



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 10:05 AM JST

PDB ID : 7VY3 / pdb_00007vy3
EMDB ID : EMD-32193
Title : STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOBACTER SPHAEROIDES LACKING PROTEIN-U
Authors : Tani, K.; Kanno, R.; Kawamura, S.; Kikuchi, R.; Nagashima, K.V.P.; Hall, M.; Takahashi, A.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2021-11-13
Resolution : 2.63 Å(reported)
Based on initial model : 7F0L

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

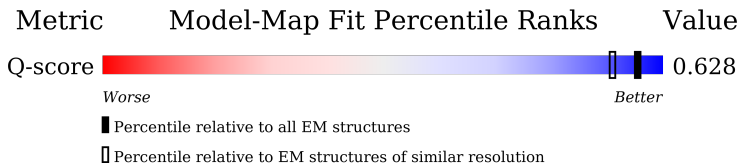
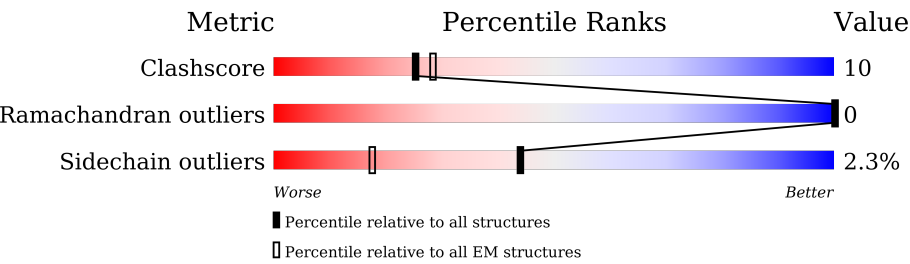
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.63 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	8888 (2.13 - 3.13)

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	L	281	80%19%.
2	M	307	79%19%.
3	H	260	82%13%5%

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Mol	Chain	Length	Quality of chain
4	1	54	
4	A	54	
4	D	54	
4	F	54	
4	I	54	
4	K	54	
4	O	54	
4	Q	54	
4	S	54	
4	V	54	
4	Y	54	
5	B	48	
5	E	48	
5	G	48	
5	J	48	
5	N	48	
5	P	48	
5	R	48	
5	T	48	
5	W	48	
5	Z	48	
6	X	81	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 18831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2233	1508	355	362	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	306	Total	C	N	O	S	0	0
			2437	1627	398	401	11		

- Molecule 3 is a protein called Photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	246	Total	C	N	O	S	1	0
			1867	1199	314	344	10		

- Molecule 4 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	45	Total	C	N	O	S	0	0
			386	266	59	58	3		
4	D	54	Total	C	N	O	S	0	0
			455	309	73	70	3		
4	F	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	I	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	K	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	O	54	Total	C	N	O	S	0	0
			453	308	72	70	3		
4	Q	54	Total	C	N	O	S	0	0
			457	311	73	70	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	54	Total	C	N	O	S	0	0
			454	309	73	70	2		
4	V	52	Total	C	N	O	S	0	0
			441	302	71	66	2		
4	Y	39	Total	C	N	O	S	0	0
			318	217	50	50	1		
4	1	27	Total	C	N	O	S	0	0
			216	147	36	32	1		

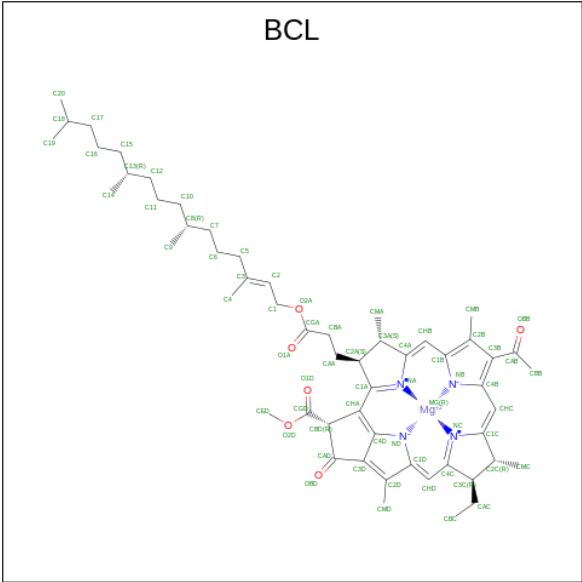
- Molecule 5 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	P	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	R	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	T	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	W	42	Total	C	N	O	S	0	0
			339	228	54	56	1		
5	Z	31	Total	C	N	O	S	0	0
			261	181	41	38	1		

- Molecule 6 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	52	Total	C	N	O	S	0	0
			401	267	68	63	3		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



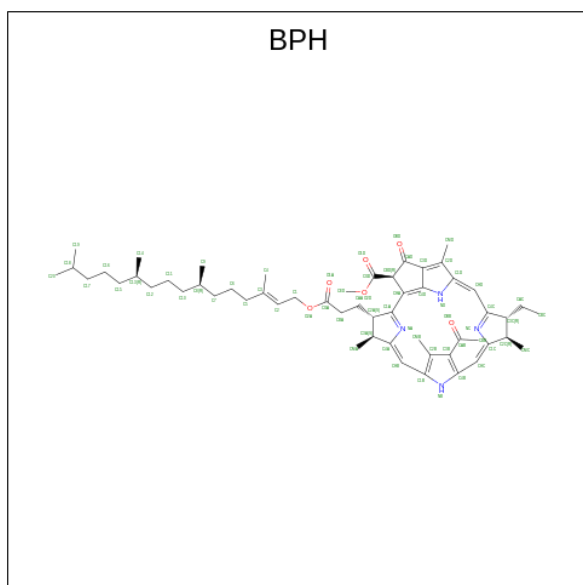
Mol	Chain	Residues	Atoms					AltConf
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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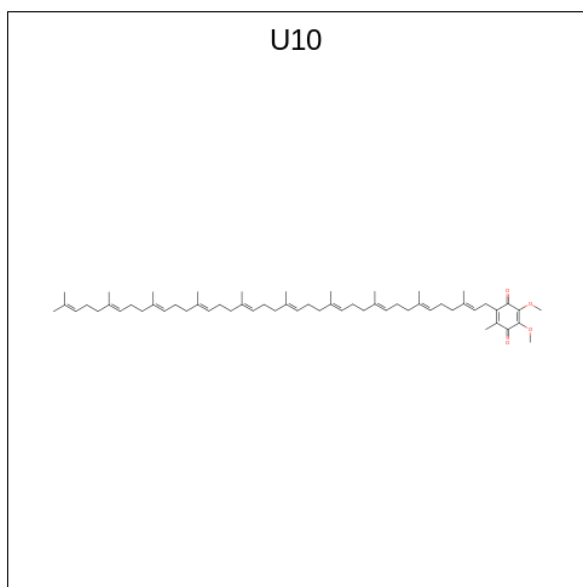
Mol	Chain	Residues	Atoms					AltConf
7	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



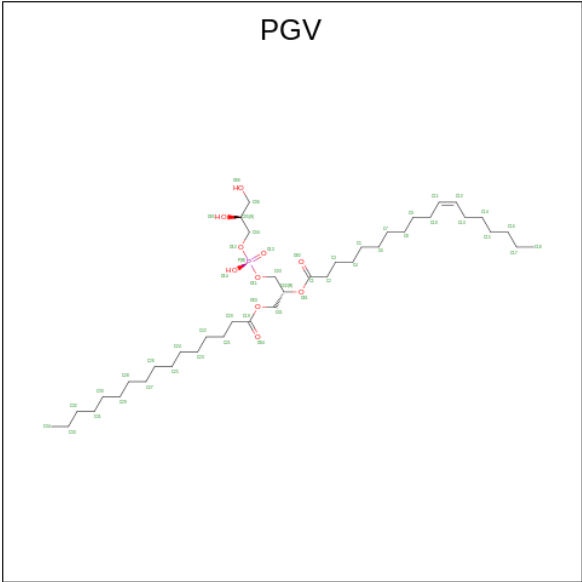
Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	N	O	0
			65	55	4	6	
8	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



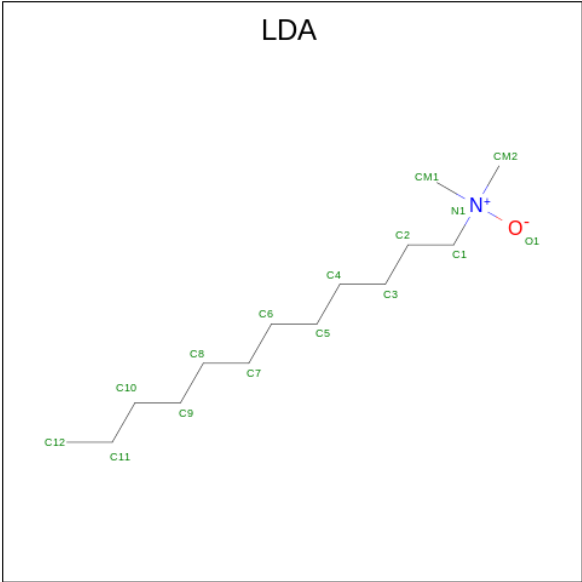
Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			35	31	4	
9	L	1	Total	C	O	0
			28	24	4	
9	M	1	Total	C	O	0
			63	59	4	
9	D	1	Total	C	O	0
			63	59	4	

- Molecule 10 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



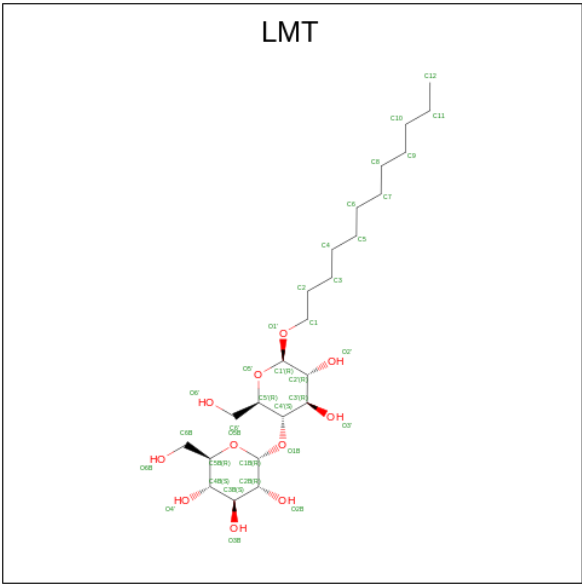
Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	O	P	0
			39	28	10	1	
10	M	1	Total	C	O	P	0
			38	27	10	1	
10	H	1	Total	C	O	P	0
			47	36	10	1	
10	F	1	Total	C	O	P	0
			40	29	10	1	
10	F	1	Total	C	O	P	0
			47	36	10	1	
10	K	1	Total	C	O	P	0
			41	34	6	1	
10	Q	1	Total	C	O	P	0
			39	28	10	1	
10	Y	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 11 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				AltConf
11	L	1	Total	C	N	O	0
			16	14	1	1	
11	H	1	Total	C	N	O	0
			16	14	1	1	
11	Y	1	Total	C	N	O	0
			12	10	1	1	
11	X	1	Total	C	N	O	0
			13	11	1	1	

- Molecule 12 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

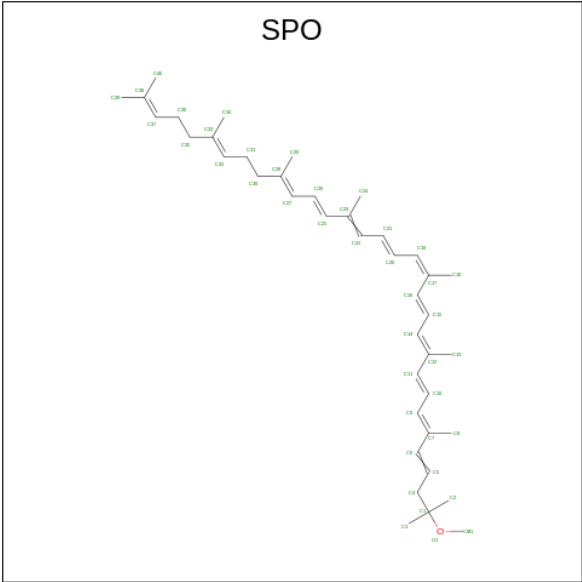


Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			35	24	11	
12	L	1	Total	C	O	0
			34	23	11	
12	M	1	Total	C	O	0
			27	20	7	
12	M	1	Total	C	O	0
			25	19	6	
12	H	1	Total	C	O	0
			35	24	11	
12	H	1	Total	C	O	0
			35	24	11	
12	H	1	Total	C	O	0
			30	19	11	
12	A	1	Total	C	O	0
			35	24	11	
12	A	1	Total	C	O	0
			35	24	11	
12	B	1	Total	C	O	0
			27	16	11	
12	D	1	Total	C	O	0
			27	16	11	
12	F	1	Total	C	O	0
			17	11	6	
12	I	1	Total	C	O	0
			26	16	10	
12	I	1	Total	C	O	0
			27	16	11	
12	K	1	Total	C	O	0
			35	24	11	
12	Q	1	Total	C	O	0
			24	18	6	
12	Q	1	Total	C	O	0
			19	13	6	

- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 14 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



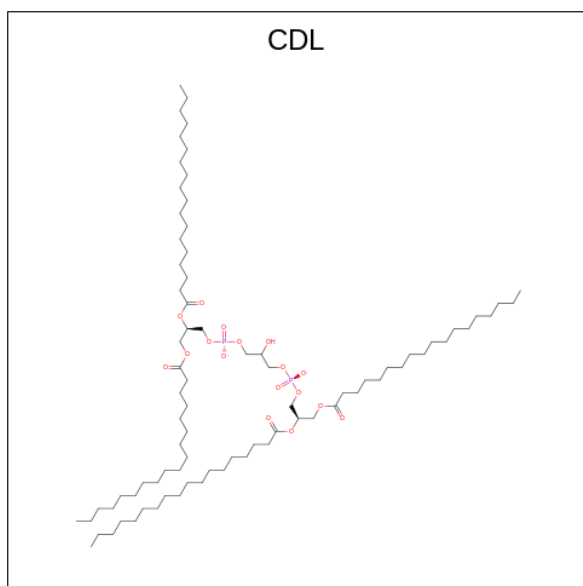
Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			42	41	1	
14	B	1	Total	C	O	0
			42	41	1	
14	B	1	Total	C	O	0
			42	41	1	
14	D	1	Total	C	O	0
			42	41	1	
14	D	1	Total	C	O	0
			42	41	1	
14	F	1	Total	C	O	0
			42	41	1	
14	G	1	Total	C	O	0
			42	41	1	
14	G	1	Total	C	O	0
			42	41	1	
14	J	1	Total	C	O	0
			42	41	1	
14	K	1	Total	C	O	0
			42	41	1	
14	K	1	Total	C	O	0
			42	41	1	
14	O	1	Total	C	O	0
			42	41	1	
14	P	1	Total	C	O	0
			42	41	1	
14	Q	1	Total	C	O	0
			42	41	1	

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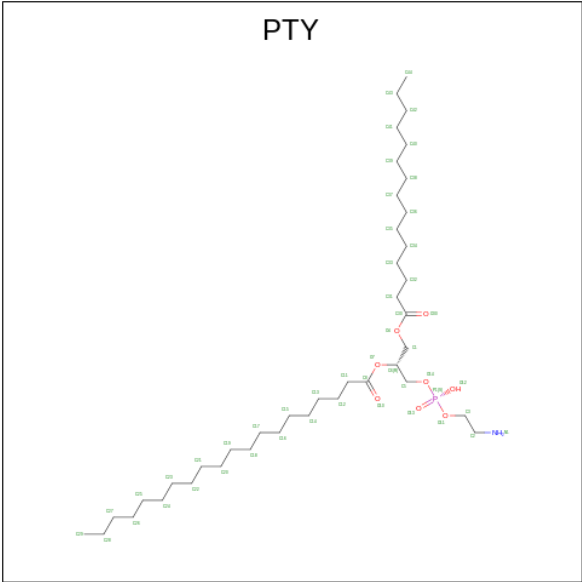
Mol	Chain	Residues	Atoms			AltConf
14	S	1	Total	C	O	0
			42	41	1	
14	S	1	Total	C	O	0
			42	41	1	
14	V	1	Total	C	O	0
			42	41	1	
14	V	1	Total	C	O	0
			42	41	1	
14	Z	1	Total	C	O	0
			42	41	1	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			79	60	17	2	
15	H	1	Total	C	O	P	0
			61	42	17	2	
15	Y	1	Total	C	O	P	0
			35	19	14	2	

- Molecule 16 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).

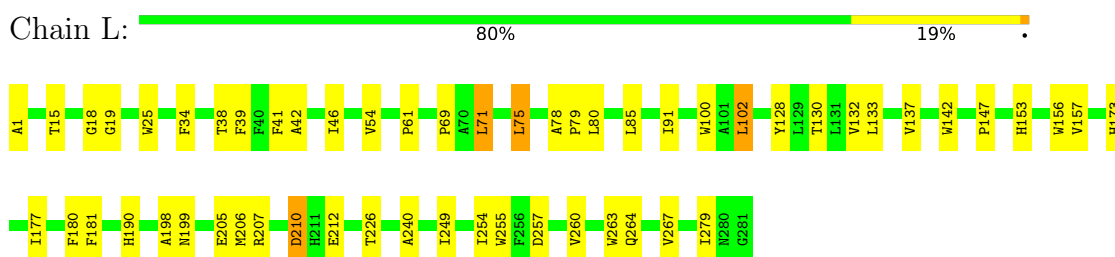


Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
16	F	1	Total	C	N	O	P	0
			48	38	1	8	1	

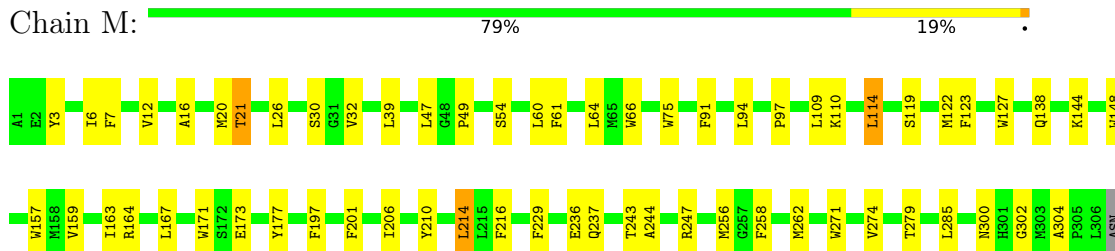
3 Residue-property plots

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

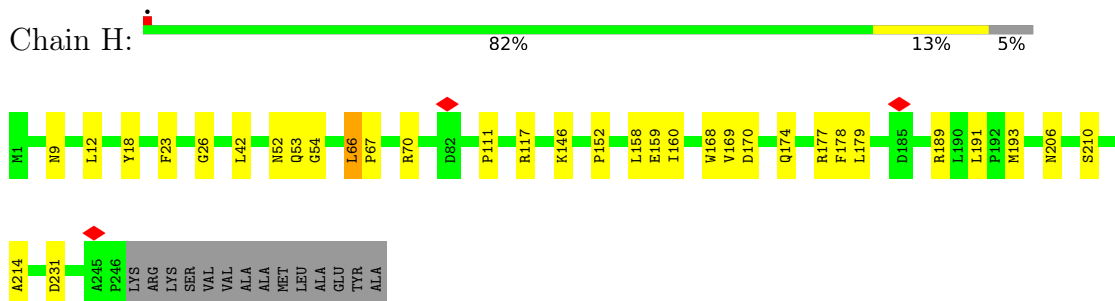
- Molecule 1: Photosynthetic reaction center L subunit



- Molecule 2: Reaction center protein M chain

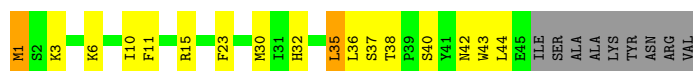


- Molecule 3: Photosynthetic reaction center subunit H



- Molecule 4: Antenna pigment protein alpha chain

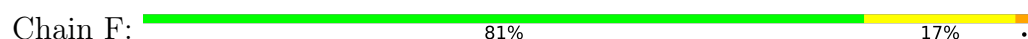




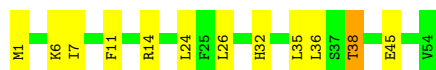
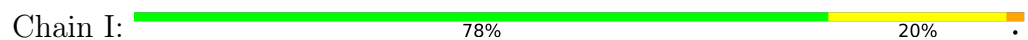
- Molecule 4: Antenna pigment protein alpha chain



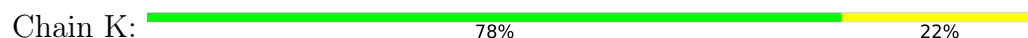
- Molecule 4: Antenna pigment protein alpha chain



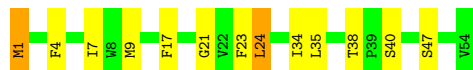
- Molecule 4: Antenna pigment protein alpha chain



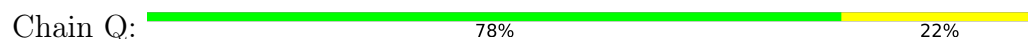
- Molecule 4: Antenna pigment protein alpha chain



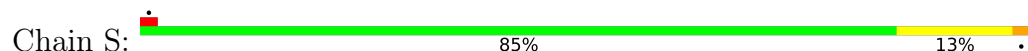
- Molecule 4: Antenna pigment protein alpha chain

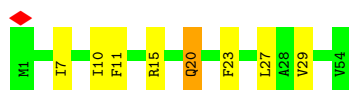


- Molecule 4: Antenna pigment protein alpha chain

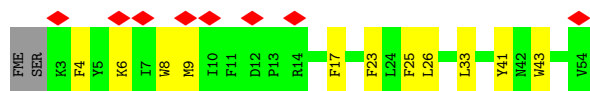
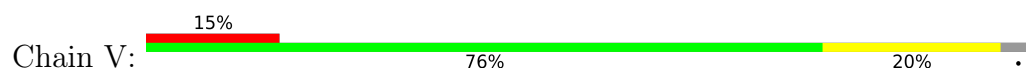


- Molecule 4: Antenna pigment protein alpha chain





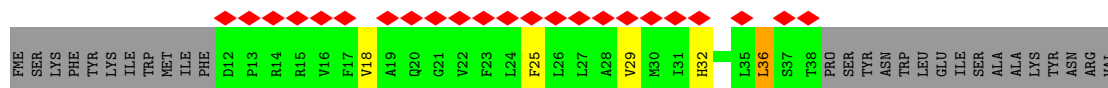
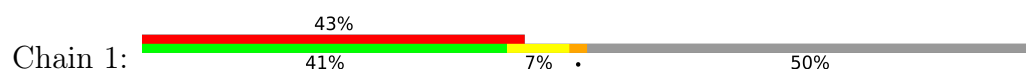
- Molecule 4: Antenna pigment protein alpha chain



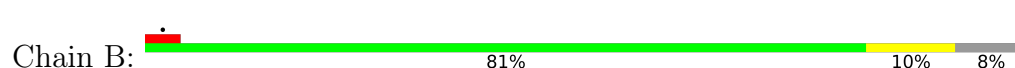
- Molecule 4: Antenna pigment protein alpha chain



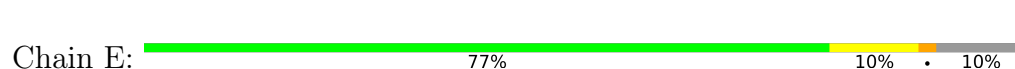
- Molecule 4: Antenna pigment protein alpha chain



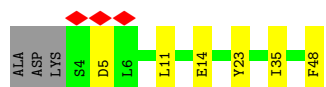
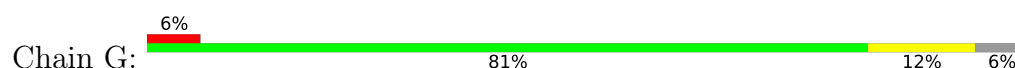
- Molecule 5: Antenna pigment protein beta chain



- Molecule 5: Antenna pigment protein beta chain



- Molecule 5: Antenna pigment protein beta chain



- Molecule 5: Antenna pigment protein beta chain

Chain J:  79% 10% 10%



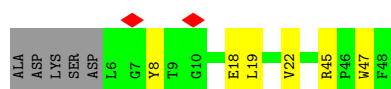
- Molecule 5: Antenna pigment protein beta chain

Chain N:  69% 19% 10%



- Molecule 5: Antenna pigment protein beta chain

Chain P:  77% 12% 10%



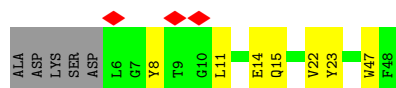
- Molecule 5: Antenna pigment protein beta chain

Chain R:  73% 17% 10%



- Molecule 5: Antenna pigment protein beta chain

Chain T:  6% 75% 15% 10%



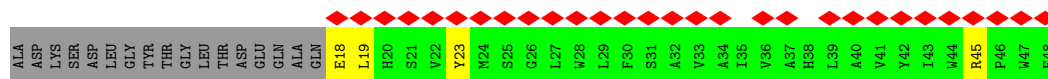
- Molecule 5: Antenna pigment protein beta chain

Chain W:  23% 75% 12% 12%

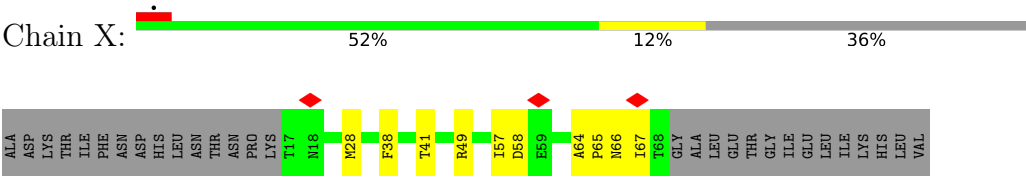


- Molecule 5: Antenna pigment protein beta chain

Chain Z:  60% 56% 8% 35%



● Molecule 6: PufX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124589	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.265	Depositor
Minimum map value	-0.146	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82000005, 0.82000005, 0.82000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, PTY, BPH, LDA, PGV, FE, LMT, SPO, FME, U10, CDL

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	L	0.13	0/2321	0.24	0/3177
2	M	0.13	0/2530	0.25	0/3455
3	H	0.12	0/1920	0.26	0/2615
4	1	0.06	0/220	0.16	0/298
4	A	0.12	0/389	0.21	0/528
4	D	0.14	0/459	0.25	0/622
4	F	0.13	0/461	0.22	0/625
4	I	0.14	0/461	0.21	0/625
4	K	0.13	0/461	0.22	0/625
4	O	0.12	0/457	0.21	0/621
4	Q	0.11	0/461	0.22	0/625
4	S	0.11	0/461	0.20	0/625
4	V	0.11	0/455	0.21	0/617
4	Y	0.08	0/327	0.21	0/446
5	B	0.10	0/372	0.18	0/510
5	E	0.11	0/364	0.18	0/499
5	G	0.12	0/378	0.20	0/518
5	J	0.11	0/364	0.19	0/499
5	N	0.12	0/364	0.20	0/499
5	P	0.11	0/364	0.25	0/499
5	R	0.10	0/360	0.18	0/494
5	T	0.08	0/364	0.16	0/499
5	W	0.08	0/352	0.18	0/483
5	Z	0.06	0/273	0.16	0/375
6	X	0.10	0/413	0.25	0/561
All	All	0.12	0/15351	0.23	0/20940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2233	0	2189	41	0
2	M	2437	0	2355	45	0
3	H	1867	0	1867	23	0
4	1	216	0	236	5	0
4	A	386	0	400	14	0
4	D	455	0	469	15	0
4	F	457	0	476	11	0
4	I	457	0	476	12	0
4	K	457	0	476	15	0
4	O	453	0	465	15	0
4	Q	457	0	476	10	0
4	S	454	0	469	8	0
4	V	441	0	460	11	0
4	Y	318	0	331	7	0
5	B	359	0	340	3	0
5	E	351	0	336	6	0
5	G	365	0	345	4	0
5	J	351	0	336	6	0
5	N	351	0	336	10	0
5	P	351	0	336	8	0
5	R	347	0	332	8	0
5	T	351	0	336	9	0
5	W	339	0	321	6	0
5	Z	261	0	254	6	0
6	X	401	0	409	8	0
7	1	66	0	74	8	0
7	A	61	0	61	5	0
7	B	66	0	74	4	0
7	D	66	0	74	12	0
7	E	66	0	74	2	0
7	F	66	0	74	8	0
7	G	66	0	74	3	0
7	I	66	0	74	3	0
7	J	66	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	66	0	74	5	0
7	L	132	0	148	4	0
7	M	132	0	148	7	0
7	N	66	0	74	6	0
7	O	66	0	74	4	0
7	P	66	0	74	5	0
7	Q	132	0	148	16	0
7	S	66	0	74	6	0
7	T	66	0	74	5	0
7	V	66	0	74	3	0
7	W	66	0	74	2	0
7	Y	66	0	74	5	0
7	Z	66	0	74	4	0
8	L	65	0	76	3	0
8	M	65	0	76	8	0
9	D	63	0	90	11	0
9	L	63	0	74	4	0
9	M	63	0	90	6	0
10	F	87	0	110	6	0
10	H	47	0	65	1	0
10	K	41	0	60	2	0
10	L	39	0	47	2	0
10	M	38	0	45	4	0
10	Q	39	0	48	2	0
10	Y	43	0	54	3	0
11	H	16	0	31	1	0
11	L	16	0	31	0	0
11	X	13	0	22	0	0
11	Y	12	0	20	2	0
12	A	70	0	92	4	0
12	B	27	0	27	0	0
12	D	27	0	27	1	0
12	F	17	0	16	0	0
12	H	100	0	125	10	0
12	I	53	0	51	4	0
12	K	35	0	46	4	0
12	L	69	0	87	2	0
12	M	52	0	71	1	0
12	Q	43	0	55	3	0
13	M	1	0	0	0	0
14	B	84	0	120	11	0
14	D	84	0	120	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	F	42	0	60	6	0
14	G	84	0	120	11	0
14	J	42	0	60	6	0
14	K	84	0	120	11	0
14	M	42	0	60	5	0
14	O	42	0	60	4	0
14	P	42	0	60	8	0
14	Q	42	0	60	6	0
14	S	84	0	120	9	0
14	V	84	0	120	10	0
14	Z	42	0	60	11	0
15	H	61	0	66	5	0
15	M	79	0	105	5	0
15	Y	35	0	32	2	0
16	F	48	0	72	4	0
16	H	46	0	68	6	0
All	All	18831	0	19682	399	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 10.

All (399) 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)
14:B:104:SPO:H342	9:D:105:U10:H38	1.61	0.81
4:F:1:FME:HCN	4:F:3:LYS:H	1.47	0.78
2:M:109:LEU:HB2	11:Y:101:LDA:H11	1.63	0.78
2:M:119:SER:HB3	14:M:405:SPO:H311	1.66	0.76
14:Z:101:SPO:HM11	4:1:29:VAL:HG13	1.69	0.74
7:P:101:BCL:H43	14:P:102:SPO:H292	1.69	0.73
2:M:110:LYS:HG3	11:Y:101:LDA:H12	1.71	0.73
2:M:75:TRP:HE1	14:M:405:SPO:HM12	1.54	0.72
4:V:25:PHE:HB2	7:V:101:BCL:H62	1.71	0.72
5:Z:19:LEU:HD12	14:Z:101:SPO:H351	1.70	0.71
2:M:243:THR:OG1	2:M:247:ARG:NH1	2.22	0.70
4:F:15:ARG:NH1	10:F:102:PGV:O13	2.24	0.70
7:S:101:BCL:HED3	14:S:103:SPO:H25	1.73	0.70
4:A:37:SER:OG	12:A:102:LMT:O2'	2.10	0.70
3:H:53:GLN:O	16:H:306:PTY:N1	2.25	0.69
12:H:304:LMT:H82	4:K:26:LEU:HD22	1.73	0.69
4:A:3:LYS:HE2	4:A:6:LYS:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:147:PRO:HD3	6:X:66:ASN:HD21	1.57	0.68
15:M:408:CDL:HA61	15:M:408:CDL:HB62	1.75	0.67
2:M:247:ARG:NH2	3:H:111:PRO:O	2.28	0.67
14:D:104:SPO:H293	14:F:105:SPO:H37	1.75	0.67
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.77	0.67
2:M:201:PHE:HD1	2:M:279:THR:HG23	1.58	0.67
14:K:105:SPO:H401	5:N:6:LEU:HD21	1.77	0.67
4:Q:24:LEU:HD13	7:Q:106:BCL:HED1	1.77	0.67
7:D:101:BCL:H142	9:D:105:U10:H271	1.77	0.66
4:I:26:LEU:HD22	12:K:101:LMT:H101	1.78	0.66
1:L:199:ASN:HB3	15:M:408:CDL:HA22	1.78	0.66
4:F:20:GLN:NE2	5:G:23:TYR:OH	2.29	0.66
4:Q:40:SER:O	5:R:45:ARG:NH1	2.30	0.65
14:P:102:SPO:H25	7:Q:104:BCL:HED3	1.79	0.65
9:M:410:U10:H353	9:M:410:U10:H502	1.77	0.65
15:H:307:CDL:H181	4:K:26:LEU:HD11	1.79	0.64
8:L:302:BPH:HHC	8:L:302:BPH:HBB3	1.80	0.64
3:H:170:ASP:HB2	3:H:177:ARG:HE	1.62	0.64
14:D:104:SPO:H6	7:I:102:BCL:HMB2	1.80	0.64
1:L:61:PRO:HG3	10:L:305:PGV:H62	1.81	0.63
5:E:48:PHE:HB3	14:F:105:SPO:H82	1.80	0.63
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.64	0.63
4:I:36:LEU:HB3	12:I:101:LMT:H3'	1.81	0.63
4:A:10:ILE:HD11	14:D:102:SPO:H37	1.80	0.62
7:L:309:BCL:HHC	7:M:402:BCL:H42	1.82	0.62
5:W:8:TYR:HB3	4:Y:14:ARG:HD3	1.82	0.62
10:M:409:PGV:H061	10:Q:103:PGV:H202	1.81	0.61
4:F:35:LEU:HD11	7:G:101:BCL:HHD	1.81	0.61
5:Z:18:GLU:HB3	14:Z:101:SPO:H393	1.82	0.61
4:I:35:LEU:HD11	7:J:101:BCL:HHD	1.83	0.61
10:Y:104:PGV:H061	4:I:18:VAL:HG21	1.84	0.60
8:M:403:BPH:HBB3	8:M:403:BPH:HHC	1.84	0.60
4:K:3:LYS:NZ	5:P:18:GLU:OE2	2.35	0.60
1:L:210:ASP:N	1:L:210:ASP:OD1	2.35	0.59
4:I:32:HIS:NE2	7:I:101:BCL:ND	2.51	0.59
5:G:35:ILE:HG12	7:G:101:BCL:H92	1.85	0.59
2:M:6:ILE:HD11	11:H:302:LDA:H121	1.85	0.58
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.85	0.58
14:Q:105:SPO:H6	7:S:101:BCL:HMB1	1.85	0.58
14:V:102:SPO:H392	5:W:19:LEU:HA	1.84	0.58
1:L:79:PRO:HG3	12:A:102:LMT:H1B	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:20:GLN:HE22	5:T:23:TYR:HE1	1.51	0.58
10:Y:104:PGV:H271	10:Y:104:PGV:H102	1.85	0.58
14:K:105:SPO:H352	5:P:22:VAL:HB	1.84	0.58
4:Q:33:LEU:HD22	12:Q:102:LMT:H21	1.86	0.58
1:L:205:GLU:HB3	3:H:67:PRO:HA	1.86	0.58
14:K:105:SPO:H351	5:P:19:LEU:HG	1.86	0.58
4:Q:35:LEU:HD11	7:Q:106:BCL:HHD	1.85	0.58
1:L:226:THR:HA	9:L:303:U10:H3M2	1.87	0.57
14:B:104:SPO:H343	7:D:101:BCL:H92	1.87	0.57
4:D:42:ASN:HB3	4:D:45:GLU:HG2	1.87	0.57
4:O:35:LEU:HD11	7:P:101:BCL:HHD	1.87	0.57
3:H:152:PRO:HB2	3:H:160:ILE:HD12	1.86	0.57
14:S:102:SPO:H352	5:T:22:VAL:HB	1.86	0.57
2:M:12:VAL:HG11	3:H:169:VAL:HG11	1.86	0.56
1:L:42:ALA:O	1:L:46:ILE:HG12	2.05	0.56
1:L:133:LEU:HD13	12:A:101:LMT:H112	1.87	0.56
4:I:45:GLU:OE2	12:I:101:LMT:O3B	2.23	0.56
5:R:48:PHE:HB3	14:S:103:SPO:H82	1.88	0.56
4:D:1:FME:O	12:D:103:LMT:O2B	2.23	0.55
4:Y:15:ARG:NH2	15:Y:102:CDL:OA2	2.34	0.55
1:L:39:PHE:HB2	9:M:410:U10:H361	1.87	0.55
2:M:30:SER:HB2	15:Y:102:CDL:H1	1.88	0.55
7:A:103:BCL:H92	6:X:28:MET:HG2	1.87	0.55
9:D:105:U10:H553	5:E:33:VAL:HG13	1.88	0.55
14:G:102:SPO:H31	7:K:102:BCL:HBB2	1.88	0.55
9:M:410:U10:H23	16:H:306:PTY:H321	1.89	0.55
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.89	0.55
5:R:6:LEU:HD12	5:T:15:GLN:HE21	1.72	0.55
3:H:189:ARG:NH1	3:H:214:ALA:O	2.39	0.54
5:G:48:PHE:HB3	14:G:103:SPO:H82	1.89	0.54
10:F:102:PGV:H05	4:I:14:ARG:HB3	1.89	0.54
14:D:102:SPO:H292	9:D:105:U10:H411	1.90	0.54
12:H:305:LMT:H21	4:O:34:ILE:HG12	1.90	0.54
7:V:101:BCL:H43	14:V:103:SPO:H32	1.90	0.54
8:M:403:BPH:HBC3	8:M:403:BPH:HHD	1.89	0.53
12:M:407:LMT:H102	14:Q:105:SPO:HM12	1.91	0.53
15:M:408:CDL:H202	3:H:26:GLY:HA3	1.91	0.53
3:H:18:TYR:HD1	12:H:304:LMT:H112	1.72	0.53
15:M:408:CDL:H191	3:H:23:PHE:HA	1.91	0.53
2:M:256:MET:HE1	9:M:410:U10:H102	1.89	0.53
12:H:304:LMT:O1B	12:H:304:LMT:O6'	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:24:LEU:HB2	7:I:102:BCL:H42	1.89	0.53
4:Q:20:GLN:OE1	5:R:23:TYR:OH	2.20	0.53
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.44	0.52
12:H:303:LMT:H5B	12:H:303:LMT:H6D	1.91	0.52
2:M:159:VAL:HA	2:M:163:ILE:HB	1.89	0.52
10:Q:103:PGV:H51	7:S:101:BCL:H93	1.90	0.52
2:M:300:ASN:O	3:H:9:ASN:ND2	2.42	0.52
4:A:36:LEU:HD11	4:A:44:LEU:HG	1.91	0.52
14:Z:101:SPO:H31	7:1:101:BCL:HBB2	1.91	0.52
4:D:35:LEU:HD11	7:E:101:BCL:HHD	1.92	0.52
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.45	0.52
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.91	0.52
8:M:403:BPH:H18	8:M:403:BPH:H13	1.91	0.52
4:K:20:GLN:NE2	5:N:23:TYR:OH	2.22	0.52
14:G:102:SPO:H41	4:K:32:HIS:CG	2.45	0.51
10:L:305:PGV:H252	12:K:101:LMT:H102	1.93	0.51
14:G:102:SPO:H392	5:J:19:LEU:HA	1.91	0.51
4:V:8:TRP:CG	5:W:19:LEU:HD23	2.45	0.51
4:A:36:LEU:O	4:A:42:ASN:ND2	2.44	0.51
14:J:102:SPO:H10	5:N:44:TRP:HB2	1.92	0.51
4:O:7:ILE:HB	14:Q:105:SPO:H343	1.92	0.51
10:H:301:PGV:H132	16:H:306:PTY:H443	1.92	0.51
9:D:105:U10:H253	9:D:105:U10:H201	1.92	0.51
4:K:35:LEU:HD11	7:N:101:BCL:HHD	1.93	0.51
7:Z:102:BCL:HHB	7:1:101:BCL:HHB	1.93	0.51
16:H:306:PTY:H371	16:H:306:PTY:H411	1.91	0.51
4:Y:20:GLN:NE2	5:Z:23:TYR:OH	2.43	0.51
10:M:409:PGV:H92	4:S:23:PHE:HD1	1.76	0.50
3:H:159:GLU:HB2	3:H:210:SER:HB2	1.93	0.50
4:A:38:THR:HG21	4:D:44:LEU:HD13	1.94	0.50
4:S:20:GLN:OE1	5:T:23:TYR:OH	2.18	0.50
3:H:191:LEU:HD11	3:H:213:PHE:HE2	1.76	0.50
7:Z:102:BCL:HBB3	7:1:101:BCL:HMC3	1.94	0.50
4:A:40:SER:HB2	4:D:53:ARG:HD2	1.92	0.50
4:Q:10:ILE:HD11	14:S:102:SPO:H393	1.93	0.50
1:L:255:TRP:NE1	1:L:257:ASP:O	2.45	0.50
3:H:66:LEU:HB3	3:H:70:ARG:HB2	1.94	0.50
4:I:6:LYS:NZ	5:N:18:GLU:OE2	2.43	0.50
7:T:101:BCL:H172	14:V:103:SPO:H14	1.93	0.50
2:M:302:GLY:O	2:M:304:ALA:N	2.45	0.49
14:D:102:SPO:H6	7:F:101:BCL:HMB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:41:PHE:CE1	9:D:105:U10:H1M2	2.47	0.49
4:I:7:ILE:HB	14:K:103:SPO:H343	1.93	0.49
12:H:305:LMT:H5'	4:O:38:THR:HG22	1.94	0.49
14:B:101:SPO:H6	7:D:101:BCL:HMB2	1.94	0.49
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.47	0.49
14:V:102:SPO:H9	7:Y:103:BCL:HHB	1.95	0.49
4:F:19:ALA:HB2	10:F:103:PGV:H61	1.94	0.49
7:N:101:BCL:H42	14:O:102:SPO:H293	1.95	0.49
4:Q:37:SER:HA	12:Q:102:LMT:H2'	1.95	0.49
14:B:104:SPO:H351	7:D:101:BCL:H52	1.94	0.49
5:N:48:PHE:HB3	14:O:102:SPO:H82	1.95	0.48
2:M:237:GLN:HB2	2:M:262:MET:HG2	1.95	0.48
7:N:101:BCL:H92	7:N:101:BCL:HAA1	1.94	0.48
3:H:179:LEU:HD21	3:H:193:MET:HE2	1.94	0.48
4:K:11:PHE:HE2	4:O:17:PHE:HD2	1.61	0.48
4:O:1:FME:SD	4:O:1:FME:N	2.80	0.48
2:M:236:GLU:OE1	3:H:117:ARG:NH2	2.46	0.48
4:V:6:LYS:HB3	14:Z:101:SPO:H402	1.96	0.48
5:Z:23:TYR:HA	14:Z:101:SPO:H27	1.96	0.48
14:K:103:SPO:H341	14:K:103:SPO:H361	1.58	0.48
4:A:35:LEU:HD22	7:B:103:BCL:HHD	1.96	0.48
14:V:102:SPO:H41	4:Y:32:HIS:CG	2.49	0.48
4:D:4:PHE:HB3	7:F:101:BCL:H201	1.95	0.47
4:O:23:PHE:HE1	4:Q:25:PHE:CE1	2.32	0.47
2:M:94:LEU:HB3	2:M:177:TYR:HB2	1.96	0.47
2:M:123:PHE:HA	2:M:157:TRP:HH2	1.79	0.47
4:D:21:GLY:HA3	9:D:105:U10:H222	1.95	0.47
2:M:39:LEU:HD12	2:M:47:LEU:HD11	1.96	0.47
14:G:102:SPO:H341	14:G:102:SPO:H361	1.57	0.47
5:W:9:THR:HG23	5:W:11:LEU:HB2	1.97	0.47
7:O:101:BCL:H192	7:O:101:BCL:H161	1.77	0.47
4:Y:42:ASN:O	4:Y:46:ILE:N	2.38	0.47
2:M:21:THR:HB	2:M:26:LEU:HD21	1.96	0.47
12:I:103:LMT:H2'	5:J:24:MET:HE2	1.96	0.47
14:P:102:SPO:H351	7:Q:104:BCL:H43	1.97	0.47
5:W:48:PHE:HD2	7:W:101:BCL:H202	1.78	0.47
14:V:102:SPO:H6	7:Y:103:BCL:CHB	2.45	0.47
1:L:78:ALA:C	12:A:102:LMT:H2'	2.39	0.47
12:H:305:LMT:H6D	12:Q:102:LMT:H6D	1.97	0.47
14:K:103:SPO:H352	5:N:22:VAL:HB	1.96	0.46
8:L:302:BPH:HBB2	2:M:210:TYR:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:11:PHE:HZ	4:O:17:PHE:HB2	1.80	0.46
14:K:103:SPO:H6	7:O:101:BCL:HMB2	1.97	0.46
7:P:101:BCL:H61	7:P:101:BCL:H2	1.63	0.46
4:A:1:FME:HE3	5:E:29:LEU:HD22	1.96	0.46
1:L:18:GLY:O	4:A:15:ARG:NH1	2.48	0.46
5:T:47:TRP:CE2	7:T:101:BCL:H2C	2.50	0.46
1:L:25:TRP:O	4:D:15:ARG:NH1	2.44	0.46
7:Q:106:BCL:H143	7:Q:106:BCL:H111	1.64	0.46
7:Z:102:BCL:HHB	7:1:101:BCL:CHB	2.45	0.46
4:F:1:FME:HE1	5:J:29:LEU:HD22	1.97	0.46
7:Q:106:BCL:H92	5:R:35:ILE:HA	1.96	0.46
14:D:104:SPO:H291	7:F:101:BCL:H193	1.97	0.46
4:F:15:ARG:NH2	16:F:104:PTY:O12	2.49	0.46
4:I:11:PHE:HZ	4:K:17:PHE:HB2	1.79	0.46
14:J:102:SPO:H20	14:J:102:SPO:H181	1.79	0.46
4:O:40:SER:O	5:P:45:ARG:NH1	2.47	0.46
4:I:32:HIS:CE1	7:J:101:BCL:HMD1	2.51	0.46
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.97	0.46
7:A:103:BCL:H13	7:A:103:BCL:H102	1.56	0.46
10:K:104:PGV:H251	4:O:21:GLY:HA3	1.97	0.46
2:M:60:LEU:O	2:M:64:LEU:HB2	2.16	0.45
5:N:47:TRP:O	4:O:47:SER:OG	2.34	0.45
7:S:101:BCL:H161	7:S:101:BCL:H202	1.68	0.45
14:Z:101:SPO:H10	14:Z:101:SPO:H81	1.83	0.45
2:M:167:LEU:HD22	2:M:285:LEU:HD11	1.99	0.45
3:H:170:ASP:O	3:H:174:GLN:N	2.49	0.45
4:F:25:PHE:CD2	10:F:103:PGV:H302	2.51	0.45
4:I:38:THR:HG21	4:K:44:LEU:HD13	1.99	0.45
14:J:102:SPO:H22	7:K:102:BCL:O1D	2.16	0.45
5:P:18:GLU:O	5:P:22:VAL:HG23	2.15	0.45
7:B:103:BCL:HBA1	7:B:103:BCL:H3A	1.78	0.45
4:K:45:GLU:OE2	12:K:101:LMT:O4'	2.29	0.45
14:K:105:SPO:H20	14:K:105:SPO:H181	1.82	0.45
7:O:101:BCL:H2A	14:O:102:SPO:H25	1.97	0.45
7:Y:103:BCL:H61	7:Y:103:BCL:H41	1.69	0.45
1:L:34:PHE:CE1	1:L:102:LEU:HD23	2.52	0.45
4:O:17:PHE:HB3	14:O:102:SPO:H391	1.99	0.45
14:Q:105:SPO:H20	14:Q:105:SPO:H181	1.87	0.45
4:1:25:PHE:HB2	7:1:101:BCL:H2	1.99	0.45
1:L:263:TRP:HE3	9:L:304:U10:H3M3	1.81	0.45
2:M:61:PHE:CD2	4:V:26:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:101:BCL:H141	7:T:101:BCL:H162	1.80	0.45
4:O:24:LEU:HB3	7:O:101:BCL:H12	1.99	0.45
14:S:103:SPO:H20	14:S:103:SPO:H181	1.82	0.45
14:V:102:SPO:H26	14:V:102:SPO:H241	1.79	0.45
7:D:101:BCL:HMD3	5:E:38:HIS:CE1	2.53	0.44
14:J:102:SPO:H15	14:J:102:SPO:H131	1.83	0.44
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.99	0.44
7:M:402:BCL:HAA2	7:M:402:BCL:HBD	1.99	0.44
14:B:101:SPO:H20	14:B:101:SPO:H181	1.79	0.44
7:F:101:BCL:H41	14:F:105:SPO:H351	1.98	0.44
14:P:102:SPO:H27	14:P:102:SPO:H311	1.85	0.44
2:M:148:TRP:CD1	15:M:408:CDL:HB32	2.53	0.44
14:G:102:SPO:H341	5:J:19:LEU:HD12	1.99	0.44
2:M:54:SER:HB2	4:S:15:ARG:HH22	1.81	0.44
14:P:102:SPO:H20	14:P:102:SPO:H181	1.86	0.44
1:L:279:ILE:HG21	2:M:91:PHE:HB3	1.99	0.44
2:M:3:TYR:OH	2:M:7:PHE:O	2.33	0.44
2:M:138:GLN:HB2	2:M:144:LYS:HE3	2.00	0.44
9:M:410:U10:H372	9:M:410:U10:H351	1.57	0.44
5:T:47:TRP:CD2	7:T:101:BCL:H2C	2.53	0.44
7:I:101:BCL:H13	7:I:101:BCL:H172	1.79	0.44
7:A:103:BCL:H41	7:A:103:BCL:H62	1.75	0.44
14:B:101:SPO:H132	7:D:101:BCL:H42	1.98	0.44
16:F:104:PTY:HC12	16:F:104:PTY:H312	1.76	0.44
5:J:47:TRP:CE2	7:J:101:BCL:H2C	2.53	0.44
5:P:47:TRP:CE2	7:P:101:BCL:H2C	2.53	0.44
4:S:27:LEU:HD23	7:T:101:BCL:HED3	1.99	0.44
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.99	0.44
7:D:101:BCL:H121	9:D:105:U10:H28	1.99	0.44
14:B:104:SPO:H25	7:D:101:BCL:HED3	1.99	0.43
14:K:105:SPO:H6	7:Q:104:BCL:HMB2	2.00	0.43
4:V:4:PHE:HD1	14:Z:101:SPO:H302	1.83	0.43
1:L:1:ALA:N	10:F:103:PGV:O06	2.41	0.43
3:H:191:LEU:HD11	3:H:213:PHE:CE2	2.53	0.43
7:M:402:BCL:H162	7:M:402:BCL:H121	1.77	0.43
7:J:101:BCL:H172	14:J:102:SPO:H14	1.99	0.43
7:Y:103:BCL:HBC3	7:Y:103:BCL:H2C	1.78	0.43
12:H:304:LMT:H3'	12:H:304:LMT:H1B	1.86	0.43
2:M:127:TRP:CG	10:M:409:PGV:H232	2.54	0.43
15:H:307:CDL:H351	4:K:23:PHE:HA	2.00	0.43
5:B:47:TRP:O	4:D:47:SER:OG	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:104:SPO:H10	14:B:104:SPO:H81	1.75	0.43
9:D:105:U10:H472	9:D:105:U10:H451	1.78	0.43
7:Q:106:BCL:H93	7:Q:106:BCL:H62	1.72	0.43
4:S:11:PHE:HZ	4:V:17:PHE:HB2	1.83	0.43
10:K:104:PGV:H172	10:K:104:PGV:H142	1.93	0.43
14:K:105:SPO:H32	5:P:22:VAL:HG12	2.01	0.43
14:S:102:SPO:H32	5:T:22:VAL:HG12	2.00	0.43
3:H:54:GLY:HA3	16:H:306:PTY:N1	2.34	0.43
14:V:102:SPO:H15	14:V:102:SPO:H131	1.88	0.43
7:N:101:BCL:H202	7:N:101:BCL:H162	1.78	0.43
6:X:49:ARG:HD2	6:X:49:ARG:HA	1.86	0.43
6:X:57:ILE:O	6:X:58:ASP:HB2	2.19	0.43
4:A:11:PHE:HZ	4:D:17:PHE:HB2	1.84	0.43
7:W:101:BCL:H192	7:W:101:BCL:H162	1.81	0.43
14:Z:101:SPO:H341	14:Z:101:SPO:H362	1.72	0.43
1:L:207:ARG:HD3	1:L:207:ARG:HA	1.86	0.43
4:D:24:LEU:HB3	7:D:101:BCL:H12	2.01	0.43
1:L:75:LEU:HD21	1:L:137:VAL:HG22	2.00	0.42
1:L:198:ALA:HA	1:L:206:MET:HG3	2.00	0.42
12:K:101:LMT:H3'	12:K:101:LMT:H1B	1.67	0.42
1:L:71:LEU:HD22	6:X:64:ALA:HB2	2.01	0.42
14:B:104:SPO:H15	14:B:104:SPO:H131	1.74	0.42
14:F:105:SPO:H15	14:F:105:SPO:H131	1.91	0.42
7:K:102:BCL:H152	7:K:102:BCL:H111	1.88	0.42
4:Y:46:ILE:HD13	5:Z:45:ARG:NE	2.33	0.42
1:L:190:HIS:HA	9:L:303:U10:O2	2.19	0.42
15:H:307:CDL:H141	15:H:307:CDL:H172	1.84	0.42
7:Y:103:BCL:H62	7:Y:103:BCL:H101	1.38	0.42
4:O:4:PHE:CE1	14:Q:105:SPO:H302	2.54	0.42
5:Z:19:LEU:HA	14:Z:101:SPO:H37	2.01	0.42
1:L:128:TYR:O	1:L:132:VAL:HG22	2.19	0.42
2:M:114:LEU:HD23	2:M:114:LEU:HA	1.79	0.42
14:D:102:SPO:H392	5:E:19:LEU:HA	2.01	0.42
4:A:23:PHE:CD2	7:D:101:BCL:H102	2.54	0.42
4:F:32:HIS:CE1	7:G:101:BCL:HMD1	2.54	0.42
5:G:5:ASP:HB2	5:J:11:LEU:HG	2.01	0.42
10:Y:104:PGV:H22	7:1:101:BCL:H102	2.01	0.42
1:L:91:ILE:HG22	9:D:105:U10:H1M3	2.01	0.42
12:L:308:LMT:H51	12:L:308:LMT:H22	1.78	0.42
8:M:403:BPH:H143	8:M:403:BPH:H112	1.76	0.42
10:M:409:PGV:H82	10:M:409:PGV:H51	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:103:BCL:H41	14:B:104:SPO:H241	2.00	0.42
14:P:102:SPO:H15	14:P:102:SPO:H131	1.88	0.42
2:M:64:LEU:HD12	2:M:64:LEU:HA	1.89	0.42
4:A:32:HIS:CE1	7:B:103:BCL:HMD1	2.54	0.42
4:K:32:HIS:CE1	7:N:101:BCL:HMD1	2.55	0.42
1:L:69:PRO:HB3	1:L:78:ALA:CB	2.50	0.42
7:F:101:BCL:H61	14:F:105:SPO:H343	2.02	0.42
14:K:105:SPO:H15	14:K:105:SPO:H131	1.94	0.42
7:Q:104:BCL:H61	7:Q:104:BCL:H102	1.47	0.42
4:S:10:ILE:HA	5:T:8:TYR:HD2	1.84	0.42
1:L:147:PRO:HD3	6:X:66:ASN:ND2	2.29	0.42
14:M:405:SPO:H181	14:M:405:SPO:H20	1.82	0.42
3:H:52:ASN:HD22	16:F:104:PTY:HC21	1.85	0.42
4:D:8:TRP:CD1	5:E:20:HIS:HB2	2.54	0.42
7:F:101:BCL:H91	7:F:101:BCL:H111	1.84	0.42
2:M:164:ARG:HH12	2:M:173:GLU:HB3	1.85	0.41
4:A:43:TRP:CZ3	7:A:103:BCL:HAC2	2.55	0.41
14:B:101:SPO:HM11	4:D:29:VAL:HG13	2.02	0.41
7:Q:106:BCL:HBB3	7:S:101:BCL:C1C	2.50	0.41
14:S:102:SPO:H20	14:S:102:SPO:H181	1.86	0.41
7:Z:102:BCL:H2	7:Z:102:BCL:H61	1.83	0.41
7:L:301:BCL:H151	7:L:301:BCL:H18	1.94	0.41
2:M:214:LEU:HD21	9:M:410:U10:H172	2.02	0.41
7:M:401:BCL:H18	7:M:401:BCL:H151	1.71	0.41
14:M:405:SPO:H391	4:V:33:LEU:HD21	2.02	0.41
4:D:32:HIS:CE1	7:E:101:BCL:HMD1	2.55	0.41
7:Q:104:BCL:HAC1	7:Q:104:BCL:HHH	1.86	0.41
8:M:403:BPH:HBA2	8:M:403:BPH:H3A	1.88	0.41
7:D:101:BCL:H72	9:D:105:U10:H253	2.01	0.41
4:F:34:ILE:HD11	12:I:101:LMT:H22	2.02	0.41
14:G:102:SPO:H26	14:G:102:SPO:H241	1.88	0.41
7:I:102:BCL:H162	7:I:102:BCL:H192	1.72	0.41
14:V:102:SPO:H20	14:V:102:SPO:H181	1.85	0.41
1:L:130:THR:HG23	1:L:249:ILE:HD13	2.03	0.41
8:L:302:BPH:HHH	8:L:302:BPH:CBB	2.49	0.41
7:A:103:BCL:HHH	5:B:41:VAL:HG21	2.02	0.41
6:X:38:PHE:O	6:X:41:THR:OG1	2.28	0.41
1:L:156:TRP:CD1	6:X:65:PRO:HB2	2.55	0.41
7:F:101:BCL:H121	7:F:101:BCL:H162	1.89	0.41
5:T:11:LEU:HG	5:T:15:GLN:HB3	2.02	0.41
1:L:15:THR:OG1	1:L:19:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:LEU:HD12	1:L:85:LEU:HD23	2.02	0.41
15:H:307:CDL:HB31	4:I:11:PHE:HD1	1.85	0.41
5:B:14:GLU:CD	5:B:14:GLU:H	2.29	0.41
16:F:104:PTY:H402	16:F:104:PTY:H443	2.01	0.41
7:K:102:BCL:H192	7:K:102:BCL:H162	1.87	0.41
14:P:102:SPO:H22	7:Q:104:BCL:O1D	2.20	0.41
4:Q:6:LYS:HB3	14:S:102:SPO:H392	2.03	0.41
1:L:212:GLU:HB3	9:L:303:U10:H4M3	2.02	0.41
2:M:271:TRP:HA	2:M:274:VAL:HG22	2.03	0.41
2:M:274:VAL:HA	8:M:403:BPH:HBC1	2.02	0.41
14:G:103:SPO:H20	14:G:103:SPO:H181	1.83	0.41
1:L:181:PHE:HB3	8:M:403:BPH:HBB2	2.03	0.41
2:M:94:LEU:HD11	2:M:114:LEU:HB3	2.03	0.41
2:M:197:PHE:CE1	7:M:402:BCL:HMC2	2.56	0.41
7:F:101:BCL:HED3	14:F:105:SPO:H25	2.01	0.41
4:O:9:MET:O	5:P:8:TYR:HB2	2.20	0.41
4:V:9:MET:HE3	4:V:9:MET:HB2	1.90	0.41
4:V:43:TRP:CE3	7:V:101:BCL:HBC2	2.56	0.41
7:L:309:BCL:H192	8:M:403:BPH:H202	2.03	0.41
14:M:405:SPO:H26	14:M:405:SPO:H241	1.85	0.41
3:H:146:LYS:N	12:H:303:LMT:O3B	2.52	0.41
14:J:102:SPO:H10	14:J:102:SPO:H81	1.82	0.41
7:P:101:BCL:HBB3	7:Q:104:BCL:C1C	2.51	0.41
4:Q:36:LEU:HD13	4:Q:43:TRP:CH2	2.56	0.41
7:Q:106:BCL:H161	5:R:48:PHE:HE2	1.86	0.41
7:Q:106:BCL:H2C	5:R:47:TRP:CE2	2.55	0.41
2:M:258:PHE:CG	16:H:306:PTY:H122	2.55	0.41
15:H:307:CDL:H352	4:K:26:LEU:HD12	2.03	0.41
14:G:102:SPO:H10	14:G:102:SPO:H81	1.96	0.41
5:N:39:LEU:O	5:N:43:ILE:HG12	2.21	0.41
14:Q:105:SPO:H6	7:S:101:BCL:CMB	2.49	0.41
1:L:254:ILE:O	12:L:308:LMT:O2'	2.39	0.40
7:K:102:BCL:HHH	5:N:41:VAL:HG21	2.03	0.40
4:V:23:PHE:HE1	4:Y:25:PHE:CE1	2.39	0.40
4:D:33:LEU:HA	4:D:33:LEU:HD12	1.83	0.40
4:K:3:LYS:HG3	4:K:6:LYS:HG3	2.03	0.40
2:M:206:ILE:HD13	7:M:401:BCL:HMD2	2.03	0.40
5:N:47:TRP:CE2	7:N:101:BCL:H2C	2.56	0.40
4:S:7:ILE:HB	14:V:102:SPO:H352	2.04	0.40
14:S:102:SPO:H10	14:S:102:SPO:H81	1.97	0.40
4:V:41:TYR:OH	5:W:47:TRP:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:153:HIS:O	1:L:157:VAL:HG23	2.21	0.40
7:L:301:BCL:CGA	7:M:401:BCL:HBC1	2.51	0.40
12:H:305:LMT:O6B	12:H:305:LMT:O4'	2.36	0.40
14:G:102:SPO:H15	14:G:102:SPO:H131	1.97	0.40
14:G:103:SPO:H15	14:G:103:SPO:H131	1.85	0.40
7:Q:104:BCL:H143	7:Q:104:BCL:H111	1.78	0.40
14:Z:101:SPO:H20	14:Z:101:SPO:H181	1.92	0.40
3:H:12:LEU:HD12	3:H:12:LEU:HA	1.96	0.40
7:D:101:BCL:H92	7:D:101:BCL:H61	1.73	0.40
14:D:104:SPO:H26	14:D:104:SPO:H241	1.92	0.40
4:F:14:ARG:CZ	10:F:103:PGV:H042	2.52	0.40
14:P:102:SPO:H10	5:R:44:TRP:HB2	2.03	0.40
4:1:32:HIS:O	4:1:36:LEU:N	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
2	M	304/307 (99%)	292 (96%)	12 (4%)	0	100	100
3	H	245/260 (94%)	238 (97%)	7 (3%)	0	100	100
4	1	25/54 (46%)	25 (100%)	0	0	100	100
4	A	43/54 (80%)	43 (100%)	0	0	100	100
4	D	52/54 (96%)	52 (100%)	0	0	100	100
4	F	52/54 (96%)	52 (100%)	0	0	100	100
4	I	52/54 (96%)	52 (100%)	0	0	100	100
4	K	52/54 (96%)	52 (100%)	0	0	100	100
4	O	52/54 (96%)	52 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	52/54 (96%)	52 (100%)	0	0	100	100
4	S	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	V	50/54 (93%)	49 (98%)	1 (2%)	0	100	100
4	Y	37/54 (68%)	37 (100%)	0	0	100	100
5	B	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
5	E	41/48 (85%)	41 (100%)	0	0	100	100
5	G	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
5	J	41/48 (85%)	41 (100%)	0	0	100	100
5	N	41/48 (85%)	41 (100%)	0	0	100	100
5	P	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
5	R	41/48 (85%)	41 (100%)	0	0	100	100
5	T	41/48 (85%)	41 (100%)	0	0	100	100
5	W	40/48 (83%)	39 (98%)	1 (2%)	0	100	100
5	Z	29/48 (60%)	29 (100%)	0	0	100	100
6	X	50/81 (62%)	48 (96%)	2 (4%)	0	100	100
All	All	1797/2003 (90%)	1761 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	214 (97%)	6 (3%)	39	60
2	M	239/240 (100%)	234 (98%)	5 (2%)	47	67
3	H	198/208 (95%)	193 (98%)	5 (2%)	42	63
4	1	24/48 (50%)	23 (96%)	1 (4%)	26	44
4	A	41/48 (85%)	39 (95%)	2 (5%)	22	37
4	D	47/48 (98%)	46 (98%)	1 (2%)	47	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	48/48 (100%)	48 (100%)	0	100	100
4	I	48/48 (100%)	47 (98%)	1 (2%)	47	67
4	K	48/48 (100%)	48 (100%)	0	100	100
4	O	47/48 (98%)	46 (98%)	1 (2%)	47	67
4	Q	48/48 (100%)	48 (100%)	0	100	100
4	S	48/48 (100%)	46 (96%)	2 (4%)	26	44
4	V	47/48 (98%)	47 (100%)	0	100	100
4	Y	35/48 (73%)	33 (94%)	2 (6%)	18	31
5	B	36/39 (92%)	34 (94%)	2 (6%)	19	31
5	E	35/39 (90%)	34 (97%)	1 (3%)	37	57
5	G	37/39 (95%)	35 (95%)	2 (5%)	20	33
5	J	35/39 (90%)	35 (100%)	0	100	100
5	N	35/39 (90%)	34 (97%)	1 (3%)	37	57
5	P	35/39 (90%)	35 (100%)	0	100	100
5	R	34/39 (87%)	33 (97%)	1 (3%)	37	57
5	T	35/39 (90%)	34 (97%)	1 (3%)	37	57
5	W	33/39 (85%)	33 (100%)	0	100	100
5	Z	26/39 (67%)	26 (100%)	0	100	100
6	X	40/65 (62%)	39 (98%)	1 (2%)	42	63
All	All	1519/1651 (92%)	1484 (98%)	35 (2%)	44	65

