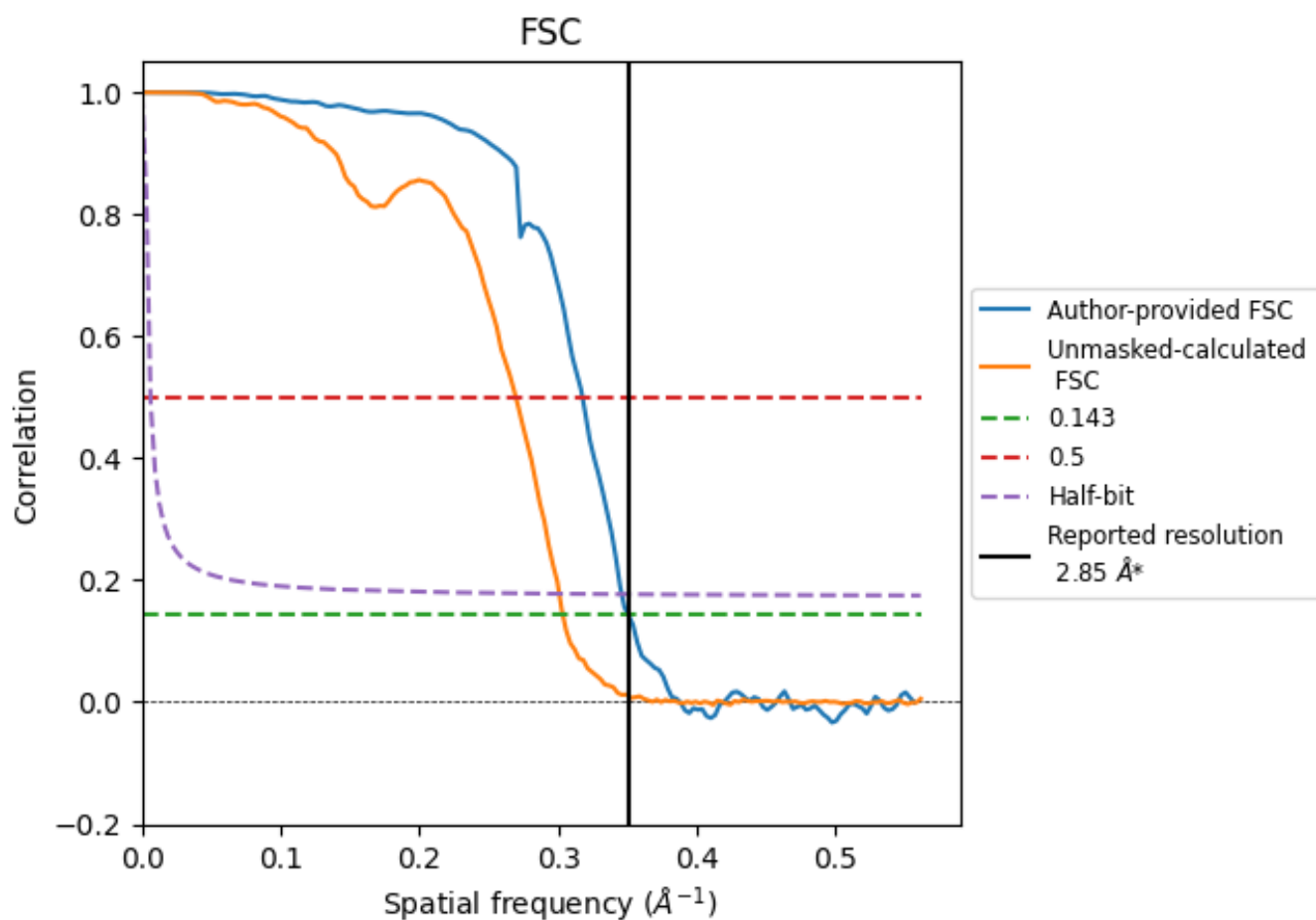


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

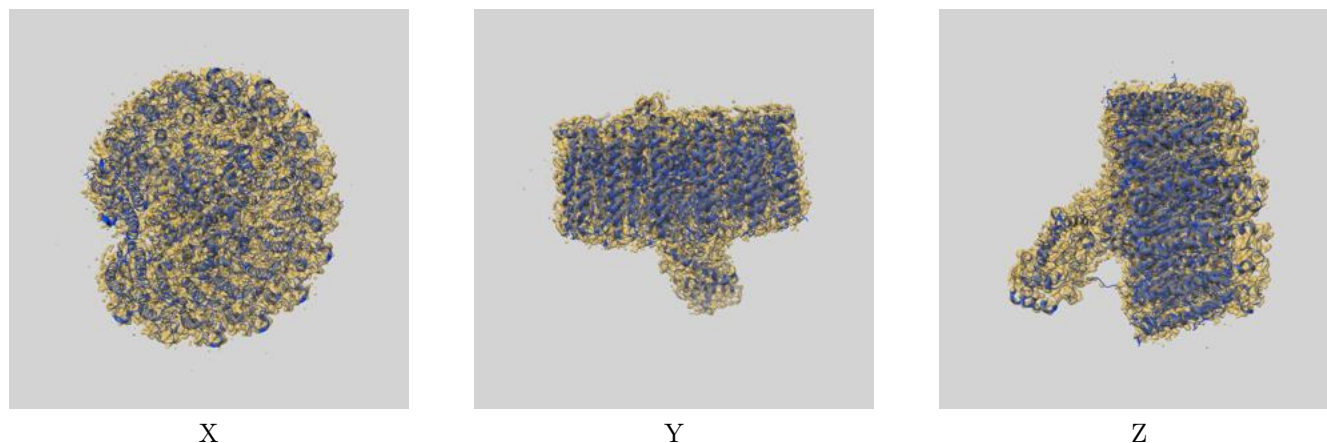
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.15	2.89
Unmasked-calculated*	3.29	3.71	3.32