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

Mol	Chain	Res	Type
1	L	54	VAL
1	L	71	LEU
1	L	75	LEU
1	L	102	LEU
1	L	210	ASP
1	L	260	VAL
2	M	20	MET
2	M	21	THR
2	M	114	LEU
2	M	214	LEU
2	M	216	PHE

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Mol	Chain	Res	Type
3	H	42	LEU
3	H	66	LEU
3	H	158	LEU
3	H	206	ASN
3	H	231	ASP
4	A	30	MET
4	A	35	LEU
5	B	11	LEU
5	B	19	LEU
4	D	33	LEU
5	E	19	LEU
5	G	11	LEU
5	G	14	GLU
4	I	38	THR
5	N	39	LEU
4	O	24	LEU
5	R	39	LEU
4	S	20	GLN
4	S	29	VAL
5	T	14	GLU
4	Y	33	LEU
4	Y	36	LEU
4	1	36	LEU
6	X	67	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	28	ASN
2	M	202	HIS
2	M	299	GLN
2	M	301	HIS
3	H	44	ASN
3	H	199	GLN
4	D	52	ASN
4	F	20	GLN
5	G	17	GLN
5	J	15	GLN
4	K	20	GLN
5	N	17	GLN
4	S	20	GLN
4	1	20	GLN

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Mol	Chain	Res	Type
6	X	60	ASN
6	X	66	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FME	A	1	4	8,9,10	0.53	0	7,9,11	0.92	1 (14%)
4	FME	S	1	4	5,6,10	0.79	0	3,6,11	0.75	0
4	FME	O	1	4	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
4	FME	K	1	4	8,9,10	0.52	0	7,9,11	1.05	1 (14%)
4	FME	D	1	4	8,9,10	0.50	0	7,9,11	1.07	1 (14%)
4	FME	F	1	4	8,9,10	0.50	0	7,9,11	1.07	1 (14%)
4	FME	I	1	4	8,9,10	0.52	0	7,9,11	0.99	1 (14%)
4	FME	Q	1	4	8,9,10	0.52	0	7,9,11	0.94	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	A	1	4	-	3/7/9/11	-
4	FME	S	1	4	-	1/2/5/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	K	1	4	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	D	1	4	-	0/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-
4	FME	Q	1	4	-	0/7/9/11	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	FME	O-C-CA	-2.59	117.98	124.78
4	O	1	FME	O-C-CA	-2.56	118.06	124.78
4	K	1	FME	O-C-CA	-2.56	118.07	124.78
4	F	1	FME	O-C-CA	-2.51	118.20	124.78
4	I	1	FME	O-C-CA	-2.44	118.37	124.78
4	A	1	FME	O-C-CA	-2.40	118.49	124.78
4	Q	1	FME	O-C-CA	-2.29	118.79	124.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	A	1	FME	N-CA-CB-CG
4	F	1	FME	O1-CN-N-CA
4	O	1	FME	O1-CN-N-CA
4	S	1	FME	O1-CN-N-CA
4	I	1	FME	CA-CB-CG-SD
4	A	1	FME	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	FME	1	0
4	O	1	FME	1	0
4	D	1	FME	1	0
4	F	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 1 is monoatomic - leaving 84 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
7	BCL	D	101	4	69,74,74	1.79	19 (27%)	83,115,115	2.56	25 (30%)
9	U10	L	304	-	28,28,63	0.85	2 (7%)	34,37,79	0.78	2 (5%)
14	SPO	B	101	-	40,41,41	0.64	0	47,50,50	1.78	11 (23%)
7	BCL	G	101	5	69,74,74	1.79	17 (24%)	83,115,115	2.46	25 (30%)
11	LDA	L	306	-	12,15,15	2.08	1 (8%)	14,17,17	0.49	0
11	LDA	Y	101	-	8,11,15	2.53	1 (12%)	10,13,17	0.43	0
12	LMT	H	304	-	36,36,36	0.39	0	47,47,47	0.88	1 (2%)
8	BPH	M	403	-	59,70,70	0.74	3 (5%)	61,101,101	0.96	2 (3%)
14	SPO	Q	105	-	40,41,41	0.65	0	47,50,50	1.76	14 (29%)
9	U10	D	105	-	63,63,63	0.62	2 (3%)	76,79,79	0.62	0
10	PGV	Q	103	-	38,38,50	1.04	2 (5%)	41,44,56	1.08	3 (7%)
10	PGV	F	103	-	46,46,50	0.96	2 (4%)	49,52,56	1.06	3 (6%)
8	BPH	L	302	-	59,70,70	0.78	3 (5%)	61,101,101	0.94	3 (4%)
15	CDL	M	408	-	78,78,99	1.05	4 (5%)	84,90,111	1.13	6 (7%)
7	BCL	T	101	5	69,74,74	1.78	17 (24%)	83,115,115	2.48	24 (28%)
12	LMT	D	103	-	28,28,36	0.46	0	39,39,47	0.67	1 (2%)
11	LDA	X	101	-	9,12,15	2.41	1 (11%)	11,14,17	0.50	0
10	PGV	L	305	-	38,38,50	1.06	2 (5%)	41,44,56	1.11	2 (4%)
14	SPO	G	102	-	40,41,41	0.64	0	47,50,50	1.74	10 (21%)
15	CDL	H	307	-	60,60,99	1.18	4 (6%)	66,72,111	1.12	5 (7%)
14	SPO	D	102	-	40,41,41	0.63	0	47,50,50	1.73	12 (25%)
14	SPO	B	104	-	40,41,41	0.64	0	47,50,50	2.10	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	SPO	D	104	-	40,41,41	0.62	0	47,50,50	1.70	11 (23%)
7	BCL	V	101	4	69,74,74	1.79	18 (26%)	83,115,115	2.58	26 (31%)
7	BCL	W	101	5	69,74,74	1.85	17 (24%)	83,115,115	2.35	21 (25%)
12	LMT	Q	102	-	19,19,36	0.44	0	24,24,47	0.54	0
7	BCL	Z	102	5	69,74,74	1.90	17 (24%)	83,115,115	2.43	24 (28%)
12	LMT	I	101	-	27,27,36	0.47	0	38,38,47	0.80	1 (2%)
9	U10	M	410	-	63,63,63	0.62	2 (3%)	76,79,79	0.53	0
12	LMT	M	406	-	27,27,36	0.49	0	32,33,47	0.71	1 (3%)
7	BCL	E	101	5	69,74,74	1.79	18 (26%)	83,115,115	2.43	24 (28%)
15	CDL	Y	102	-	34,34,99	0.85	1 (2%)	37,43,111	0.74	1 (2%)
14	SPO	J	102	-	40,41,41	0.65	0	47,50,50	1.89	13 (27%)
7	BCL	P	101	5	69,74,74	1.81	18 (26%)	83,115,115	2.42	23 (27%)
12	LMT	M	407	-	25,25,36	0.41	0	30,30,47	0.64	0
14	SPO	K	103	-	40,41,41	0.64	0	47,50,50	1.71	11 (23%)
7	BCL	O	101	4	69,74,74	1.79	17 (24%)	83,115,115	2.60	28 (33%)
7	BCL	M	402	2	69,74,74	1.80	17 (24%)	83,115,115	2.56	25 (30%)
12	LMT	H	303	-	36,36,36	0.37	0	47,47,47	0.79	2 (4%)
11	LDA	H	302	-	12,15,15	2.08	1 (8%)	14,17,17	0.51	0
12	LMT	L	307	-	36,36,36	0.42	0	47,47,47	1.07	3 (6%)
7	BCL	A	103	4	64,69,74	1.90	17 (26%)	77,109,115	2.52	23 (29%)
12	LMT	H	305	-	31,31,36	0.48	0	42,42,47	0.93	1 (2%)
12	LMT	L	308	-	35,35,36	0.42	0	46,46,47	0.78	1 (2%)
12	LMT	B	102	-	28,28,36	0.44	0	39,39,47	0.69	1 (2%)
10	PGV	Y	104	-	42,42,50	1.01	2 (4%)	44,48,56	1.06	3 (6%)
14	SPO	G	103	-	40,41,41	0.63	0	47,50,50	1.81	12 (25%)
7	BCL	L	309	2	69,74,74	1.84	17 (24%)	83,115,115	2.39	23 (27%)
14	SPO	K	105	-	40,41,41	0.64	0	47,50,50	1.67	12 (25%)
7	BCL	I	102	4	69,74,74	1.77	18 (26%)	83,115,115	2.55	26 (31%)
10	PGV	M	409	-	37,37,50	1.05	2 (5%)	40,43,56	1.14	3 (7%)
12	LMT	F	106	-	17,17,36	0.46	0	22,22,47	0.52	0
7	BCL	N	101	5	69,74,74	1.79	18 (26%)	83,115,115	2.44	24 (28%)
7	BCL	Y	103	4	69,74,74	1.82	17 (24%)	83,115,115	2.37	22 (26%)
12	LMT	Q	101	-	24,24,36	0.40	0	29,29,47	0.71	0
12	LMT	K	101	-	36,36,36	0.39	0	47,47,47	0.84	2 (4%)
10	PGV	K	104	-	38,40,50	1.03	2 (5%)	40,42,56	1.08	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PGV	H	301	-	46,46,50	0.94	2 (4%)	49,52,56	1.05	4 (8%)
9	U10	L	303	-	35,35,63	0.83	2 (5%)	42,45,79	0.69	0
7	BCL	Q	106	5	69,74,74	1.80	18 (26%)	83,115,115	2.45	24 (28%)
16	PTY	F	104	-	47,47,49	0.28	0	50,52,54	0.56	1 (2%)
14	SPO	V	102	-	40,41,41	0.63	0	47,50,50	1.83	13 (27%)
7	BCL	S	101	4	69,74,74	1.78	18 (26%)	83,115,115	2.53	26 (31%)
7	BCL	J	101	5	69,74,74	1.78	17 (24%)	83,115,115	2.43	25 (30%)
14	SPO	S	103	-	40,41,41	0.62	0	47,50,50	1.85	13 (27%)
7	BCL	K	102	4	69,74,74	1.77	18 (26%)	83,115,115	2.55	25 (30%)
14	SPO	S	102	-	40,41,41	0.64	0	47,50,50	1.72	12 (25%)
7	BCL	M	401	1	69,74,74	1.78	18 (26%)	83,115,115	2.49	26 (31%)
7	BCL	L	301	1	69,74,74	1.80	19 (27%)	83,115,115	2.57	26 (31%)
14	SPO	Z	101	-	40,41,41	0.64	0	47,50,50	1.74	12 (25%)
7	BCL	F	101	4	69,74,74	1.77	18 (26%)	83,115,115	2.57	25 (30%)
7	BCL	1	101	4	69,74,74	1.87	17 (24%)	83,115,115	2.34	21 (25%)
12	LMT	A	101	-	36,36,36	0.37	0	47,47,47	0.69	0
7	BCL	B	103	5	69,74,74	1.81	17 (24%)	83,115,115	2.44	23 (27%)
14	SPO	V	103	-	40,41,41	0.64	0	47,50,50	1.81	13 (27%)
14	SPO	M	405	-	40,41,41	0.63	0	47,50,50	1.64	12 (25%)
14	SPO	P	102	-	40,41,41	0.65	0	47,50,50	3.67	16 (34%)
12	LMT	A	102	-	36,36,36	0.39	0	47,47,47	0.74	1 (2%)
14	SPO	F	105	-	40,41,41	0.63	0	47,50,50	1.92	16 (34%)
7	BCL	Q	104	4	69,74,74	1.78	17 (24%)	83,115,115	2.49	25 (30%)
14	SPO	O	102	-	40,41,41	0.63	0	47,50,50	1.76	13 (27%)
12	LMT	I	103	-	28,28,36	0.44	0	39,39,47	0.57	1 (2%)
10	PGV	F	102	-	39,39,50	1.04	2 (5%)	42,45,56	1.26	5 (11%)
16	PTY	H	306	-	45,45,49	0.29	0	48,50,54	0.42	0

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
7	BCL	D	101	4	-	10/41/137/137	-
9	U10	L	304	-	-	3/21/45/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SPO	B	101	-	-	1/47/47/47	-
7	BCL	G	101	5	-	12/41/137/137	-
11	LDA	L	306	-	-	2/13/13/13	-
11	LDA	Y	101	-	-	1/9/9/13	-
12	LMT	H	304	-	-	8/21/61/61	0/2/2/2
8	BPH	M	403	-	-	7/37/105/105	0/5/6/6
14	SPO	Q	105	-	-	2/47/47/47	-
9	U10	D	105	-	-	20/63/87/87	0/1/1/1
10	PGV	Q	103	-	-	10/43/43/55	-
10	PGV	F	103	-	-	12/51/51/55	-
8	BPH	L	302	-	-	5/37/105/105	0/5/6/6
15	CDL	M	408	-	-	26/89/89/110	-
7	BCL	T	101	5	-	16/41/137/137	-
12	LMT	D	103	-	-	4/13/53/61	0/2/2/2
11	LDA	X	101	-	-	0/10/10/13	-
10	PGV	L	305	-	-	9/43/43/55	-
14	SPO	G	102	-	-	3/47/47/47	-
15	CDL	H	307	-	-	19/71/71/110	-
14	SPO	D	102	-	-	2/47/47/47	-
14	SPO	B	104	-	-	11/47/47/47	-
14	SPO	D	104	-	-	4/47/47/47	-
7	BCL	V	101	4	-	12/41/137/137	-
7	BCL	W	101	5	-	12/41/137/137	-
12	LMT	Q	102	-	-	2/11/31/61	0/1/1/2
7	BCL	Z	102	5	-	14/41/137/137	-
12	LMT	I	101	-	-	3/11/51/61	0/2/2/2
9	U10	M	410	-	-	6/63/87/87	0/1/1/1
12	LMT	M	406	-	-	2/19/39/61	0/1/1/2
7	BCL	E	101	5	-	14/41/137/137	-
15	CDL	Y	102	-	-	15/40/40/110	-
14	SPO	J	102	-	-	9/47/47/47	-
7	BCL	P	101	5	-	15/41/137/137	-
12	LMT	M	407	-	-	5/17/37/61	0/1/1/2
14	SPO	K	103	-	-	6/47/47/47	-
7	BCL	O	101	4	-	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	M	402	2	-	3/41/137/137	-
12	LMT	H	303	-	-	6/21/61/61	0/2/2/2
11	LDA	H	302	-	-	1/13/13/13	-
12	LMT	L	307	-	-	6/21/61/61	0/2/2/2
7	BCL	A	103	4	-	13/35/131/137	-
12	LMT	H	305	-	-	7/16/56/61	0/2/2/2
12	LMT	L	308	-	-	6/20/60/61	0/2/2/2
12	LMT	B	102	-	-	1/13/53/61	0/2/2/2
10	PGV	Y	104	-	-	8/47/47/55	-
14	SPO	G	103	-	-	8/47/47/47	-
7	BCL	L	309	2	-	17/41/137/137	-
14	SPO	K	105	-	-	2/47/47/47	-
7	BCL	I	102	4	-	13/41/137/137	-
10	PGV	M	409	-	-	20/42/42/55	-
12	LMT	F	106	-	-	0/9/29/61	0/1/1/2
7	BCL	N	101	5	-	17/41/137/137	-
7	BCL	Y	103	4	-	20/41/137/137	-
12	LMT	Q	101	-	-	3/15/35/61	0/1/1/2
12	LMT	K	101	-	-	4/21/61/61	0/2/2/2
10	PGV	K	104	-	-	12/40/42/55	-
10	PGV	H	301	-	-	12/51/51/55	-
9	U10	L	303	-	-	7/30/54/87	0/1/1/1
7	BCL	Q	106	5	-	18/41/137/137	-
16	PTY	F	104	-	-	10/51/51/53	-
14	SPO	V	102	-	-	5/47/47/47	-
7	BCL	S	101	4	-	12/41/137/137	-
7	BCL	J	101	5	-	17/41/137/137	-
14	SPO	S	103	-	-	7/47/47/47	-
7	BCL	K	102	4	-	3/41/137/137	-
14	SPO	S	102	-	-	2/47/47/47	-
7	BCL	M	401	1	-	12/41/137/137	-
7	BCL	L	301	1	-	10/41/137/137	-
14	SPO	Z	101	-	-	5/47/47/47	-
7	BCL	F	101	4	-	12/41/137/137	-
7	BCL	1	101	4	-	12/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LMT	A	101	-	-	6/21/61/61	0/2/2/2
7	BCL	B	103	5	-	12/41/137/137	-
14	SPO	V	103	-	-	5/47/47/47	-
14	SPO	M	405	-	-	2/47/47/47	-
14	SPO	P	102	-	-	14/47/47/47	-
12	LMT	A	102	-	-	4/21/61/61	0/2/2/2
14	SPO	F	105	-	-	6/47/47/47	-
7	BCL	Q	104	4	-	14/41/137/137	-
14	SPO	O	102	-	-	5/47/47/47	-
12	LMT	I	103	-	-	4/13/53/61	0/2/2/2
10	PGV	F	102	-	-	11/44/44/55	-
16	PTY	H	306	-	-	8/49/49/53	-