*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 3.29 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

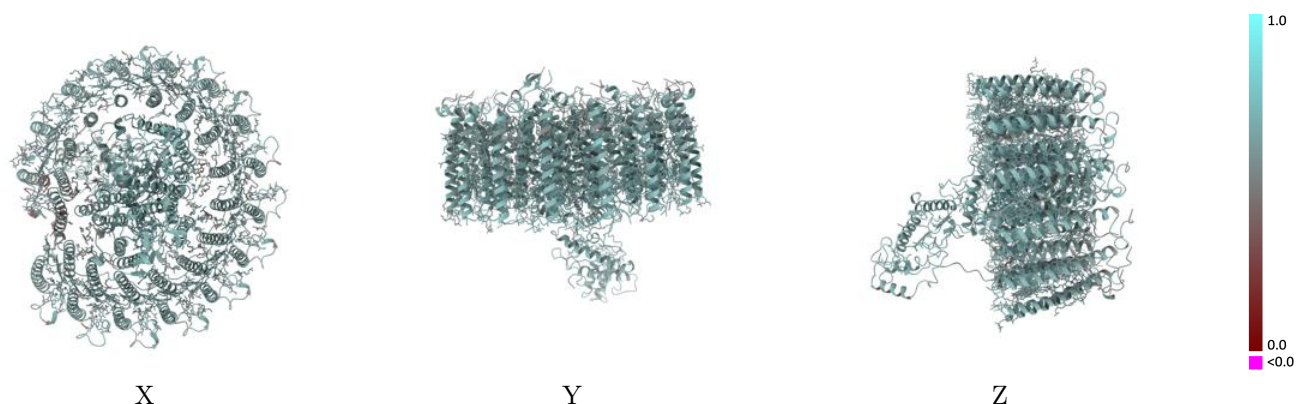
This section contains information regarding the fit between EMDB map EMD-35727 and PDB model 8IUN. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



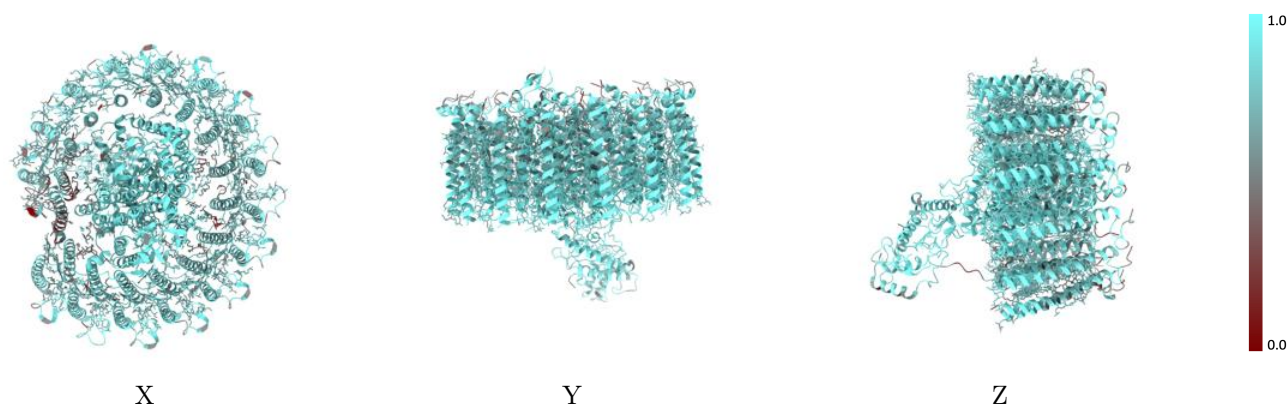
The images above show the 3D surface view of the map at the recommended contour level 0.307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