All (482) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	101	LDA	O1-N1	-7.19	1.25	1.42
11	L	306	LDA	O1-N1	-7.18	1.25	1.42
11	H	302	LDA	O1-N1	-7.16	1.25	1.42
11	Y	101	LDA	O1-N1	-7.12	1.25	1.42
7	L	301	BCL	O2D-CGD	5.20	1.45	1.33
7	A	103	BCL	O2D-CGD	5.18	1.45	1.33
7	M	402	BCL	O2D-CGD	5.17	1.45	1.33
7	W	101	BCL	O2D-CGD	5.17	1.45	1.33
7	1	101	BCL	O2D-CGD	5.16	1.45	1.33
7	Q	104	BCL	O2D-CGD	5.15	1.45	1.33
7	B	103	BCL	O2D-CGD	5.14	1.45	1.33
7	Z	102	BCL	O2D-CGD	5.13	1.45	1.33
7	Y	103	BCL	O2D-CGD	5.12	1.45	1.33
7	N	101	BCL	O2D-CGD	5.12	1.45	1.33
7	D	101	BCL	O2D-CGD	5.09	1.45	1.33
7	J	101	BCL	O2D-CGD	5.08	1.45	1.33
7	G	101	BCL	O2D-CGD	5.08	1.45	1.33
7	T	101	BCL	O2D-CGD	5.08	1.45	1.33
7	E	101	BCL	O2D-CGD	5.07	1.45	1.33
7	P	101	BCL	O2D-CGD	5.06	1.45	1.33
7	O	101	BCL	O2D-CGD	5.05	1.45	1.33
7	V	101	BCL	O2D-CGD	5.03	1.45	1.33
7	S	101	BCL	O2D-CGD	5.03	1.45	1.33
7	F	101	BCL	O2D-CGD	5.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	102	BCL	O2D-CGD	5.01	1.45	1.33
7	M	401	BCL	O2D-CGD	5.00	1.45	1.33
7	K	102	BCL	O2D-CGD	5.00	1.45	1.33
7	L	309	BCL	O2D-CGD	4.97	1.45	1.33
7	Q	106	BCL	O2D-CGD	4.96	1.45	1.33
7	P	101	BCL	C3D-C4D	-4.71	1.33	1.44
7	M	401	BCL	C3D-C4D	-4.71	1.33	1.44
7	L	309	BCL	C3D-C4D	-4.69	1.33	1.44
7	Q	106	BCL	C3D-C4D	-4.69	1.33	1.44
7	A	103	BCL	C3D-C4D	-4.68	1.33	1.44
7	L	301	BCL	C3D-C4D	-4.68	1.33	1.44
7	M	402	BCL	C3D-C4D	-4.67	1.33	1.44
7	E	101	BCL	C3D-C4D	-4.66	1.33	1.44
7	O	101	BCL	C3D-C4D	-4.65	1.33	1.44
7	Z	102	BCL	C3D-C4D	-4.63	1.33	1.44
7	D	101	BCL	C3D-C4D	-4.62	1.33	1.44
7	W	101	BCL	C3D-C4D	-4.62	1.33	1.44
7	N	101	BCL	C3D-C4D	-4.61	1.33	1.44
7	1	101	BCL	C3D-C4D	-4.61	1.33	1.44
7	G	101	BCL	C3D-C4D	-4.60	1.33	1.44
7	Y	103	BCL	C3D-C4D	-4.59	1.33	1.44
7	B	103	BCL	C3D-C4D	-4.59	1.33	1.44
7	Q	104	BCL	C3D-C4D	-4.58	1.33	1.44
7	T	101	BCL	C3D-C4D	-4.57	1.33	1.44
7	K	102	BCL	C3D-C4D	-4.55	1.33	1.44
7	I	102	BCL	C3D-C4D	-4.54	1.33	1.44
7	S	101	BCL	C3D-C4D	-4.54	1.33	1.44
7	V	101	BCL	C3D-C4D	-4.54	1.33	1.44
7	J	101	BCL	C3D-C4D	-4.54	1.33	1.44
7	F	101	BCL	C3D-C4D	-4.51	1.34	1.44
7	1	101	BCL	CHD-C1D	4.50	1.47	1.38
15	M	408	CDL	OA8-CA7	4.41	1.46	1.33
7	M	401	BCL	O2A-CGA	4.37	1.46	1.33
7	L	301	BCL	C3B-C4B	4.37	1.49	1.41
7	O	101	BCL	C3B-C4B	4.36	1.49	1.41
7	Z	102	BCL	CHD-C1D	4.34	1.46	1.38
7	S	101	BCL	O2A-CGA	4.32	1.46	1.33
15	H	307	CDL	OA8-CA7	4.32	1.46	1.33
7	1	101	BCL	C3B-C4B	4.31	1.49	1.41
7	Z	102	BCL	O2A-CGA	4.31	1.45	1.33
7	1	101	BCL	O2A-CGA	4.30	1.45	1.33
15	Y	102	CDL	OA8-CA7	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	102	BCL	C3B-C4B	4.29	1.49	1.41
10	F	103	PGV	O03-C19	4.29	1.45	1.33
7	V	101	BCL	O2A-CGA	4.29	1.45	1.33
10	F	102	PGV	O03-C19	4.28	1.45	1.33
7	F	101	BCL	C3B-C4B	4.28	1.49	1.41
10	Y	104	PGV	O03-C19	4.27	1.45	1.33
7	D	101	BCL	O2A-CGA	4.27	1.45	1.33
7	M	402	BCL	C3B-C4B	4.27	1.49	1.41
7	Y	103	BCL	O2A-CGA	4.26	1.45	1.33
7	J	101	BCL	O2A-CGA	4.26	1.45	1.33
10	L	305	PGV	O03-C19	4.26	1.45	1.33
7	V	101	BCL	C3B-C4B	4.26	1.49	1.41
7	W	101	BCL	O2A-CGA	4.26	1.45	1.33
7	Q	106	BCL	O2A-CGA	4.23	1.45	1.33
7	L	309	BCL	C3B-C4B	4.23	1.49	1.41
15	H	307	CDL	OB8-CB7	4.23	1.45	1.33
7	A	103	BCL	O2A-CGA	4.22	1.45	1.33
10	K	104	PGV	O03-C19	4.22	1.45	1.33
7	K	102	BCL	O2A-CGA	4.22	1.45	1.33
7	E	101	BCL	O2A-CGA	4.22	1.45	1.33
10	Q	103	PGV	O03-C19	4.21	1.45	1.33
7	Y	103	BCL	CHD-C1D	4.20	1.46	1.38
10	M	409	PGV	O03-C19	4.20	1.45	1.33
15	M	408	CDL	OB8-CB7	4.20	1.45	1.33
7	L	309	BCL	O2A-CGA	4.20	1.45	1.33
7	I	102	BCL	O2A-CGA	4.20	1.45	1.33
7	Q	104	BCL	O2A-CGA	4.20	1.45	1.33
7	T	101	BCL	O2A-CGA	4.19	1.45	1.33
7	D	101	BCL	C3B-C4B	4.19	1.48	1.41
10	L	305	PGV	O01-C1	4.18	1.46	1.34
7	G	101	BCL	O2A-CGA	4.18	1.45	1.33
7	B	103	BCL	O2A-CGA	4.17	1.45	1.33
7	T	101	BCL	C3B-C4B	4.17	1.48	1.41
7	Y	103	BCL	C3B-C4B	4.17	1.48	1.41
7	L	301	BCL	O2A-CGA	4.16	1.45	1.33
7	F	101	BCL	O2A-CGA	4.16	1.45	1.33
7	P	101	BCL	O2A-CGA	4.16	1.45	1.33
15	M	408	CDL	OB6-CB5	4.16	1.46	1.34
7	S	101	BCL	C3B-C4B	4.16	1.48	1.41
7	N	101	BCL	O2A-CGA	4.14	1.45	1.33
15	H	307	CDL	OA6-CA5	4.12	1.45	1.34
7	O	101	BCL	O2A-CGA	4.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	103	BCL	C3B-C4B	4.10	1.48	1.41
10	Y	104	PGV	O01-C1	4.10	1.45	1.34
10	H	301	PGV	O03-C19	4.10	1.45	1.33
7	Z	102	BCL	C3B-C4B	4.09	1.48	1.41
7	A	103	BCL	CHD-C1D	4.09	1.46	1.38
7	Q	104	BCL	C3B-C4B	4.08	1.48	1.41
7	G	101	BCL	C3B-C4B	4.08	1.48	1.41
7	J	101	BCL	C3B-C4B	4.07	1.48	1.41
7	Q	106	BCL	C3B-C4B	4.07	1.48	1.41
7	M	402	BCL	O2A-CGA	4.06	1.45	1.33
10	Q	103	PGV	O01-C1	4.06	1.45	1.34
7	P	101	BCL	C3B-C4B	4.05	1.48	1.41
15	M	408	CDL	OA6-CA5	4.05	1.45	1.34
10	H	301	PGV	O01-C1	4.04	1.45	1.34
10	K	104	PGV	O01-C1	4.04	1.45	1.34
10	F	103	PGV	O01-C1	4.04	1.45	1.34
15	H	307	CDL	OB6-CB5	4.03	1.45	1.34
10	M	409	PGV	O01-C1	4.02	1.45	1.34
10	F	102	PGV	O01-C1	4.00	1.45	1.34
7	W	101	BCL	CHD-C1D	3.99	1.46	1.38
7	E	101	BCL	C3B-C4B	3.98	1.48	1.41
7	K	102	BCL	C3B-C4B	3.96	1.48	1.41
7	A	103	BCL	C3B-C4B	3.95	1.48	1.41
7	M	401	BCL	C3B-C4B	3.93	1.48	1.41
7	L	309	BCL	CHD-C1D	3.92	1.46	1.38
7	N	101	BCL	C3B-C4B	3.92	1.48	1.41
7	W	101	BCL	C3B-C4B	3.88	1.48	1.41
7	1	101	BCL	CHB-C1B	3.75	1.47	1.39
7	1	101	BCL	OBD-CAD	3.75	1.28	1.22
7	Y	103	BCL	OBD-CAD	3.73	1.28	1.22
7	B	103	BCL	CHD-C1D	3.71	1.45	1.38
7	P	101	BCL	CHD-C1D	3.70	1.45	1.38
7	Z	102	BCL	OBD-CAD	3.70	1.28	1.22
7	Z	102	BCL	CHB-C1B	3.69	1.47	1.39
7	Q	104	BCL	CHD-C1D	3.65	1.45	1.38
7	L	301	BCL	CHD-C1D	3.64	1.45	1.38
7	Z	102	BCL	CHC-C4B	3.64	1.47	1.39
7	L	309	BCL	CHB-C1B	3.63	1.47	1.39
7	Q	106	BCL	CHD-C1D	3.63	1.45	1.38
7	S	101	BCL	OBD-CAD	3.63	1.28	1.22
7	T	101	BCL	OBD-CAD	3.62	1.28	1.22
7	Y	103	BCL	CHB-C1B	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	101	BCL	CHD-C1D	3.61	1.45	1.38
7	W	101	BCL	OBD-CAD	3.61	1.28	1.22
7	D	101	BCL	OBD-CAD	3.59	1.28	1.22
7	1	101	BCL	CHC-C4B	3.59	1.47	1.39
7	E	101	BCL	OBD-CAD	3.59	1.28	1.22
7	W	101	BCL	CHB-C1B	3.58	1.47	1.39
7	M	401	BCL	CHD-C1D	3.58	1.45	1.38
7	Q	104	BCL	OBD-CAD	3.58	1.28	1.22
7	D	101	BCL	CHD-C1D	3.57	1.45	1.38
7	V	101	BCL	OBD-CAD	3.57	1.28	1.22
7	M	402	BCL	CHD-C1D	3.57	1.45	1.38
7	A	103	BCL	OBD-CAD	3.57	1.28	1.22
7	L	301	BCL	OBD-CAD	3.56	1.28	1.22
7	T	101	BCL	CHD-C1D	3.56	1.45	1.38
7	A	103	BCL	CHB-C1B	3.56	1.47	1.39
7	F	101	BCL	OBD-CAD	3.56	1.28	1.22
7	P	101	BCL	OBD-CAD	3.56	1.28	1.22
7	O	101	BCL	OBD-CAD	3.55	1.28	1.22
7	N	101	BCL	OBD-CAD	3.55	1.28	1.22
7	K	102	BCL	OBD-CAD	3.55	1.28	1.22
7	J	101	BCL	OBD-CAD	3.54	1.28	1.22
7	Q	106	BCL	OBD-CAD	3.54	1.28	1.22
7	O	101	BCL	CHD-C1D	3.54	1.45	1.38
7	E	101	BCL	CHD-C1D	3.53	1.45	1.38
7	V	101	BCL	CHD-C1D	3.53	1.45	1.38
7	L	309	BCL	OBD-CAD	3.53	1.28	1.22
7	F	101	BCL	CHD-C1D	3.52	1.45	1.38
7	M	402	BCL	OBD-CAD	3.51	1.28	1.22
7	S	101	BCL	CHD-C1D	3.51	1.45	1.38
7	G	101	BCL	CHD-C1D	3.50	1.45	1.38
7	G	101	BCL	OBD-CAD	3.49	1.28	1.22
7	B	103	BCL	OBD-CAD	3.48	1.28	1.22
7	I	102	BCL	CHD-C1D	3.47	1.45	1.38
7	J	101	BCL	CHD-C1D	3.46	1.45	1.38
7	I	102	BCL	OBD-CAD	3.45	1.28	1.22
7	M	401	BCL	OBD-CAD	3.44	1.28	1.22
7	M	401	BCL	CHB-C1B	3.44	1.47	1.39
7	Y	103	BCL	CHC-C4B	3.44	1.47	1.39
7	W	101	BCL	CHC-C4B	3.43	1.47	1.39
7	K	102	BCL	CHD-C1D	3.43	1.45	1.38
7	S	101	BCL	CHB-C1B	3.43	1.47	1.39
7	J	101	BCL	CHB-C1B	3.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	101	BCL	CHB-C1B	3.39	1.47	1.39
7	M	402	BCL	CHB-C1B	3.39	1.47	1.39
7	P	101	BCL	CHB-C1B	3.37	1.47	1.39
7	T	101	BCL	CHB-C1B	3.37	1.47	1.39
7	Q	106	BCL	CHB-C1B	3.37	1.47	1.39
7	E	101	BCL	CHB-C1B	3.36	1.46	1.39
7	N	101	BCL	CHB-C1B	3.35	1.46	1.39
7	B	103	BCL	CHC-C4B	3.35	1.46	1.39
7	G	101	BCL	CHB-C1B	3.35	1.46	1.39
7	I	102	BCL	CHB-C1B	3.34	1.46	1.39
7	K	102	BCL	CHB-C1B	3.32	1.46	1.39
7	G	101	BCL	CHC-C4B	3.32	1.46	1.39
7	Q	104	BCL	CHB-C1B	3.32	1.46	1.39
7	T	101	BCL	CHC-C4B	3.31	1.46	1.39
7	M	402	BCL	CHC-C4B	3.31	1.46	1.39
7	L	309	BCL	CHC-C4B	3.30	1.46	1.39
7	J	101	BCL	CHC-C4B	3.30	1.46	1.39
7	D	101	BCL	CHB-C1B	3.28	1.46	1.39
7	L	301	BCL	CHB-C1B	3.28	1.46	1.39
7	B	103	BCL	CHB-C1B	3.27	1.46	1.39
7	A	103	BCL	CHC-C4B	3.26	1.46	1.39
7	L	309	BCL	C4B-NB	-3.25	1.33	1.37
7	F	101	BCL	CHB-C1B	3.25	1.46	1.39
7	Q	106	BCL	CHC-C4B	3.24	1.46	1.39
7	E	101	BCL	CHC-C4B	3.24	1.46	1.39
7	L	301	BCL	CHC-C4B	3.24	1.46	1.39
7	O	101	BCL	CHC-C4B	3.23	1.46	1.39
7	O	101	BCL	CHB-C1B	3.22	1.46	1.39
7	Q	104	BCL	CHC-C4B	3.19	1.46	1.39
7	P	101	BCL	CHC-C4B	3.18	1.46	1.39
7	1	101	BCL	C3D-C2D	3.16	1.47	1.39
7	W	101	BCL	C4B-NB	-3.15	1.33	1.37
7	Z	102	BCL	C3D-C2D	3.15	1.47	1.39
7	W	101	BCL	C3D-C2D	3.14	1.47	1.39
7	S	101	BCL	CHC-C4B	3.14	1.46	1.39
7	N	101	BCL	CHC-C4B	3.13	1.46	1.39
7	F	101	BCL	CHC-C4B	3.12	1.46	1.39
7	A	103	BCL	C4B-NB	-3.12	1.34	1.37
7	1	101	BCL	MG-NC	-3.09	1.98	2.06
7	M	401	BCL	CHC-C4B	3.09	1.46	1.39
7	1	101	BCL	CHD-C4C	3.09	1.48	1.39
7	V	101	BCL	CHC-C4B	3.08	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	103	BCL	C3D-C2D	3.08	1.47	1.39
7	I	102	BCL	CHC-C4B	3.08	1.46	1.39
7	L	309	BCL	C3D-C2D	3.07	1.47	1.39
7	K	102	BCL	CHC-C4B	3.06	1.46	1.39
7	K	102	BCL	C4B-NB	-3.06	1.34	1.37
7	1	101	BCL	C1D-C2D	3.05	1.51	1.45
7	Z	102	BCL	CHD-C4C	3.05	1.47	1.39
7	Z	102	BCL	C4B-NB	-3.05	1.34	1.37
7	B	103	BCL	C3D-C2D	3.05	1.47	1.39
7	Y	103	BCL	CHD-C4C	3.04	1.47	1.39
7	J	101	BCL	C3D-C2D	3.04	1.47	1.39
7	A	103	BCL	C3D-C2D	3.04	1.47	1.39
8	L	302	BPH	C4D-CHA	3.04	1.44	1.39
7	D	101	BCL	CHC-C4B	3.04	1.46	1.39
7	G	101	BCL	C3D-C2D	3.03	1.47	1.39
7	K	102	BCL	C3D-C2D	3.02	1.47	1.39
7	Z	102	BCL	MG-NA	-3.01	1.99	2.06
7	Y	103	BCL	C1D-C2D	3.00	1.51	1.45
7	E	101	BCL	C3D-C2D	3.00	1.47	1.39
7	F	101	BCL	C3D-C2D	2.99	1.47	1.39
7	M	401	BCL	C3D-C2D	2.99	1.47	1.39
7	I	102	BCL	C3D-C2D	2.99	1.47	1.39
7	T	101	BCL	C3D-C2D	2.98	1.47	1.39
7	P	101	BCL	C4B-NB	-2.98	1.34	1.37
7	P	101	BCL	C1D-ND	-2.97	1.34	1.37
7	D	101	BCL	C3D-C2D	2.96	1.47	1.39
7	N	101	BCL	C3D-C2D	2.96	1.47	1.39
7	V	101	BCL	C3D-C2D	2.95	1.47	1.39
7	Q	106	BCL	C3D-C2D	2.95	1.47	1.39
7	B	103	BCL	C4B-NB	-2.95	1.34	1.37
7	G	101	BCL	C4B-NB	-2.95	1.34	1.37
7	M	401	BCL	C4B-NB	-2.94	1.34	1.37
7	O	101	BCL	C3D-C2D	2.94	1.47	1.39
7	P	101	BCL	C3D-C2D	2.94	1.47	1.39
7	L	301	BCL	C3D-C2D	2.93	1.47	1.39
7	Q	104	BCL	C3D-C2D	2.93	1.47	1.39
7	S	101	BCL	C3D-C2D	2.93	1.47	1.39
7	Z	102	BCL	MG-NC	-2.93	1.99	2.06
7	E	101	BCL	C1D-ND	-2.93	1.34	1.37
7	Z	102	BCL	C1D-C2D	2.92	1.51	1.45
7	N	101	BCL	C4B-NB	-2.91	1.34	1.37
7	Q	106	BCL	C4B-NB	-2.91	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	101	BCL	C1D-ND	-2.90	1.34	1.37
7	W	101	BCL	CHD-C4C	2.90	1.47	1.39
9	L	303	U10	C3-C2	-2.90	1.40	1.48
7	M	402	BCL	C3D-C2D	2.90	1.47	1.39
7	J	101	BCL	C1D-ND	-2.89	1.34	1.37
7	V	101	BCL	C4B-NB	-2.89	1.34	1.37
8	M	403	BPH	C4D-CHA	2.88	1.44	1.39
7	A	103	BCL	CHD-C4C	2.85	1.47	1.39
7	Q	106	BCL	C1D-ND	-2.84	1.34	1.37
7	L	309	BCL	C1D-ND	-2.82	1.34	1.37
7	L	309	BCL	CHD-C4C	2.82	1.47	1.39
7	G	101	BCL	C1D-ND	-2.80	1.34	1.37
7	Z	102	BCL	C1B-NB	-2.79	1.34	1.37
7	B	103	BCL	C1D-ND	-2.79	1.34	1.37
7	W	101	BCL	C1D-ND	-2.78	1.34	1.37
7	E	101	BCL	C4B-NB	-2.77	1.34	1.37
7	A	103	BCL	C1D-C2D	2.76	1.50	1.45
7	O	101	BCL	C1D-ND	-2.75	1.34	1.37
7	Y	103	BCL	MG-NC	-2.75	1.99	2.06
7	S	101	BCL	C4B-NB	-2.75	1.34	1.37
7	D	101	BCL	C4B-NB	-2.75	1.34	1.37
7	I	102	BCL	C4B-NB	-2.74	1.34	1.37
7	Z	102	BCL	C1D-ND	-2.74	1.34	1.37
9	L	304	U10	C3-C2	-2.74	1.41	1.48
7	Z	102	BCL	C1B-C2B	2.74	1.49	1.43
7	M	401	BCL	C1D-ND	-2.73	1.34	1.37
7	A	103	BCL	MG-NC	-2.73	1.99	2.06
7	B	103	BCL	CHD-C4C	2.72	1.46	1.39
7	V	101	BCL	C1D-C2D	2.71	1.50	1.45
7	W	101	BCL	C1B-C2B	2.71	1.49	1.43
7	K	102	BCL	C1D-ND	-2.71	1.34	1.37
7	Q	104	BCL	C4B-NB	-2.71	1.34	1.37
7	T	101	BCL	C4B-NB	-2.70	1.34	1.37
7	T	101	BCL	C1D-ND	-2.70	1.34	1.37
7	D	101	BCL	C1D-ND	-2.70	1.34	1.37
7	V	101	BCL	CHD-C4C	2.69	1.46	1.39
7	Q	104	BCL	CHD-C4C	2.69	1.46	1.39
7	Q	104	BCL	C1D-ND	-2.69	1.34	1.37
7	F	101	BCL	C4B-NB	-2.69	1.34	1.37
7	S	101	BCL	C1D-ND	-2.69	1.34	1.37
7	Q	106	BCL	CHD-C4C	2.68	1.46	1.39
7	I	102	BCL	C1D-ND	-2.68	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	402	BCL	C4B-NB	-2.68	1.34	1.37
7	F	101	BCL	C1D-ND	-2.68	1.34	1.37
7	N	101	BCL	CHD-C4C	2.67	1.46	1.39
7	T	101	BCL	CHD-C4C	2.67	1.46	1.39
7	M	401	BCL	CHD-C4C	2.66	1.46	1.39
7	P	101	BCL	C1B-NB	-2.66	1.34	1.37
7	M	402	BCL	C1D-C2D	2.66	1.50	1.45
7	D	101	BCL	CHD-C4C	2.65	1.46	1.39
7	J	101	BCL	C4B-NB	-2.65	1.34	1.37
7	O	101	BCL	CHD-C4C	2.65	1.46	1.39
7	W	101	BCL	C1D-C2D	2.65	1.50	1.45
7	L	301	BCL	C4B-NB	-2.64	1.34	1.37
7	O	101	BCL	C4B-NB	-2.64	1.34	1.37
7	P	101	BCL	CHD-C4C	2.63	1.46	1.39
7	M	402	BCL	CHD-C4C	2.63	1.46	1.39
7	F	101	BCL	C1B-NB	-2.63	1.34	1.37
7	D	101	BCL	C1B-NB	-2.63	1.34	1.37
7	W	101	BCL	C1B-NB	-2.63	1.34	1.37
7	S	101	BCL	CHD-C4C	2.62	1.46	1.39
7	M	402	BCL	C1B-NB	-2.62	1.34	1.37
7	W	101	BCL	MG-NA	-2.62	2.00	2.06
7	L	309	BCL	C1D-C2D	2.62	1.50	1.45
9	D	105	U10	C3-C2	-2.62	1.41	1.48
7	E	101	BCL	C1B-NB	-2.61	1.34	1.37
7	L	301	BCL	CHD-C4C	2.61	1.46	1.39
7	L	301	BCL	C1D-C2D	2.61	1.50	1.45
7	O	101	BCL	C1B-NB	-2.61	1.34	1.37
7	G	101	BCL	CHD-C4C	2.61	1.46	1.39
7	F	101	BCL	CHD-C4C	2.61	1.46	1.39
7	A	103	BCL	C1B-C2B	2.59	1.49	1.43
7	K	102	BCL	CHD-C4C	2.59	1.46	1.39
7	1	101	BCL	MG-NA	-2.58	2.00	2.06
7	E	101	BCL	CHD-C4C	2.58	1.46	1.39
7	1	101	BCL	C1B-C2B	2.58	1.49	1.43
7	I	102	BCL	CHD-C4C	2.58	1.46	1.39
7	Q	104	BCL	C1D-C2D	2.57	1.50	1.45
7	J	101	BCL	CHD-C4C	2.57	1.46	1.39
7	W	101	BCL	MG-NC	-2.56	2.00	2.06
7	M	402	BCL	C1D-ND	-2.56	1.34	1.37
7	O	101	BCL	C1D-C2D	2.56	1.50	1.45
7	P	101	BCL	C1B-C2B	2.55	1.49	1.43
7	Q	106	BCL	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	106	BCL	C1B-NB	-2.55	1.34	1.37
7	L	309	BCL	MG-NC	-2.54	2.00	2.06
7	V	101	BCL	C1D-ND	-2.54	1.34	1.37
7	L	301	BCL	C1D-ND	-2.54	1.34	1.37
9	M	410	U10	C4-C5	-2.53	1.41	1.48
7	Y	103	BCL	C1B-C2B	2.53	1.49	1.43
7	J	101	BCL	C1B-C2B	2.52	1.49	1.43
7	S	101	BCL	C1D-C2D	2.52	1.50	1.45
7	F	101	BCL	C1D-C2D	2.52	1.50	1.45
7	N	101	BCL	C1B-C2B	2.52	1.49	1.43
7	B	103	BCL	C1B-NB	-2.52	1.34	1.37
7	B	103	BCL	C1D-C2D	2.51	1.50	1.45
7	T	101	BCL	C1B-C2B	2.51	1.49	1.43
7	B	103	BCL	C1B-C2B	2.51	1.49	1.43
7	A	103	BCL	C1D-ND	-2.50	1.34	1.37
7	M	401	BCL	C1D-C2D	2.50	1.50	1.45
7	E	101	BCL	C1B-C2B	2.49	1.49	1.43
7	L	309	BCL	MG-NA	-2.49	2.00	2.06
7	K	102	BCL	C1D-C2D	2.48	1.50	1.45
7	L	309	BCL	C1B-NB	-2.47	1.34	1.37
7	K	102	BCL	C1B-NB	-2.47	1.34	1.37
7	I	102	BCL	C1D-C2D	2.46	1.50	1.45
9	D	105	U10	C4-C5	-2.46	1.41	1.48
7	N	101	BCL	C1D-C2D	2.45	1.50	1.45
7	D	101	BCL	C1D-C2D	2.45	1.50	1.45
7	T	101	BCL	C1D-C2D	2.45	1.50	1.45
7	P	101	BCL	C1D-C2D	2.45	1.50	1.45
7	A	103	BCL	MG-NA	-2.45	2.00	2.06
7	S	101	BCL	C1B-C2B	2.45	1.49	1.43
7	Q	106	BCL	C1D-C2D	2.44	1.50	1.45
7	B	103	BCL	MG-NC	-2.43	2.00	2.06
7	G	101	BCL	C1B-C2B	2.43	1.49	1.43
7	L	301	BCL	C1B-NB	-2.42	1.34	1.37
7	I	102	BCL	C1B-NB	-2.42	1.34	1.37
7	M	402	BCL	C1B-C2B	2.42	1.48	1.43
7	G	101	BCL	C1B-NB	-2.41	1.34	1.37
7	Q	104	BCL	C1B-NB	-2.41	1.34	1.37
9	M	410	U10	C3-C2	-2.40	1.42	1.48
7	Y	103	BCL	C4B-NB	-2.39	1.34	1.37
7	Q	104	BCL	C1B-C2B	2.39	1.48	1.43
7	L	309	BCL	C1B-C2B	2.38	1.48	1.43
9	L	303	U10	C4-C5	-2.37	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	101	BCL	MG-NA	-2.37	2.00	2.06
7	L	301	BCL	C1B-C2B	2.37	1.48	1.43
7	A	103	BCL	C1B-NB	-2.36	1.34	1.37
7	V	101	BCL	C1B-C2B	2.35	1.48	1.43
7	B	103	BCL	MG-NA	-2.35	2.00	2.06
7	Y	103	BCL	MG-NA	-2.34	2.00	2.06
7	T	101	BCL	C1B-NB	-2.33	1.34	1.37
7	P	101	BCL	MG-NC	-2.33	2.00	2.06
7	K	102	BCL	C1B-C2B	2.33	1.48	1.43
7	I	102	BCL	C1B-C2B	2.33	1.48	1.43
7	F	101	BCL	C1B-C2B	2.33	1.48	1.43
7	M	401	BCL	C1B-NB	-2.33	1.34	1.37
7	Q	106	BCL	MG-NA	-2.32	2.00	2.06
7	V	101	BCL	C1B-NB	-2.32	1.34	1.37
7	M	401	BCL	C1B-C2B	2.32	1.48	1.43
7	P	101	BCL	MG-NA	-2.32	2.00	2.06
7	M	401	BCL	MG-NA	-2.31	2.00	2.06
7	N	101	BCL	C1B-NB	-2.31	1.34	1.37
7	G	101	BCL	MG-NA	-2.30	2.00	2.06
7	I	101	BCL	C1B-NB	-2.30	1.35	1.37
7	G	101	BCL	C1D-C2D	2.30	1.49	1.45
7	J	101	BCL	C1B-NB	-2.29	1.35	1.37
7	O	101	BCL	MG-NA	-2.29	2.00	2.06
7	D	101	BCL	C1B-C2B	2.29	1.48	1.43
7	J	101	BCL	C1D-C2D	2.29	1.49	1.45
7	M	401	BCL	MG-NC	-2.28	2.00	2.06
7	E	101	BCL	C1D-C2D	2.27	1.49	1.45
7	M	402	BCL	MG-NC	-2.27	2.00	2.06
7	S	101	BCL	C1B-NB	-2.26	1.35	1.37
7	N	101	BCL	MG-NA	-2.25	2.00	2.06
7	N	101	BCL	MG-NC	-2.24	2.00	2.06
7	O	101	BCL	C1B-C2B	2.24	1.48	1.43
7	K	102	BCL	MG-NA	-2.24	2.01	2.06
7	I	101	BCL	C4B-NB	-2.24	1.35	1.37
7	Q	106	BCL	MG-NC	-2.23	2.01	2.06
7	L	301	BCL	MG-NC	-2.21	2.01	2.06
8	M	403	BPH	C3A-C2A	-2.20	1.52	1.54
7	S	101	BCL	MG-NA	-2.20	2.01	2.06
7	Y	103	BCL	C1B-NB	-2.18	1.35	1.37
7	G	101	BCL	MG-NC	-2.17	2.01	2.06
7	E	101	BCL	MG-NA	-2.16	2.01	2.06
7	T	101	BCL	MG-NC	-2.16	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	402	BCL	MG-NA	-2.16	2.01	2.06
7	Y	103	BCL	C1D-ND	-2.15	1.35	1.37
7	D	101	BCL	MG-NA	-2.15	2.01	2.06
8	L	302	BPH	CBD-CGD	-2.14	1.49	1.52
7	E	101	BCL	MG-NC	-2.13	2.01	2.06
7	O	101	BCL	MG-NC	-2.13	2.01	2.06
7	Q	104	BCL	MG-NA	-2.13	2.01	2.06
7	Q	104	BCL	MG-NC	-2.13	2.01	2.06
7	L	301	BCL	CHB-C4A	-2.13	1.32	1.37
8	L	302	BPH	C1B-C2B	2.12	1.41	1.39
7	S	101	BCL	MG-NC	-2.11	2.01	2.06
7	K	102	BCL	CHC-C1C	-2.11	1.32	1.37
7	F	101	BCL	MG-NA	-2.10	2.01	2.06
7	I	102	BCL	MG-NA	-2.10	2.01	2.06
7	P	101	BCL	CHC-C1C	-2.10	1.32	1.37
7	J	101	BCL	MG-NC	-2.09	2.01	2.06
7	M	401	BCL	CHC-C1C	-2.09	1.32	1.37
7	T	101	BCL	MG-NA	-2.08	2.01	2.06
7	V	101	BCL	CHC-C1C	-2.08	1.32	1.37
7	F	101	BCL	MG-NC	-2.07	2.01	2.06
7	V	101	BCL	MG-NC	-2.07	2.01	2.06
7	Q	106	BCL	CHC-C1C	-2.07	1.32	1.37
9	L	304	U10	C4-C5	-2.07	1.42	1.48
7	D	101	BCL	CHC-C1C	-2.07	1.32	1.37
7	D	101	BCL	MG-NC	-2.07	2.01	2.06
8	M	403	BPH	C1B-C2B	2.06	1.41	1.39
7	F	101	BCL	CHC-C1C	-2.06	1.32	1.37
7	N	101	BCL	CHC-C1C	-2.06	1.32	1.37
7	I	102	BCL	CHC-C1C	-2.06	1.32	1.37
7	L	301	BCL	MG-NA	-2.06	2.01	2.06
7	I	102	BCL	MG-NC	-2.05	2.01	2.06
7	J	101	BCL	MG-NA	-2.04	2.01	2.06
7	L	301	BCL	CHC-C1C	-2.03	1.32	1.37
7	D	101	BCL	CHB-C4A	-2.03	1.32	1.37
7	E	101	BCL	CHC-C1C	-2.03	1.32	1.37
7	S	101	BCL	CHC-C1C	-2.03	1.32	1.37
7	K	102	BCL	CHB-C4A	-2.02	1.32	1.37
7	1	101	BCL	C1D-ND	-2.02	1.35	1.37

All (910) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	102	SPO	C2-C1-C4	-16.52	85.50	110.86
14	P	102	SPO	C3-C1-C4	-13.75	89.74	110.86
7	O	101	BCL	C2B-C1B-NB	10.76	117.45	110.23
7	L	301	BCL	C2B-C1B-NB	10.58	117.33	110.23
7	F	101	BCL	C2B-C1B-NB	10.49	117.27	110.23
7	I	102	BCL	C2B-C1B-NB	10.41	117.21	110.23
7	K	102	BCL	C2B-C1B-NB	10.37	117.19	110.23
7	D	101	BCL	C2B-C1B-NB	10.33	117.16	110.23
7	Q	104	BCL	C2B-C1B-NB	10.14	117.03	110.23
7	V	101	BCL	C2B-C1B-NB	10.12	117.01	110.23
7	M	402	BCL	C2B-C1B-NB	10.01	116.94	110.23
7	T	101	BCL	C2B-C1B-NB	10.01	116.94	110.23
7	G	101	BCL	C2B-C1B-NB	9.94	116.90	110.23
7	B	103	BCL	C2B-C1B-NB	9.90	116.87	110.23
7	J	101	BCL	C2B-C1B-NB	9.89	116.86	110.23
7	S	101	BCL	C2B-C1B-NB	9.86	116.84	110.23
7	N	101	BCL	C2B-C1B-NB	9.80	116.80	110.23
7	E	101	BCL	C2B-C1B-NB	9.74	116.76	110.23
7	Q	106	BCL	C2B-C1B-NB	9.72	116.75	110.23
7	M	401	BCL	C2B-C1B-NB	9.68	116.72	110.23
7	P	101	BCL	C2B-C1B-NB	9.61	116.67	110.23
7	L	309	BCL	C2B-C1B-NB	9.28	116.45	110.23
7	A	103	BCL	C2B-C1B-NB	9.23	116.42	110.23
7	Y	103	BCL	C2B-C1B-NB	9.10	116.33	110.23
7	1	101	BCL	C2B-C1B-NB	8.72	116.08	110.23
7	Z	102	BCL	CHD-C1D-ND	-8.71	116.45	124.45
7	Y	103	BCL	CHD-C1D-ND	-8.68	116.48	124.45
7	1	101	BCL	CHD-C1D-ND	-8.52	116.62	124.45
7	V	101	BCL	CHD-C1D-ND	-8.52	116.63	124.45
7	M	402	BCL	CHD-C1D-ND	-8.43	116.71	124.45
7	L	301	BCL	CHD-C1D-ND	-8.39	116.75	124.45
7	S	101	BCL	CHD-C1D-ND	-8.37	116.76	124.45
7	O	101	BCL	CHD-C1D-ND	-8.36	116.78	124.45
7	A	103	BCL	CHD-C1D-ND	-8.30	116.82	124.45
7	W	101	BCL	C2B-C1B-NB	8.28	115.78	110.23
7	1	101	BCL	CMD-C2D-C1D	8.22	139.21	124.71
7	L	309	BCL	CHD-C1D-ND	-8.20	116.92	124.45
7	M	402	BCL	CMD-C2D-C1D	8.19	139.15	124.71
7	Y	103	BCL	CMD-C2D-C1D	8.19	139.15	124.71
7	L	301	BCL	CMD-C2D-C1D	8.18	139.13	124.71
7	B	103	BCL	CHD-C1D-ND	-8.15	116.96	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	102	BCL	CHD-C1D-ND	-8.14	116.98	124.45
7	Q	104	BCL	CHD-C1D-ND	-8.13	116.98	124.45
7	M	401	BCL	CHD-C1D-ND	-8.13	116.98	124.45
7	W	101	BCL	CHD-C1D-ND	-8.12	116.99	124.45
7	A	103	BCL	CMD-C2D-C1D	8.07	138.93	124.71
7	D	101	BCL	CHD-C1D-ND	-8.07	117.04	124.45
7	V	101	BCL	CMD-C2D-C1D	8.04	138.88	124.71
7	I	102	BCL	CHD-C1D-ND	-8.03	117.07	124.45
7	F	101	BCL	CHD-C1D-ND	-8.03	117.08	124.45
7	Z	102	BCL	C2B-C1B-NB	8.01	115.61	110.23
7	P	101	BCL	CHD-C1D-ND	-7.97	117.13	124.45
7	Q	106	BCL	CHD-C1D-ND	-7.96	117.14	124.45
7	T	101	BCL	CHD-C1D-ND	-7.95	117.15	124.45
7	S	101	BCL	CMD-C2D-C1D	7.94	138.71	124.71
7	O	101	BCL	CMD-C2D-C1D	7.92	138.67	124.71
7	Z	102	BCL	CMD-C2D-C1D	7.84	138.52	124.71
7	G	101	BCL	CHD-C1D-ND	-7.82	117.27	124.45
7	D	101	BCL	CMD-C2D-C1D	7.80	138.46	124.71
7	Q	104	BCL	CMD-C2D-C1D	7.77	138.41	124.71
7	N	101	BCL	CHD-C1D-ND	-7.76	117.33	124.45
7	I	102	BCL	CMD-C2D-C1D	7.67	138.22	124.71
7	E	101	BCL	CHD-C1D-ND	-7.66	117.41	124.45
7	F	101	BCL	CMD-C2D-C1D	7.65	138.19	124.71
7	J	101	BCL	CHD-C1D-ND	-7.54	117.53	124.45
7	M	401	BCL	CMD-C2D-C1D	7.50	137.93	124.71
7	K	102	BCL	CMD-C2D-C1D	7.49	137.92	124.71
7	L	309	BCL	CMD-C2D-C1D	7.43	137.80	124.71
7	Q	106	BCL	CMD-C2D-C1D	7.40	137.75	124.71
7	B	103	BCL	CMD-C2D-C1D	7.39	137.75	124.71
7	P	101	BCL	CMD-C2D-C1D	7.31	137.60	124.71
7	W	101	BCL	CMD-C2D-C1D	7.29	137.57	124.71
7	T	101	BCL	CMD-C2D-C1D	7.29	137.56	124.71
7	N	101	BCL	CMD-C2D-C1D	7.19	137.38	124.71
7	E	101	BCL	CMD-C2D-C1D	7.11	137.24	124.71
7	G	101	BCL	CMD-C2D-C1D	7.09	137.22	124.71
7	J	101	BCL	CMD-C2D-C1D	6.81	136.71	124.71
7	Z	102	BCL	CHB-C1B-NB	-6.19	117.70	124.26
7	Z	102	BCL	CHC-C4B-NB	-5.72	118.20	124.26
7	M	401	BCL	O2D-CGD-CBD	5.71	121.42	111.27
14	V	102	SPO	C21-C22-C23	-5.50	119.46	127.31
7	S	101	BCL	C2D-C1D-ND	5.37	114.06	110.10
7	I	102	BCL	C2D-C1D-ND	5.33	114.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	101	BCL	C2D-C1D-ND	5.32	114.03	110.10
7	K	102	BCL	C2D-C1D-ND	5.29	114.00	110.10
7	A	103	BCL	CHB-C1B-NB	-5.28	118.67	124.26
7	J	101	BCL	C2D-C1D-ND	5.22	113.95	110.10
7	G	101	BCL	C2D-C1D-ND	5.19	113.93	110.10
7	W	101	BCL	CHB-C1B-NB	-5.15	118.81	124.26
7	M	402	BCL	C2D-C1D-ND	5.13	113.89	110.10
7	D	101	BCL	C2D-C1D-ND	5.12	113.88	110.10
7	M	402	BCL	C3D-C2D-C1D	-5.12	98.84	105.83
7	L	309	BCL	CHC-C4B-NB	-5.11	118.84	124.26
7	I	101	BCL	O2D-CGD-CBD	5.10	120.33	111.27
7	Y	103	BCL	O2D-CGD-CBD	5.09	120.32	111.27
14	B	104	SPO	C5-C6-C7	-5.08	118.22	125.89
7	L	301	BCL	C2D-C1D-ND	5.07	113.84	110.10
7	T	101	BCL	C2D-C1D-ND	5.05	113.83	110.10
14	B	104	SPO	C10-C9-C7	-5.04	120.12	127.31
7	L	301	BCL	C3D-C2D-C1D	-5.03	98.96	105.83
7	O	101	BCL	C2D-C1D-ND	5.03	113.81	110.10
7	S	101	BCL	C3D-C2D-C1D	-5.02	98.98	105.83
7	E	101	BCL	C2D-C1D-ND	5.01	113.80	110.10
7	Q	104	BCL	C2D-C1D-ND	5.00	113.79	110.10
7	F	101	BCL	C3D-C2D-C1D	-5.00	99.01	105.83
7	V	101	BCL	O2D-CGD-CBD	4.99	120.13	111.27
7	K	102	BCL	C3D-C2D-C1D	-4.97	99.05	105.83
7	I	102	BCL	C3D-C2D-C1D	-4.97	99.05	105.83
14	Q	105	SPO	C21-C22-C23	-4.97	120.22	127.31
7	V	101	BCL	C2D-C1D-ND	4.96	113.76	110.10
14	B	104	SPO	C15-C14-C12	-4.96	120.23	127.31
14	P	102	SPO	C3-C1-C2	4.95	119.69	110.37
7	V	101	BCL	C3D-C2D-C1D	-4.95	99.08	105.83
7	O	101	BCL	C3D-C2D-C1D	-4.93	99.10	105.83
7	D	101	BCL	C3D-C2D-C1D	-4.92	99.11	105.83
14	B	101	SPO	C21-C22-C23	-4.90	120.32	127.31
7	Q	106	BCL	O2D-CGD-CBD	4.88	119.94	111.27
7	N	101	BCL	C2D-C1D-ND	4.87	113.69	110.10
7	Q	104	BCL	C3D-C2D-C1D	-4.87	99.18	105.83
14	F	105	SPO	C10-C9-C7	-4.86	120.38	127.31
7	B	103	BCL	C2D-C1D-ND	4.85	113.68	110.10
7	A	103	BCL	C3D-C2D-C1D	-4.83	99.24	105.83
7	G	101	BCL	C3D-C2D-C1D	-4.81	99.26	105.83
14	S	102	SPO	C21-C22-C23	-4.81	120.45	127.31
7	P	101	BCL	C2D-C1D-ND	4.80	113.64	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	401	BCL	C2D-C1D-ND	4.78	113.63	110.10
7	B	103	BCL	C3D-C2D-C1D	-4.75	99.35	105.83
7	P	101	BCL	C3D-C2D-C1D	-4.73	99.37	105.83
7	M	401	BCL	C3D-C2D-C1D	-4.73	99.38	105.83
7	E	101	BCL	C3D-C2D-C1D	-4.73	99.38	105.83
7	T	101	BCL	C3D-C2D-C1D	-4.72	99.39	105.83
7	W	101	BCL	CHC-C4B-NB	-4.72	119.26	124.26
7	O	101	BCL	O2D-CGD-CBD	4.72	119.65	111.27
7	J	101	BCL	C3D-C2D-C1D	-4.71	99.40	105.83
7	D	101	BCL	O2D-CGD-CBD	4.71	119.63	111.27
7	Q	106	BCL	C3D-C2D-C1D	-4.69	99.43	105.83
7	N	101	BCL	C3D-C2D-C1D	-4.68	99.44	105.83
7	F	101	BCL	O2D-CGD-CBD	4.68	119.59	111.27
7	Q	106	BCL	C2D-C1D-ND	4.67	113.55	110.10
7	M	402	BCL	CHD-C4C-NC	4.67	130.26	125.08
7	I	102	BCL	O2D-CGD-CBD	4.65	119.54	111.27
7	A	103	BCL	CHC-C4B-NB	-4.65	119.33	124.26
7	L	309	BCL	C3D-C2D-C1D	-4.64	99.49	105.83
7	Y	103	BCL	C3D-C2D-C1D	-4.63	99.51	105.83
7	G	101	BCL	CHD-C4C-NC	4.62	130.21	125.08
14	F	105	SPO	C5-C6-C7	-4.61	118.92	125.89
7	L	309	BCL	O2D-CGD-CBD	4.60	119.45	111.27
7	T	101	BCL	CHD-C4C-NC	4.59	130.17	125.08
7	S	101	BCL	CHD-C4C-NC	4.58	130.16	125.08
7	K	102	BCL	CHD-C4C-NC	4.57	130.15	125.08
7	D	101	BCL	CHD-C4C-NC	4.54	130.12	125.08
14	V	103	SPO	C21-C22-C23	-4.53	120.84	127.31
7	J	101	BCL	CHD-C4C-NC	4.53	130.11	125.08
7	F	101	BCL	CHD-C4C-NC	4.53	130.11	125.08
7	1	101	BCL	C3D-C2D-C1D	-4.53	99.65	105.83
14	P	102	SPO	C21-C22-C23	-4.53	120.85	127.31
7	N	101	BCL	CHD-C4C-NC	4.52	130.10	125.08
7	Q	104	BCL	O2D-CGD-CBD	4.51	119.29	111.27
7	K	102	BCL	C3C-C4C-CHD	-4.51	113.75	123.39
7	W	101	BCL	C3D-C2D-C1D	-4.49	99.70	105.83
7	S	101	BCL	O2D-CGD-CBD	4.47	119.21	111.27
7	K	102	BCL	O2D-CGD-CBD	4.47	119.21	111.27
7	P	101	BCL	O2D-CGD-CBD	4.47	119.21	111.27
7	I	102	BCL	CHD-C4C-NC	4.46	130.03	125.08
7	V	101	BCL	CHD-C4C-NC	4.45	130.02	125.08
7	F	101	BCL	C3C-C4C-CHD	-4.45	113.88	123.39
14	S	103	SPO	C5-C6-C7	-4.45	119.17	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	101	BCL	CHD-C4C-NC	4.44	130.01	125.08
10	F	102	PGV	O01-C1-C2	4.44	121.06	111.50
7	L	301	BCL	CHD-C4C-NC	4.42	129.99	125.08
7	G	101	BCL	C3C-C4C-CHD	-4.42	113.94	123.39
7	A	103	BCL	O2D-CGD-CBD	4.42	119.12	111.27
7	M	401	BCL	CHD-C4C-NC	4.40	129.96	125.08
7	T	101	BCL	O2D-CGD-CBD	4.40	119.08	111.27
15	M	408	CDL	OB6-CB5-C51	4.39	120.97	111.50
7	S	101	BCL	C3C-C4C-CHD	-4.39	114.01	123.39
7	D	101	BCL	C3C-C4C-CHD	-4.39	114.02	123.39
7	J	101	BCL	C3C-C4C-CHD	-4.38	114.03	123.39
7	Q	106	BCL	CHD-C4C-NC	4.37	129.93	125.08
7	I	102	BCL	C3C-C4C-CHD	-4.37	114.06	123.39
7	Z	102	BCL	C3D-C2D-C1D	-4.35	99.89	105.83
14	K	103	SPO	C21-C22-C23	-4.35	121.10	127.31
8	L	302	BPH	C4D-CHA-CBD	-4.35	106.55	108.52
14	J	102	SPO	C10-C9-C7	-4.35	121.10	127.31
14	J	102	SPO	C5-C6-C7	-4.35	119.32	125.89
7	T	101	BCL	C3C-C4C-CHD	-4.34	114.11	123.39
7	O	101	BCL	CHD-C4C-NC	4.34	129.89	125.08
7	Z	102	BCL	O2D-CGD-CBD	4.33	118.97	111.27
14	D	104	SPO	C21-C22-C23	-4.33	121.13	127.31
7	E	101	BCL	O2D-CGD-CBD	4.32	118.94	111.27
7	Q	104	BCL	CHD-C4C-NC	4.32	129.87	125.08
7	B	103	BCL	O2D-CGD-CBD	4.29	118.88	111.27
7	W	101	BCL	O2D-CGD-CBD	4.28	118.87	111.27
7	L	301	BCL	C3C-C4C-CHD	-4.28	114.26	123.39
7	B	103	BCL	CHB-C1B-NB	-4.27	119.74	124.26
7	E	101	BCL	C3C-C4C-CHD	-4.26	114.28	123.39
7	N	101	BCL	C3C-C4C-CHD	-4.26	114.30	123.39
7	B	103	BCL	CHD-C4C-NC	4.23	129.77	125.08
14	D	102	SPO	C21-C22-C23	-4.22	121.29	127.31
7	L	309	BCL	C2D-C1D-ND	4.22	113.21	110.10
10	F	103	PGV	O01-C1-C2	4.21	120.58	111.50
7	P	101	BCL	CHD-C4C-NC	4.21	129.75	125.08
7	V	101	BCL	C3C-C4C-CHD	-4.19	114.43	123.39
7	M	402	BCL	C3C-C4C-CHD	-4.19	114.44	123.39
7	T	101	BCL	C1D-ND-C4D	-4.16	103.38	106.33
7	Q	104	BCL	C3C-C4C-CHD	-4.15	114.53	123.39
7	Q	106	BCL	C3C-C4C-CHD	-4.15	114.53	123.39
7	P	101	BCL	CHC-C4B-NB	-4.15	119.87	124.26
14	B	104	SPO	C20-C19-C17	-4.14	121.39	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	101	BCL	O2D-CGD-CBD	4.14	118.63	111.27
7	P	101	BCL	CHB-C1B-NB	-4.13	119.88	124.26
14	G	102	SPO	C21-C22-C23	-4.12	121.43	127.31
7	J	101	BCL	C1D-ND-C4D	-4.12	103.41	106.33
7	V	101	BCL	CHC-C4B-NB	-4.11	119.90	124.26
15	M	408	CDL	OA6-CA5-C11	4.11	120.36	111.50
7	M	402	BCL	C1D-ND-C4D	-4.11	103.42	106.33
7	S	101	BCL	C1D-ND-C4D	-4.10	103.42	106.33
7	I	102	BCL	C1D-ND-C4D	-4.10	103.42	106.33
14	K	105	SPO	C21-C22-C23	-4.09	121.47	127.31
7	N	101	BCL	O2D-CGD-CBD	4.09	118.54	111.27
7	G	101	BCL	O2D-CGD-CBD	4.09	118.53	111.27
7	A	103	BCL	C2D-C1D-ND	4.08	113.11	110.10
14	M	405	SPO	C21-C22-C23	-4.08	121.49	127.31
7	O	101	BCL	CHC-C4B-NB	-4.08	119.94	124.26
7	O	101	BCL	C3C-C4C-CHD	-4.07	114.69	123.39
10	M	409	PGV	O01-C1-C2	4.07	120.28	111.50
7	B	103	BCL	CHC-C4B-NB	-4.06	119.96	124.26
7	I	101	BCL	CHC-C4B-NB	-4.05	119.97	124.26
7	P	101	BCL	C3C-C4C-CHD	-4.03	114.79	123.39
7	G	101	BCL	C1D-ND-C4D	-4.02	103.48	106.33
7	F	101	BCL	C1D-ND-C4D	-4.01	103.48	106.33
14	G	102	SPO	C20-C19-C17	-4.01	121.59	127.31
7	L	301	BCL	C1D-ND-C4D	-4.00	103.49	106.33
7	K	102	BCL	C1D-ND-C4D	-4.00	103.49	106.33
7	F	101	BCL	CHC-C4B-NB	-4.00	120.03	124.26
14	J	102	SPO	C20-C19-C17	-3.99	121.61	127.31
7	M	401	BCL	C3C-C4C-CHD	-3.98	114.89	123.39
7	M	401	BCL	C1D-ND-C4D	-3.98	103.51	106.33
14	B	101	SPO	C29-C28-C30	3.97	121.94	115.27
14	B	101	SPO	C20-C19-C17	-3.96	121.66	127.31
10	L	305	PGV	O01-C1-C2	3.94	119.99	111.50
7	B	103	BCL	C3C-C4C-CHD	-3.93	114.99	123.39
10	H	301	PGV	O01-C1-C2	3.93	119.98	111.50
7	W	101	BCL	C2D-C1D-ND	3.93	113.00	110.10
7	Q	104	BCL	C1D-ND-C4D	-3.93	103.54	106.33
7	N	101	BCL	C1D-ND-C4D	-3.93	103.55	106.33
7	D	101	BCL	C1-C2-C3	-3.92	119.26	126.04
10	Y	104	PGV	O01-C1-C2	3.92	119.96	111.50
7	Q	106	BCL	CHB-C1B-NB	-3.92	120.11	124.26
10	Q	103	PGV	O01-C1-C2	3.92	119.94	111.50
7	W	101	BCL	CHD-C4C-NC	3.92	129.43	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	101	BCL	C1D-ND-C4D	-3.91	103.56	106.33
14	K	103	SPO	C20-C19-C17	-3.90	121.75	127.31
7	O	101	BCL	C1D-ND-C4D	-3.89	103.57	106.33
7	Q	106	BCL	CHC-C4B-NB	-3.88	120.15	124.26
8	M	403	BPH	C4D-CHA-CBD	-3.87	106.77	108.52
14	G	103	SPO	C5-C6-C7	-3.85	120.07	125.89
7	E	101	BCL	C1D-ND-C4D	-3.85	103.60	106.33
7	Y	103	BCL	C2D-C1D-ND	3.84	112.94	110.10
14	M	405	SPO	C20-C19-C17	-3.83	121.84	127.31
7	V	101	BCL	C1D-ND-C4D	-3.82	103.62	106.33
7	M	402	BCL	CHC-C4B-NB	-3.81	120.22	124.26
7	M	402	BCL	O2D-CGD-CBD	3.81	118.04	111.27
7	I	102	BCL	CHC-C4B-NB	-3.80	120.24	124.26
10	K	104	PGV	O01-C1-C2	3.80	119.68	111.50
7	P	101	BCL	C1D-ND-C4D	-3.80	103.64	106.33
7	L	309	BCL	CHB-C1B-NB	-3.79	120.25	124.26
14	S	103	SPO	C20-C19-C17	-3.78	121.92	127.31
7	L	301	BCL	CHC-C4B-NB	-3.77	120.26	124.26
14	Z	101	SPO	C20-C19-C17	-3.76	121.94	127.31
14	D	102	SPO	C20-C19-C17	-3.76	121.94	127.31
14	K	105	SPO	C20-C19-C17	-3.76	121.94	127.31
7	D	101	BCL	CHC-C4B-NB	-3.75	120.28	124.26
7	B	103	BCL	C1D-ND-C4D	-3.75	103.67	106.33
14	O	102	SPO	C20-C19-C17	-3.72	122.00	127.31
7	G	101	BCL	CHC-C4B-NB	-3.71	120.33	124.26
15	H	307	CDL	OB6-CB5-C51	3.71	119.49	111.50
7	Q	106	BCL	C1D-ND-C4D	-3.70	103.71	106.33
14	V	103	SPO	C5-C6-C7	-3.68	120.33	125.89
14	B	104	SPO	C21-C22-C23	-3.67	122.08	127.31
14	G	103	SPO	C10-C9-C7	-3.66	122.08	127.31
15	H	307	CDL	OA6-CA5-C11	3.66	119.39	111.50
14	V	103	SPO	C10-C9-C7	-3.63	122.13	127.31
7	G	101	BCL	CHB-C1B-NB	-3.60	120.44	124.26
7	N	101	BCL	CHB-C1B-NB	-3.60	120.44	124.26
7	K	102	BCL	CHC-C4B-NB	-3.60	120.45	124.26
14	G	103	SPO	C20-C19-C17	-3.59	122.18	127.31
7	Z	102	BCL	CHD-C4C-NC	3.59	129.07	125.08
7	L	309	BCL	C1-C2-C3	-3.57	119.87	126.04
7	I	101	BCL	CHB-C1B-NB	-3.55	120.50	124.26
14	V	102	SPO	C20-C19-C17	-3.55	122.24	127.31
7	E	101	BCL	CHB-C1B-NB	-3.54	120.51	124.26
14	Z	101	SPO	C10-C9-C7	-3.53	122.27	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	101	BCL	CHC-C4B-NB	-3.53	120.53	124.26
7	L	301	BCL	O2D-CGD-CBD	3.52	117.53	111.27
12	L	307	LMT	O5B-C5B-C4B	3.52	116.08	109.69
14	S	103	SPO	C31-C32-C33	-3.51	119.20	127.66
7	L	309	BCL	CHD-C4C-NC	3.51	128.97	125.08
7	N	101	BCL	CHC-C4B-NB	-3.49	120.56	124.26
14	J	102	SPO	C15-C14-C12	-3.49	122.33	127.31
7	M	401	BCL	C3D-C4D-ND	3.47	115.86	110.24
7	M	401	BCL	C1-C2-C3	-3.46	120.06	126.04
7	S	101	BCL	CHC-C4B-NB	-3.46	120.60	124.26
14	G	103	SPO	C21-C22-C23	-3.46	122.38	127.31
14	D	104	SPO	C20-C19-C17	-3.45	122.39	127.31
14	F	105	SPO	C21-C22-C23	-3.44	122.40	127.31
7	F	101	BCL	C1-C2-C3	-3.43	120.11	126.04
7	Y	103	BCL	CHC-C4B-NB	-3.43	120.63	124.26
14	B	104	SPO	C29-C28-C30	3.43	121.04	115.27
7	T	101	BCL	CHC-C4B-NB	-3.43	120.63	124.26
7	Q	104	BCL	CHC-C4B-NB	-3.42	120.64	124.26
14	P	102	SPO	C20-C19-C17	-3.42	122.43	127.31
14	O	102	SPO	C5-C6-C7	-3.40	120.75	125.89
7	M	401	BCL	CHC-C4B-NB	-3.39	120.67	124.26
7	T	101	BCL	C3D-C4D-ND	3.39	115.72	110.24
10	F	102	PGV	C02-O01-C1	-3.38	109.46	117.79
7	J	101	BCL	C3D-C4D-ND	3.36	115.68	110.24
7	O	101	BCL	C4-C3-C5	3.36	120.92	115.27
14	F	105	SPO	C20-C19-C17	-3.36	122.52	127.31
14	G	103	SPO	C15-C14-C12	-3.36	122.52	127.31
14	G	103	SPO	C29-C28-C30	3.36	120.92	115.27
7	N	101	BCL	C3D-C4D-ND	3.36	115.67	110.24
14	S	102	SPO	C20-C19-C17	-3.35	122.53	127.31
7	W	101	BCL	C3C-C4C-CHD	-3.34	116.26	123.39
14	Z	101	SPO	C29-C28-C30	3.34	120.88	115.27
14	F	105	SPO	C29-C28-C30	3.33	120.87	115.27
7	M	402	BCL	C3D-C4D-ND	3.32	115.61	110.24
7	J	101	BCL	CHC-C4B-NB	-3.32	120.74	124.26
7	L	309	BCL	C3D-C4D-ND	3.31	115.60	110.24
14	O	102	SPO	C29-C28-C30	3.31	120.85	115.27
7	M	402	BCL	CHB-C1B-NB	-3.31	120.75	124.26
14	Z	101	SPO	C21-C22-C23	-3.31	122.58	127.31
7	P	101	BCL	C3D-C4D-ND	3.30	115.58	110.24
14	O	102	SPO	C10-C9-C7	-3.30	122.61	127.31
7	V	101	BCL	C4A-NA-C1A	3.29	108.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	103	BCL	C3D-C4D-ND	3.28	115.55	110.24
7	B	103	BCL	C3D-C4D-ND	3.28	115.54	110.24
14	P	102	SPO	C34-C33-C35	3.28	120.78	115.27
14	Q	105	SPO	C20-C19-C17	-3.28	122.63	127.31
7	G	101	BCL	C3D-C4D-ND	3.27	115.53	110.24
14	S	103	SPO	C21-C22-C23	-3.27	122.64	127.31
7	Q	106	BCL	C3D-C4D-ND	3.26	115.51	110.24
7	L	301	BCL	O2A-CGA-CBA	3.26	122.13	111.91
14	G	102	SPO	C31-C32-C33	-3.25	119.83	127.66
14	V	103	SPO	C29-C28-C30	3.25	120.74	115.27
7	L	301	BCL	C3D-C4D-ND	3.25	115.49	110.24
14	D	104	SPO	C34-C33-C35	3.24	120.72	115.27
7	J	101	BCL	C4-C3-C5	3.24	120.72	115.27
7	Q	104	BCL	C3D-C4D-ND	3.23	115.47	110.24
12	A	102	LMT	C1B-O1B-C4'	-3.23	109.96	117.96
12	L	307	LMT	C3B-C4B-C5B	3.23	116.01	110.24
7	Z	102	BCL	C2D-C1D-ND	3.23	112.49	110.10
7	Z	102	BCL	C4A-NA-C1A	3.23	108.16	106.71
7	L	309	BCL	C1D-ND-C4D	-3.22	104.04	106.33
7	1	101	BCL	C2D-C1D-ND	3.22	112.47	110.10
7	E	101	BCL	C3D-C4D-ND	3.21	115.43	110.24
7	A	103	BCL	CHD-C4C-NC	3.21	128.64	125.08
7	I	102	BCL	C3D-C4D-ND	3.20	115.42	110.24
7	A	103	BCL	C1-C2-C3	-3.20	120.51	126.04
7	A	103	BCL	C4A-NA-C1A	3.19	108.14	106.71
7	S	101	BCL	C4-C3-C5	3.19	120.64	115.27
7	Y	103	BCL	C1D-ND-C4D	-3.19	104.07	106.33
7	P	101	BCL	O2A-CGA-CBA	3.19	121.91	111.91
7	K	102	BCL	C3D-C4D-ND	3.19	115.39	110.24
7	Z	102	BCL	C1C-NC-C4C	3.19	108.14	106.71
14	G	102	SPO	C34-C33-C35	3.18	120.63	115.27
14	J	102	SPO	C21-C22-C23	-3.18	122.77	127.31
7	W	101	BCL	C3D-C4D-ND	3.18	115.38	110.24
7	E	101	BCL	O2A-CGA-CBA	3.17	121.87	111.91
7	T	101	BCL	C1-C2-C3	-3.17	120.56	126.04
14	O	102	SPO	C21-C22-C23	-3.17	122.79	127.31
7	F	101	BCL	C3D-C4D-ND	3.16	115.34	110.24
8	M	403	BPH	C2B-C1B-NB	-3.15	107.35	109.53
14	J	102	SPO	C29-C28-C30	3.15	120.57	115.27
7	J	101	BCL	CHB-C1B-NB	-3.15	120.92	124.26
7	O	101	BCL	C3D-C4D-ND	3.15	115.33	110.24
7	S	101	BCL	C3D-C4D-ND	3.14	115.32	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	102	SPO	C34-C33-C35	3.14	120.55	115.27
7	Y	103	BCL	CHB-C1B-NB	-3.13	120.94	124.26
7	D	101	BCL	C3D-C4D-ND	3.13	115.30	110.24
7	E	101	BCL	C4-C3-C5	3.12	120.53	115.27
7	G	101	BCL	C4-C3-C5	3.11	120.51	115.27
14	G	103	SPO	C34-C33-C35	3.11	120.51	115.27
7	T	101	BCL	CHB-C1B-NB	-3.11	120.97	124.26
7	Z	102	BCL	C3D-C4D-ND	3.11	115.27	110.24
14	F	105	SPO	C34-C33-C35	3.11	120.50	115.27
8	L	302	BPH	C2B-C1B-NB	-3.10	107.38	109.53
7	F	101	BCL	O2A-CGA-CBA	3.10	121.63	111.91
7	V	101	BCL	C3D-C4D-ND	3.10	115.25	110.24
14	V	102	SPO	C31-C32-C33	-3.10	120.20	127.66
7	W	101	BCL	C1-C2-C3	-3.09	120.69	126.04
7	I	102	BCL	C1-C2-C3	-3.09	120.69	126.04
7	A	103	BCL	C3D-C4D-ND	3.09	115.24	110.24
14	M	405	SPO	C31-C32-C33	-3.09	120.23	127.66
7	1	101	BCL	C4A-NA-C1A	3.07	108.09	106.71
7	F	101	BCL	CHB-C1B-NB	-3.07	121.01	124.26
7	G	101	BCL	O2A-CGA-CBA	3.06	121.52	111.91
7	J	101	BCL	O2A-CGA-CBA	3.06	121.51	111.91
7	Q	104	BCL	O2A-CGA-CBA	3.06	121.51	111.91
7	Q	104	BCL	CHB-C1B-NB	-3.06	121.02	124.26
7	K	102	BCL	C1-C2-C3	-3.05	120.76	126.04
14	K	103	SPO	C31-C32-C33	-3.05	120.31	127.66
7	L	309	BCL	C3C-C4C-CHD	-3.05	116.87	123.39
7	A	103	BCL	C4-C3-C5	3.05	120.40	115.27
14	D	102	SPO	C34-C33-C35	3.05	120.39	115.27
14	Q	105	SPO	C31-C32-C33	-3.04	120.34	127.66
7	I	102	BCL	CHB-C1B-NB	-3.04	121.04	124.26
7	N	101	BCL	C4-C3-C5	3.04	120.38	115.27
14	S	103	SPO	C10-C9-C7	-3.03	122.98	127.31
7	1	101	BCL	C3D-C4D-ND	3.03	115.14	110.24
14	O	102	SPO	C34-C33-C35	3.03	120.37	115.27
7	O	101	BCL	O2A-CGA-CBA	3.03	121.42	111.91
7	D	101	BCL	C4B-C3B-C2B	-3.02	103.50	108.36
7	V	101	BCL	C1C-NC-C4C	-3.02	105.35	106.71
7	F	101	BCL	C4B-C3B-C2B	-3.01	103.51	108.36
7	K	102	BCL	CHC-C1C-NC	3.01	128.68	124.51
7	L	301	BCL	CHB-C1B-NB	-3.01	121.07	124.26
7	Z	102	BCL	O2A-CGA-CBA	3.00	121.34	111.91
14	K	105	SPO	C34-C33-C35	3.00	120.32	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	V	103	SPO	C21-C20-C19	-2.99	117.34	123.47
14	B	104	SPO	C34-C33-C35	2.99	120.31	115.27
7	S	101	BCL	CHB-C1B-NB	-2.99	121.09	124.26
7	I	102	BCL	O2A-CGA-CBA	2.99	121.29	111.91
7	I	102	BCL	C4B-C3B-C2B	-2.97	103.58	108.36
14	D	104	SPO	C31-C32-C33	-2.97	120.51	127.66
14	S	103	SPO	C29-C28-C30	2.97	120.27	115.27
14	K	103	SPO	C29-C28-C30	2.97	120.26	115.27
7	I	101	BCL	C1D-CHD-C4C	-2.96	119.47	126.62
14	K	105	SPO	C29-C28-C30	2.96	120.26	115.27
14	P	102	SPO	C15-C14-C12	-2.96	123.08	127.31
14	K	103	SPO	C9-C10-C11	-2.96	113.99	123.22
7	Q	106	BCL	O2A-CGA-CBA	2.95	121.16	111.91
7	M	402	BCL	C1-C2-C3	-2.94	120.95	126.04
14	D	102	SPO	C29-C28-C30	2.94	120.22	115.27
7	A	103	BCL	C1D-ND-C4D	-2.94	104.25	106.33
7	V	101	BCL	C1-C2-C3	-2.94	120.96	126.04
7	V	101	BCL	CHB-C1B-NB	-2.94	121.15	124.26
7	K	102	BCL	C1C-NC-C4C	-2.94	105.39	106.71
12	H	304	LMT	O1B-C4'-C3'	2.93	115.08	107.28
14	V	102	SPO	C15-C14-C12	-2.93	123.13	127.31
14	V	103	SPO	C15-C14-C12	-2.93	123.13	127.31
14	B	104	SPO	C10-C11-C12	-2.93	118.19	126.42
7	Q	104	BCL	C4-C3-C5	2.92	120.19	115.27
7	F	101	BCL	CHC-C1C-NC	2.92	128.56	124.51
14	V	103	SPO	C34-C33-C35	2.92	120.19	115.27
7	M	402	BCL	C4B-C3B-C2B	-2.92	103.66	108.36
7	T	101	BCL	O2A-CGA-CBA	2.92	121.06	111.91
7	N	101	BCL	C1-C2-C3	-2.91	121.00	126.04
14	D	104	SPO	C29-C28-C30	2.91	120.17	115.27
7	P	101	BCL	C4-C3-C5	2.90	120.15	115.27
7	L	301	BCL	C4B-C3B-C2B	-2.90	103.69	108.36
7	D	101	BCL	CHB-C1B-NB	-2.90	121.19	124.26
7	L	301	BCL	C1-C2-C3	-2.90	121.03	126.04
7	S	101	BCL	O2A-CGA-CBA	2.89	120.99	111.91
10	K	104	PGV	O03-C19-C20	2.89	120.98	111.91
14	D	102	SPO	C31-C32-C33	-2.89	120.70	127.66
7	I	101	BCL	C4-C3-C5	2.89	120.13	115.27
7	O	101	BCL	C4B-C3B-C2B	-2.89	103.72	108.36
10	F	102	PGV	O03-C19-C20	2.88	120.95	111.91
14	D	102	SPO	C9-C10-C11	-2.88	114.24	123.22
7	V	101	BCL	CHC-C1C-NC	2.88	128.49	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	103	BCL	C4-C3-C5	2.88	120.11	115.27
7	O	101	BCL	C1-C2-C3	-2.88	121.07	126.04
10	L	305	PGV	O03-C19-C20	2.88	120.93	111.91
7	W	101	BCL	C1D-ND-C4D	-2.87	104.29	106.33
14	Q	105	SPO	C29-C28-C30	2.87	120.10	115.27
7	S	101	BCL	CHC-C1C-NC	2.87	128.48	124.51
7	D	101	BCL	CHC-C1C-NC	2.86	128.47	124.51
14	V	102	SPO	C34-C33-C35	2.85	120.07	115.27
7	M	401	BCL	O2D-CGD-O1D	-2.84	118.28	123.84
7	W	101	BCL	O2A-CGA-CBA	2.84	120.83	111.91
14	Z	101	SPO	C31-C32-C33	-2.84	120.82	127.66
7	L	309	BCL	O2A-CGA-CBA	2.84	120.82	111.91
7	O	101	BCL	CMB-C2B-C3B	2.83	133.57	125.93
14	B	101	SPO	C9-C10-C11	-2.83	114.40	123.22
7	K	102	BCL	CHB-C1B-NB	-2.83	121.27	124.26
14	S	102	SPO	C29-C28-C30	2.82	120.02	115.27
7	L	301	BCL	C4-C3-C5	2.82	120.01	115.27
10	H	301	PGV	O03-C19-C20	2.81	120.74	111.91
7	I	101	BCL	CMD-C2D-C3D	-2.81	121.14	127.61
7	P	101	BCL	C4B-C3B-C2B	-2.80	103.85	108.36
7	K	102	BCL	C4-C3-C5	2.80	119.99	115.27
7	D	101	BCL	O2A-CGA-CBA	2.80	120.70	111.91
7	M	402	BCL	C4-C3-C5	2.80	119.98	115.27
14	S	103	SPO	C9-C10-C11	-2.80	114.48	123.22
7	B	103	BCL	C4-C3-C5	2.79	119.97	115.27
7	Z	102	BCL	C4-C3-C5	2.79	119.97	115.27
7	I	102	BCL	CHC-C1C-NC	2.79	128.37	124.51
7	O	101	BCL	CHB-C1B-NB	-2.79	121.31	124.26
7	L	309	BCL	C4A-NA-C1A	2.78	107.96	106.71
7	B	103	BCL	C1-C2-C3	-2.78	121.24	126.04
7	Z	102	BCL	C3C-C4C-CHD	-2.78	117.46	123.39
14	Q	105	SPO	C21-C20-C19	-2.77	117.79	123.47
7	L	309	BCL	CMB-C2B-C3B	2.77	133.42	125.93
7	Y	103	BCL	C1D-CHD-C4C	-2.77	119.95	126.62
7	Q	106	BCL	C4-C3-C5	2.76	119.91	115.27
7	O	101	BCL	CHB-C4A-NA	2.76	128.33	124.51
7	V	101	BCL	C4B-C3B-C2B	-2.75	103.94	108.36
7	S	101	BCL	C4B-C3B-C2B	-2.75	103.94	108.36
7	N	101	BCL	O2A-CGA-CBA	2.75	120.52	111.91
14	F	105	SPO	C15-C14-C12	-2.74	123.39	127.31
7	L	301	BCL	CHC-C1C-NC	2.74	128.31	124.51
7	O	101	BCL	CHC-C1C-NC	2.74	128.29	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	101	BCL	CHB-C4A-NA	2.74	128.29	124.51
7	I	101	BCL	C1-C2-C3	-2.74	121.31	126.04
7	J	101	BCL	CHB-C4A-NA	2.73	128.29	124.51
10	Q	103	PGV	O03-C19-C20	2.73	120.49	111.91
7	Y	103	BCL	CMD-C2D-C3D	-2.73	121.34	127.61
14	D	104	SPO	C9-C10-C11	-2.73	114.71	123.22
14	S	102	SPO	C9-C10-C11	-2.72	114.72	123.22
7	V	101	BCL	C4-C3-C5	2.72	119.85	115.27
10	M	409	PGV	O03-C19-C20	2.72	120.44	111.91
7	E	101	BCL	C4B-C3B-C2B	-2.72	103.99	108.36
12	I	101	LMT	O1B-C4'-C3'	2.72	114.51	107.28
10	F	103	PGV	C02-O01-C1	-2.72	111.10	117.79
7	M	401	BCL	C4-C3-C5	2.71	119.84	115.27
7	B	103	BCL	C4B-C3B-C2B	-2.71	104.00	108.36
14	G	102	SPO	C29-C28-C30	2.71	119.83	115.27
7	L	309	BCL	C4B-C3B-C2B	-2.71	104.00	108.36
7	Q	104	BCL	C4B-C3B-C2B	-2.71	104.00	108.36
7	Q	104	BCL	CHC-C1C-NC	2.71	128.25	124.51
14	D	102	SPO	C14-C15-C16	-2.71	114.77	123.22
7	W	101	BCL	C4-C3-C5	2.70	119.82	115.27
7	F	101	BCL	CHB-C4A-NA	2.70	128.25	124.51
7	A	103	BCL	C3C-C4C-CHD	-2.70	117.63	123.39
7	Q	106	BCL	C4B-C3B-C2B	-2.70	104.02	108.36
7	K	102	BCL	CHB-C4A-NA	2.69	128.24	124.51
7	M	402	BCL	CED-O2D-CGD	2.69	122.03	115.94
14	P	102	SPO	C21-C20-C19	-2.69	117.96	123.47
7	F	101	BCL	CMB-C2B-C3B	2.69	133.19	125.93
14	V	102	SPO	C21-C20-C19	-2.69	117.97	123.47
7	M	401	BCL	C4B-C3B-C2B	-2.69	104.04	108.36
7	T	101	BCL	C4-C3-C5	2.68	119.78	115.27
7	I	101	BCL	C4B-C3B-C2B	-2.68	104.05	108.36
14	B	101	SPO	C14-C15-C16	-2.68	114.86	123.22
14	O	102	SPO	C15-C14-C12	-2.68	123.49	127.31
16	F	104	PTY	O7-C8-C11	2.67	117.27	111.50
7	J	101	BCL	C4B-C3B-C2B	-2.67	104.06	108.36
15	H	307	CDL	OB8-CB7-C71	2.67	120.28	111.91
7	W	101	BCL	C4B-C3B-C2B	-2.66	104.08	108.36
7	M	402	BCL	CMB-C2B-C3B	2.66	133.11	125.93
7	Z	102	BCL	CHD-C1D-C2D	2.66	131.05	125.48
14	P	102	SPO	C5-C6-C7	-2.66	121.88	125.89
7	T	101	BCL	C4B-C3B-C2B	-2.65	104.09	108.36
7	L	301	BCL	CED-O2D-CGD	2.65	121.93	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	401	BCL	CHB-C1B-NB	-2.65	121.45	124.26
7	S	101	BCL	CHB-C4A-NA	2.64	128.17	124.51
14	S	103	SPO	C14-C15-C16	-2.64	114.97	123.22
7	Q	106	BCL	C1-C2-C3	-2.64	121.47	126.04
14	V	102	SPO	C29-C28-C30	2.64	119.72	115.27
7	Z	102	BCL	C4B-C3B-C2B	-2.64	104.11	108.36
7	Q	106	BCL	O2D-CGD-O1D	-2.64	118.68	123.84
7	Q	106	BCL	CHB-C4A-NA	2.63	128.16	124.51
7	I	102	BCL	CHB-C4A-NA	2.63	128.15	124.51
7	G	101	BCL	C4B-C3B-C2B	-2.63	104.14	108.36
7	Y	103	BCL	O2A-CGA-CBA	2.62	120.14	111.91
7	Z	102	BCL	CMD-C2D-C3D	-2.62	121.59	127.61
14	S	102	SPO	C15-C14-C12	-2.62	123.57	127.31
7	N	101	BCL	C4B-C3B-C2B	-2.61	104.15	108.36
12	H	303	LMT	C1-O1'-C1'	-2.61	109.51	113.84
14	K	105	SPO	C9-C10-C11	-2.61	115.08	123.22
14	G	102	SPO	C9-C10-C11	-2.61	115.09	123.22
7	K	102	BCL	O2A-CGA-CBA	2.61	120.08	111.91
12	H	305	LMT	O1B-C1B-C2B	2.60	114.85	108.10
7	M	401	BCL	CHC-C1C-NC	2.60	128.11	124.51
7	M	402	BCL	CAA-C2A-C3A	-2.60	105.65	112.78
7	V	101	BCL	CHB-C4A-NA	2.60	128.11	124.51
10	M	409	PGV	C02-O01-C1	-2.60	111.39	117.79
7	F	101	BCL	C4-C3-C5	2.60	119.64	115.27
14	V	103	SPO	C20-C19-C17	-2.60	123.60	127.31
7	D	101	BCL	CMB-C2B-C3B	2.59	132.94	125.93
14	K	103	SPO	C34-C33-C35	2.59	119.63	115.27
7	L	301	BCL	CMB-C2B-C3B	2.59	132.92	125.93
7	1	101	BCL	CHD-C1D-C2D	2.59	130.90	125.48
7	K	102	BCL	C4B-C3B-C2B	-2.58	104.20	108.36
7	A	103	BCL	O2A-CGA-CBA	2.58	120.01	111.91
7	1	101	BCL	O2A-CGA-CBA	2.58	120.00	111.91
7	N	101	BCL	CHB-C4A-NA	2.58	128.08	124.51
7	Y	103	BCL	O2D-CGD-O1D	-2.57	118.81	123.84
7	I	102	BCL	CMB-C2B-C3B	2.56	132.84	125.93
14	O	102	SPO	C27-C26-C25	-2.56	115.23	123.22
7	V	101	BCL	O2D-CGD-O1D	-2.56	118.84	123.84
10	Y	104	PGV	O03-C19-C20	2.56	119.94	111.91
7	S	101	BCL	C1C-NC-C4C	-2.56	105.56	106.71
7	D	101	BCL	CHB-C4A-NA	2.56	128.05	124.51
7	Y	103	BCL	C1-C2-C3	-2.56	121.62	126.04
14	Z	101	SPO	C5-C6-C7	-2.55	122.03	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	S	103	SPO	C34-C33-C35	2.55	119.56	115.27
7	F	101	BCL	O2D-CGD-O1D	-2.55	118.86	123.84
14	Q	105	SPO	C9-C10-C11	-2.55	115.27	123.22
12	D	103	LMT	C1B-O1B-C4'	-2.55	111.67	117.96
7	K	102	BCL	C4A-NA-C1A	2.54	107.85	106.71
14	S	103	SPO	C13-C12-C11	2.54	122.08	118.08
7	Y	103	BCL	C4B-C3B-C2B	-2.53	104.29	108.36
7	T	101	BCL	CHC-C1C-NC	2.53	128.01	124.51
7	J	101	BCL	C2A-C1A-CHA	-2.53	119.44	123.86
7	E	101	BCL	CHB-C4A-NA	2.53	128.00	124.51
7	M	401	BCL	O2A-CGA-CBA	2.52	119.83	111.91
7	M	402	BCL	O2A-CGA-CBA	2.52	119.83	111.91
14	M	405	SPO	C5-C6-C7	-2.52	122.09	125.89
7	A	103	BCL	CMD-C2D-C3D	-2.52	121.83	127.61
14	S	102	SPO	C34-C33-C35	2.51	119.50	115.27
14	B	101	SPO	C34-C33-C35	2.51	119.50	115.27
14	M	405	SPO	C34-C33-C35	2.50	119.48	115.27
14	M	405	SPO	C10-C9-C7	-2.50	123.75	127.31
7	E	101	BCL	O2D-CGD-O1D	-2.49	118.98	123.84
14	P	102	SPO	C31-C32-C33	-2.49	121.67	127.66
7	M	402	BCL	CHB-C4A-NA	2.48	127.95	124.51
7	I	101	BCL	O2D-CGD-O1D	-2.48	118.98	123.84
7	Q	104	BCL	C1-C2-C3	-2.48	121.75	126.04
7	G	101	BCL	CHB-C4A-NA	2.48	127.94	124.51
7	L	301	BCL	CMD-C2D-C3D	-2.48	121.91	127.61
7	M	402	BCL	CHC-C1C-NC	2.48	127.94	124.51
14	Q	105	SPO	C15-C14-C12	-2.47	123.78	127.31
7	G	101	BCL	C1-C2-C3	-2.47	121.77	126.04
7	B	103	BCL	CHB-C4A-NA	2.47	127.92	124.51
14	S	103	SPO	C40-C38-C39	2.47	120.05	114.60
10	F	103	PGV	O03-C19-C20	2.46	119.64	111.91
7	V	101	BCL	CMB-C2B-C3B	2.46	132.58	125.93
7	V	101	BCL	O2A-CGA-CBA	2.46	119.63	111.91
14	M	405	SPO	C15-C14-C12	-2.46	123.80	127.31
14	Q	105	SPO	C34-C33-C35	2.46	119.40	115.27
7	V	101	BCL	C1D-CHD-C4C	-2.45	120.70	126.62
14	F	105	SPO	C40-C38-C39	2.45	120.01	114.60
7	G	101	BCL	CMB-C2B-C3B	2.45	132.54	125.93
7	Q	104	BCL	CMB-C2B-C3B	2.44	132.53	125.93
7	J	101	BCL	CHC-C1C-NC	2.44	127.89	124.51
7	M	401	BCL	CHB-C4A-NA	2.44	127.89	124.51
12	B	102	LMT	C1B-O1B-C4'	-2.44	111.92	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	307	CDL	OA8-CA7-C31	2.44	119.56	111.91
14	Q	105	SPO	C14-C15-C16	-2.44	115.61	123.22
7	D	101	BCL	O2D-CGD-O1D	-2.44	119.07	123.84
7	I	102	BCL	C1C-NC-C4C	-2.44	105.61	106.71
14	Z	101	SPO	C14-C15-C16	-2.44	115.61	123.22
14	G	102	SPO	C14-C15-C16	-2.44	115.61	123.22
14	J	102	SPO	C40-C38-C39	2.44	119.98	114.60
7	M	402	BCL	CMD-C2D-C3D	-2.44	122.01	127.61
14	S	103	SPO	C20-C21-C22	-2.44	118.48	123.47
14	D	104	SPO	C40-C38-C39	2.43	119.98	114.60
7	M	401	BCL	C2A-C1A-CHA	-2.43	119.61	123.86
10	H	301	PGV	C02-O01-C1	-2.43	111.81	117.79
7	Y	103	BCL	CHD-C1D-C2D	2.43	130.58	125.48
15	Y	102	CDL	OA8-CA7-C31	2.43	119.53	111.91
7	W	101	BCL	O2D-CGD-O1D	-2.43	119.09	123.84
14	P	102	SPO	C10-C9-C7	-2.43	123.85	127.31
7	M	401	BCL	CMB-C2B-C3B	2.42	132.47	125.93
7	V	101	BCL	CMD-C2D-C3D	-2.42	122.05	127.61
14	K	105	SPO	C14-C15-C16	-2.42	115.67	123.22
7	O	101	BCL	O2D-CGD-O1D	-2.42	119.11	123.84
7	T	101	BCL	C2A-C1A-CHA	-2.42	119.63	123.86
14	G	103	SPO	C31-C32-C33	-2.42	121.84	127.66
7	N	101	BCL	CHC-C1C-NC	2.42	127.85	124.51
15	M	408	CDL	OB8-CB7-C71	2.41	119.48	111.91
7	E	101	BCL	CMB-C2B-C3B	2.41	132.45	125.93
7	J	101	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
14	B	101	SPO	C21-C20-C19	-2.41	118.53	123.47
7	L	301	BCL	O2A-CGA-O1A	-2.41	117.52	123.59
14	B	104	SPO	C40-C38-C39	2.41	119.92	114.60
14	G	103	SPO	C27-C26-C25	-2.40	115.71	123.22
7	Q	104	BCL	CHB-C4A-NA	2.40	127.83	124.51
7	B	103	BCL	O2D-CGD-O1D	-2.40	119.14	123.84
14	O	102	SPO	C40-C38-C39	2.40	119.90	114.60
14	Z	101	SPO	C34-C33-C35	2.40	119.30	115.27
7	I	102	BCL	C4-C3-C5	2.39	119.30	115.27
14	V	102	SPO	C9-C10-C11	-2.39	115.75	123.22
7	I	102	BCL	O2D-CGD-O1D	-2.39	119.16	123.84
14	D	102	SPO	C40-C38-C39	2.38	119.87	114.60
7	Z	102	BCL	C1-C2-C3	-2.38	121.92	126.04
7	1	101	BCL	C1D-ND-C4D	-2.38	104.64	106.33
14	D	102	SPO	C13-C12-C11	2.38	121.83	118.08
14	P	102	SPO	C29-C28-C30	2.38	119.27	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	K	103	SPO	C14-C15-C16	-2.37	115.82	123.22
7	O	101	BCL	C1C-NC-C4C	-2.37	105.64	106.71
14	P	102	SPO	C9-C10-C11	-2.37	115.83	123.22
14	F	105	SPO	C31-C32-C33	-2.37	121.96	127.66
14	V	102	SPO	C10-C9-C7	-2.36	123.94	127.31
7	B	103	BCL	CMB-C2B-C3B	2.36	132.31	125.93
14	G	102	SPO	C40-C38-C39	2.36	119.82	114.60
12	L	308	LMT	C1B-O1B-C4'	-2.36	112.12	117.96
14	B	101	SPO	C40-C38-C39	2.36	119.82	114.60
7	Y	103	BCL	CHD-C4C-NC	2.35	127.69	125.08
7	M	401	BCL	C1D-CHD-C4C	-2.35	120.94	126.62
14	B	104	SPO	C27-C26-C25	-2.35	115.89	123.22
14	O	102	SPO	C31-C32-C33	-2.35	122.01	127.66
14	F	105	SPO	C14-C15-C16	-2.34	115.90	123.22
7	O	101	BCL	CMD-C2D-C3D	-2.34	122.23	127.61
14	Z	101	SPO	C20-C21-C22	-2.34	118.68	123.47
14	Q	105	SPO	C13-C12-C11	2.34	121.76	118.08
14	V	102	SPO	C40-C38-C39	2.33	119.76	114.60
15	M	408	CDL	OA8-CA7-C31	2.33	119.23	111.91
7	K	102	BCL	CMB-C2B-C3B	2.33	132.23	125.93
7	O	101	BCL	C1D-CHD-C4C	-2.33	121.00	126.62
7	P	101	BCL	CMB-C2B-C3B	2.33	132.22	125.93
7	L	309	BCL	C4-C3-C5	2.33	119.19	115.27
7	L	309	BCL	O2D-CGD-O1D	-2.32	119.29	123.84
7	L	301	BCL	CHB-C4A-NA	2.32	127.72	124.51
7	J	101	BCL	CMB-C2B-C3B	2.32	132.20	125.93
7	T	101	BCL	CMB-C2B-C3B	2.32	132.20	125.93
7	Z	102	BCL	O2D-CGD-O1D	-2.32	119.30	123.84
12	H	303	LMT	C1B-O1B-C4'	-2.32	112.22	117.96
14	S	102	SPO	C21-C20-C19	-2.32	118.72	123.47
14	S	102	SPO	C40-C38-C39	2.32	119.73	114.60
15	H	307	CDL	CB4-OB6-CB5	-2.32	112.08	117.79
14	B	101	SPO	C13-C12-C11	2.32	121.73	118.08
14	Z	101	SPO	C40-C38-C39	2.32	119.72	114.60
14	V	103	SPO	C40-C38-C39	2.32	119.72	114.60
7	L	301	BCL	C2A-C1A-CHA	-2.31	119.82	123.86
7	N	101	BCL	C2A-C1A-CHA	-2.31	119.83	123.86
7	S	101	BCL	CMD-C2D-C3D	-2.31	122.31	127.61
7	Q	106	BCL	CMB-C2B-C3B	2.30	132.15	125.93
7	P	101	BCL	O2D-CGD-O1D	-2.30	119.33	123.84
14	G	103	SPO	C40-C38-C39	2.30	119.69	114.60
14	P	102	SPO	C40-C38-C39	2.29	119.67	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	102	BCL	C1D-CHD-C4C	-2.29	121.09	126.62
14	G	103	SPO	C21-C20-C19	-2.29	118.79	123.47
14	V	102	SPO	C36-C37-C38	-2.28	119.94	127.75
14	K	103	SPO	C8-C7-C6	2.28	121.68	118.08
7	Q	104	BCL	O2D-CGD-O1D	-2.28	119.38	123.84
7	Z	102	BCL	C1D-ND-C4D	-2.28	104.72	106.33
7	M	402	BCL	C1D-CHD-C4C	-2.28	121.12	126.62
14	B	104	SPO	C20-C21-C22	-2.28	118.81	123.47
14	J	102	SPO	C27-C26-C25	-2.27	116.12	123.22
7	S	101	BCL	O2D-CGD-O1D	-2.27	119.39	123.84
7	F	101	BCL	O2A-CGA-O1A	-2.27	117.87	123.59
7	S	101	BCL	CMB-C2B-C3B	2.26	132.04	125.93
7	Q	104	BCL	CMD-C2D-C3D	-2.26	122.41	127.61
7	A	103	BCL	C4B-C3B-C2B	-2.26	104.73	108.36
7	O	101	BCL	CAC-C3C-C4C	-2.26	107.58	112.58
14	K	105	SPO	C15-C14-C12	-2.26	124.09	127.31
14	V	103	SPO	C31-C32-C33	-2.26	122.23	127.66
14	Q	105	SPO	C40-C38-C39	2.25	119.58	114.60
14	S	102	SPO	C31-C32-C33	-2.25	122.23	127.66
7	D	101	BCL	CMD-C2D-C3D	-2.25	122.43	127.61
14	V	103	SPO	C14-C15-C16	-2.25	116.19	123.22
14	S	102	SPO	C14-C15-C16	-2.25	116.20	123.22
7	E	101	BCL	CHC-C1C-NC	2.25	127.62	124.51
7	S	101	BCL	C1D-CHD-C4C	-2.25	121.19	126.62
15	M	408	CDL	CA4-OA6-CA5	-2.25	112.25	117.79
14	B	101	SPO	C31-C32-C33	-2.24	122.26	127.66
14	S	102	SPO	C8-C7-C6	2.24	121.61	118.08
7	J	101	BCL	CHC-C4B-C3B	-2.24	124.38	132.35
14	F	105	SPO	C27-C26-C25	-2.24	116.22	123.22
7	Y	103	BCL	CHB-C4A-NA	2.24	127.61	124.51
14	D	104	SPO	C14-C15-C16	-2.24	116.23	123.22
7	N	101	BCL	CMB-C2B-C3B	2.24	131.98	125.93
7	T	101	BCL	O2D-CGD-O1D	-2.24	119.46	123.84
14	M	405	SPO	C40-C38-C39	2.24	119.55	114.60
14	O	102	SPO	C14-C15-C16	-2.23	116.25	123.22
7	W	101	BCL	C1D-CHD-C4C	-2.23	121.24	126.62
10	K	104	PGV	C02-O01-C1	-2.23	112.31	117.79
7	E	101	BCL	O2A-CGA-O1A	-2.22	117.98	123.59
7	G	101	BCL	O2D-CGD-O1D	-2.22	119.49	123.84
7	P	101	BCL	O2A-CGA-O1A	-2.22	117.98	123.59
7	L	301	BCL	C1D-CHD-C4C	-2.22	121.26	126.62
7	N	101	BCL	C1D-CHD-C4C	-2.22	121.26	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	101	BCL	CHC-C4B-C3B	-2.22	124.45	132.35
7	I	101	BCL	CMB-C2B-C3B	2.22	131.92	125.93
7	Q	104	BCL	CHC-C4B-C3B	-2.21	124.48	132.35
14	G	102	SPO	C13-C12-C11	2.21	121.56	118.08
14	K	103	SPO	C13-C12-C11	2.21	121.56	118.08
7	G	101	BCL	C1D-CHD-C4C	-2.21	121.29	126.62
7	L	309	BCL	C1D-CHD-C4C	-2.21	121.29	126.62
7	D	101	BCL	CHC-C4B-C3B	-2.21	124.50	132.35
7	N	101	BCL	CHC-C4B-C3B	-2.21	124.50	132.35
7	N	101	BCL	CED-O2D-CGD	2.20	120.92	115.94
14	M	405	SPO	C9-C10-C11	-2.20	116.35	123.22
7	M	401	BCL	CHC-C4B-C3B	-2.20	124.53	132.35
7	E	101	BCL	C2A-C1A-CHA	-2.20	120.02	123.86
7	A	103	BCL	C1D-CHD-C4C	-2.20	121.33	126.62
7	J	101	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
7	T	101	BCL	CHC-C4B-C3B	-2.19	124.56	132.35
14	O	102	SPO	C21-C20-C19	-2.19	118.99	123.47
14	Z	101	SPO	C27-C26-C25	-2.19	116.39	123.22
7	M	402	BCL	C1C-NC-C4C	-2.19	105.72	106.71
7	S	101	BCL	CAC-C3C-C4C	-2.19	107.73	112.58
7	I	102	BCL	O2A-CGA-O1A	-2.19	118.07	123.59
7	I	102	BCL	CHC-C4B-C3B	-2.19	124.57	132.35
7	A	103	BCL	CHD-C1D-C2D	2.19	130.06	125.48
7	B	103	BCL	CHC-C1C-NC	2.18	127.53	124.51
14	Q	105	SPO	C18-C17-C16	2.18	121.51	118.08
14	F	105	SPO	C21-C20-C19	-2.18	119.01	123.47
7	B	103	BCL	O2A-CGA-CBA	2.18	118.74	111.91
7	K	102	BCL	CHC-C4B-C3B	-2.18	124.61	132.35
7	T	101	BCL	C1D-CHD-C4C	-2.17	121.38	126.62
7	D	101	BCL	C1D-CHD-C4C	-2.17	121.38	126.62
7	I	102	BCL	C1D-CHD-C4C	-2.17	121.38	126.62
7	G	101	BCL	CHC-C1C-NC	2.17	127.51	124.51
14	G	103	SPO	C14-C15-C16	-2.17	116.44	123.22
14	P	102	SPO	C14-C15-C16	-2.17	116.44	123.22
14	K	105	SPO	C8-C7-C6	2.17	121.49	118.08
7	Q	104	BCL	O2A-CGA-O1A	-2.17	118.12	123.59
7	L	301	BCL	CHC-C4B-C3B	-2.17	124.65	132.35
12	K	101	LMT	C1-O1'-C1'	-2.16	110.25	113.84
7	Z	102	BCL	CMB-C2B-C3B	2.16	131.77	125.93
7	E	101	BCL	CHC-C4B-C3B	-2.16	124.67	132.35
14	B	101	SPO	C18-C17-C16	2.16	121.48	118.08
7	M	401	BCL	C1-O2A-CGA	2.16	122.10	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	102	PGV	O01-C1-O02	-2.15	118.50	123.70
14	P	102	SPO	C26-C25-C23	-2.15	120.36	126.42
14	V	102	SPO	C26-C25-C23	-2.15	120.37	126.42
14	J	102	SPO	C21-C20-C19	-2.15	119.06	123.47
7	W	101	BCL	CHD-C1D-C2D	2.15	129.99	125.48
7	K	102	BCL	O2D-CGD-O1D	-2.15	119.64	123.84
14	V	103	SPO	C13-C12-C11	2.15	121.46	118.08
7	E	101	BCL	C1D-CHD-C4C	-2.15	121.44	126.62
14	K	103	SPO	C40-C38-C39	2.15	119.34	114.60
7	D	101	BCL	C1C-NC-C4C	-2.14	105.74	106.71
7	O	101	BCL	C4A-NA-C1A	2.14	107.67	106.71
7	G	101	BCL	O2A-CGA-O1A	-2.14	118.19	123.59
7	M	401	BCL	CMD-C2D-C3D	-2.14	122.69	127.61
14	S	103	SPO	C27-C26-C25	-2.14	116.54	123.22
7	Q	104	BCL	C1D-CHD-C4C	-2.14	121.46	126.62
7	P	101	BCL	C1-C2-C3	-2.14	122.35	126.04
14	D	104	SPO	C21-C20-C19	-2.14	119.10	123.47
7	Q	106	BCL	C1D-CHD-C4C	-2.14	121.47	126.62
7	L	309	BCL	CMD-C2D-C3D	-2.13	122.71	127.61
14	V	102	SPO	C24-C23-C22	-2.13	119.94	122.92
8	L	302	BPH	CMA-C3A-C4A	-2.13	109.71	114.38
7	F	101	BCL	CHC-C4B-C3B	-2.13	124.77	132.35
14	D	104	SPO	C13-C12-C11	2.13	121.43	118.08
7	E	101	BCL	C4D-CHA-C1A	-2.13	118.66	121.25
12	M	406	LMT	C1B-O1B-C4'	-2.13	112.70	117.96
7	O	101	BCL	CHB-C1B-C2B	-2.13	121.23	127.24
7	I	102	BCL	CMD-C2D-C3D	-2.12	122.73	127.61
14	K	105	SPO	C31-C32-C33	-2.12	122.55	127.66
7	W	101	BCL	CMD-C2D-C3D	-2.12	122.73	127.61
7	G	101	BCL	CED-O2D-CGD	2.12	120.73	115.94
14	G	102	SPO	C20-C21-C22	-2.12	119.14	123.47
7	F	101	BCL	C1D-CHD-C4C	-2.12	121.51	126.62
15	M	408	CDL	CB4-OB6-CB5	-2.11	112.58	117.79
7	I	101	BCL	CHB-C4A-NA	2.11	127.43	124.51
14	B	104	SPO	C24-C23-C25	2.11	121.41	118.08
14	V	103	SPO	C27-C26-C25	-2.11	116.62	123.22
7	V	101	BCL	CAC-C3C-C4C	-2.11	107.90	112.58
7	Q	106	BCL	CHC-C1C-NC	2.11	127.43	124.51
14	J	102	SPO	C31-C32-C33	-2.11	122.58	127.66
14	B	104	SPO	C31-C32-C33	-2.11	122.58	127.66
7	P	101	BCL	CHB-C4A-NA	2.11	127.42	124.51
7	M	402	BCL	CHC-C4B-C3B	-2.11	124.86	132.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	405	SPO	C29-C28-C30	2.10	118.81	115.27
7	F	101	BCL	C1C-NC-C4C	-2.10	105.76	106.71
7	O	101	BCL	O2A-CGA-O1A	-2.10	118.29	123.59
14	D	102	SPO	C27-C26-C25	-2.10	116.67	123.22
7	F	101	BCL	CMD-C2D-C3D	-2.10	122.79	127.61
7	L	301	BCL	C4D-CHA-C1A	-2.09	118.70	121.25
14	K	103	SPO	C15-C14-C12	-2.09	124.32	127.31
14	K	105	SPO	C20-C21-C22	-2.09	119.19	123.47
7	B	103	BCL	C4D-CHA-C1A	-2.09	118.70	121.25
14	F	105	SPO	C8-C7-C9	-2.09	119.99	122.92
7	L	309	BCL	CHD-C1D-C2D	2.09	129.87	125.48
14	Z	101	SPO	C13-C12-C11	2.09	121.37	118.08
12	L	307	LMT	C1B-O5B-C5B	2.09	117.79	113.69
14	Q	105	SPO	C8-C7-C6	2.09	121.37	118.08
7	W	101	BCL	C4A-NA-C1A	2.09	107.64	106.71
7	A	103	BCL	CED-O2D-CGD	2.09	120.66	115.94
7	S	101	BCL	C1-C2-C3	-2.08	122.44	126.04
7	D	101	BCL	C6-C5-C3	-2.08	107.99	113.45
7	Q	106	BCL	CMD-C2D-C3D	-2.08	122.82	127.61
7	Z	102	BCL	C1D-CHD-C4C	-2.08	121.60	126.62
7	P	101	BCL	CHC-C1C-NC	2.08	127.39	124.51
7	G	101	BCL	CHC-C4B-C3B	-2.08	124.96	132.35
7	N	101	BCL	O2D-CGD-O1D	-2.08	119.78	123.84
7	Q	106	BCL	C16-C15-C13	-2.07	109.22	115.92
10	Y	104	PGV	C02-O01-C1	-2.07	112.69	117.79
7	I	102	BCL	CAC-C3C-C4C	-2.07	107.99	112.58
12	K	101	LMT	O1B-C4'-C3'	2.07	112.78	107.28
14	F	105	SPO	C24-C23-C25	2.07	121.33	118.08
7	D	101	BCL	C4-C3-C5	2.07	118.75	115.27
14	S	102	SPO	C24-C23-C22	-2.07	120.03	122.92
7	Q	106	BCL	CHC-C4B-C3B	-2.06	125.02	132.35
14	M	405	SPO	C14-C15-C16	-2.06	116.79	123.22
7	J	101	BCL	O2A-CGA-O1A	-2.06	118.40	123.59
7	J	101	BCL	C4D-CHA-C1A	-2.06	118.75	121.25
7	P	101	BCL	C1D-CHD-C4C	-2.06	121.66	126.62
9	L	304	U10	O3-C3-C4	2.06	131.39	123.64
14	D	102	SPO	C8-C7-C6	2.06	121.31	118.08
7	L	309	BCL	O2A-CGA-O1A	-2.05	118.41	123.59
14	J	102	SPO	C14-C15-C16	-2.05	116.81	123.22
7	Q	104	BCL	C1C-NC-C4C	-2.05	105.78	106.71
14	F	105	SPO	C13-C12-C11	2.05	121.30	118.08
7	B	103	BCL	CMD-C2D-C3D	-2.05	122.91	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	103	BCL	CHC-C4B-C3B	-2.04	125.08	132.35
7	M	401	BCL	O1D-CGD-CBD	-2.04	120.30	124.48
10	H	301	PGV	O03-C19-O04	-2.04	118.44	123.59
14	J	102	SPO	C20-C21-C22	-2.04	119.30	123.47
7	S	101	BCL	C4A-NA-C1A	2.04	107.62	106.71
7	O	101	BCL	CHC-C4B-C3B	-2.03	125.12	132.35
10	Q	103	PGV	C02-O01-C1	-2.03	112.78	117.79
14	D	102	SPO	C21-C20-C19	-2.03	119.31	123.47
14	K	105	SPO	C13-C12-C11	2.03	121.28	118.08
14	D	104	SPO	C8-C7-C6	2.03	121.28	118.08
7	A	103	BCL	O2D-CGD-O1D	-2.03	119.87	123.84
14	F	105	SPO	C9-C10-C11	-2.03	116.89	123.22
7	A	103	BCL	CMB-C2B-C1B	2.03	128.45	125.37
14	O	102	SPO	C24-C23-C25	2.03	121.27	118.08
7	T	101	BCL	O2A-CGA-O1A	-2.02	118.49	123.59
14	Q	105	SPO	C36-C37-C38	-2.02	120.84	127.75
12	I	103	LMT	O1B-C4'-C3'	2.02	112.65	107.28
7	J	101	BCL	C6-C5-C3	-2.02	108.17	113.45
7	Y	103	BCL	CMB-C2B-C3B	2.02	131.37	125.93
7	K	102	BCL	CHB-C1B-C2B	-2.02	121.54	127.24
14	K	105	SPO	C18-C17-C16	2.02	121.25	118.08
14	M	405	SPO	C13-C12-C11	2.01	121.25	118.08
7	G	101	BCL	C2A-C1A-CHA	-2.01	120.34	123.86
9	L	304	U10	O3-C3-C2	-2.01	109.76	116.56
7	B	103	BCL	CHC-C4B-C3B	-2.01	125.20	132.35
10	F	102	PGV	O03-C19-O04	-2.01	118.52	123.59
7	Z	102	BCL	O2A-CGA-O1A	-2.01	118.53	123.59
7	P	101	BCL	CHC-C4B-C3B	-2.01	125.22	132.35
7	V	101	BCL	CHC-C4B-C3B	-2.00	125.22	132.35

There are no chirality outliers.