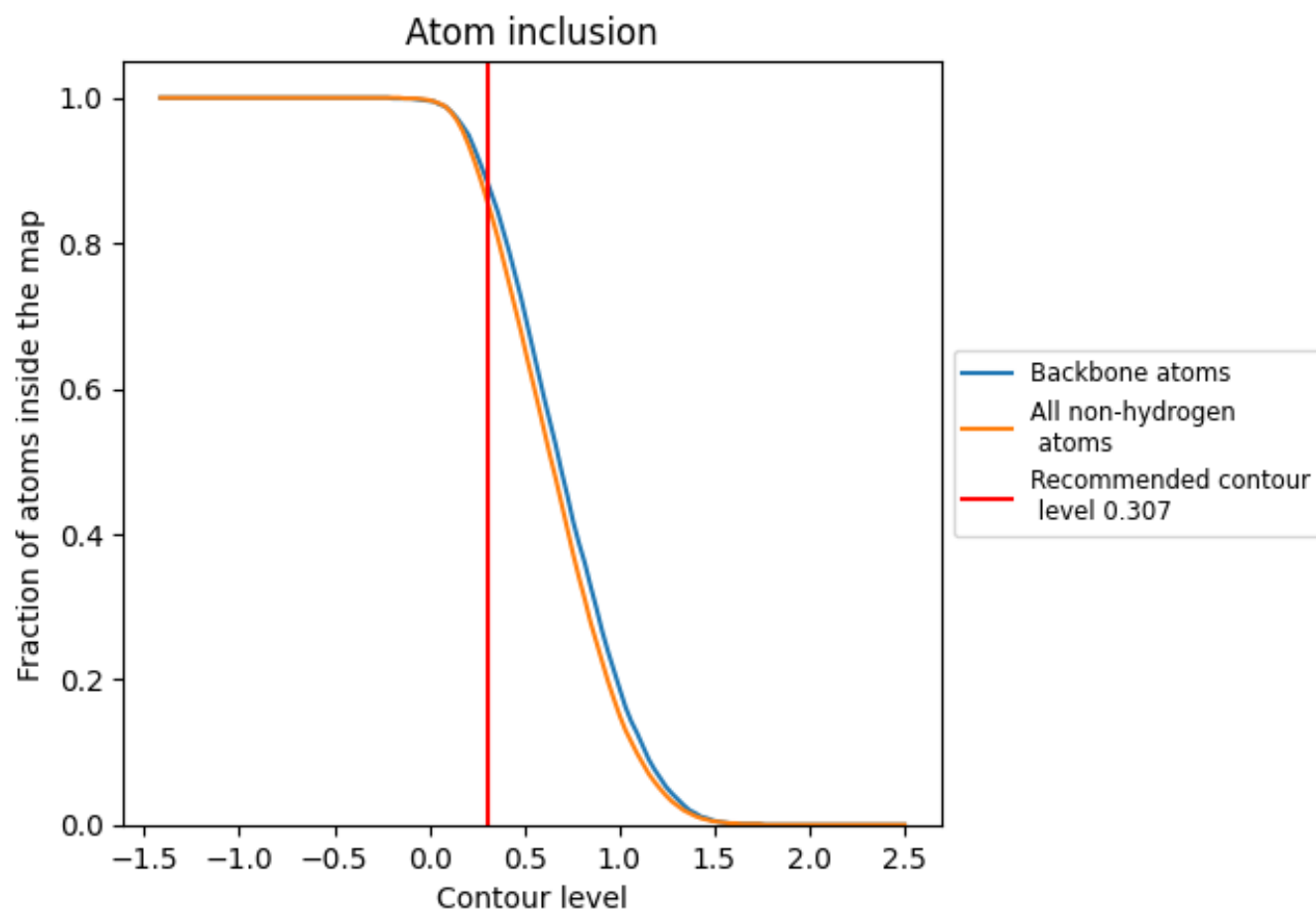
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.307).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.307) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.6130
0	 0.8280	 0.6020
1	 0.6870	 0.5670
2	 0.6600	 0.5410
3	 0.7690	 0.5950
4	 0.7800	 0.5820
5	 0.8130	 0.5950
6	 0.8250	 0.6050
7	 0.8320	 0.6040
8	 0.8370	 0.6020
9	 0.8410	 0.5980
A	 0.9260	 0.6340
B	 0.8940	 0.6170
C	 0.8680	 0.6150
D	 0.8570	 0.6190
E	 0.8290	 0.6040
F	 0.8300	 0.6040
G	 0.8440	 0.6080
H	 0.7660	 0.5880
I	 0.8210	 0.5970
J	 0.8530	 0.6170
K	 0.8160	 0.6020
L	 0.9320	 0.6380
M	 0.9460	 0.6440
N	 0.8450	 0.6170
O	 0.8350	 0.6090
P	 0.8690	 0.6180
Q	 0.8500	 0.6080
R	 0.8900	 0.6280
S	 0.8440	 0.6070
T	 0.8620	 0.6050
U	 0.8240	 0.6010
V	 0.7400	 0.5740
W	 0.7860	 0.5940
Y	 0.8450	 0.6080



Continued on next page...

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Chain	Atom inclusion	Q-score
Z	 0.9610	 0.6370
h	 0.8750	 0.6210