All (712) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	301	BCL	C2-C3-C5-C6
7	A	103	BCL	C1A-C2A-CAA-CBA
7	A	103	BCL	C3A-C2A-CAA-CBA
7	A	103	BCL	C2C-C3C-CAC-CBC
7	A	103	BCL	C4C-C3C-CAC-CBC
7	B	103	BCL	C6-C7-C8-C9
7	E	101	BCL	C1A-C2A-CAA-CBA
7	G	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
7	J	101	BCL	C1A-C2A-CAA-CBA
7	N	101	BCL	C1A-C2A-CAA-CBA
7	N	101	BCL	C3A-C2A-CAA-CBA
7	N	101	BCL	C2C-C3C-CAC-CBC
7	N	101	BCL	C4C-C3C-CAC-CBC
7	O	101	BCL	C4-C3-C5-C6
7	P	101	BCL	C1A-C2A-CAA-CBA
7	P	101	BCL	C3A-C2A-CAA-CBA
7	P	101	BCL	C2C-C3C-CAC-CBC
7	P	101	BCL	C4C-C3C-CAC-CBC
7	P	101	BCL	C11-C10-C8-C9
7	T	101	BCL	C1A-C2A-CAA-CBA
7	T	101	BCL	C2C-C3C-CAC-CBC
7	T	101	BCL	C4C-C3C-CAC-CBC
7	Y	103	BCL	C2C-C3C-CAC-CBC
7	Y	103	BCL	CHA-CBD-CGD-O1D
7	Y	103	BCL	CHA-CBD-CGD-O2D
7	1	101	BCL	C2C-C3C-CAC-CBC
7	1	101	BCL	C4C-C3C-CAC-CBC
7	1	101	BCL	CHA-CBD-CGD-O1D
7	1	101	BCL	CHA-CBD-CGD-O2D
9	L	303	U10	C7-C8-C9-C11
9	D	105	U10	C5-C6-C7-C8
9	D	105	U10	C19-C21-C22-C23
10	M	409	PGV	C03-O11-P-O14
10	M	409	PGV	C2-C1-O01-C02
10	H	301	PGV	C03-O11-P-O13
10	H	301	PGV	C03-O11-P-O14
10	H	301	PGV	C04-O12-P-O11
10	H	301	PGV	C04-O12-P-O13
10	F	102	PGV	C04-O12-P-O14
10	K	104	PGV	O01-C02-C03-O11
10	Y	104	PGV	C04-O12-P-O13
12	H	305	LMT	C2B-C1B-O1B-C4'
14	B	104	SPO	O1-C1-C4-C5
14	B	104	SPO	C2-C1-C4-C5
14	B	104	SPO	C3-C1-C4-C5
14	D	102	SPO	C28-C30-C31-C32
14	D	102	SPO	C33-C35-C36-C37
14	D	104	SPO	C28-C30-C31-C32
14	D	104	SPO	C32-C33-C35-C36
14	D	104	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
14	D	104	SPO	C33-C35-C36-C37
14	F	105	SPO	C32-C33-C35-C36
14	F	105	SPO	C34-C33-C35-C36
14	G	103	SPO	C5-C6-C7-C8
14	G	103	SPO	C32-C33-C35-C36
14	G	103	SPO	C34-C33-C35-C36
14	J	102	SPO	O1-C1-C4-C5
14	J	102	SPO	C2-C1-C4-C5
14	J	102	SPO	C3-C1-C4-C5
14	J	102	SPO	C1-C4-C5-C6
14	O	102	SPO	C29-C28-C30-C31
14	Q	105	SPO	C28-C30-C31-C32
15	M	408	CDL	CA3-OA5-PA1-OA3
15	M	408	CDL	CA3-OA5-PA1-OA4
15	M	408	CDL	OB7-CB5-OB6-CB4
15	M	408	CDL	C51-CB5-OB6-CB4
15	H	307	CDL	C11-CA5-OA6-CA4
15	H	307	CDL	CB2-OB2-PB2-OB5
15	H	307	CDL	CB3-OB5-PB2-OB3
15	H	307	CDL	CB3-OB5-PB2-OB4
15	Y	102	CDL	CA2-OA2-PA1-OA4
15	Y	102	CDL	CA3-OA5-PA1-OA3
15	Y	102	CDL	OA6-CA4-CA6-OA8
15	Y	102	CDL	CB3-OB5-PB2-OB3
16	F	104	PTY	O10-C8-O7-C6
16	F	104	PTY	C11-C8-O7-C6
16	F	104	PTY	C3-O11-P1-O13
7	Z	102	BCL	CBD-CGD-O2D-CED
12	H	304	LMT	C3'-C4'-O1B-C1B
12	I	101	LMT	O5B-C1B-O1B-C4'
16	F	104	PTY	O30-C30-O4-C1
10	M	409	PGV	O02-C1-O01-C02
12	K	101	LMT	C3'-C4'-O1B-C1B
7	D	101	BCL	C3-C5-C6-C7
7	S	101	BCL	C3-C5-C6-C7
7	Y	103	BCL	C3-C5-C6-C7
7	1	101	BCL	C3-C5-C6-C7
16	F	104	PTY	C31-C30-O4-C1
7	L	301	BCL	C4-C3-C5-C6
7	A	103	BCL	C4-C3-C5-C6
7	Y	103	BCL	C4-C3-C5-C6
14	F	105	SPO	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
14	V	103	SPO	C29-C28-C30-C31
7	O	101	BCL	C2-C3-C5-C6
7	Y	103	BCL	C2-C3-C5-C6
14	F	105	SPO	C27-C28-C30-C31
14	O	102	SPO	C27-C28-C30-C31
14	V	103	SPO	C27-C28-C30-C31
7	L	301	BCL	CBD-CGD-O2D-CED
7	G	101	BCL	C2A-CAA-CBA-CGA
7	T	101	BCL	C2A-CAA-CBA-CGA
7	J	101	BCL	C3-C5-C6-C7
15	H	307	CDL	OA7-CA5-OA6-CA4
10	L	305	PGV	C2-C1-O01-C02
12	H	304	LMT	O5'-C5'-C6'-O6'
12	A	102	LMT	O5'-C5'-C6'-O6'
9	M	410	U10	C35-C34-C36-C37
9	D	105	U10	C45-C44-C46-C47
14	G	102	SPO	C34-C33-C35-C36
14	K	103	SPO	C34-C33-C35-C36
14	P	102	SPO	C34-C33-C35-C36
14	V	102	SPO	C34-C33-C35-C36
7	A	103	BCL	C2-C3-C5-C6
9	M	410	U10	C33-C34-C36-C37
9	D	105	U10	C43-C44-C46-C47
14	G	102	SPO	C32-C33-C35-C36
14	K	103	SPO	C32-C33-C35-C36
14	P	102	SPO	C32-C33-C35-C36
14	V	102	SPO	C32-C33-C35-C36
7	J	101	BCL	C2A-CAA-CBA-CGA
9	M	410	U10	C24-C26-C27-C28
9	M	410	U10	C34-C36-C37-C38
14	G	102	SPO	C33-C35-C36-C37
14	K	103	SPO	C28-C30-C31-C32
14	K	103	SPO	C33-C35-C36-C37
14	P	102	SPO	C28-C30-C31-C32
14	V	102	SPO	C33-C35-C36-C37
14	Z	101	SPO	C28-C30-C31-C32
12	I	103	LMT	O5'-C5'-C6'-O6'
7	Z	102	BCL	O1D-CGD-O2D-CED
9	L	303	U10	C22-C23-C24-C26
7	B	103	BCL	CBA-CGA-O2A-C1
7	A	103	BCL	CBD-CGD-O2D-CED
8	M	403	BPH	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	B	103	BCL	O1A-CGA-O2A-C1
7	N	101	BCL	C10-C11-C12-C13
7	M	401	BCL	C11-C10-C8-C9
7	A	103	BCL	C6-C7-C8-C9
7	D	101	BCL	C6-C7-C8-C9
7	E	101	BCL	C6-C7-C8-C9
7	E	101	BCL	C14-C13-C15-C16
7	G	101	BCL	C14-C13-C15-C16
7	N	101	BCL	C6-C7-C8-C9
7	O	101	BCL	C11-C10-C8-C9
7	Q	104	BCL	C11-C12-C13-C14
7	Q	106	BCL	C11-C10-C8-C9
7	Q	106	BCL	C11-C12-C13-C14
7	Y	103	BCL	C11-C10-C8-C9
8	M	403	BPH	C11-C12-C13-C14
7	J	101	BCL	C10-C11-C12-C13
7	S	101	BCL	C10-C11-C12-C13
7	E	101	BCL	C2A-CAA-CBA-CGA
14	B	104	SPO	C5-C6-C7-C8
14	B	104	SPO	C10-C11-C12-C13
14	J	102	SPO	C5-C6-C7-C8
14	P	102	SPO	C5-C6-C7-C8
14	P	102	SPO	C10-C11-C12-C13
14	S	103	SPO	C24-C23-C25-C26
14	B	104	SPO	C5-C6-C7-C9
14	B	104	SPO	C10-C11-C12-C14
14	J	102	SPO	C5-C6-C7-C9
10	L	305	PGV	O02-C1-O01-C02
7	G	101	BCL	C13-C15-C16-C17
7	Q	104	BCL	C10-C11-C12-C13
12	K	101	LMT	O5'-C5'-C6'-O6'
10	F	103	PGV	C1-C2-C3-C4
7	M	402	BCL	C5-C6-C7-C8
7	M	402	BCL	C15-C16-C17-C18
7	E	101	BCL	C13-C15-C16-C17
7	O	101	BCL	C5-C6-C7-C8
7	Q	106	BCL	C10-C11-C12-C13
7	Q	106	BCL	C15-C16-C17-C18
7	T	101	BCL	C10-C11-C12-C13
7	1	101	BCL	C10-C11-C12-C13
9	L	303	U10	C7-C8-C9-C10
9	L	303	U10	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
10	L	305	PGV	C19-C20-C21-C22
10	F	102	PGV	C1-C2-C3-C4
12	H	303	LMT	O1'-C1-C2-C3
7	F	101	BCL	C5-C6-C7-C8
12	D	103	LMT	O5'-C5'-C6'-O6'
12	M	406	LMT	O1'-C1-C2-C3
7	P	101	BCL	C8-C10-C11-C12
10	L	305	PGV	C1-C2-C3-C4
7	E	101	BCL	C12-C13-C15-C16
7	Q	104	BCL	C6-C7-C8-C10
7	N	101	BCL	C2A-CAA-CBA-CGA
7	P	101	BCL	C2A-CAA-CBA-CGA
7	E	101	BCL	C8-C10-C11-C12
7	Q	106	BCL	C13-C15-C16-C17
12	L	307	LMT	O5'-C1'-O1'-C1
12	Q	101	LMT	O5'-C1'-O1'-C1
7	Y	103	BCL	C10-C11-C12-C13
9	D	105	U10	C14-C16-C17-C18
14	J	102	SPO	C33-C35-C36-C37
14	K	105	SPO	C28-C30-C31-C32
14	Q	105	SPO	C33-C35-C36-C37
14	S	102	SPO	C28-C30-C31-C32
7	J	101	BCL	C8-C10-C11-C12
7	Q	104	BCL	C13-C15-C16-C17
7	G	101	BCL	C8-C10-C11-C12
7	W	101	BCL	C5-C6-C7-C8
7	W	101	BCL	C10-C11-C12-C13
7	Y	103	BCL	C15-C16-C17-C18
10	L	305	PGV	C03-O11-P-O12
10	L	305	PGV	C04-O12-P-O11
10	M	409	PGV	C03-O11-P-O12
10	H	301	PGV	C03-O11-P-O12
15	M	408	CDL	CA3-OA5-PA1-OA2
15	M	408	CDL	CB2-OB2-PB2-OB5
15	M	408	CDL	CB3-OB5-PB2-OB2
15	H	307	CDL	CA3-OA5-PA1-OA2
15	H	307	CDL	CB3-OB5-PB2-OB2
15	Y	102	CDL	CA2-OA2-PA1-OA5
15	Y	102	CDL	CA3-OA5-PA1-OA2
15	Y	102	CDL	CB2-OB2-PB2-OB5
10	Y	104	PGV	C1-C2-C3-C4
7	S	101	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
7	J	101	BCL	C4-C3-C5-C6
14	Z	101	SPO	C34-C33-C35-C36
12	I	103	LMT	C3'-C4'-O1B-C1B
7	F	101	BCL	C15-C16-C17-C18
12	H	304	LMT	C4'-C5'-C6'-O6'
15	H	307	CDL	C31-CA7-OA8-CA6
7	S	101	BCL	C5-C6-C7-C8
12	M	407	LMT	C4-C5-C6-C7
7	L	301	BCL	O1D-CGD-O2D-CED
10	M	409	PGV	O12-C04-C05-O05
12	L	307	LMT	C2'-C1'-O1'-C1
10	K	104	PGV	C5-C6-C7-C8
15	H	307	CDL	OA9-CA7-OA8-CA6
7	E	101	BCL	C4-C3-C5-C6
7	V	101	BCL	C4-C3-C5-C6
10	Q	103	PGV	C24-C25-C26-C27
7	E	101	BCL	C2-C3-C5-C6
7	N	101	BCL	C11-C10-C8-C9
7	Q	104	BCL	C6-C7-C8-C9
7	T	101	BCL	C6-C7-C8-C9
7	W	101	BCL	C11-C10-C8-C9
7	V	101	BCL	C13-C15-C16-C17
15	M	408	CDL	C35-C36-C37-C38
15	M	408	CDL	C62-C63-C64-C65
7	N	101	BCL	C8-C10-C11-C12
7	T	101	BCL	C8-C10-C11-C12
10	K	104	PGV	C23-C24-C25-C26
12	I	101	LMT	C5'-C4'-O1B-C1B
12	A	101	LMT	O5'-C1'-O1'-C1
7	B	103	BCL	C8-C10-C11-C12
7	E	101	BCL	C3A-C2A-CAA-CBA
7	J	101	BCL	C3A-C2A-CAA-CBA
7	Q	106	BCL	C3A-C2A-CAA-CBA
7	T	101	BCL	C3A-C2A-CAA-CBA
7	Z	102	BCL	C3A-C2A-CAA-CBA
14	F	105	SPO	C11-C10-C9-C7
12	H	304	LMT	C2-C1-O1'-C1'
11	L	306	LDA	C2-C3-C4-C5
12	M	406	LMT	C1-C2-C3-C4
10	Y	104	PGV	C7-C8-C9-C10
7	G	101	BCL	C2-C3-C5-C6
7	J	101	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	V	101	BCL	C2-C3-C5-C6
7	Q	104	BCL	C15-C16-C17-C18
7	G	101	BCL	C3-C5-C6-C7
12	A	102	LMT	C4'-C5'-C6'-O6'
10	M	409	PGV	C2-C3-C4-C5
10	K	104	PGV	C13-C14-C15-C16
12	I	103	LMT	C5'-C4'-O1B-C1B
7	G	101	BCL	C4-C3-C5-C6
14	P	102	SPO	C29-C28-C30-C31
7	A	103	BCL	C6-C7-C8-C10
7	E	101	BCL	C6-C7-C8-C10
7	G	101	BCL	C12-C13-C15-C16
7	J	101	BCL	C11-C10-C8-C7
7	N	101	BCL	C6-C7-C8-C10
7	N	101	BCL	C11-C10-C8-C7
7	Q	106	BCL	C11-C12-C13-C15
7	W	101	BCL	C11-C10-C8-C7
8	M	403	BPH	C11-C12-C13-C15
14	P	102	SPO	C27-C28-C30-C31
12	I	101	LMT	C3'-C4'-O1B-C1B
10	H	301	PGV	C1-C2-C3-C4
10	M	409	PGV	C20-C19-O03-C01
10	F	103	PGV	C20-C19-O03-C01
7	Q	106	BCL	C2A-CAA-CBA-CGA
12	M	407	LMT	C6-C7-C8-C9
12	M	407	LMT	C7-C8-C9-C10
15	Y	102	CDL	CA3-CA4-CA6-OA8
7	K	102	BCL	C10-C11-C12-C13
10	M	409	PGV	C3-C4-C5-C6
12	A	101	LMT	C6-C7-C8-C9
7	Y	103	BCL	C5-C6-C7-C8
10	L	305	PGV	C3-C4-C5-C6
10	F	103	PGV	C2-C1-O01-C02
10	H	301	PGV	O01-C02-C03-O11
15	H	307	CDL	OA5-CA3-CA4-OA6
12	I	103	LMT	C4'-C5'-C6'-O6'
10	K	104	PGV	C26-C27-C28-C29
12	L	308	LMT	C3'-C4'-O1B-C1B
12	A	101	LMT	O5'-C5'-C6'-O6'
7	Q	106	BCL	C5-C6-C7-C8
7	S	101	BCL	C4-C3-C5-C6
14	Z	101	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
7	I	102	BCL	C6-C7-C8-C9
7	J	101	BCL	C11-C10-C8-C9
7	V	101	BCL	C11-C10-C8-C9
7	A	103	BCL	C2A-CAA-CBA-CGA
12	A	101	LMT	O5B-C5B-C6B-O6B
14	J	102	SPO	C10-C11-C12-C13
7	D	101	BCL	C5-C6-C7-C8
14	G	103	SPO	C5-C6-C7-C9
7	Q	106	BCL	C1A-C2A-CAA-CBA
7	Z	102	BCL	C1A-C2A-CAA-CBA
15	Y	102	CDL	C33-C34-C35-C36
7	V	101	BCL	C10-C11-C12-C13
10	K	104	PGV	C01-C02-C03-O11
15	H	307	CDL	OA5-CA3-CA4-CA6
7	A	103	BCL	O1D-CGD-O2D-CED
15	M	408	CDL	C11-C12-C13-C14
7	J	101	BCL	C2C-C3C-CAC-CBC
7	Q	106	BCL	C2C-C3C-CAC-CBC
12	H	305	LMT	C3-C4-C5-C6
7	M	401	BCL	C10-C11-C12-C13
15	H	307	CDL	C51-C52-C53-C54
7	A	103	BCL	C5-C6-C7-C8
12	Q	102	LMT	O5'-C5'-C6'-O6'
11	L	306	LDA	C1-C2-C3-C4
9	D	105	U10	C1-C6-C7-C8
7	M	401	BCL	C13-C15-C16-C17
7	W	101	BCL	CAA-CBA-CGA-O2A
12	H	305	LMT	C3'-C4'-O1B-C1B
12	B	102	LMT	O1'-C1-C2-C3
10	F	103	PGV	O04-C19-O03-C01
12	D	103	LMT	O5B-C5B-C6B-O6B
7	Z	102	BCL	C4-C3-C5-C6
12	L	308	LMT	C5'-C4'-O1B-C1B
7	V	101	BCL	C15-C16-C17-C18
16	F	104	PTY	C5-C6-O7-C8
12	H	305	LMT	O5B-C5B-C6B-O6B
10	Q	103	PGV	C22-C23-C24-C25
12	H	305	LMT	C5'-C4'-O1B-C1B
15	M	408	CDL	C17-C18-C19-C20
12	H	304	LMT	O1'-C1-C2-C3
7	I	102	BCL	C5-C6-C7-C8
14	P	102	SPO	C2-C1-O1-CM1

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Mol	Chain	Res	Type	Atoms
14	P	102	SPO	C3-C1-O1-CM1
10	F	102	PGV	O03-C01-C02-O01
15	M	408	CDL	OB6-CB4-CB6-OB8
10	F	103	PGV	O02-C1-O01-C02
10	M	409	PGV	O04-C19-O03-C01
14	G	103	SPO	C3-C1-C4-C5
14	O	102	SPO	C2-C1-C4-C5
9	M	410	U10	C32-C33-C34-C35
7	L	301	BCL	C11-C10-C8-C7
7	D	101	BCL	C12-C13-C15-C16
7	E	101	BCL	C11-C10-C8-C7
7	G	101	BCL	C11-C10-C8-C7
7	I	102	BCL	C6-C7-C8-C10
7	P	101	BCL	C11-C10-C8-C7
7	V	101	BCL	C11-C10-C8-C7
7	Y	103	BCL	C6-C7-C8-C10
7	Y	103	BCL	C11-C10-C8-C7
7	Z	102	BCL	C2-C3-C5-C6
7	L	301	BCL	C11-C10-C8-C9
7	L	309	BCL	C11-C10-C8-C9
7	E	101	BCL	C11-C10-C8-C9
7	F	101	BCL	C6-C7-C8-C9
7	Q	104	BCL	C11-C10-C8-C9
7	S	101	BCL	C11-C10-C8-C9
7	W	101	BCL	C6-C7-C8-C9
7	Z	102	BCL	C6-C7-C8-C9
14	K	103	SPO	C10-C11-C12-C13
10	F	102	PGV	C20-C21-C22-C23
11	H	302	LDA	N1-C1-C2-C3
10	M	409	PGV	C01-C02-C03-O11
10	H	301	PGV	C01-C02-C03-O11
7	Z	102	BCL	C3-C5-C6-C7
9	D	105	U10	C39-C41-C42-C43
7	O	101	BCL	C15-C16-C17-C18
7	N	101	BCL	C4-C3-C5-C6
7	P	101	BCL	C4-C3-C5-C6
7	T	101	BCL	C4-C3-C5-C6
9	D	105	U10	C15-C14-C16-C17
7	P	101	BCL	C2-C3-C5-C6
9	D	105	U10	C13-C14-C16-C17
7	P	101	BCL	C16-C17-C18-C19
10	K	104	PGV	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	M	408	CDL	C58-C59-C60-C61
15	M	408	CDL	CA5-C11-C12-C13
7	B	103	BCL	C3A-C2A-CAA-CBA
7	W	101	BCL	C3A-C2A-CAA-CBA
10	H	301	PGV	C25-C26-C27-C28
12	L	308	LMT	C2-C1-O1'-C1'
12	Q	102	LMT	C2-C1-O1'-C1'
7	L	309	BCL	C15-C16-C17-C18
8	L	302	BPH	O2A-C1-C2-C3
7	Y	103	BCL	C8-C10-C11-C12
10	F	102	PGV	C04-O12-P-O11
15	H	307	CDL	CA2-OA2-PA1-OA5
10	F	103	PGV	C2-C3-C4-C5
12	H	303	LMT	C4'-C5'-C6'-O6'
7	D	101	BCL	C8-C10-C11-C12
10	M	409	PGV	O01-C02-C03-O11
10	Q	103	PGV	O03-C01-C02-O01
7	L	309	BCL	CBD-CGD-O2D-CED
14	F	105	SPO	C28-C30-C31-C32
14	S	103	SPO	C33-C35-C36-C37
7	V	101	BCL	C2-C1-O2A-CGA
7	N	101	BCL	C2-C3-C5-C6
7	T	101	BCL	C2-C3-C5-C6
7	J	101	BCL	C6-C7-C8-C9
7	Q	106	BCL	C6-C7-C8-C9
7	W	101	BCL	C2A-CAA-CBA-CGA
14	P	102	SPO	C24-C23-C25-C26
7	M	401	BCL	C4C-C3C-CAC-CBC
14	P	102	SPO	C5-C6-C7-C9
14	P	102	SPO	C10-C11-C12-C14
12	H	303	LMT	O5'-C5'-C6'-O6'
15	Y	102	CDL	O1-C1-CA2-OA2
7	L	309	BCL	C11-C10-C8-C7
7	L	309	BCL	C11-C12-C13-C15
7	F	101	BCL	C6-C7-C8-C10
7	J	101	BCL	C6-C7-C8-C10
7	Q	104	BCL	C11-C10-C8-C7
7	Q	104	BCL	C11-C12-C13-C15
7	Q	106	BCL	C11-C10-C8-C7
7	S	101	BCL	C11-C10-C8-C7
7	W	101	BCL	C6-C7-C8-C10
7	Z	102	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	G	103	SPO	C11-C10-C9-C7
7	I	102	BCL	C16-C17-C18-C19
10	Q	103	PGV	C3-C4-C5-C6
15	M	408	CDL	C34-C35-C36-C37
7	P	101	BCL	C16-C17-C18-C20
7	A	103	BCL	C10-C11-C12-C13
7	I	102	BCL	C15-C16-C17-C18
7	L	301	BCL	CAD-CBD-CGD-O2D
8	L	302	BPH	CAD-CBD-CGD-O2D
8	M	403	BPH	CAD-CBD-CGD-O2D
7	F	101	BCL	C4-C3-C5-C6
7	Q	106	BCL	C4-C3-C5-C6
12	H	305	LMT	C2-C3-C4-C5
10	M	409	PGV	C5-C6-C7-C8
15	H	307	CDL	CA4-CA3-OA5-PA1
12	H	304	LMT	C9-C10-C11-C12
7	M	401	BCL	CHA-CBD-CGD-O1D
7	M	401	BCL	CHA-CBD-CGD-O2D
10	F	102	PGV	C2-C1-O01-C02
10	K	104	PGV	C12-C13-C14-C15
10	K	104	PGV	C4-C5-C6-C7
7	S	101	BCL	C2-C3-C5-C6
7	L	309	BCL	C11-C12-C13-C14
7	Q	104	BCL	O1D-CGD-O2D-CED
10	H	301	PGV	C27-C28-C29-C30
7	Q	106	BCL	C16-C17-C18-C19
7	Q	104	BCL	CBD-CGD-O2D-CED
14	V	102	SPO	C10-C11-C12-C13
16	F	104	PTY	C13-C14-C15-C16
7	M	401	BCL	C1A-C2A-CAA-CBA
7	G	101	BCL	C1A-C2A-CAA-CBA
7	W	101	BCL	C1A-C2A-CAA-CBA
10	F	102	PGV	C19-C20-C21-C22
10	F	102	PGV	O02-C1-O01-C02
7	L	309	BCL	O1D-CGD-O2D-CED
15	Y	102	CDL	CB3-OB5-PB2-OB2
16	F	104	PTY	C3-O11-P1-O14
12	H	303	LMT	C2-C3-C4-C5
10	L	305	PGV	C03-O11-P-O13
10	L	305	PGV	C04-O12-P-O13
10	M	409	PGV	C03-O11-P-O13
10	F	102	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
15	M	408	CDL	CB2-OB2-PB2-OB3
15	M	408	CDL	CB3-OB5-PB2-OB3
15	H	307	CDL	CA3-OA5-PA1-OA3
15	H	307	CDL	CB2-OB2-PB2-OB4
15	Y	102	CDL	CA3-OA5-PA1-OA4
15	Y	102	CDL	CB2-OB2-PB2-OB3
7	V	101	BCL	C16-C17-C18-C19
12	M	407	LMT	O5'-C1'-O1'-C1
10	Q	103	PGV	C01-C02-C03-O11
10	K	104	PGV	C27-C28-C29-C30
7	L	301	BCL	C2A-CAA-CBA-CGA
7	L	309	BCL	C3-C5-C6-C7
11	Y	101	LDA	C1-C2-C3-C4
16	F	104	PTY	C2-C3-O11-P1
7	N	101	BCL	C15-C16-C17-C18
7	1	101	BCL	C8-C10-C11-C12
12	A	101	LMT	O1'-C1-C2-C3
7	B	103	BCL	CBD-CGD-O2D-CED
7	1	101	BCL	C4-C3-C5-C6
7	L	309	BCL	C6-C7-C8-C10
7	M	401	BCL	C6-C7-C8-C10
7	M	401	BCL	C11-C10-C8-C7
7	B	103	BCL	C6-C7-C8-C10
7	D	101	BCL	C6-C7-C8-C10
8	M	403	BPH	C11-C10-C8-C7
10	Q	103	PGV	O01-C02-C03-O11
15	M	408	CDL	O1-C1-CB2-OB2
7	S	101	BCL	C8-C10-C11-C12
7	M	401	BCL	C16-C17-C18-C19
12	K	101	LMT	C4'-C5'-C6'-O6'
15	M	408	CDL	CB3-CB4-CB6-OB8
12	L	308	LMT	C3-C4-C5-C6
16	H	306	PTY	C6-C5-O14-P1
9	L	303	U10	C15-C14-C16-C17
9	D	105	U10	C35-C34-C36-C37
7	K	102	BCL	C11-C10-C8-C9
7	P	101	BCL	C14-C13-C15-C16
7	1	101	BCL	C11-C10-C8-C9
7	Y	103	BCL	O1A-CGA-O2A-C1
7	J	101	BCL	C16-C17-C18-C19
15	Y	102	CDL	C34-C35-C36-C37
14	S	103	SPO	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
7	F	101	BCL	C10-C11-C12-C13
7	Y	103	BCL	CBD-CGD-O2D-CED
7	B	103	BCL	O1D-CGD-O2D-CED
10	K	104	PGV	C25-C26-C27-C28
7	L	301	BCL	C2-C1-O2A-CGA
7	F	101	BCL	C2-C1-O2A-CGA
7	Y	103	BCL	C2-C1-O2A-CGA
7	1	101	BCL	C2-C1-O2A-CGA
12	L	308	LMT	O5B-C1B-O1B-C4'
7	T	101	BCL	C15-C16-C17-C18
7	Y	103	BCL	CBA-CGA-O2A-C1
7	Y	103	BCL	C16-C17-C18-C19
10	K	104	PGV	C9-C10-C11-C12
7	Z	102	BCL	C10-C11-C12-C13
10	M	409	PGV	C04-O12-P-O11
10	F	103	PGV	C03-O11-P-O12
10	F	103	PGV	C04-O12-P-O11
10	Q	103	PGV	C03-O11-P-O12
10	Q	103	PGV	C04-O12-P-O11
10	Y	104	PGV	C03-O11-P-O12
10	Y	104	PGV	C04-O12-P-O11
15	M	408	CDL	CA2-OA2-PA1-OA5
16	H	306	PTY	C5-O14-P1-O11
9	M	410	U10	C32-C33-C34-C36
14	O	102	SPO	C3-C1-C4-C5
14	S	103	SPO	C2-C1-C4-C5
12	D	103	LMT	C1-C2-C3-C4
10	F	102	PGV	O03-C01-C02-C03
7	F	101	BCL	C2-C3-C5-C6
7	Q	106	BCL	C2-C3-C5-C6
7	Q	106	BCL	C6-C7-C8-C10
7	T	101	BCL	C6-C7-C8-C10
7	1	101	BCL	C11-C10-C8-C7
8	L	302	BPH	C11-C12-C13-C15
15	H	307	CDL	C12-C13-C14-C15
7	D	101	BCL	C14-C13-C15-C16
7	D	101	BCL	C16-C17-C18-C19
7	Q	106	BCL	C16-C17-C18-C20
16	H	306	PTY	C11-C12-C13-C14
10	M	409	PGV	C02-C03-O11-P
12	A	102	LMT	C11-C10-C9-C8
14	P	102	SPO	C22-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
9	L	303	U10	C11-C12-C13-C14
7	V	101	BCL	C16-C17-C18-C20
12	L	307	LMT	C3'-C4'-O1B-C1B
12	A	102	LMT	O1'-C1-C2-C3
12	D	103	LMT	C4'-C5'-C6'-O6'
14	V	103	SPO	C33-C35-C36-C37
7	I	102	BCL	C8-C10-C11-C12
15	Y	102	CDL	C31-C32-C33-C34
9	D	105	U10	C36-C37-C38-C39
7	S	101	BCL	C16-C17-C18-C20
14	G	103	SPO	C29-C28-C30-C31
7	E	101	BCL	C10-C11-C12-C13
9	L	303	U10	C13-C14-C16-C17
7	L	301	BCL	C15-C16-C17-C18
7	Y	103	BCL	O1D-CGD-O2D-CED
7	D	101	BCL	C2-C1-O2A-CGA
7	W	101	BCL	CAA-CBA-CGA-O1A
7	G	101	BCL	C3A-C2A-CAA-CBA
9	D	105	U10	C2-C3-O3-C3M
9	D	105	U10	C20-C19-C21-C22
7	P	101	BCL	C6-C7-C8-C9
7	M	401	BCL	C16-C17-C18-C20
7	B	103	BCL	C1A-C2A-CAA-CBA
7	Q	104	BCL	C1A-C2A-CAA-CBA
7	T	101	BCL	C16-C17-C18-C20
12	L	307	LMT	C5-C6-C7-C8
12	L	307	LMT	C5'-C4'-O1B-C1B
7	L	309	BCL	C16-C17-C18-C19
14	M	405	SPO	C29-C28-C30-C31
12	M	407	LMT	C3-C4-C5-C6
12	Q	101	LMT	O1'-C1-C2-C3
12	L	308	LMT	C2B-C1B-O1B-C4'
15	M	408	CDL	OA6-CA4-CA6-OA8
14	S	103	SPO	C11-C10-C9-C7
14	Z	101	SPO	C17-C19-C20-C21
12	K	101	LMT	C5'-C4'-O1B-C1B
10	M	409	PGV	O12-C04-C05-C06
14	B	104	SPO	C34-C33-C35-C36
10	F	103	PGV	C20-C21-C22-C23
7	W	101	BCL	C2-C1-O2A-CGA
10	H	301	PGV	C26-C27-C28-C29
7	M	402	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
7	B	103	BCL	C14-C13-C15-C16
7	T	101	BCL	C11-C10-C8-C9
7	N	101	BCL	C3-C5-C6-C7
10	M	409	PGV	C7-C8-C9-C10
12	Q	101	LMT	C11-C10-C9-C8
14	P	102	SPO	C25-C26-C27-C28
7	I	102	BCL	C4-C3-C5-C6
9	L	304	U10	C15-C14-C16-C17
14	B	104	SPO	C29-C28-C30-C31
7	J	101	BCL	C4C-C3C-CAC-CBC
14	K	103	SPO	C10-C11-C12-C14
9	D	105	U10	C33-C34-C36-C37
7	F	101	BCL	C8-C10-C11-C12
7	Q	104	BCL	C8-C10-C11-C12
7	Z	102	BCL	CAA-CBA-CGA-O2A
7	Z	102	BCL	C16-C17-C18-C19
8	L	302	BPH	C16-C17-C18-C20
9	D	105	U10	C5-C4-O4-C4M
12	H	304	LMT	C7-C8-C9-C10
14	S	103	SPO	C28-C30-C31-C32
7	T	101	BCL	C11-C10-C8-C7
9	D	105	U10	C18-C19-C21-C22
10	F	103	PGV	C9-C10-C11-C12
7	S	101	BCL	C16-C17-C18-C19
7	Y	103	BCL	C16-C17-C18-C20
12	H	303	LMT	C3-C4-C5-C6
9	L	304	U10	C16-C17-C18-C19
7	1	101	BCL	C2-C3-C5-C6
7	L	309	BCL	C6-C7-C8-C9
7	M	401	BCL	C6-C7-C8-C9
7	F	101	BCL	C3A-C2A-CAA-CBA
7	O	101	BCL	C3A-C2A-CAA-CBA
7	Q	104	BCL	C3A-C2A-CAA-CBA
12	A	101	LMT	C9-C10-C11-C12
15	M	408	CDL	OA9-CA7-OA8-CA6
10	H	301	PGV	C9-C10-C11-C12
7	Z	102	BCL	CAD-CBD-CGD-O2D
15	H	307	CDL	CA6-CA4-OA6-CA5
9	D	105	U10	C26-C27-C28-C29
7	K	102	BCL	C2-C1-O2A-CGA
7	L	309	BCL	CAA-CBA-CGA-O2A
12	H	304	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
7	I	102	BCL	C16-C17-C18-C20
7	I	102	BCL	C2-C3-C5-C6
9	L	304	U10	C13-C14-C16-C17
14	M	405	SPO	C27-C28-C30-C31
7	J	101	BCL	CAA-CBA-CGA-O2A
14	J	102	SPO	C10-C11-C12-C14
14	V	102	SPO	C10-C11-C12-C14
10	Q	103	PGV	O03-C01-C02-C03
16	F	104	PTY	C41-C42-C43-C44
15	M	408	CDL	C12-C11-CA5-OA6
7	B	103	BCL	O2A-C1-C2-C3
15	M	408	CDL	C31-CA7-OA8-CA6
7	L	309	BCL	CHA-CBD-CGD-O1D
7	L	309	BCL	CHA-CBD-CGD-O2D
9	D	105	U10	C47-C48-C49-C51
10	M	409	PGV	O03-C19-C20-C21
10	Y	104	PGV	C24-C25-C26-C27
14	S	103	SPO	C3-C1-C4-C5
14	O	102	SPO	C34-C33-C35-C36
14	G	103	SPO	C27-C28-C30-C31
12	H	303	LMT	O5'-C1'-O1'-C1
7	N	101	BCL	CAA-CBA-CGA-O2A
8	M	403	BPH	C11-C10-C8-C9
12	L	307	LMT	C4B-C5B-C6B-O6B
8	M	403	BPH	C15-C16-C17-C18
7	L	309	BCL	C8-C10-C11-C12
7	T	101	BCL	C16-C17-C18-C19
7	P	101	BCL	C3-C5-C6-C7
7	Z	102	BCL	C2A-CAA-CBA-CGA
9	D	105	U10	C16-C17-C18-C19
14	K	105	SPO	C30-C31-C32-C33
16	H	306	PTY	C12-C11-C8-O7
14	V	103	SPO	C10-C11-C12-C13
14	V	103	SPO	C10-C11-C12-C14
7	D	101	BCL	C1A-C2A-CAA-CBA
7	F	101	BCL	C1A-C2A-CAA-CBA
7	I	102	BCL	C1A-C2A-CAA-CBA
7	O	101	BCL	C1A-C2A-CAA-CBA
7	S	101	BCL	C1A-C2A-CAA-CBA
15	M	408	CDL	C12-C11-CA5-OA7
7	J	101	BCL	CAA-CBA-CGA-O1A
10	F	102	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
7	L	309	BCL	CAA-CBA-CGA-O1A
10	M	409	PGV	C04-O12-P-O13
10	Q	103	PGV	C03-O11-P-O13
10	Y	104	PGV	C03-O11-P-O13
14	S	102	SPO	C30-C31-C32-C33
16	H	306	PTY	C38-C39-C40-C41
16	H	306	PTY	C12-C11-C8-O10
15	H	307	CDL	OB5-CB3-CB4-CB6
7	N	101	BCL	CAA-CBA-CGA-O1A
9	D	105	U10	C40-C39-C41-C42
7	L	309	BCL	C16-C17-C18-C20
16	H	306	PTY	C35-C36-C37-C38
10	M	409	PGV	O04-C19-C20-C21
7	I	102	BCL	C11-C12-C13-C14
7	V	101	BCL	C11-C12-C13-C14
10	Y	104	PGV	C23-C24-C25-C26
15	M	408	CDL	C61-C62-C63-C64
7	F	101	BCL	C13-C15-C16-C17
14	B	104	SPO	C1-C4-C5-C6
7	I	102	BCL	C13-C15-C16-C17
8	L	302	BPH	C4-C3-C5-C6
14	B	101	SPO	C29-C28-C30-C31
16	H	306	PTY	C19-C20-C21-C22
7	B	103	BCL	C11-C10-C8-C7
7	I	102	BCL	C3A-C2A-CAA-CBA
7	O	101	BCL	C11-C10-C8-C7
7	V	101	BCL	C11-C12-C13-C15
14	B	104	SPO	C27-C28-C30-C31
10	F	103	PGV	C24-C25-C26-C27
12	H	305	LMT	C2-C1-O1'-C1'
14	Z	101	SPO	C33-C35-C36-C37
10	F	103	PGV	C25-C26-C27-C28

There are no ring outliers.

77 monomers are involved in 280 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	101	BCL	12	0
9	L	304	U10	1	0
14	B	101	SPO	4	0
7	G	101	BCL	3	0
11	Y	101	LDA	2	0

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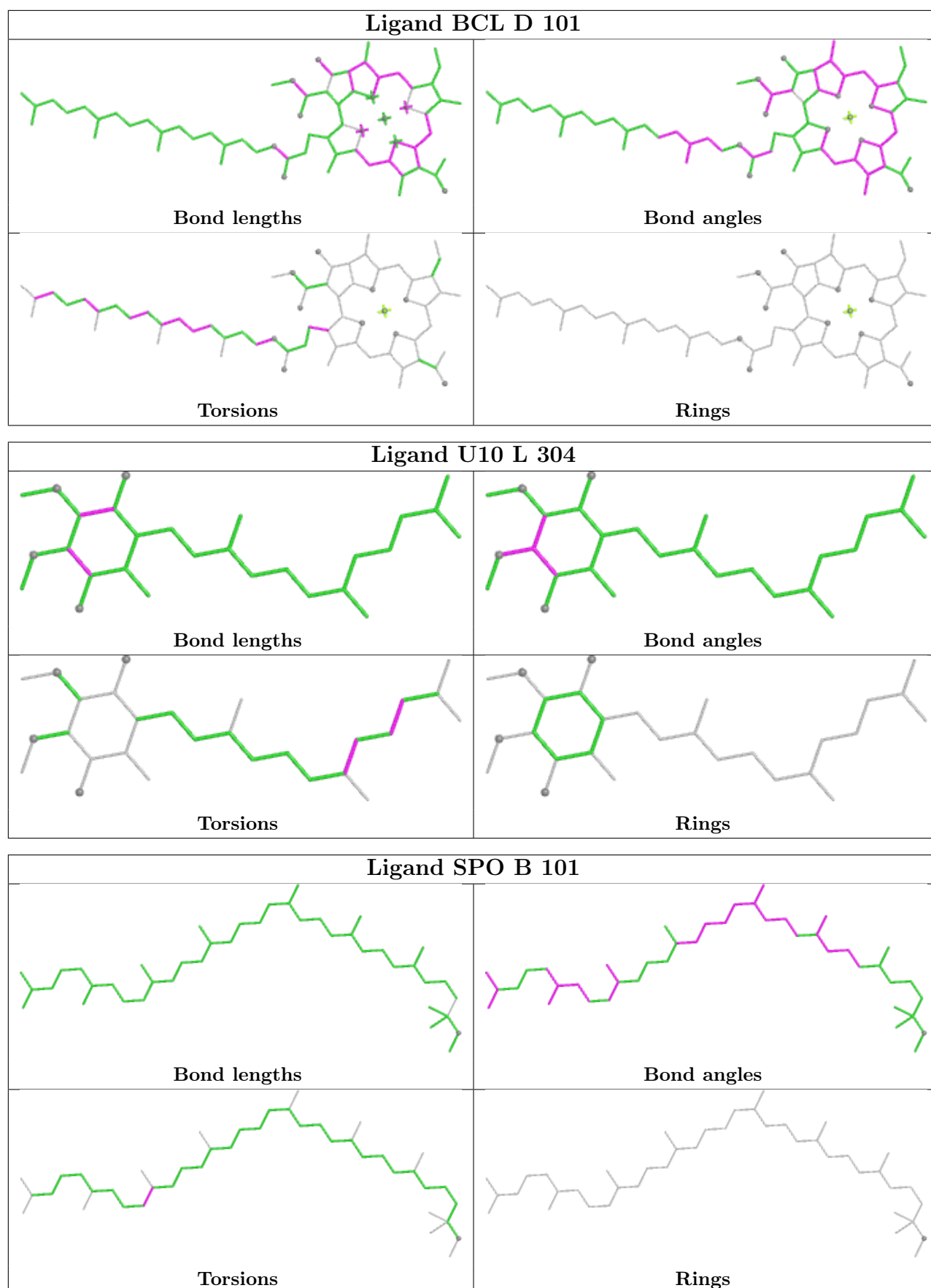
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12	H	304	LMT	4	0
8	M	403	BPH	8	0
14	Q	105	SPO	6	0
9	D	105	U10	11	0
10	Q	103	PGV	2	0
10	F	103	PGV	4	0
8	L	302	BPH	3	0
15	M	408	CDL	5	0
7	T	101	BCL	5	0
12	D	103	LMT	1	0
10	L	305	PGV	2	0
14	G	102	SPO	8	0
15	H	307	CDL	5	0
14	D	102	SPO	4	0
14	B	104	SPO	7	0
14	D	104	SPO	4	0
7	V	101	BCL	3	0
7	W	101	BCL	2	0
12	Q	102	LMT	3	0
7	Z	102	BCL	4	0
12	I	101	LMT	3	0
9	M	410	U10	6	0
7	E	101	BCL	2	0
15	Y	102	CDL	2	0
14	J	102	SPO	6	0
7	P	101	BCL	5	0
12	M	407	LMT	1	0
14	K	103	SPO	4	0
7	O	101	BCL	4	0
7	M	402	BCL	4	0
12	H	303	LMT	2	0
11	H	302	LDA	1	0
7	A	103	BCL	5	0
12	H	305	LMT	4	0
12	L	308	LMT	2	0
10	Y	104	PGV	3	0
14	G	103	SPO	3	0
7	L	309	BCL	2	0
14	K	105	SPO	7	0
7	I	102	BCL	3	0
10	M	409	PGV	4	0
7	N	101	BCL	6	0

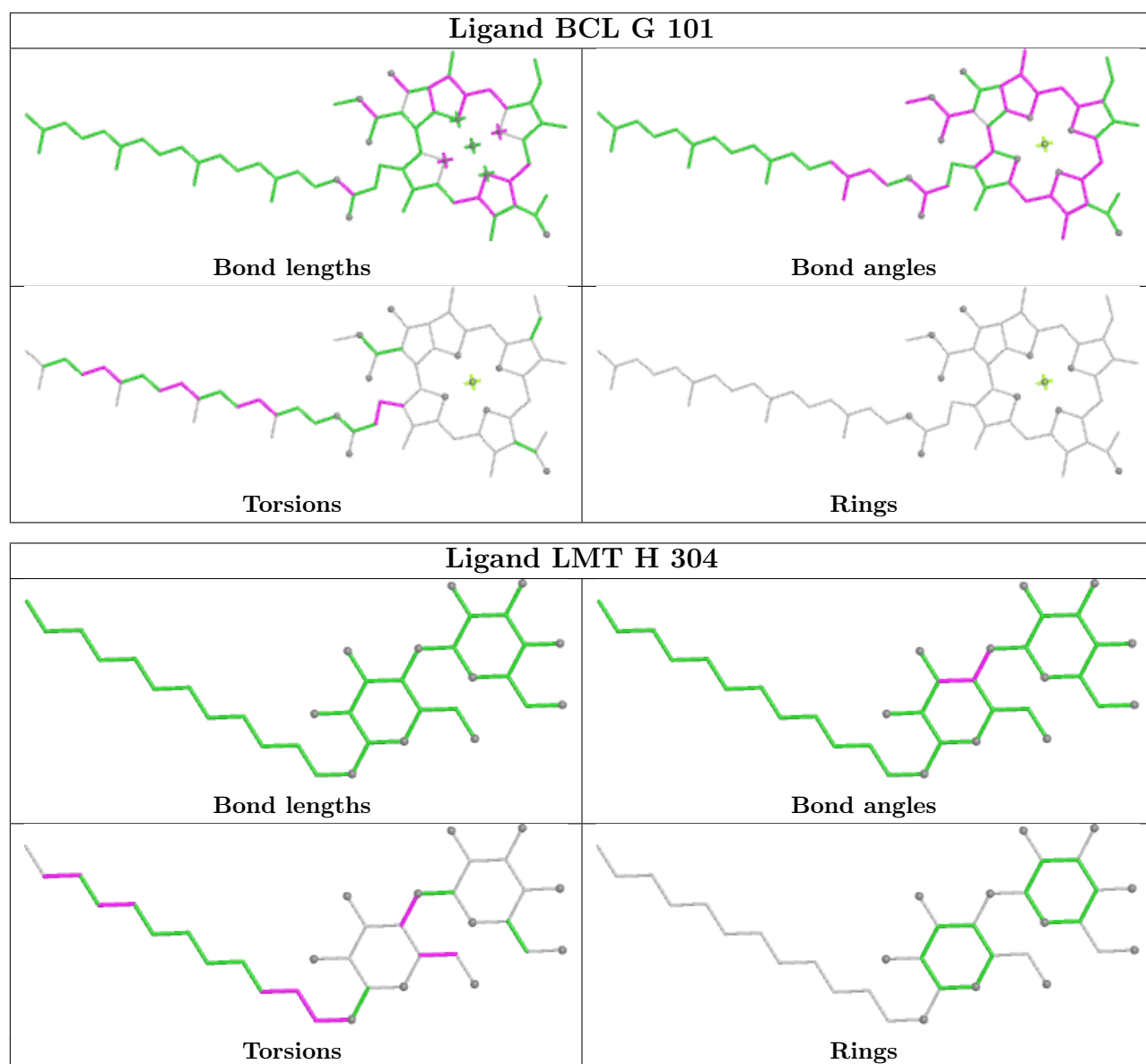
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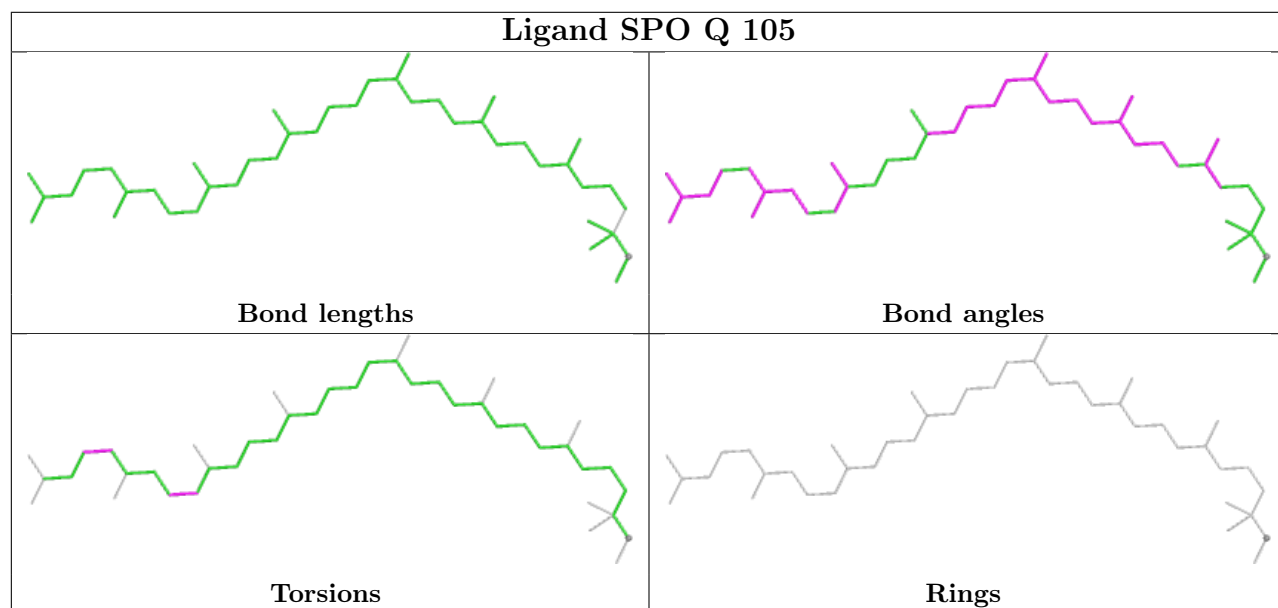
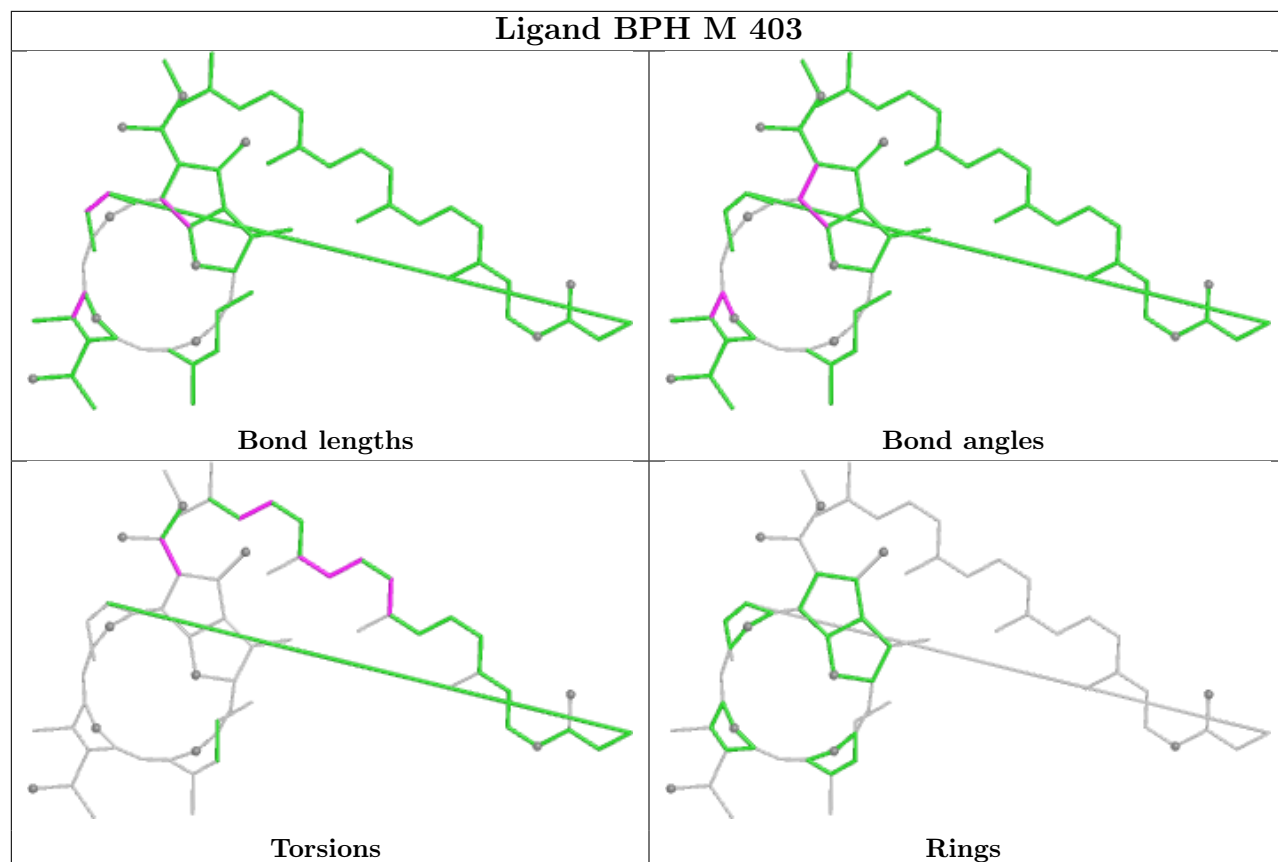
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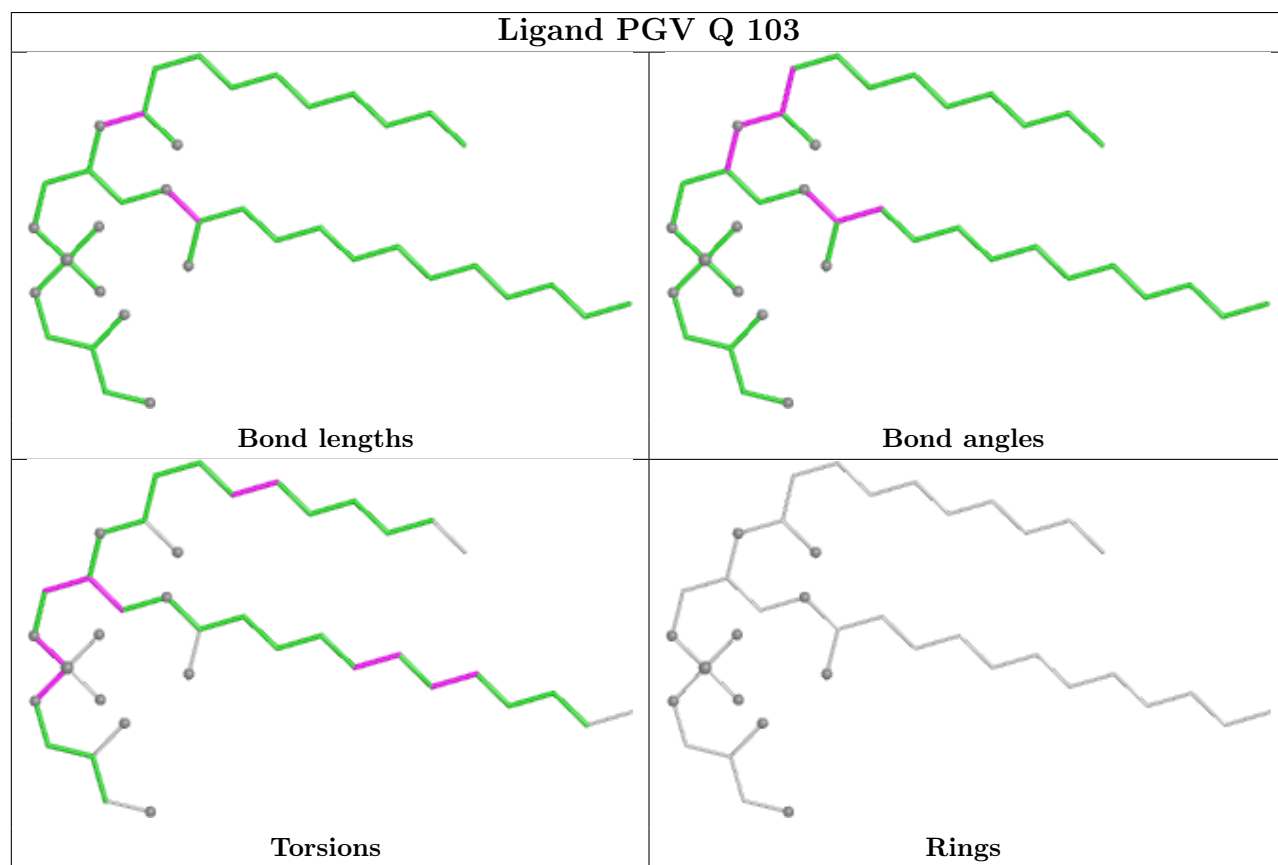
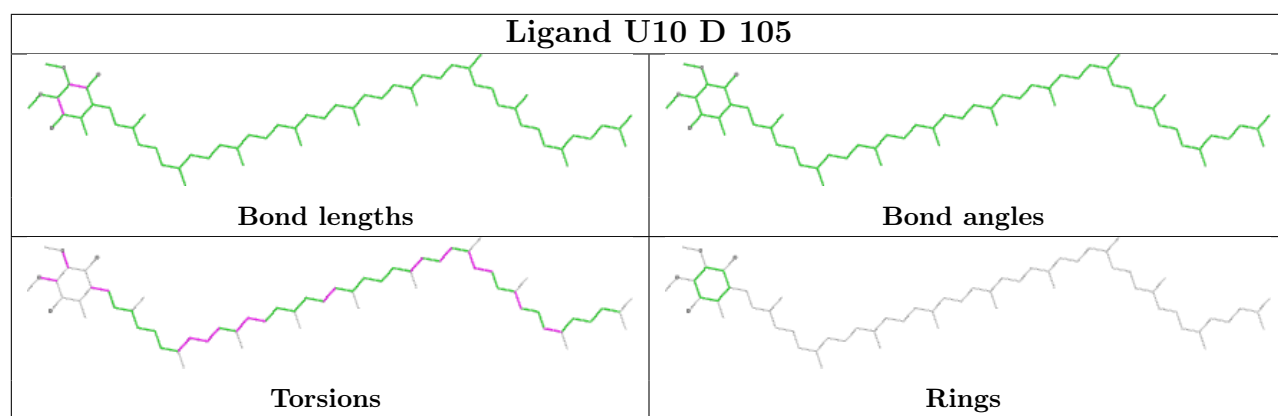
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Y	103	BCL	5	0
12	K	101	LMT	4	0
10	K	104	PGV	2	0
10	H	301	PGV	1	0
9	L	303	U10	3	0
7	Q	106	BCL	8	0
16	F	104	PTY	4	0
14	V	102	SPO	8	0
7	S	101	BCL	6	0
7	J	101	BCL	4	0
14	S	103	SPO	3	0
7	K	102	BCL	5	0
14	S	102	SPO	6	0
7	M	401	BCL	3	0
7	L	301	BCL	2	0
14	Z	101	SPO	11	0
7	F	101	BCL	8	0
7	1	101	BCL	8	0
12	A	101	LMT	1	0
7	B	103	BCL	4	0
14	V	103	SPO	2	0
14	M	405	SPO	5	0
14	P	102	SPO	8	0
12	A	102	LMT	3	0
14	F	105	SPO	6	0
7	Q	104	BCL	8	0
14	O	102	SPO	4	0
12	I	103	LMT	1	0
10	F	102	PGV	2	0
16	H	306	PTY	6	0

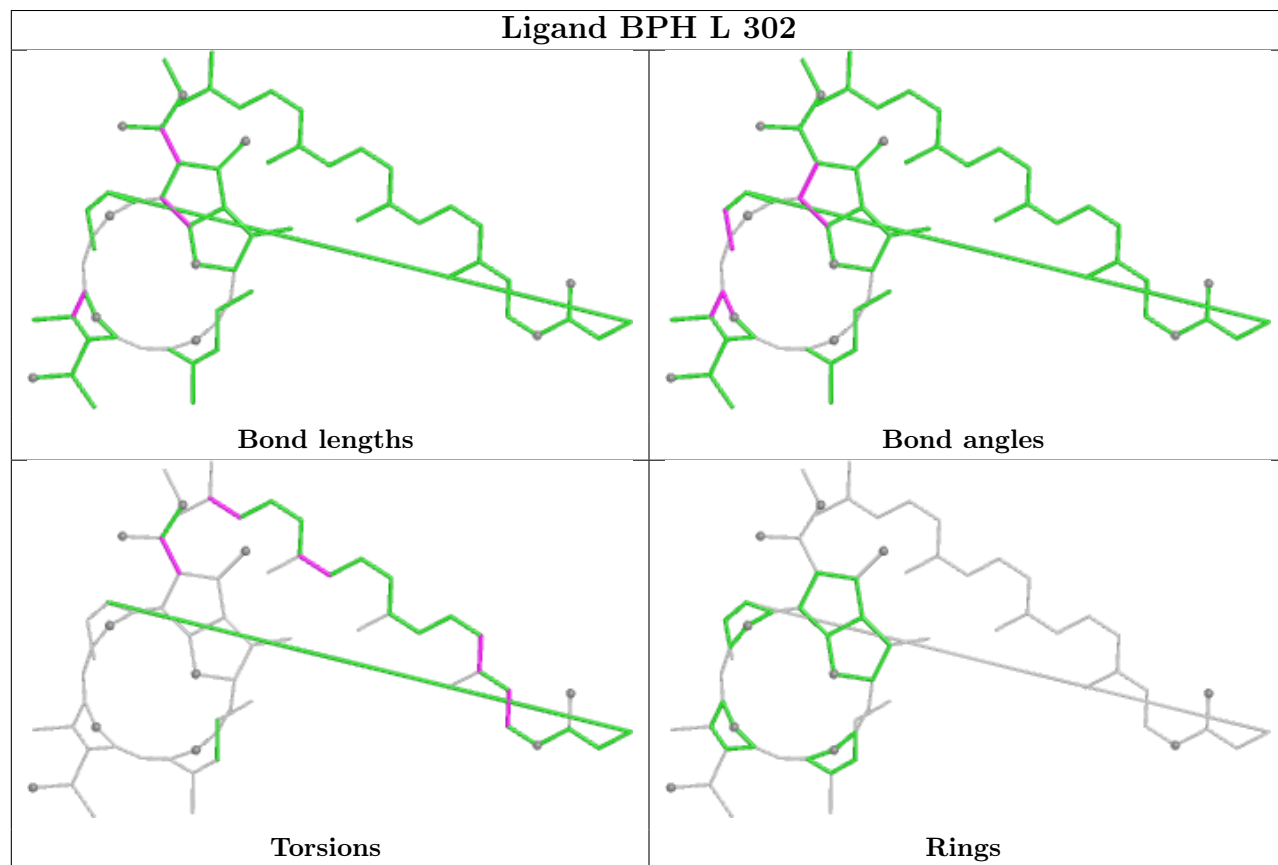
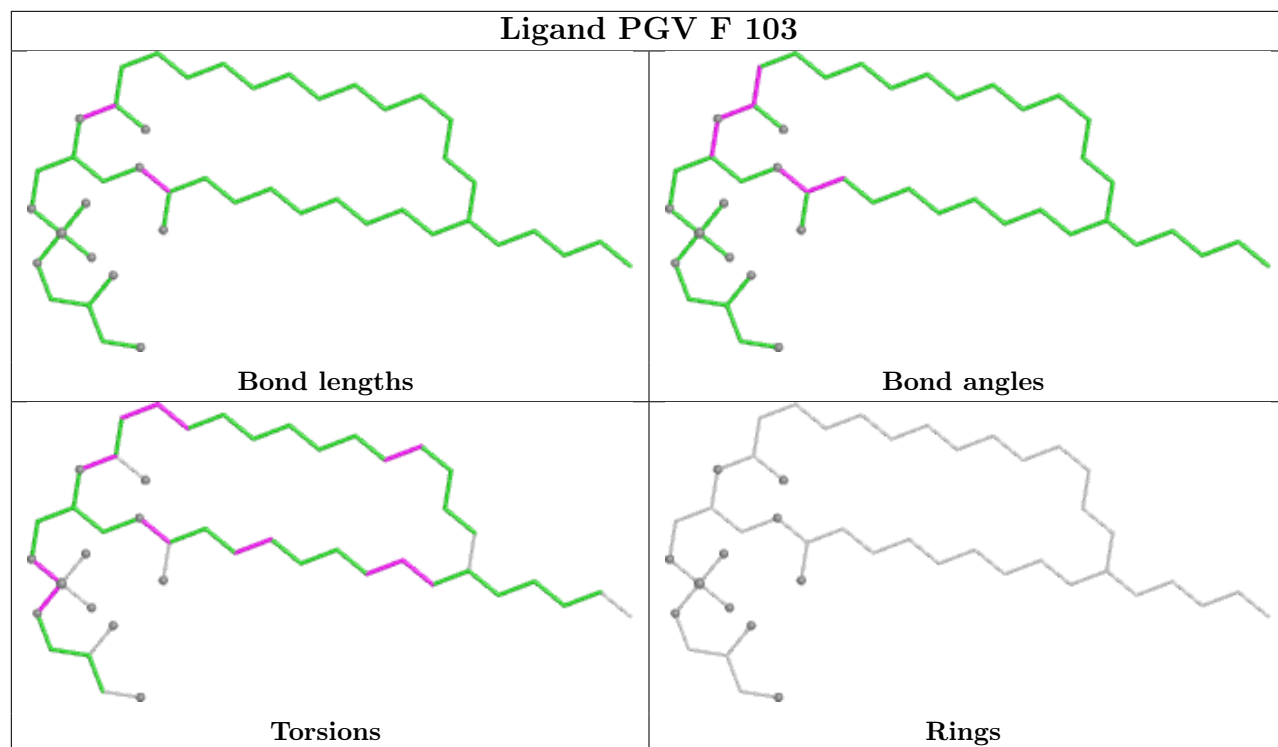
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

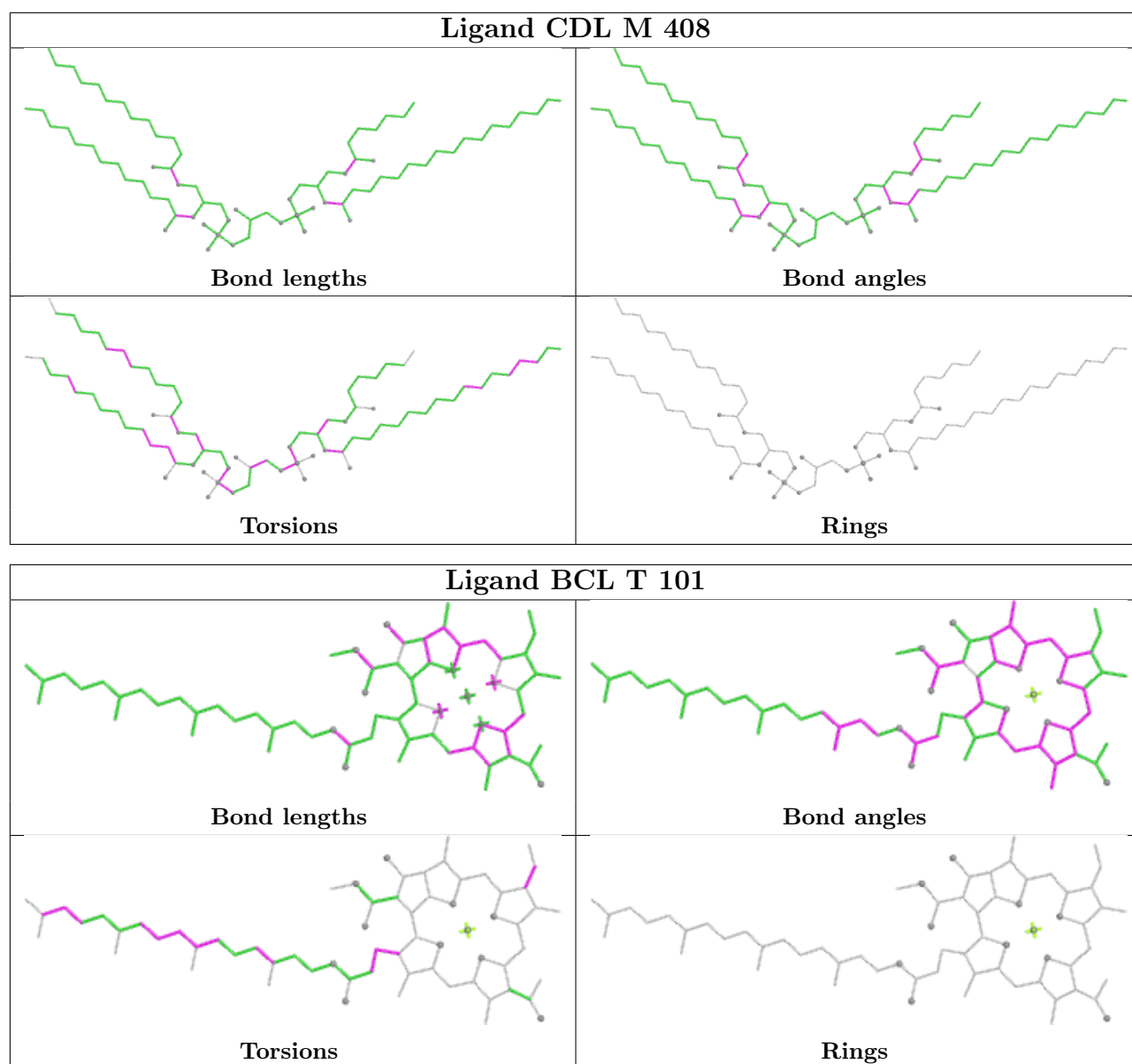


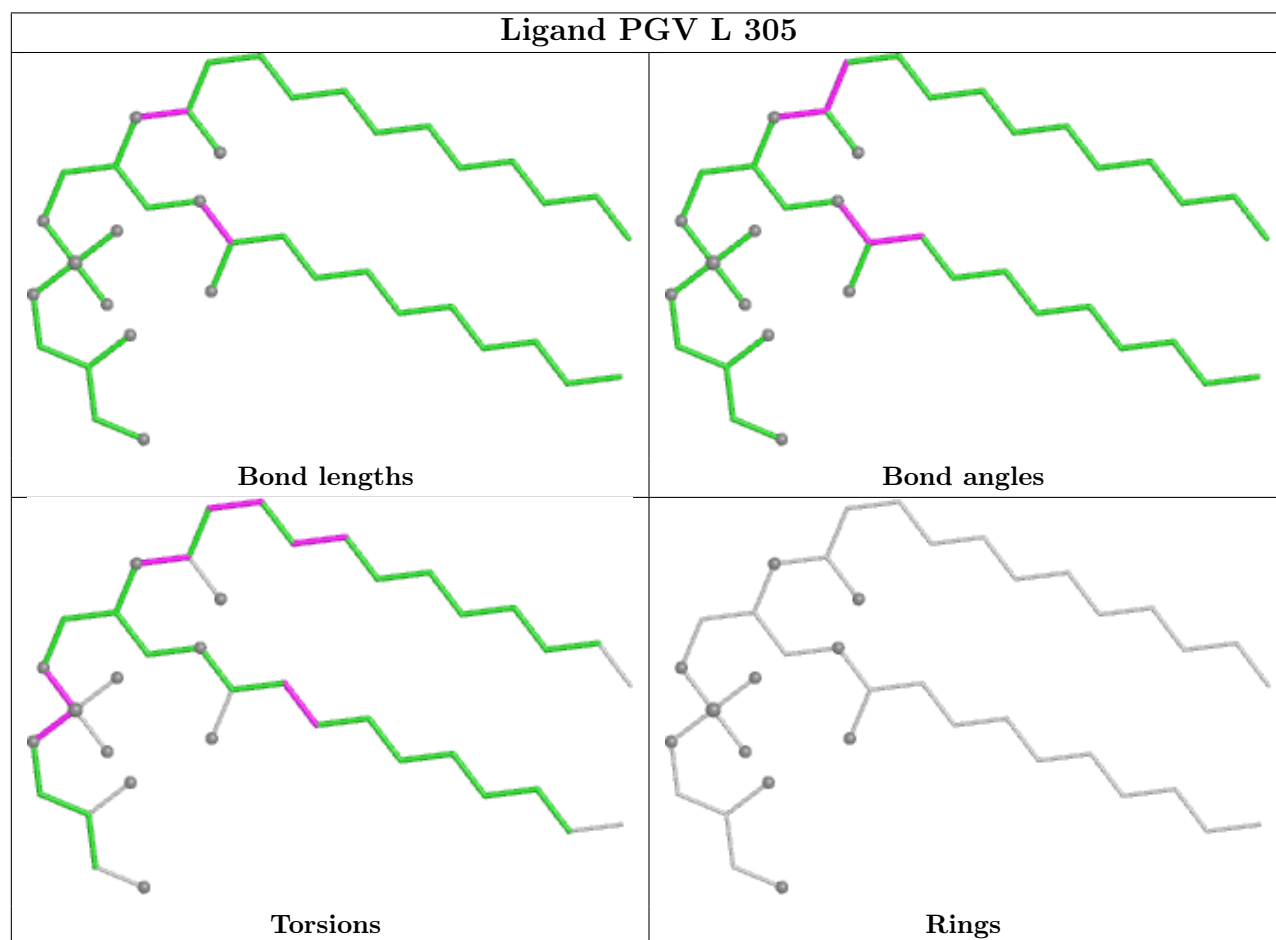
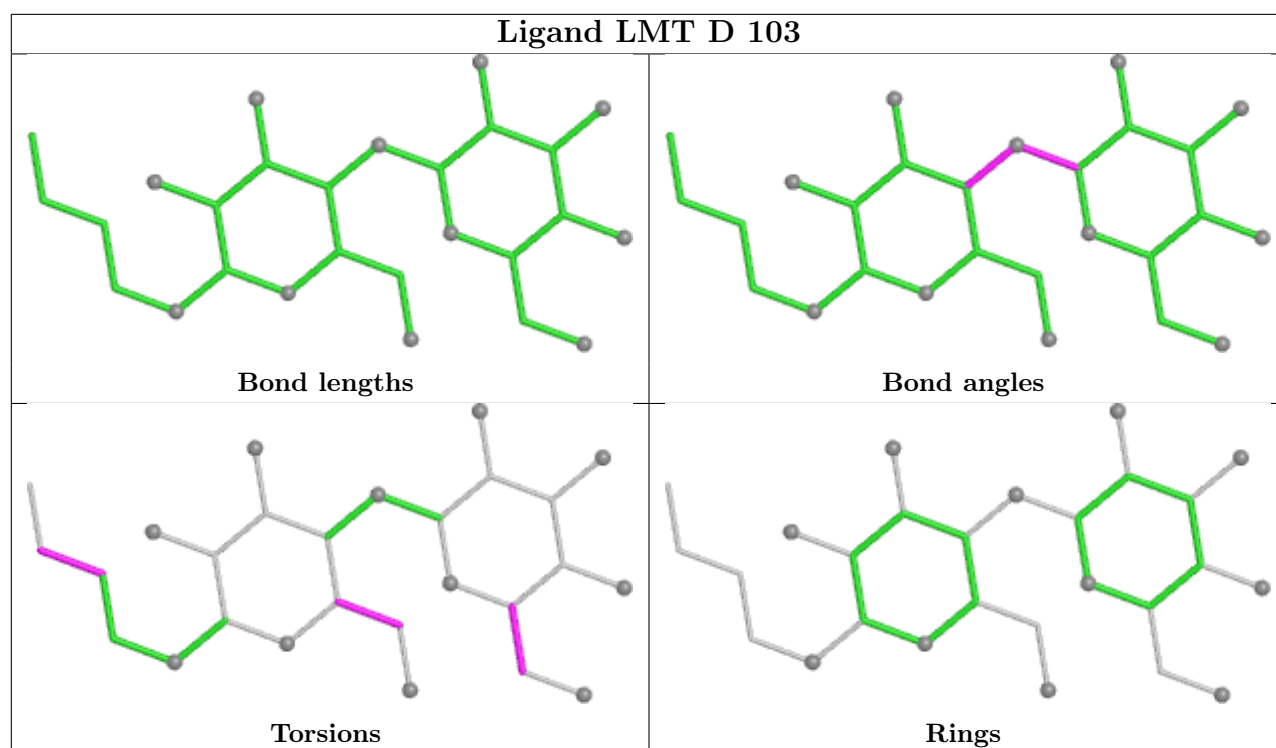


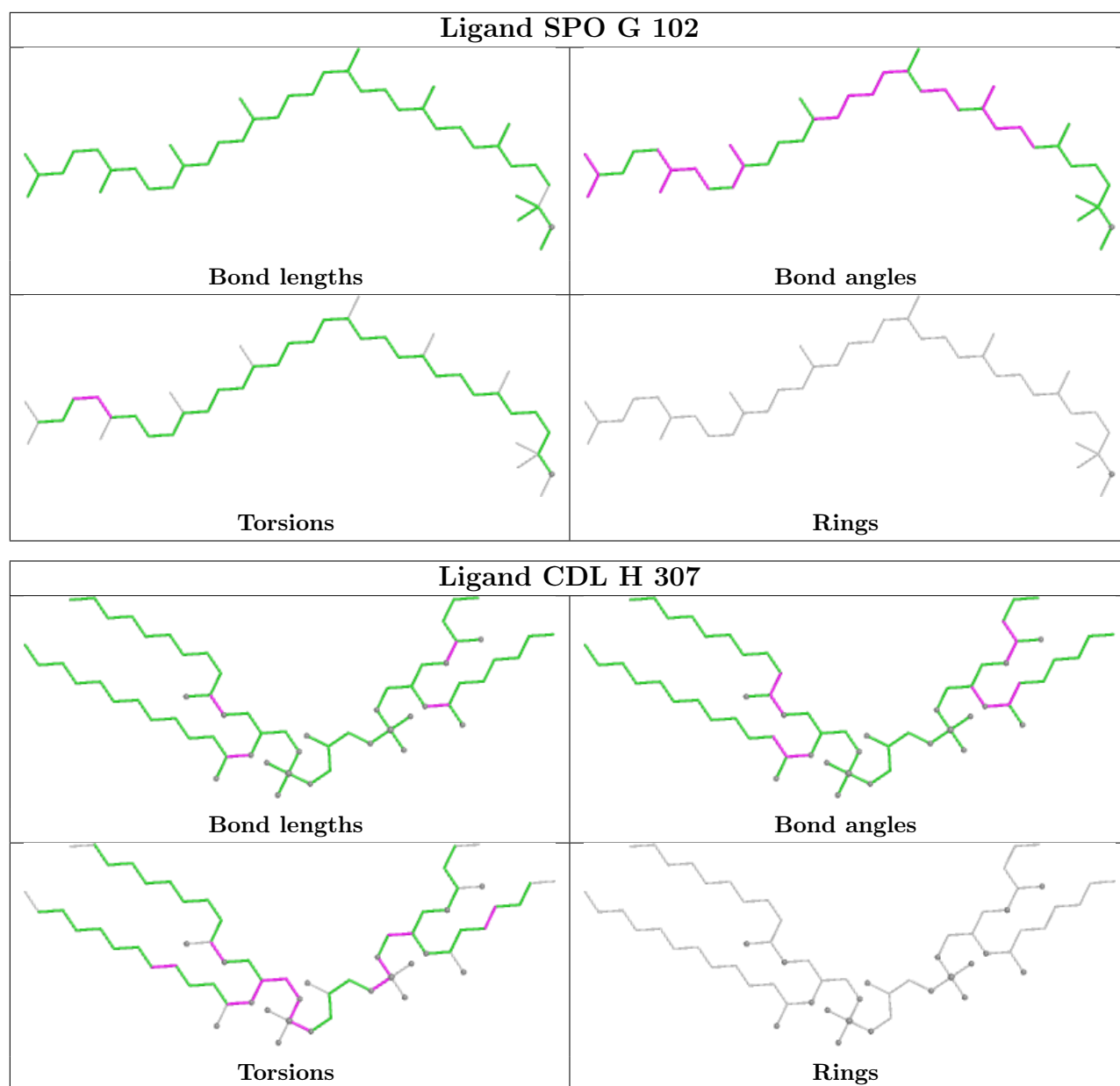


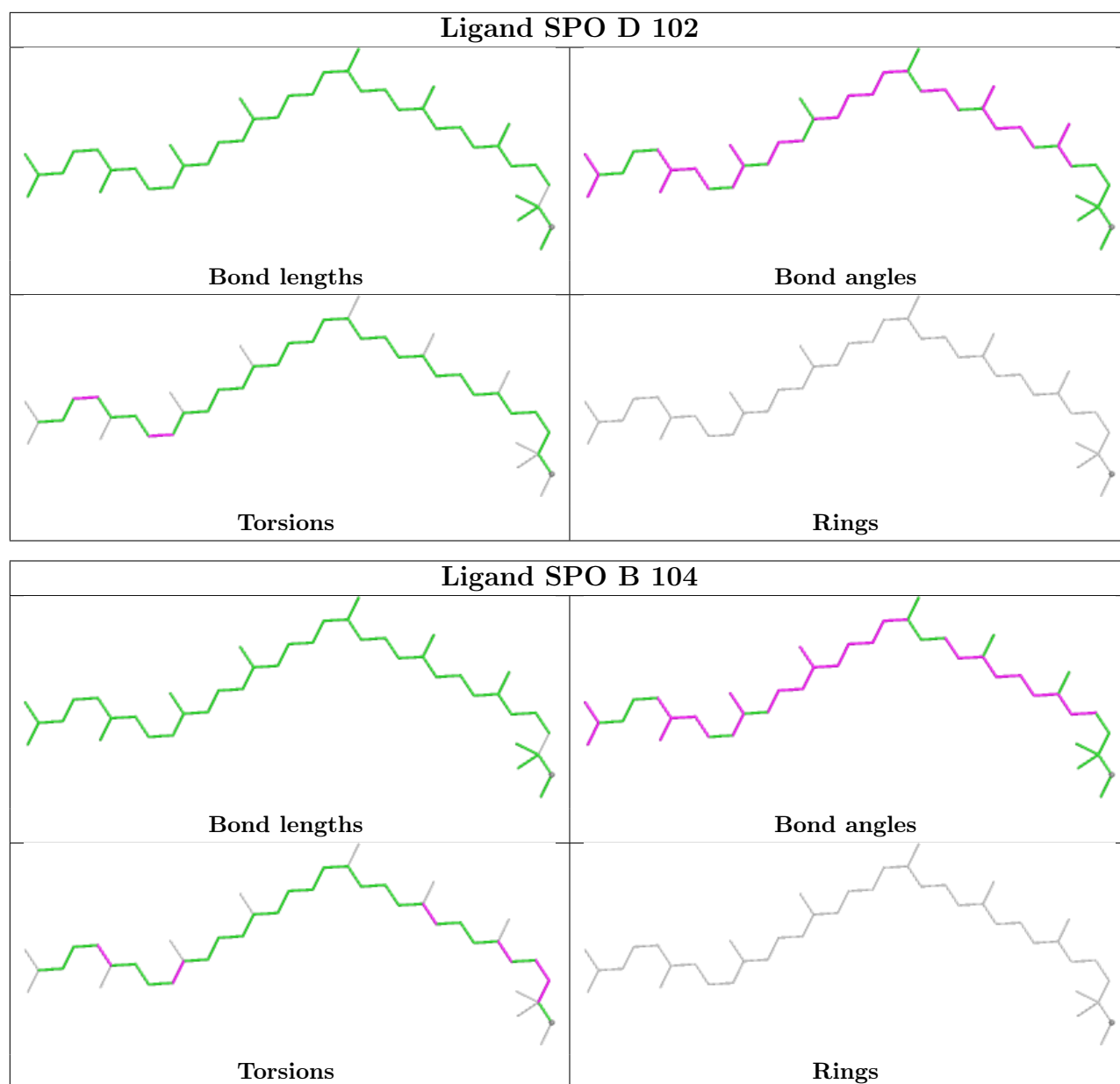


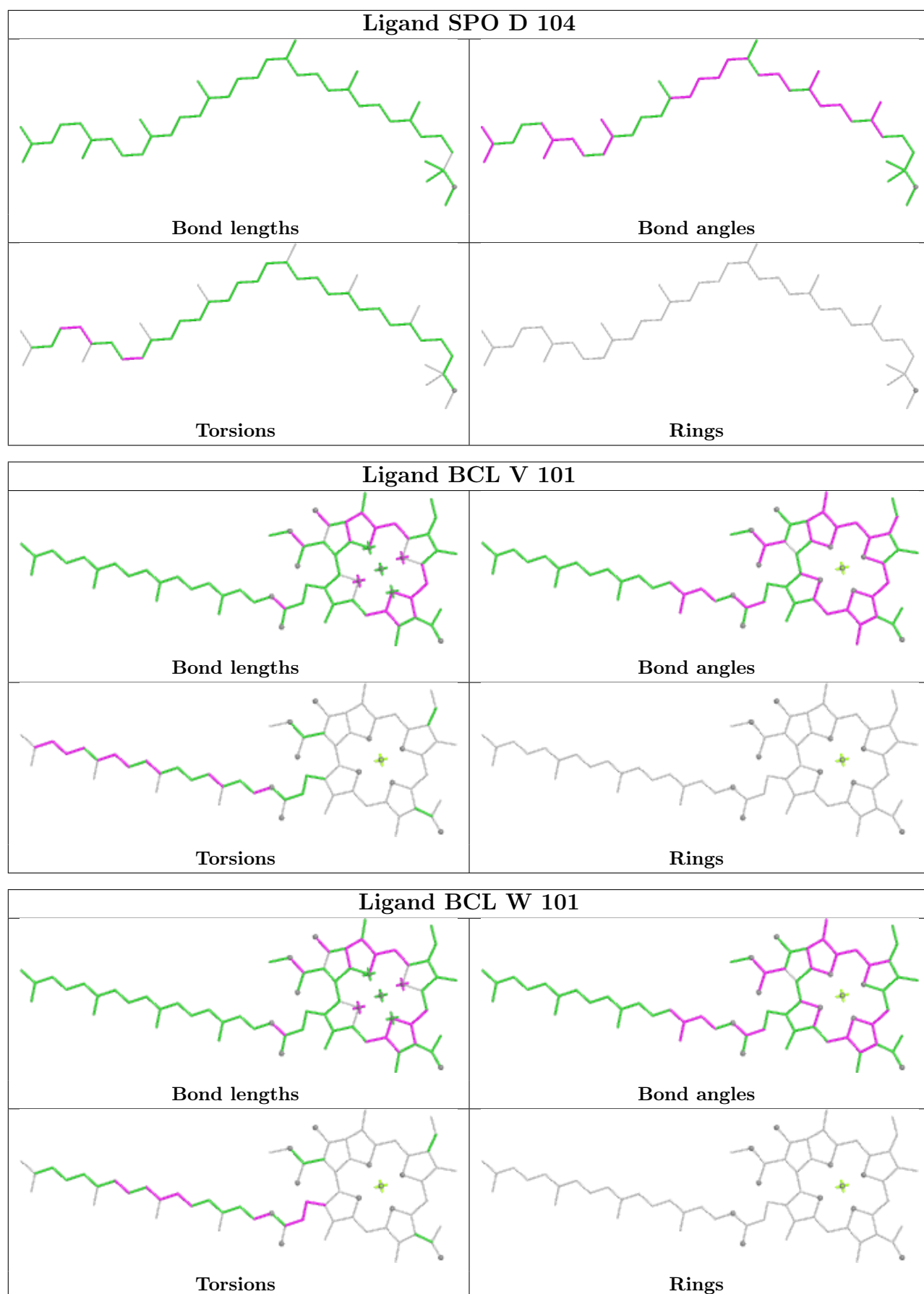


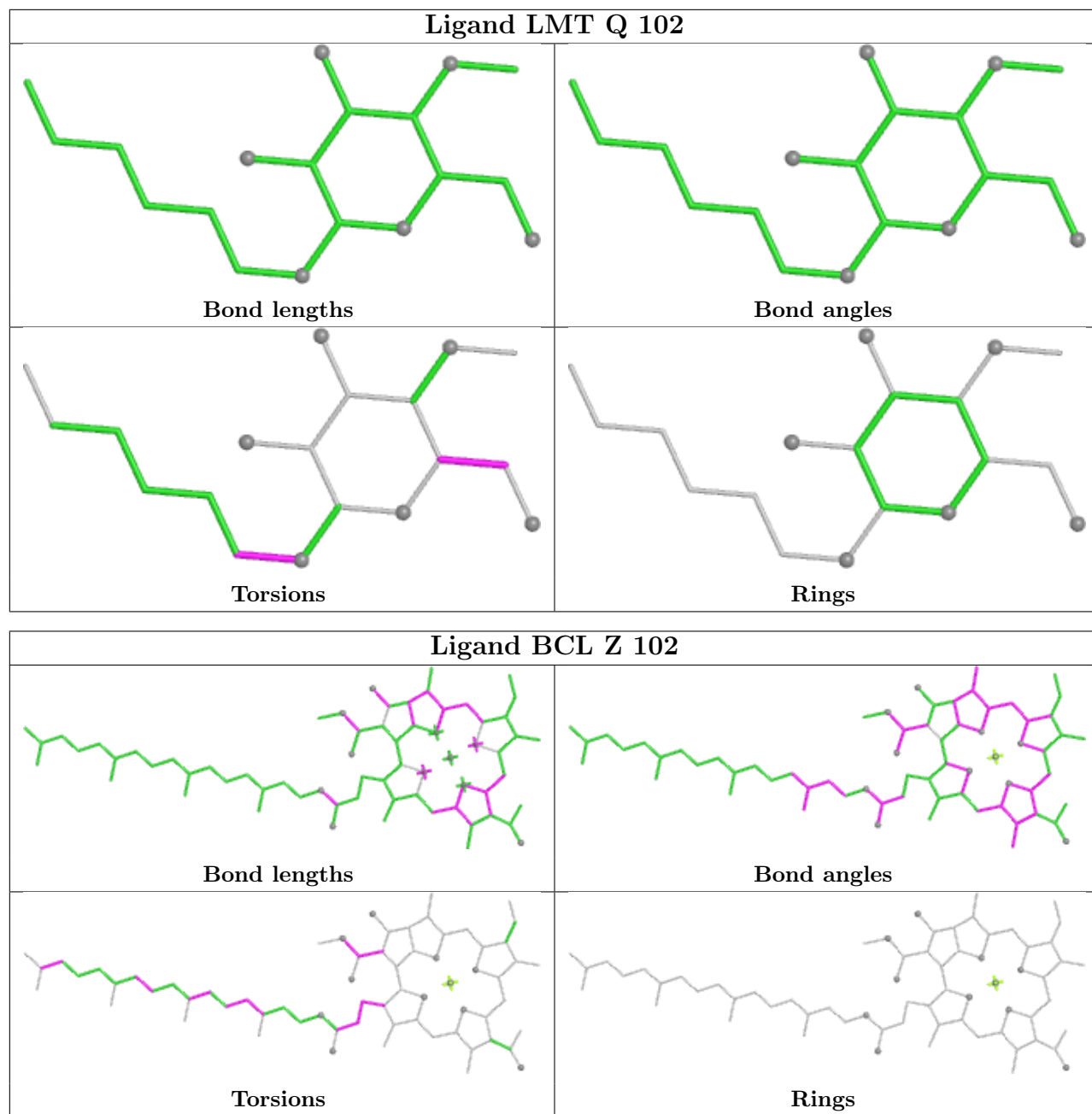


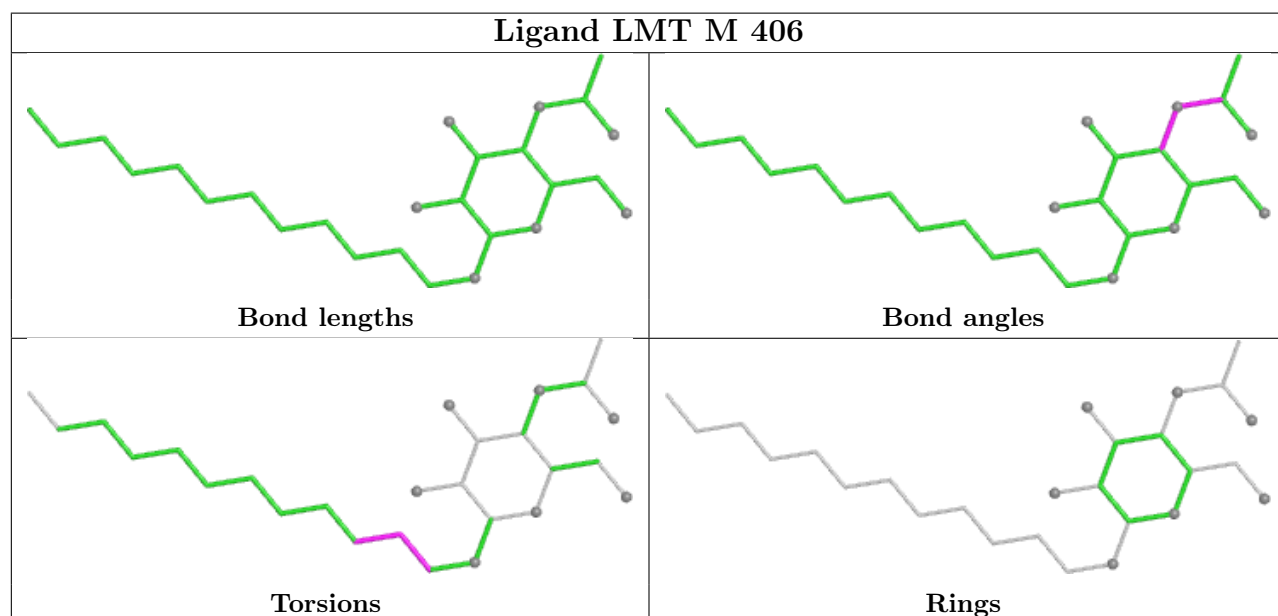
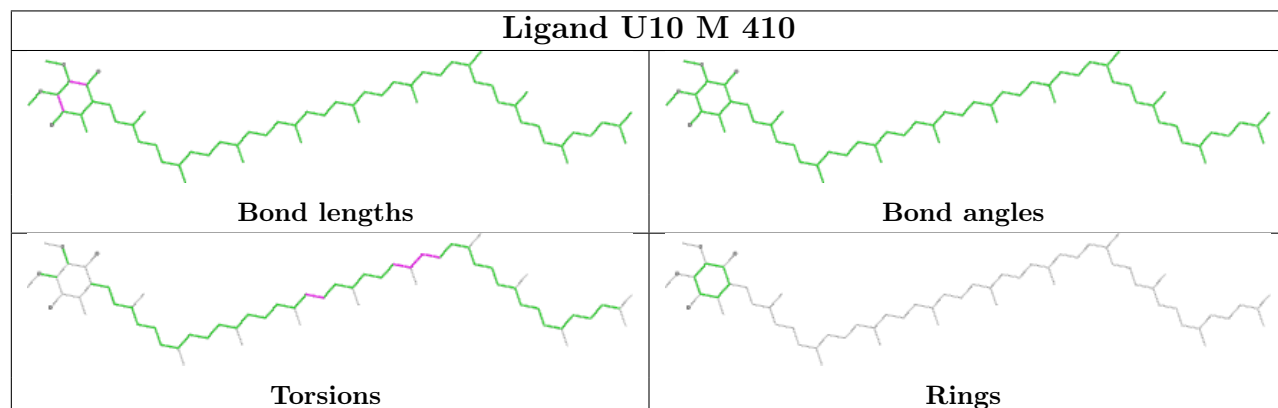
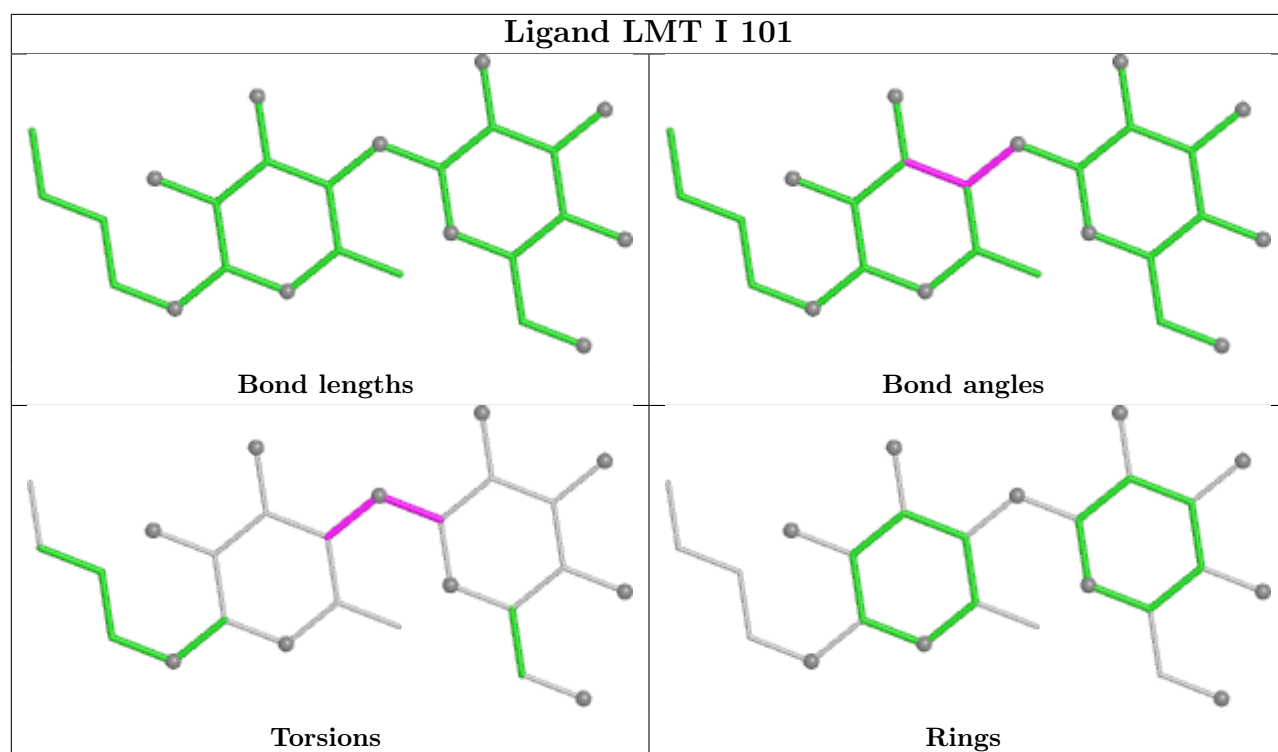


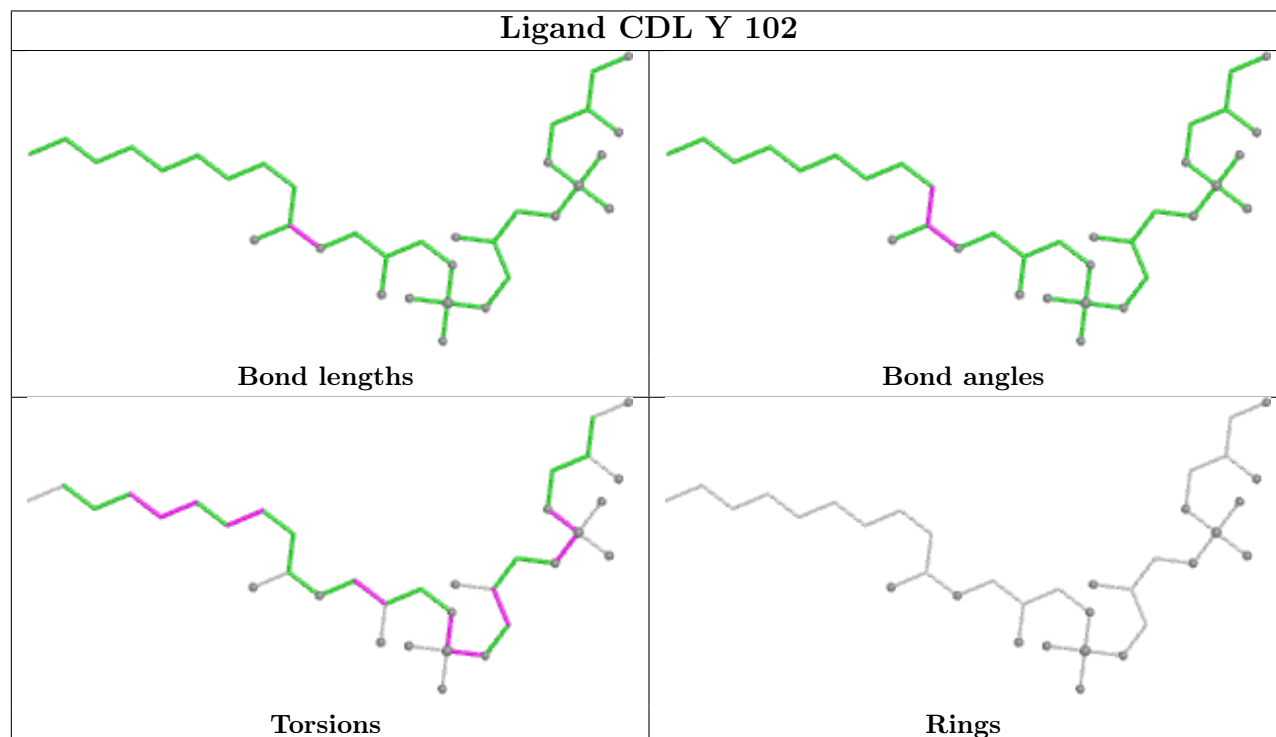
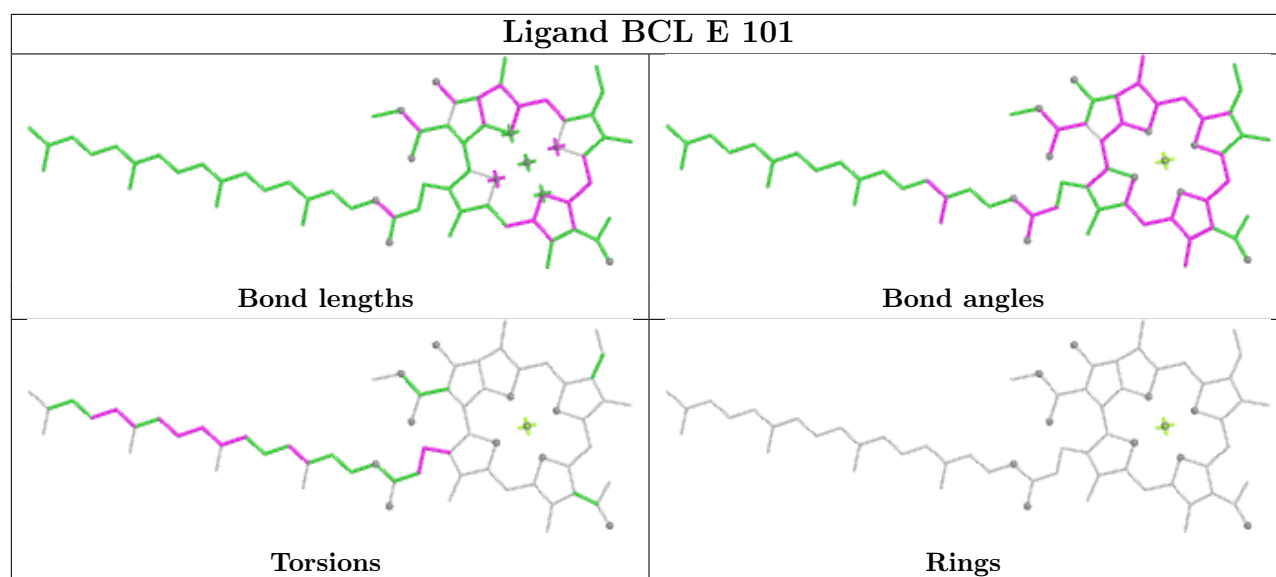


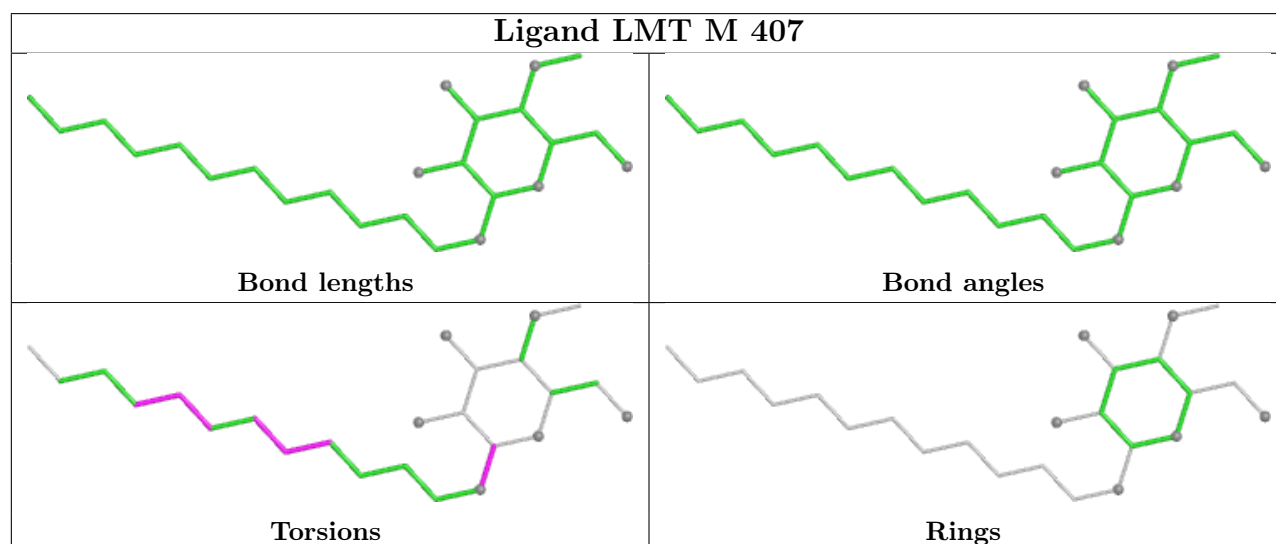
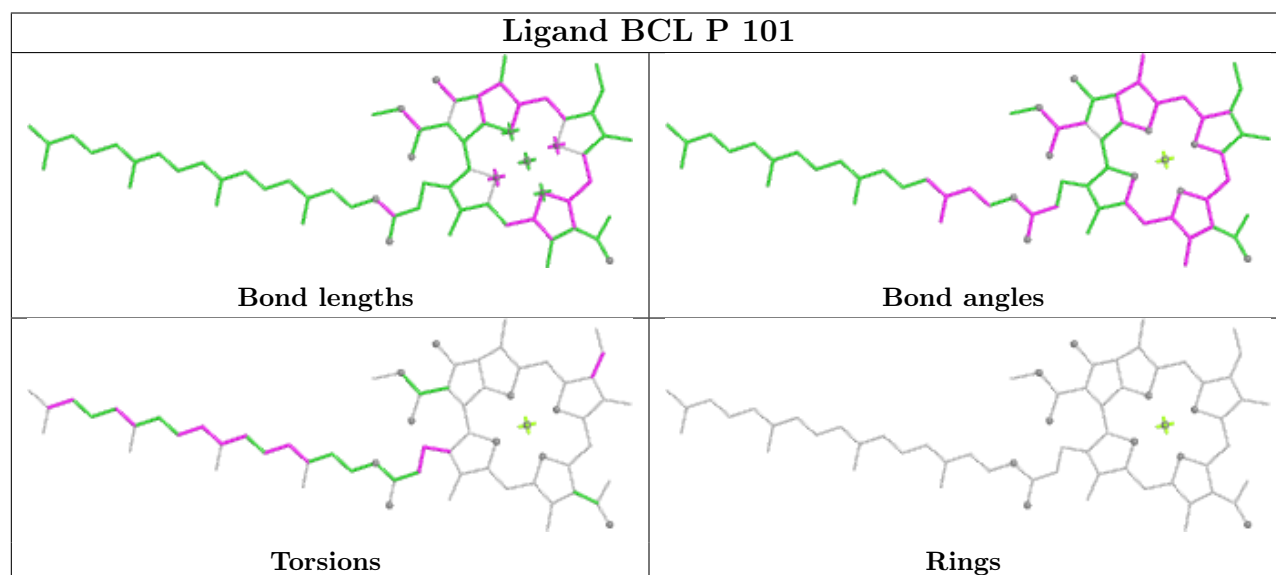
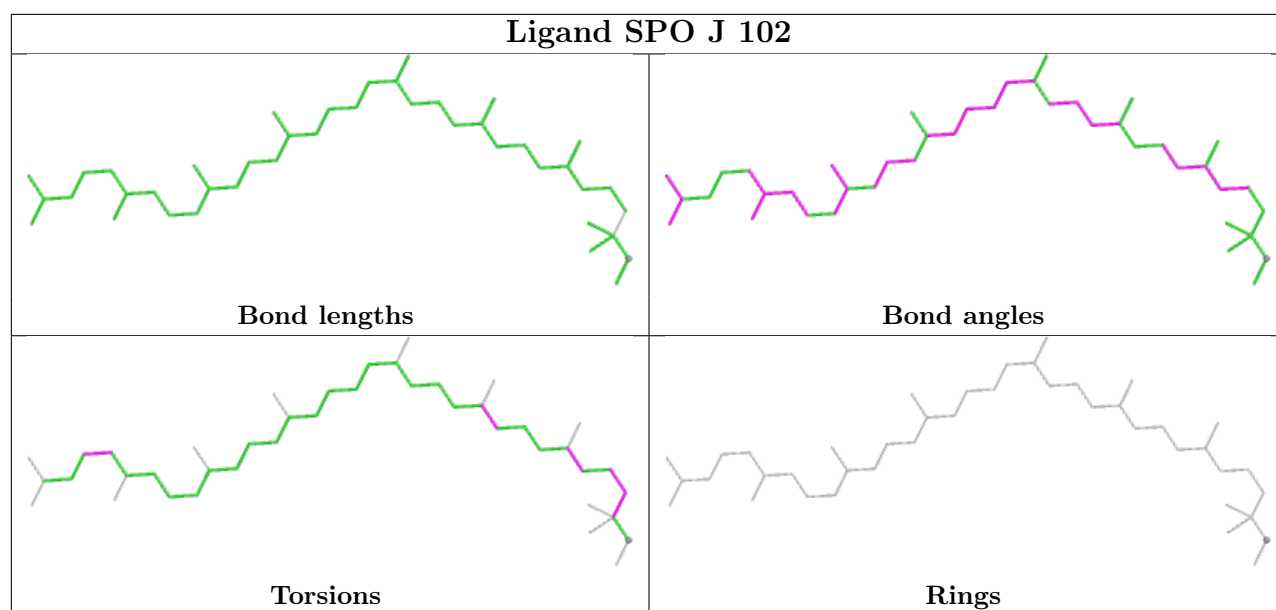


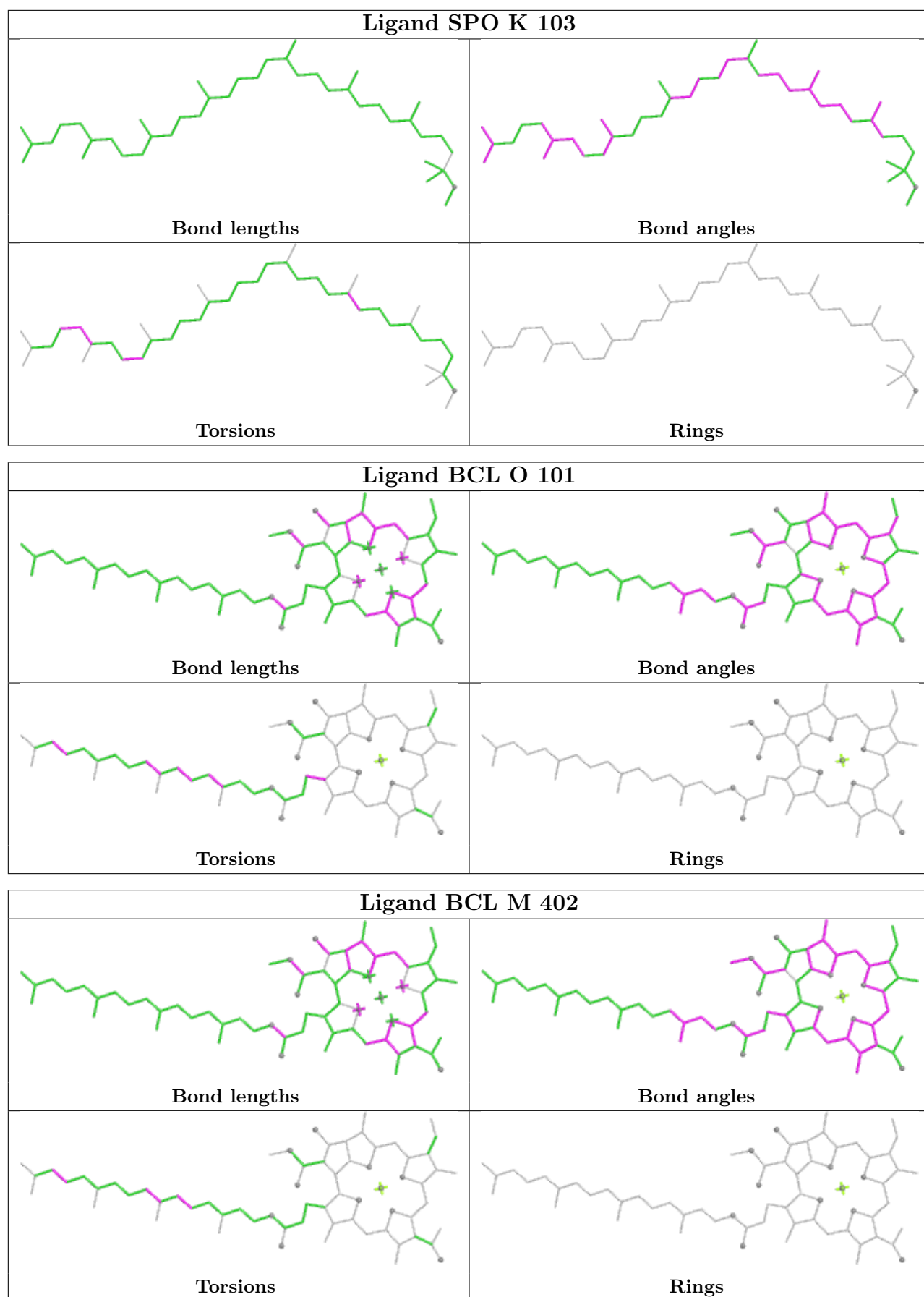


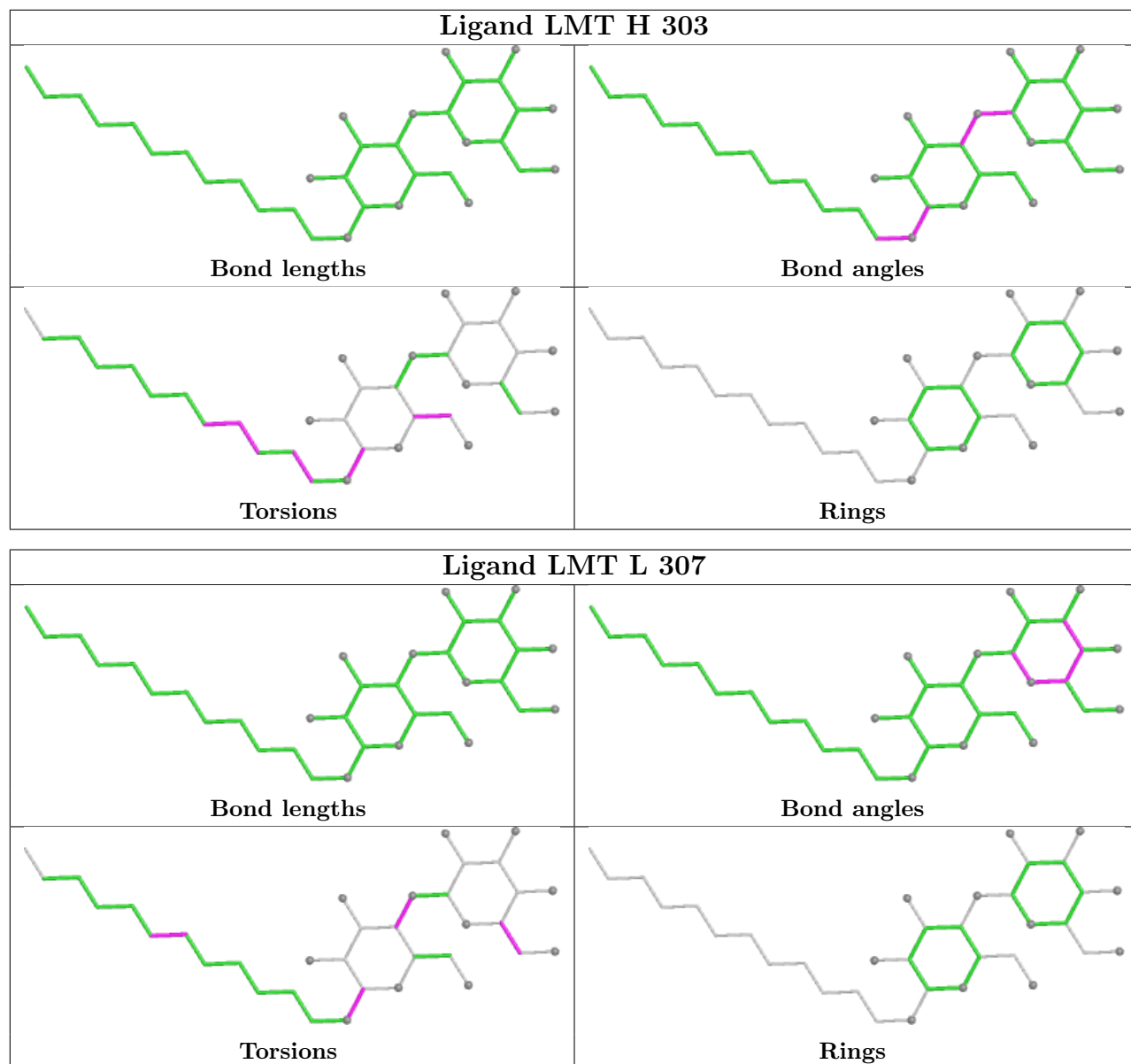


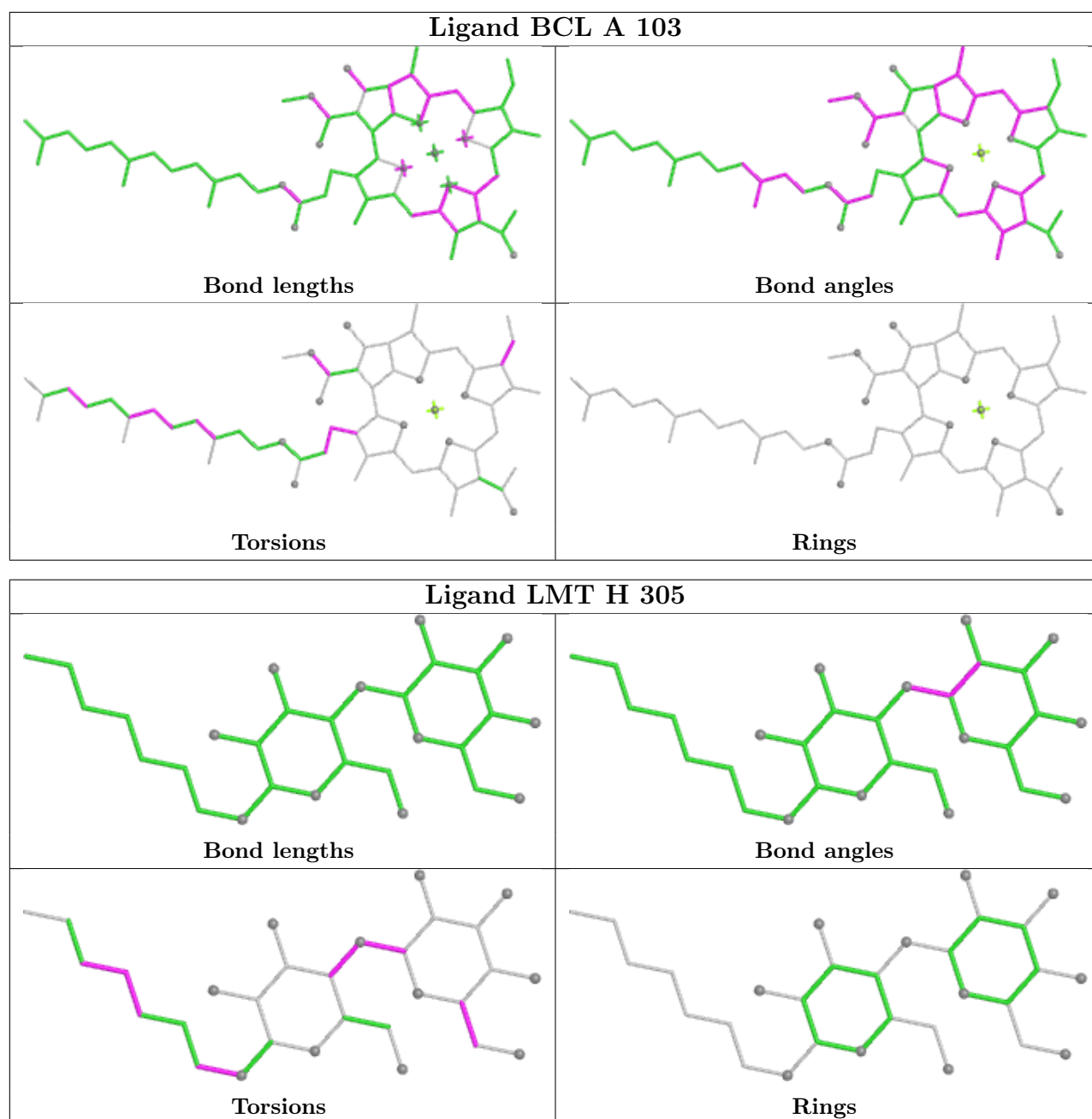


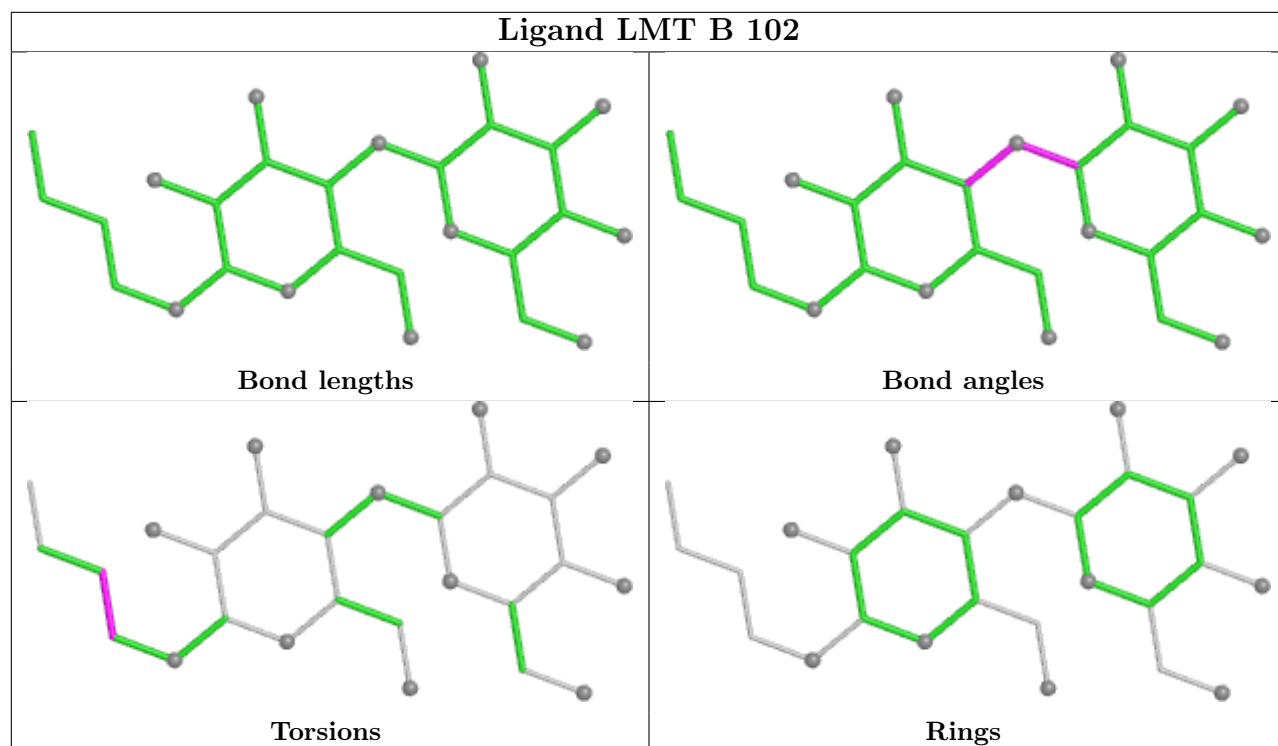
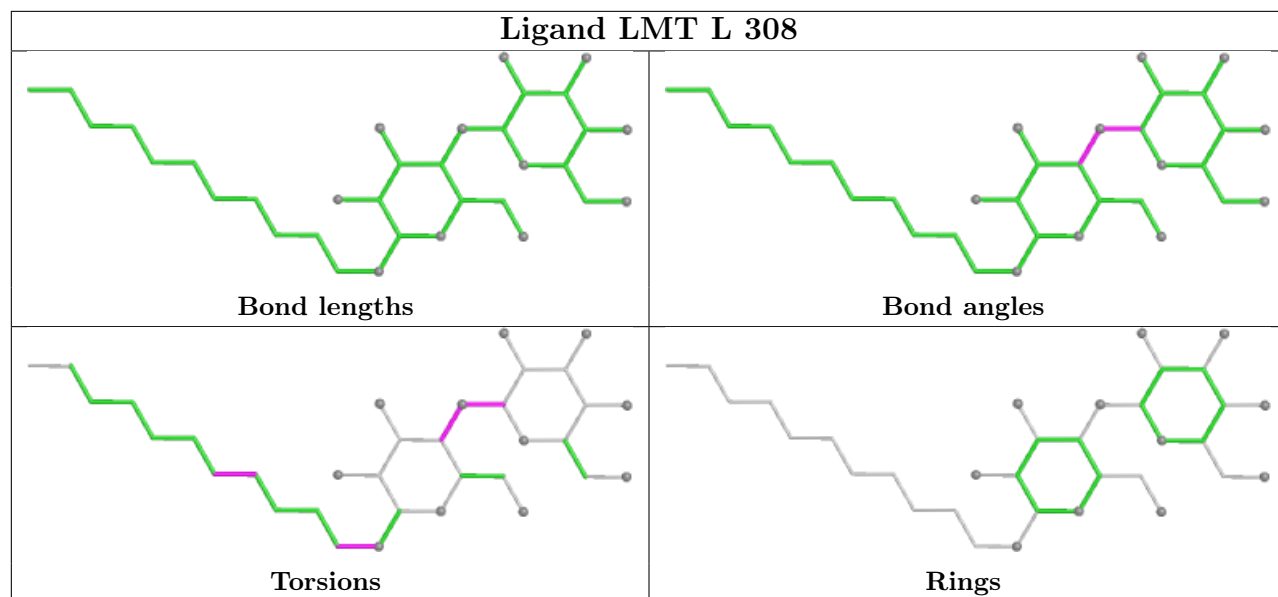


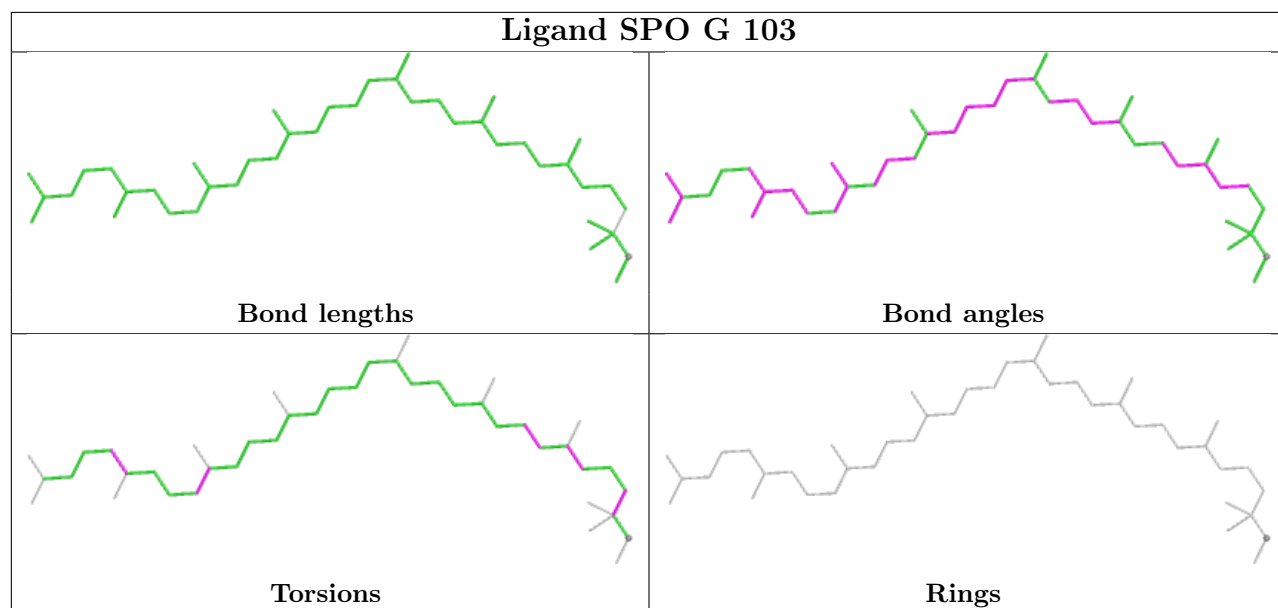
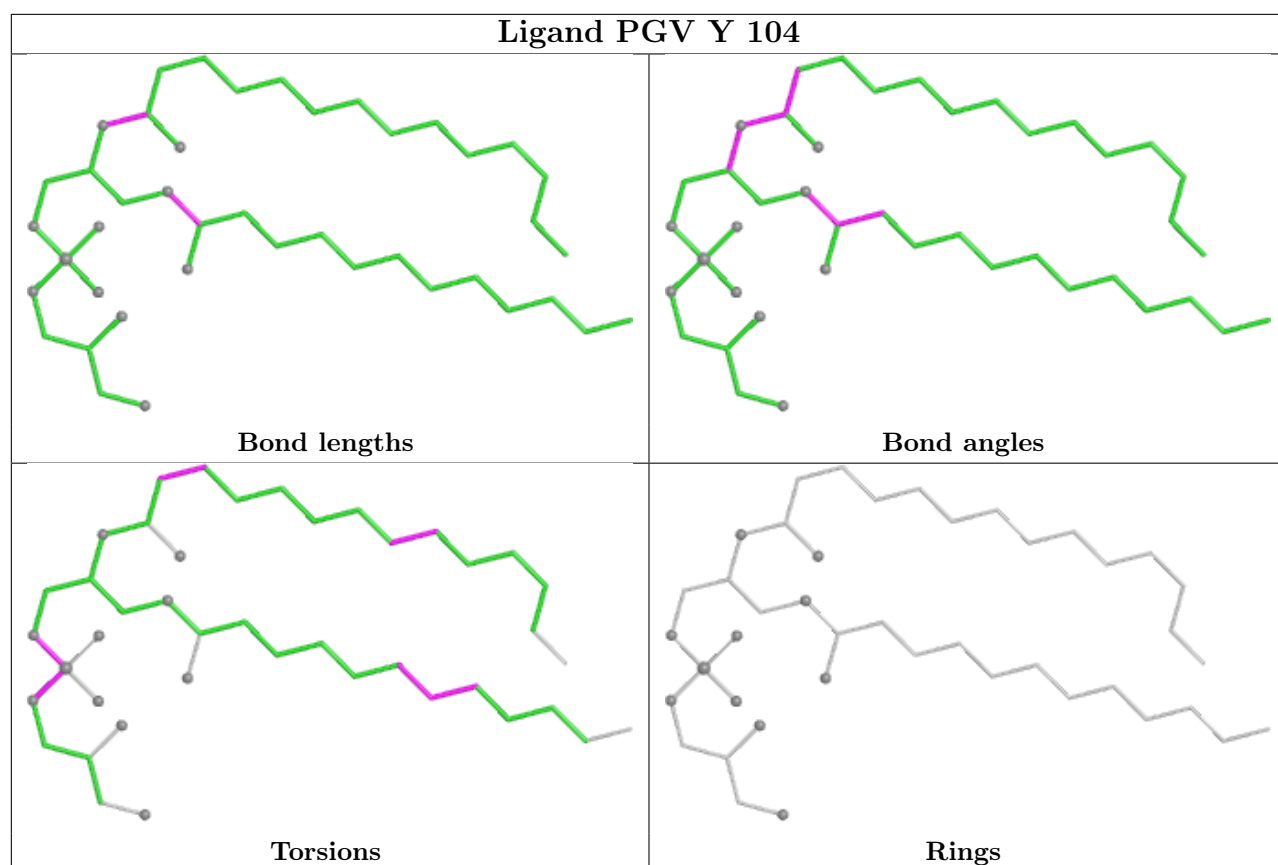


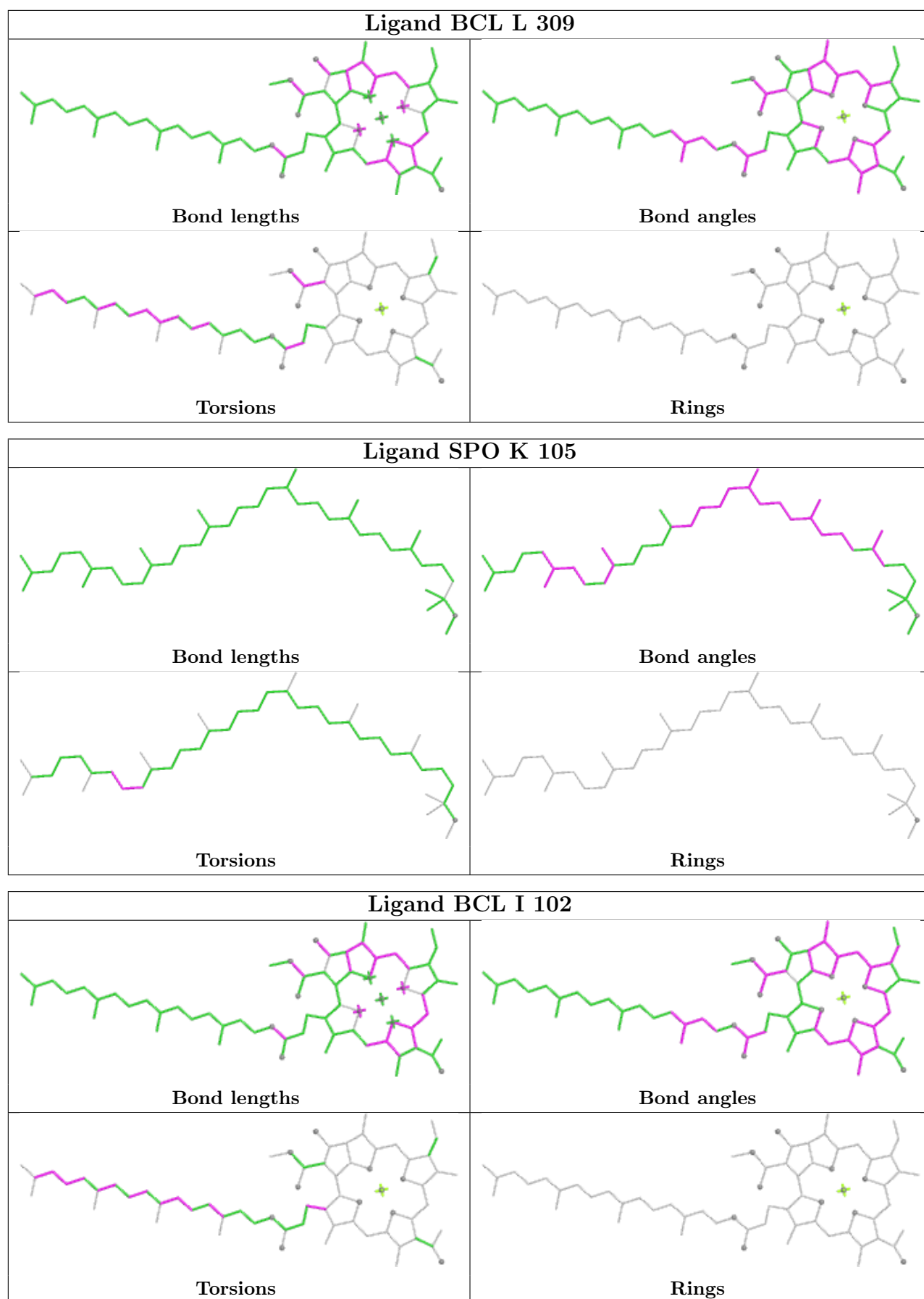


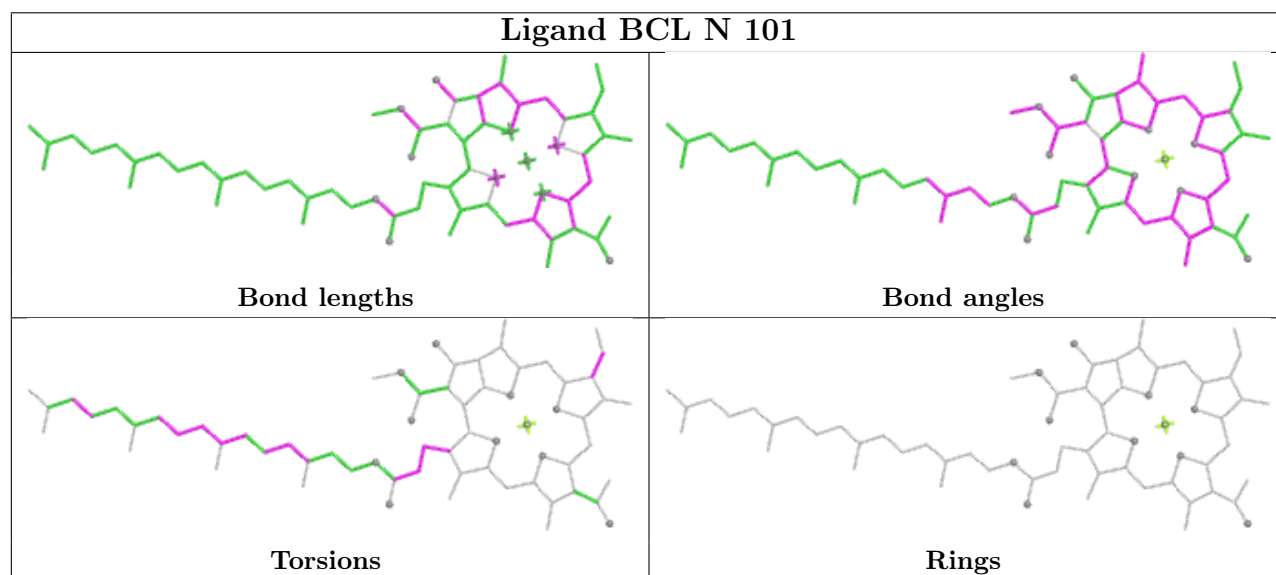
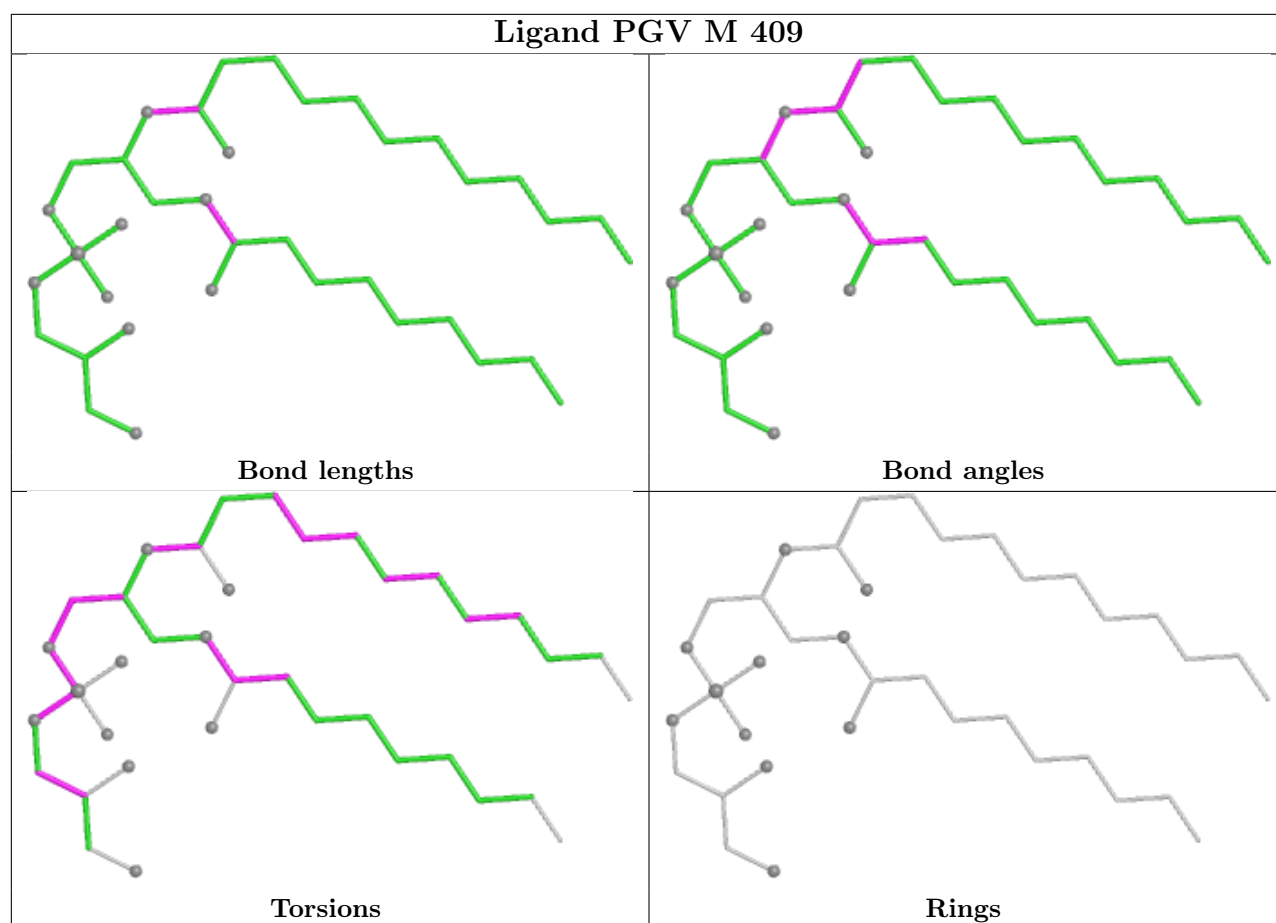


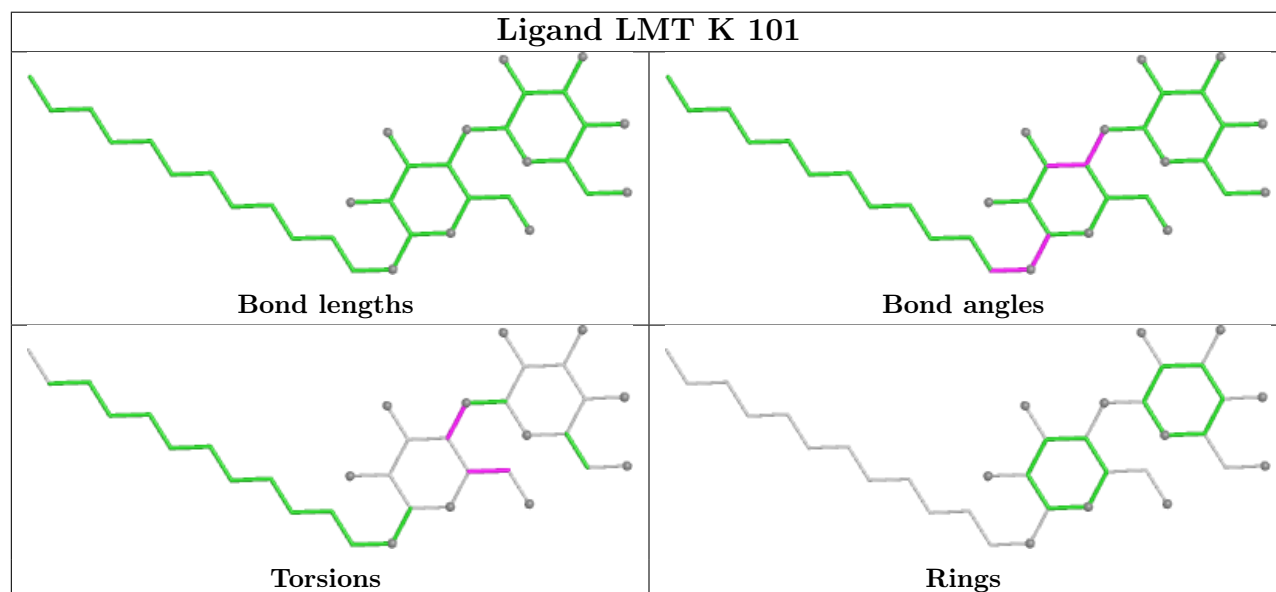
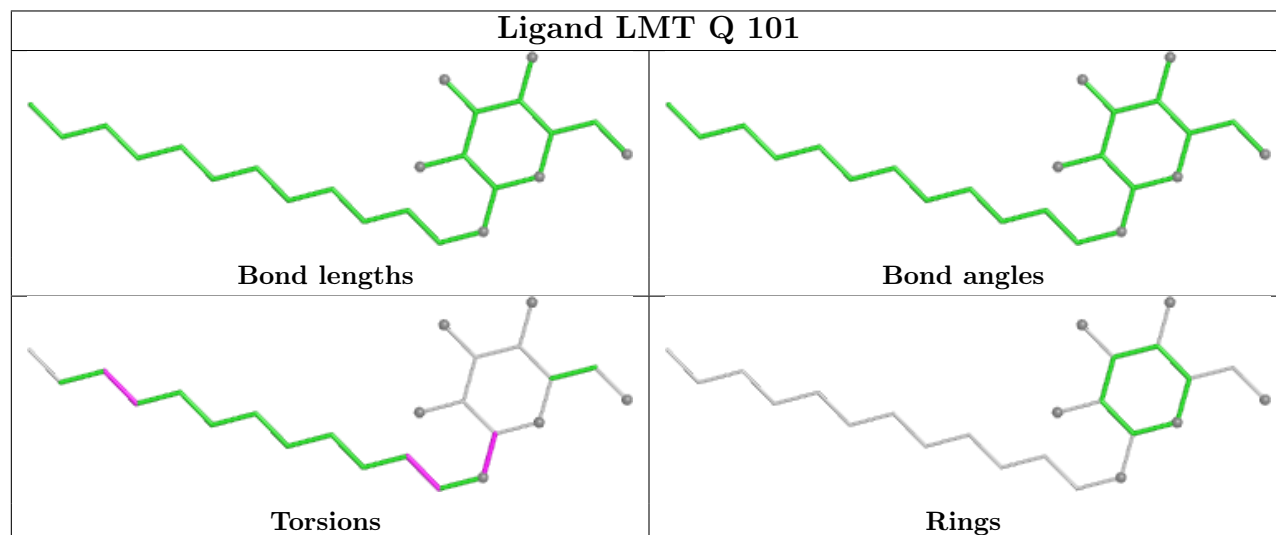
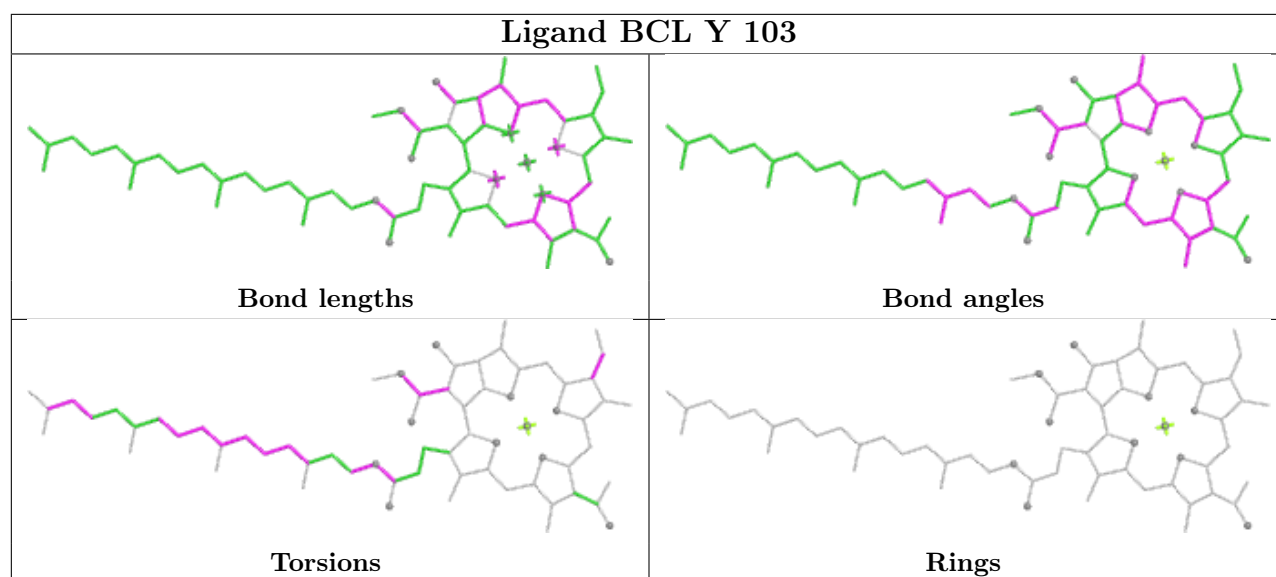


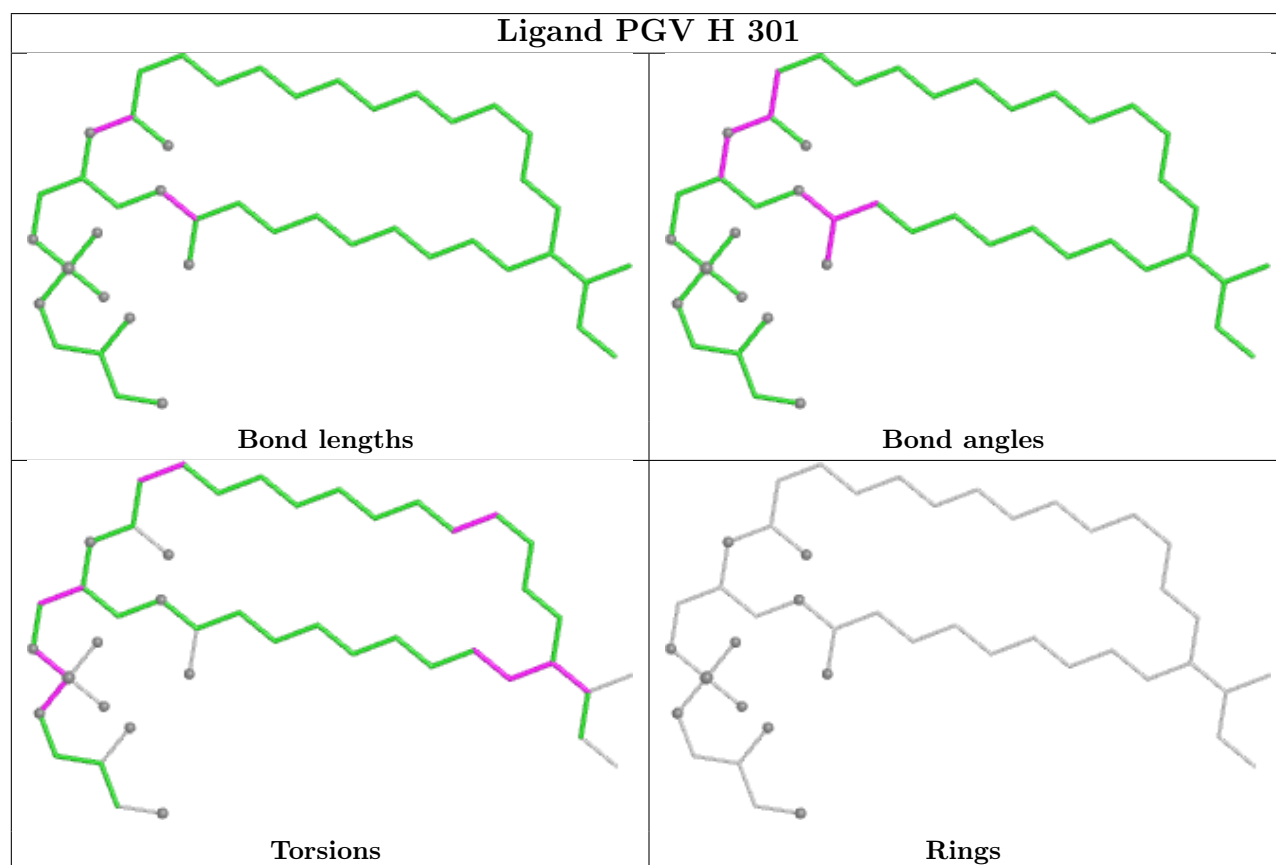
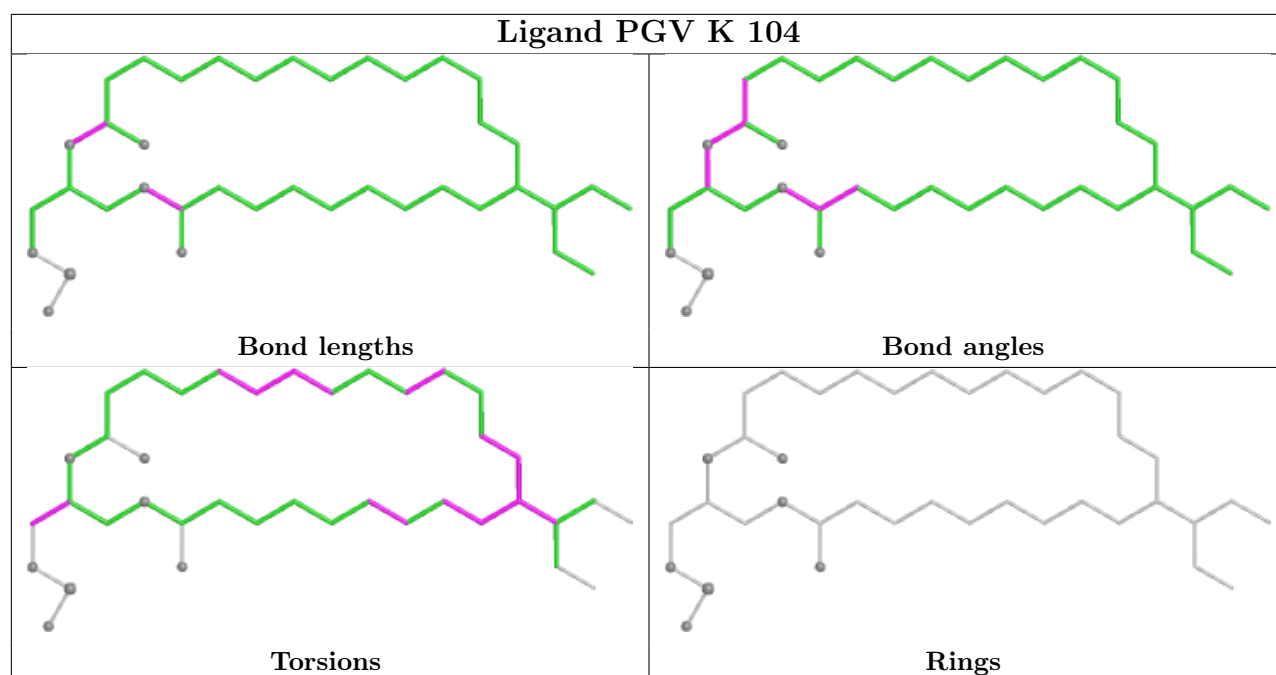


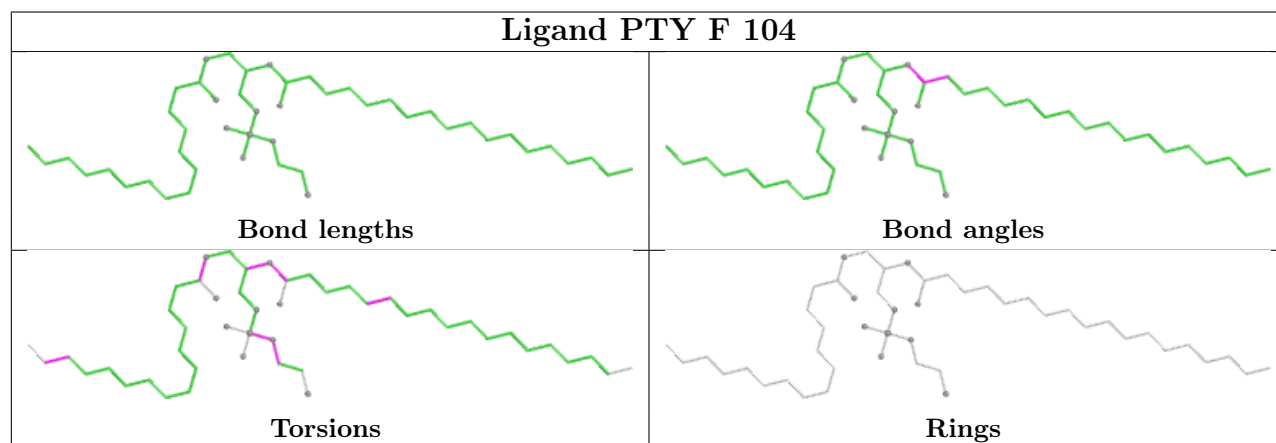
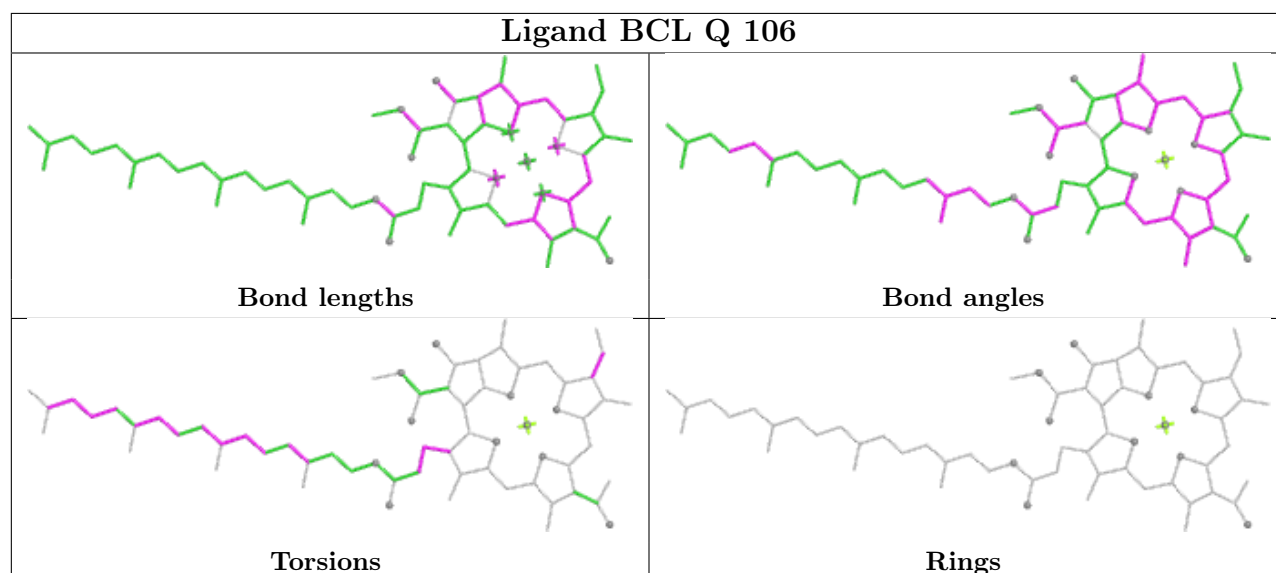
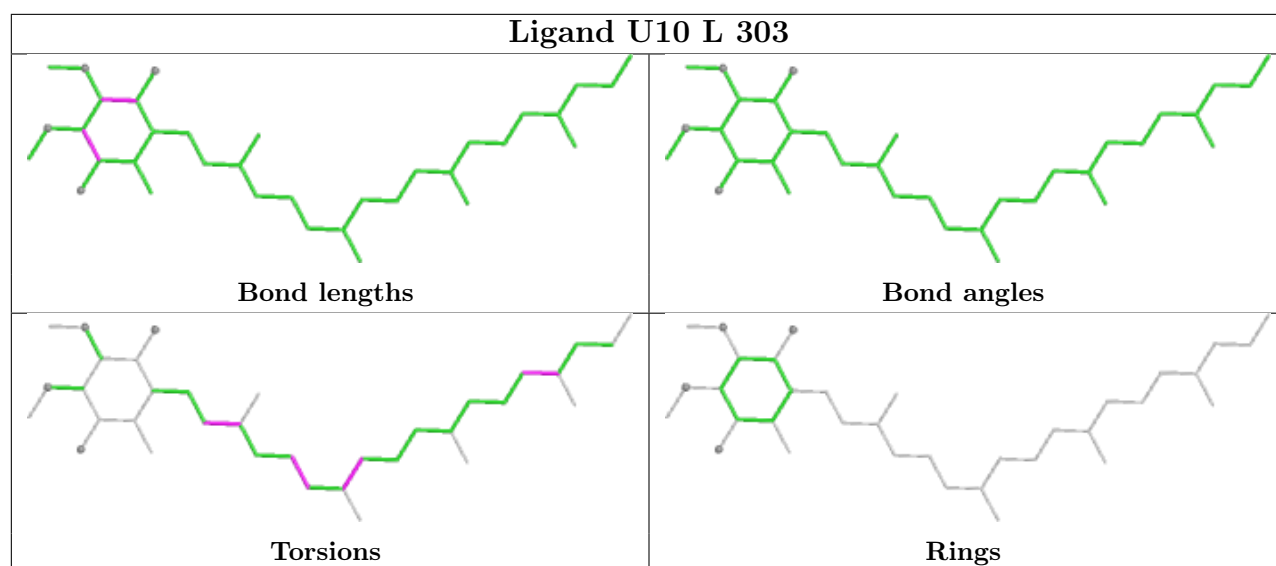


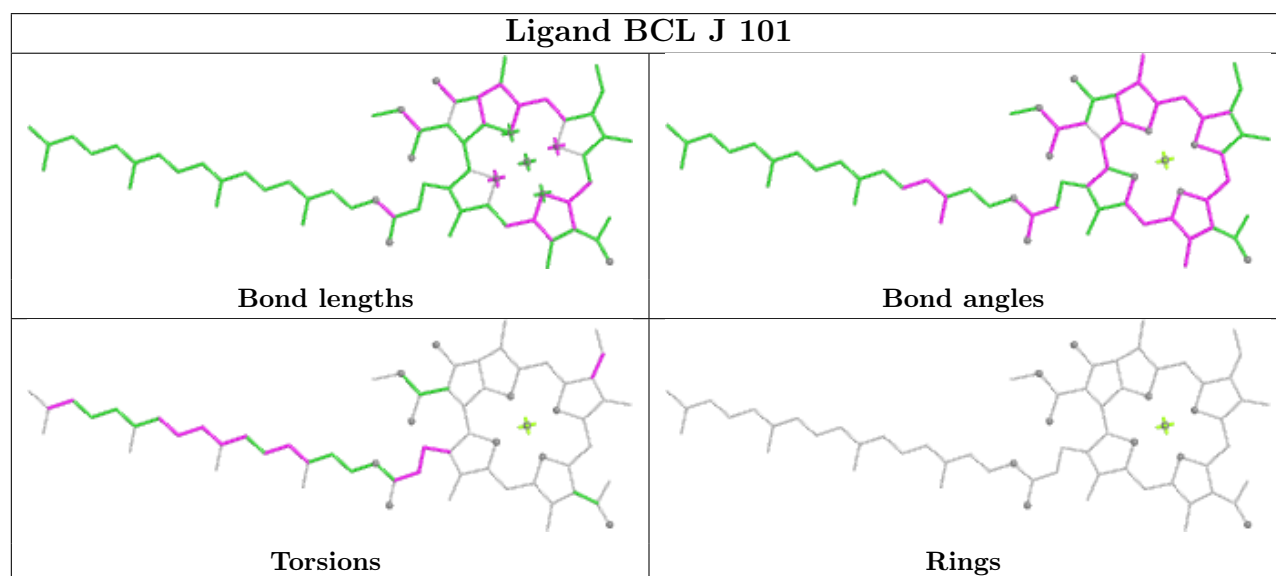
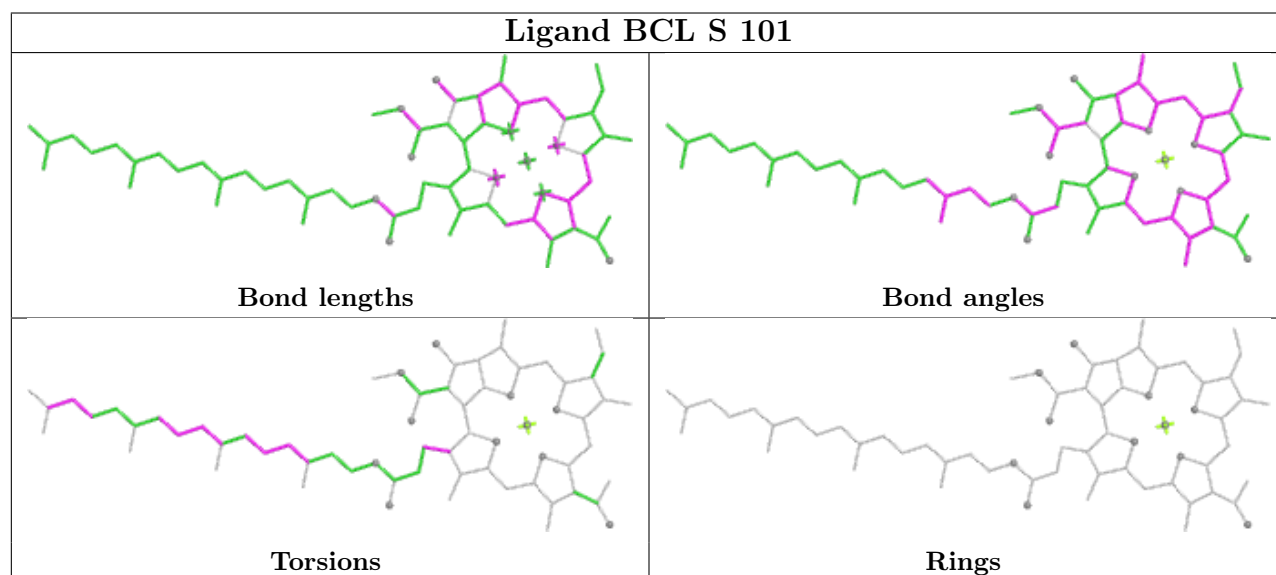
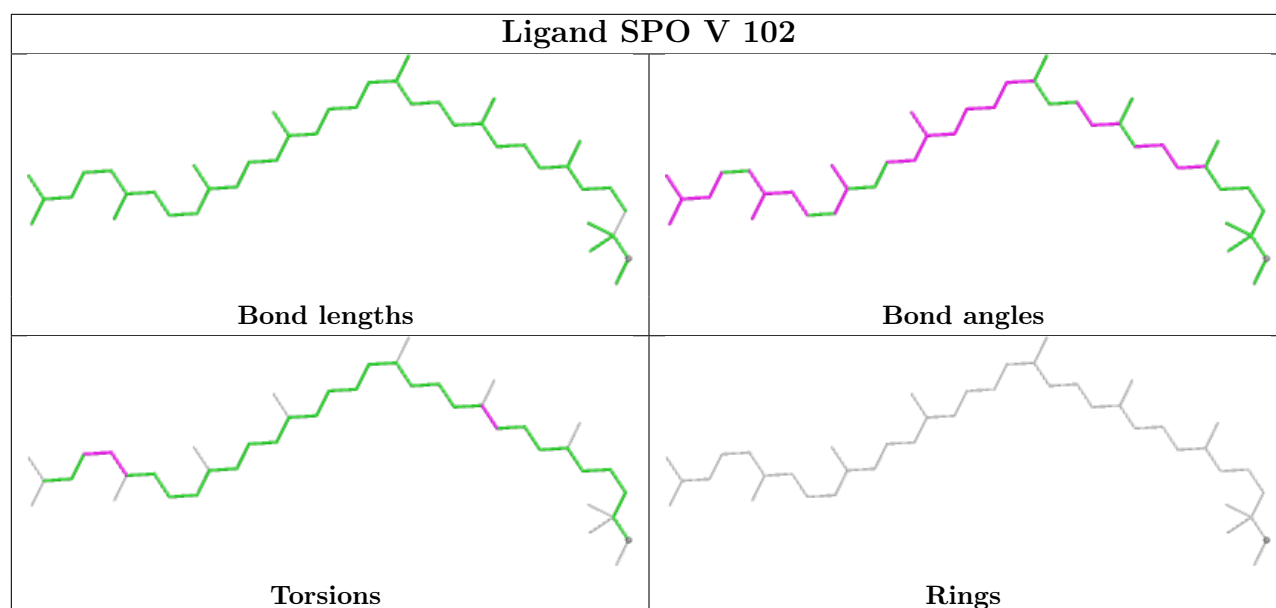


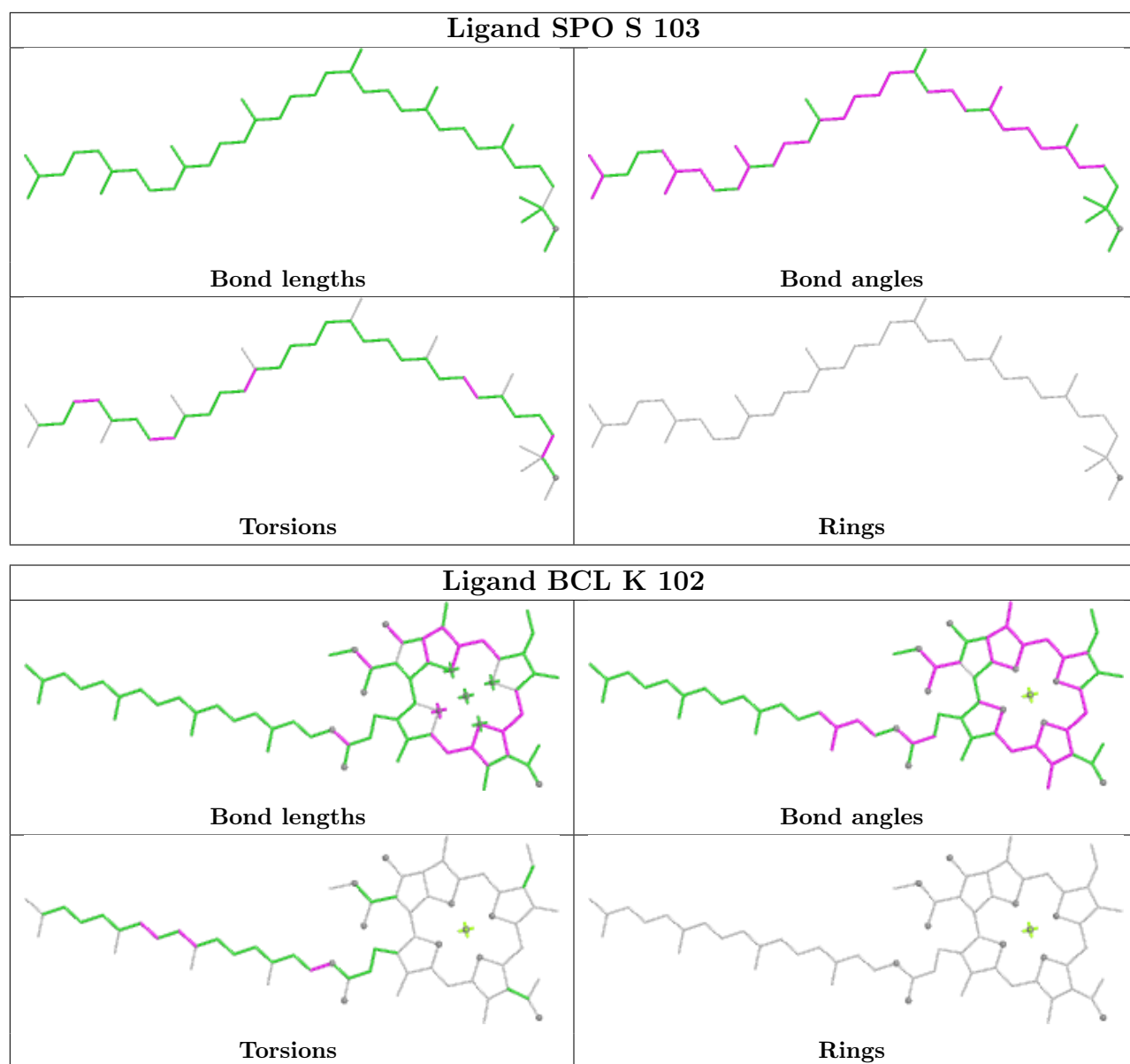


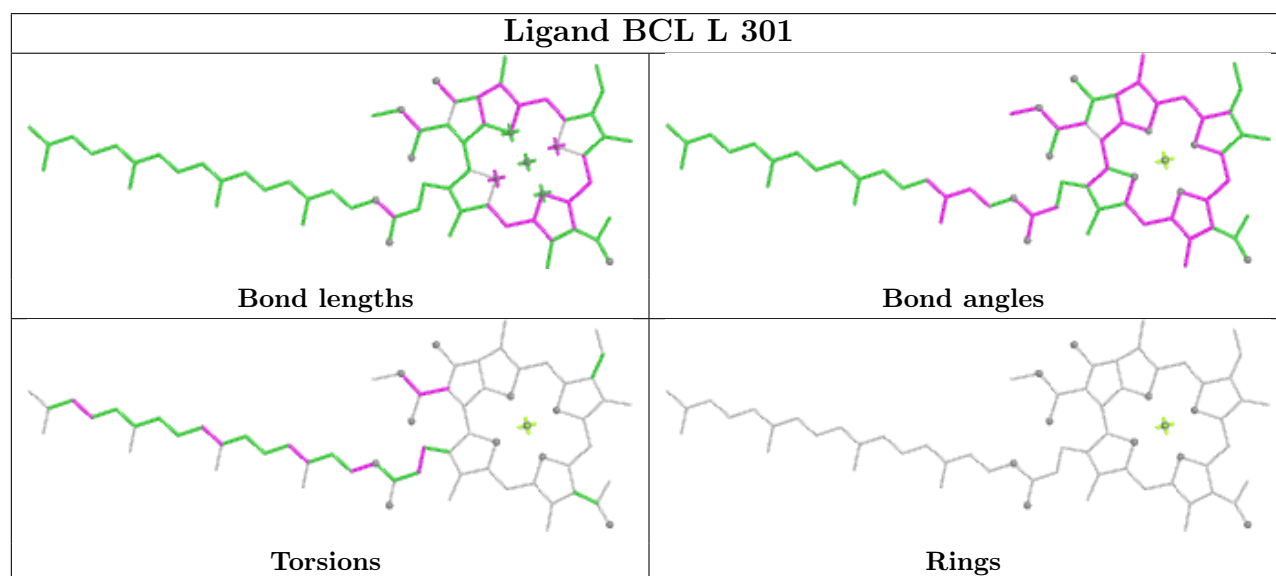
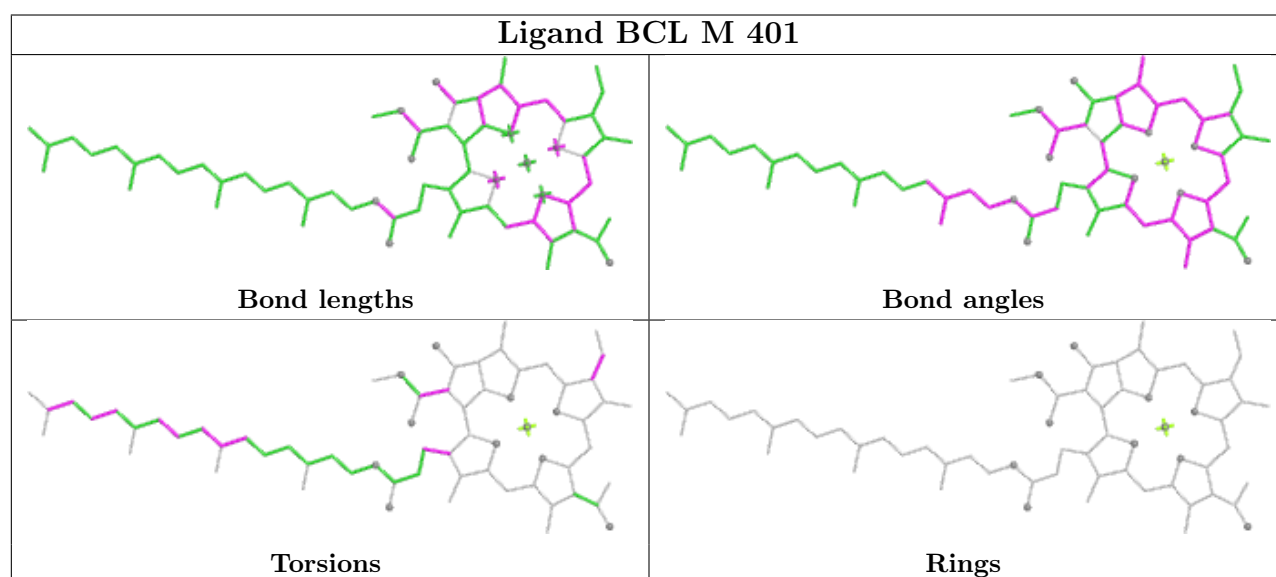
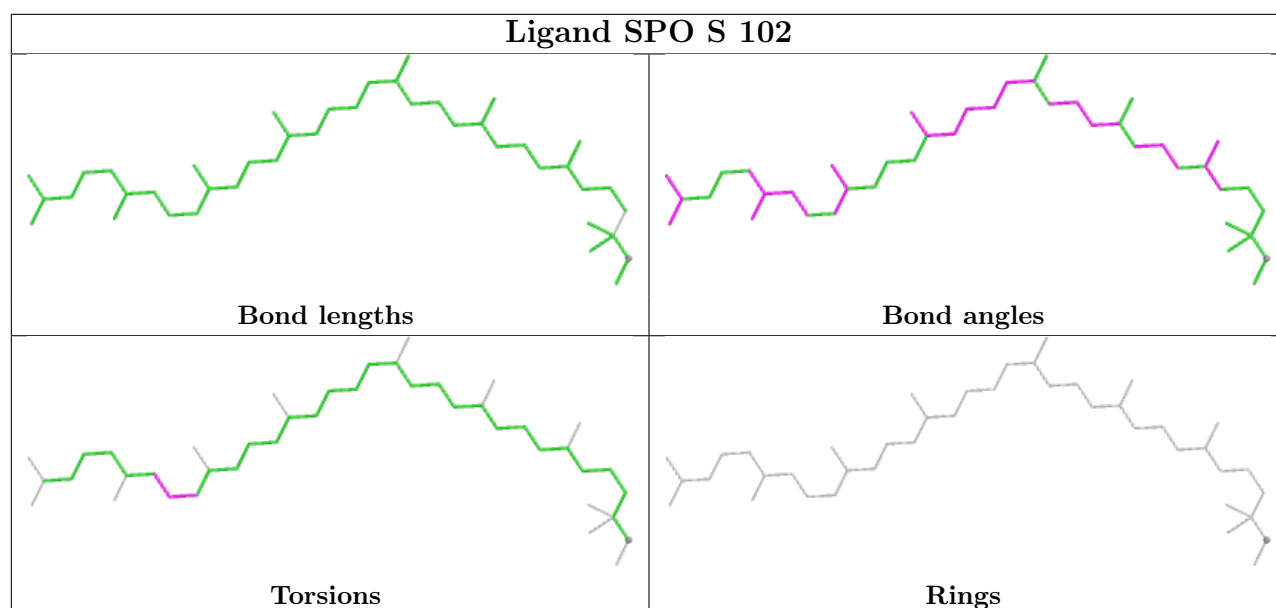


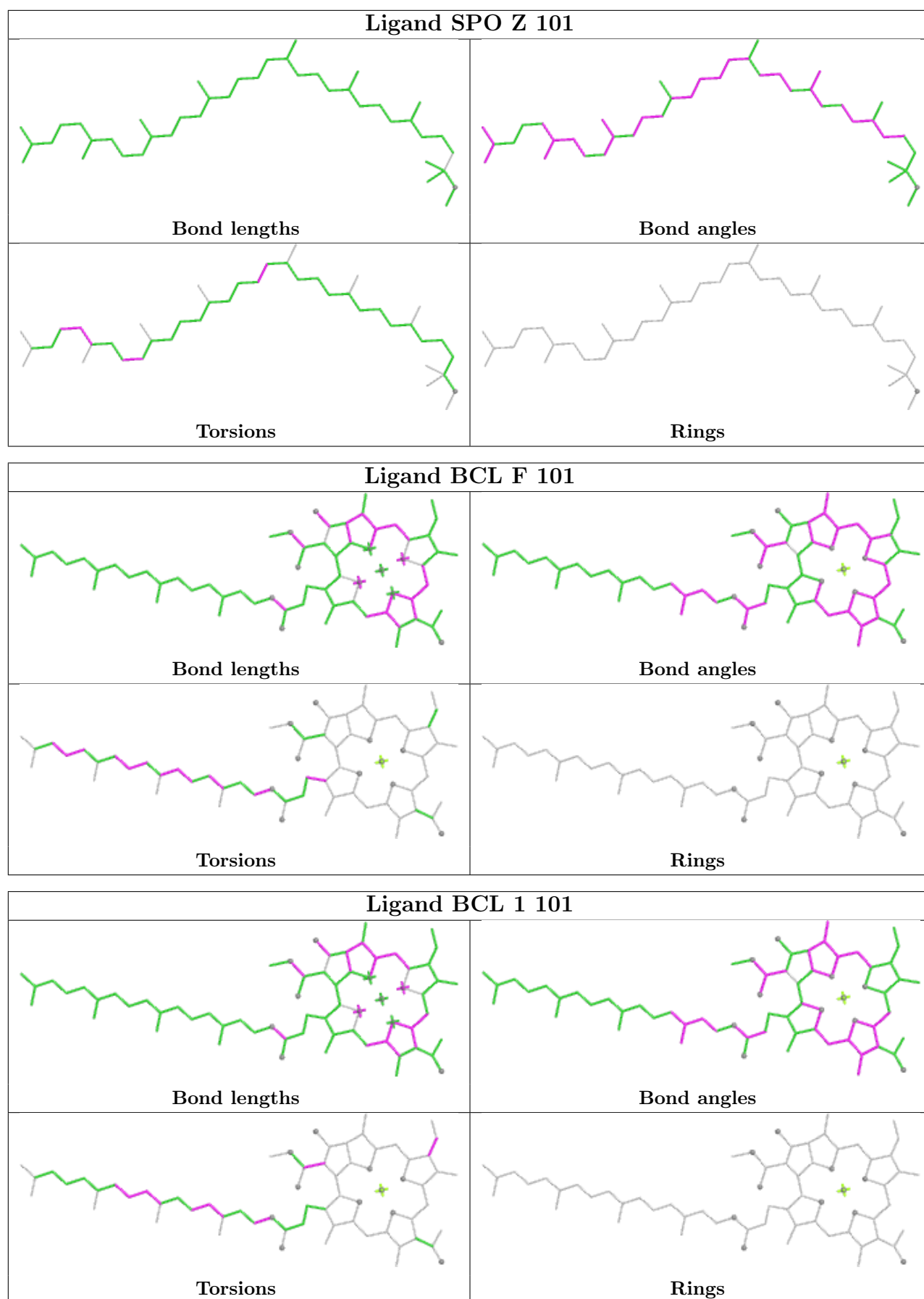


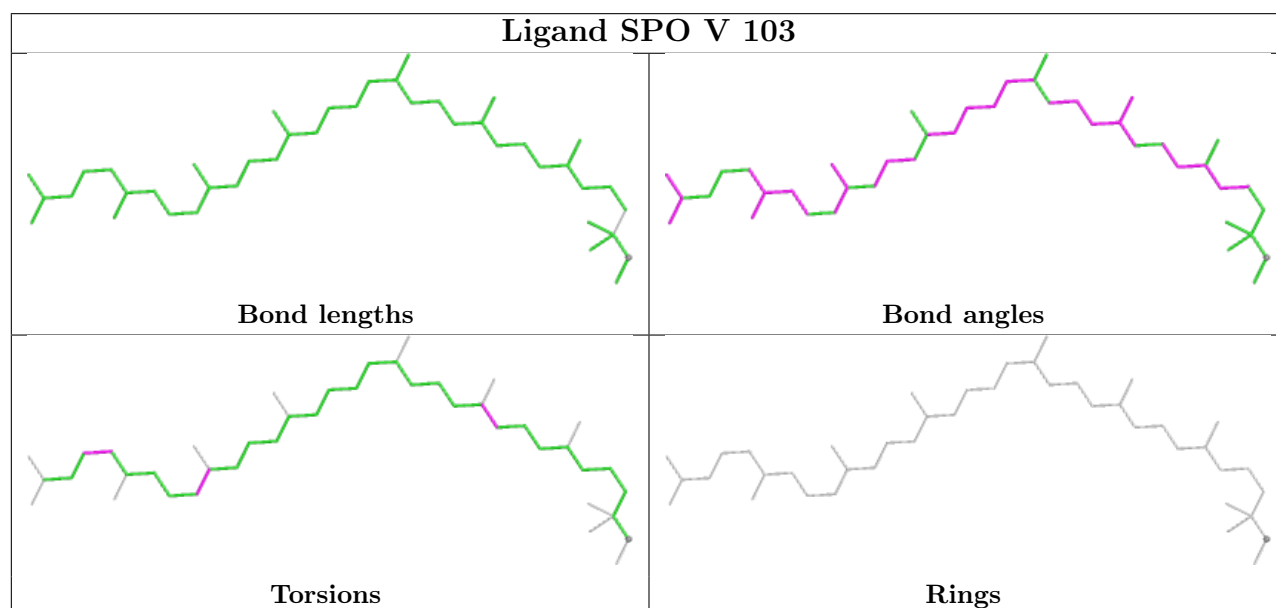
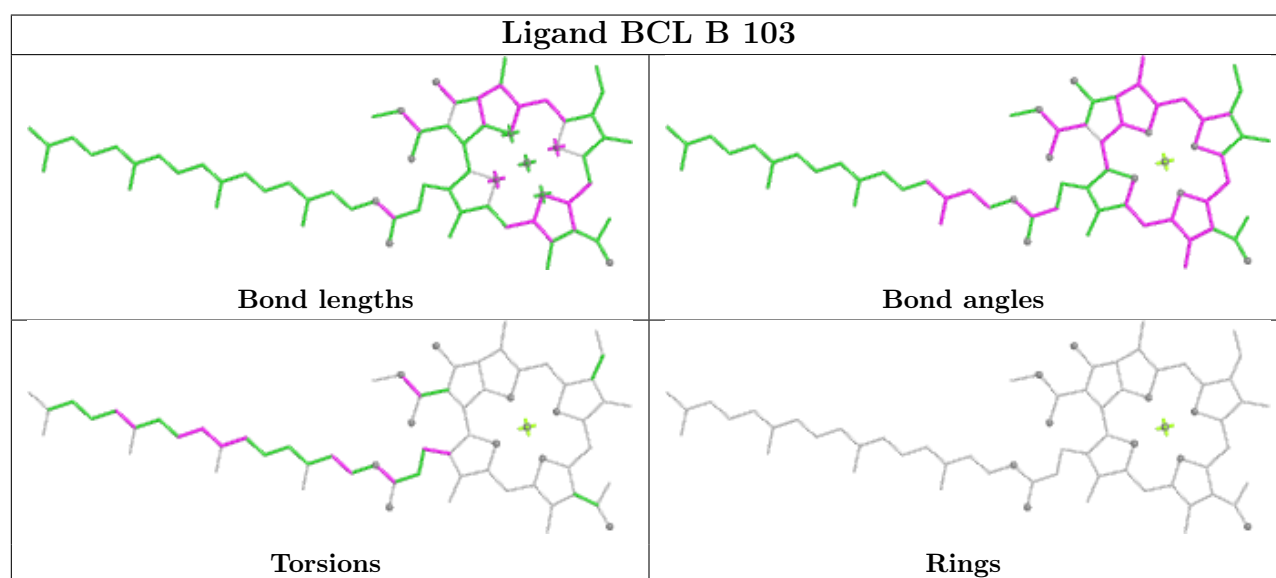
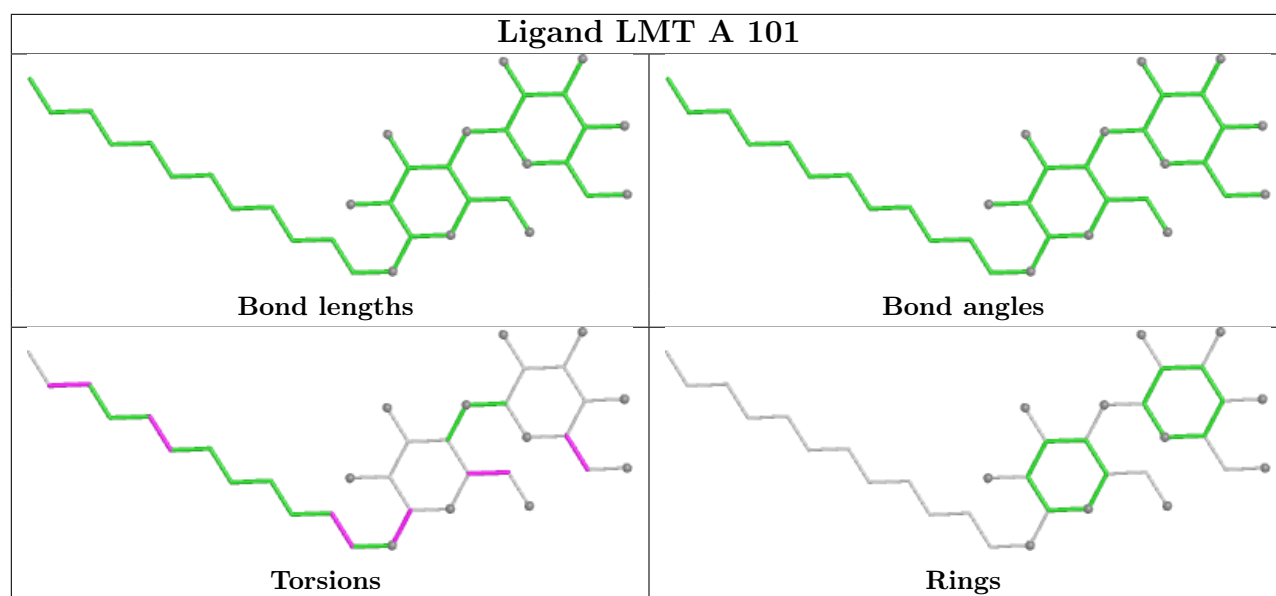


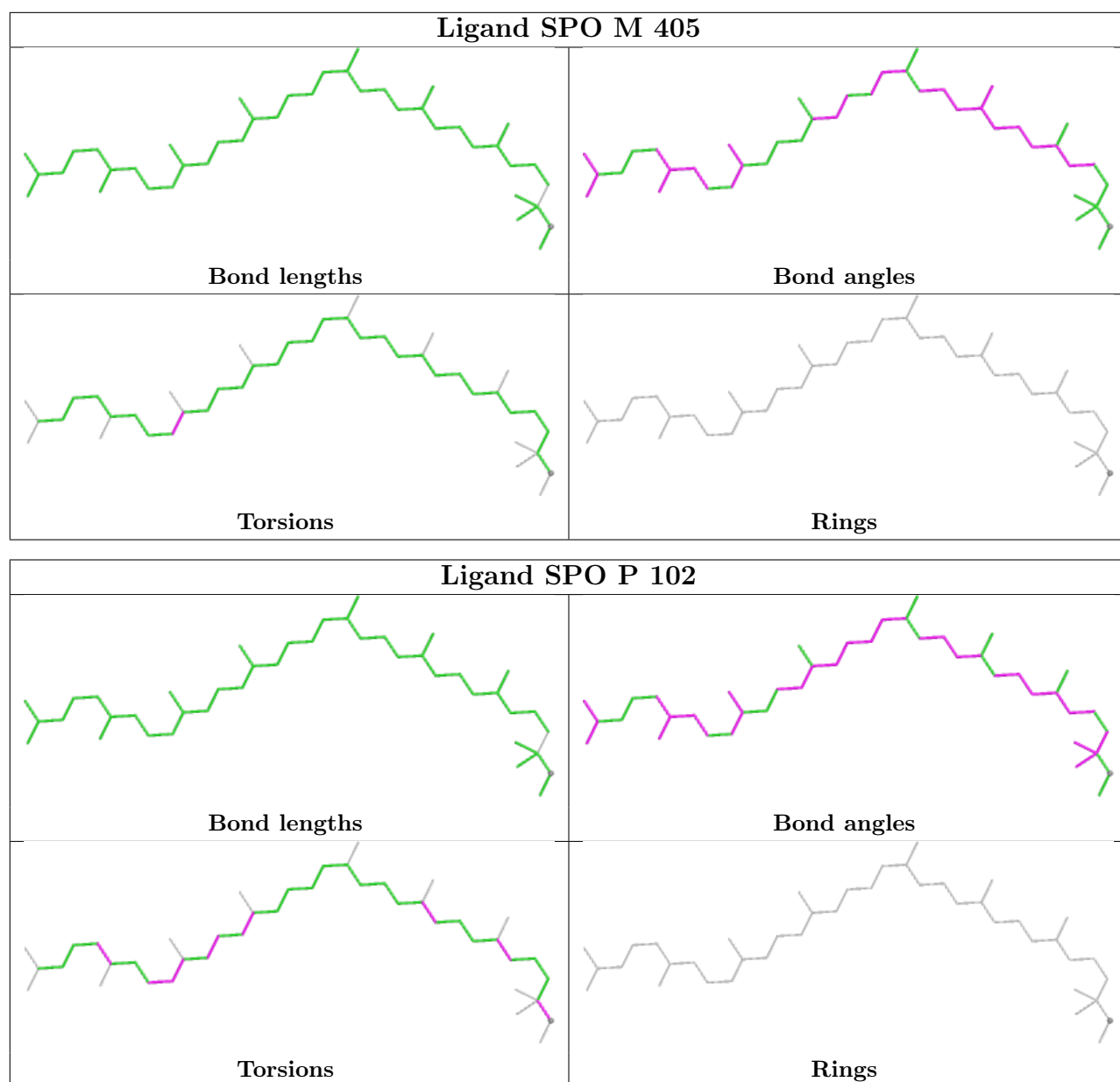


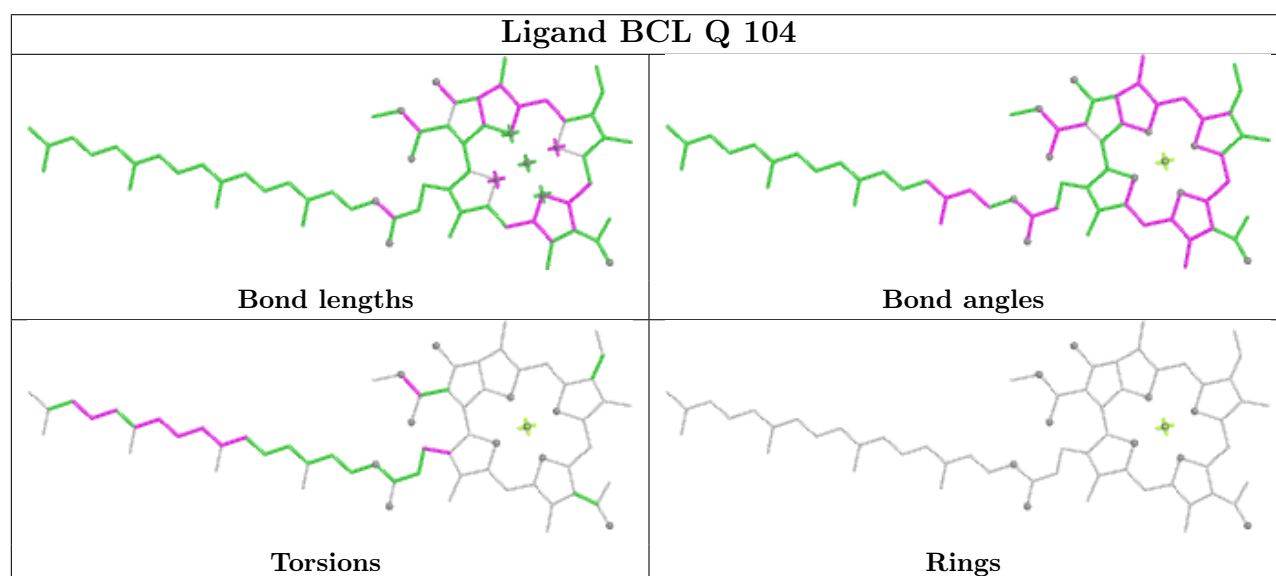
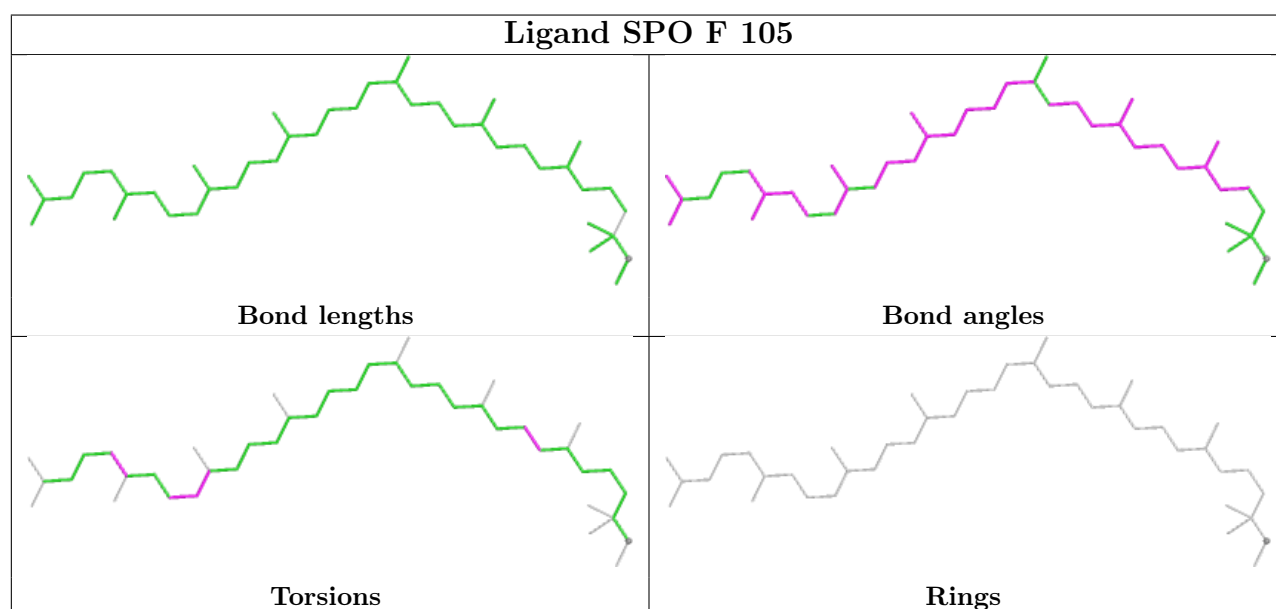
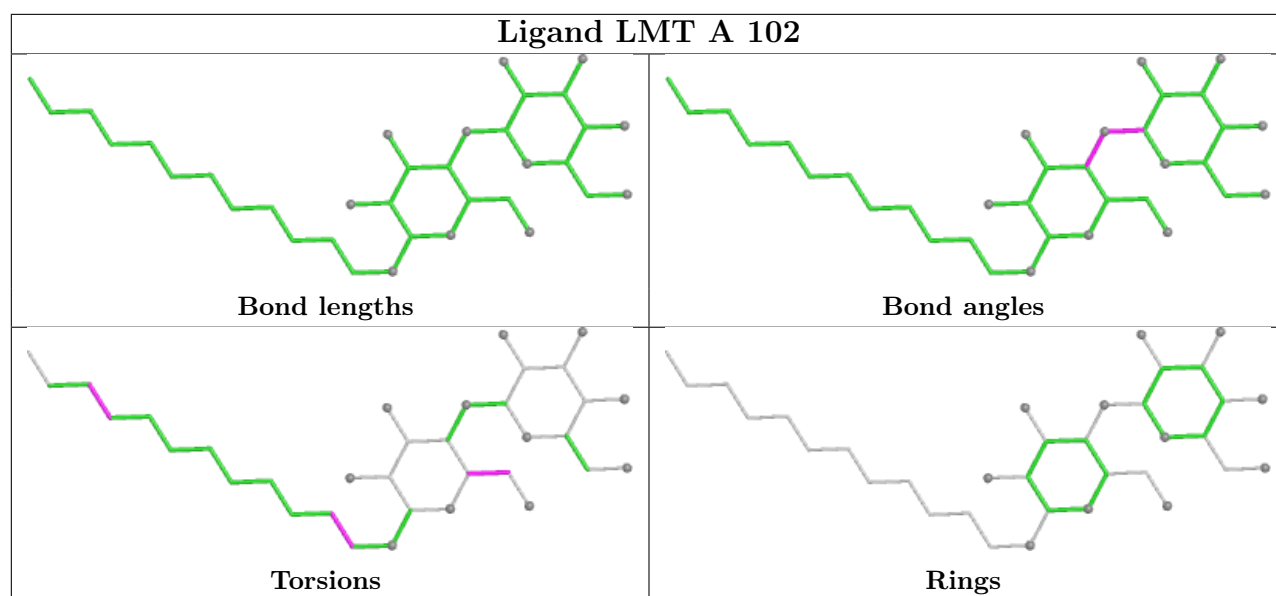


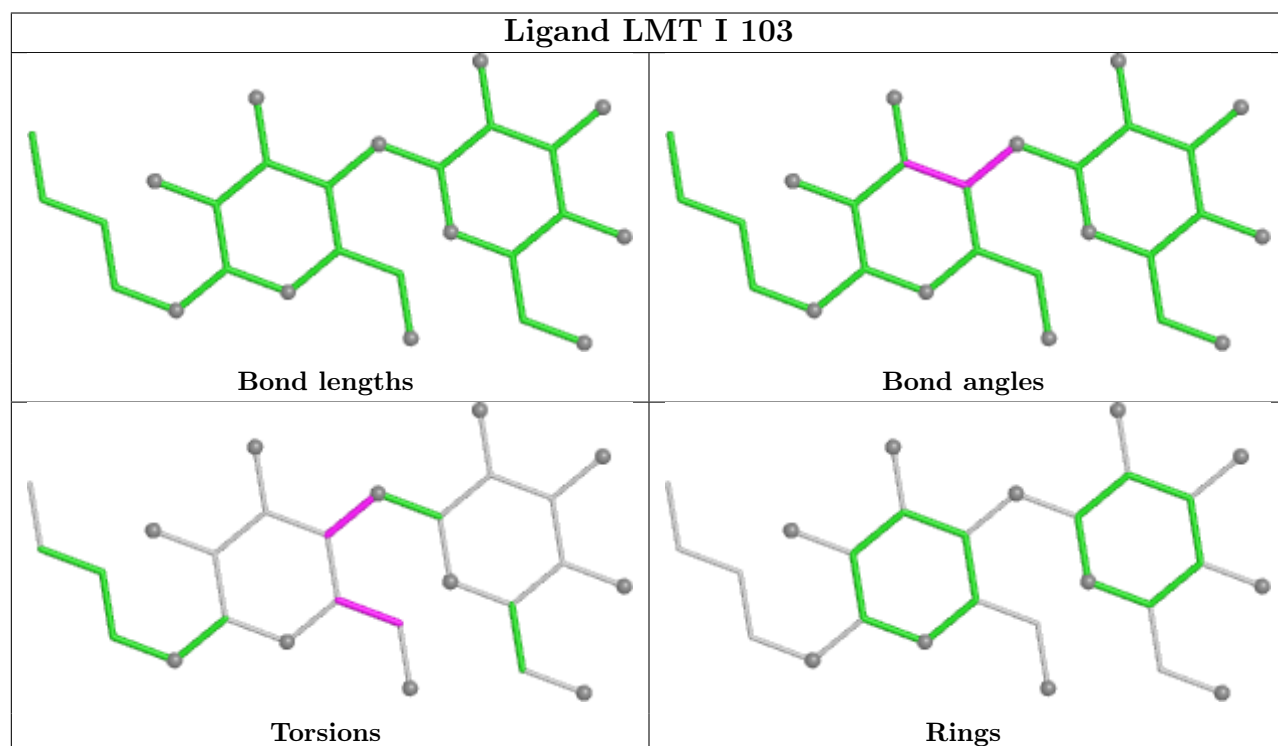
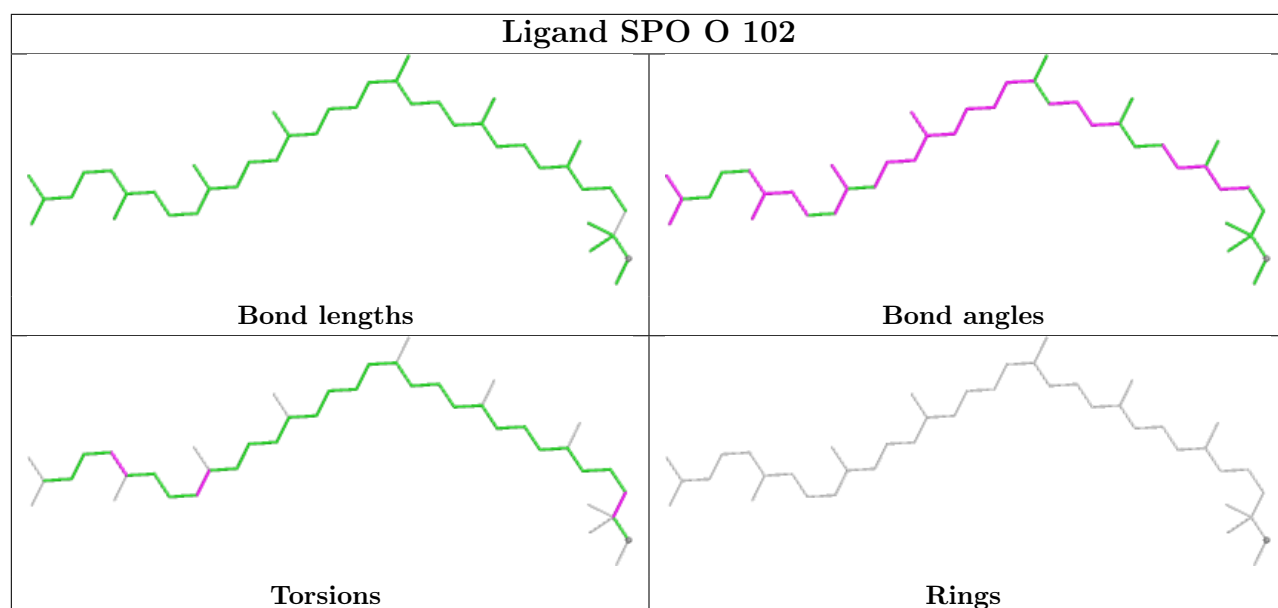


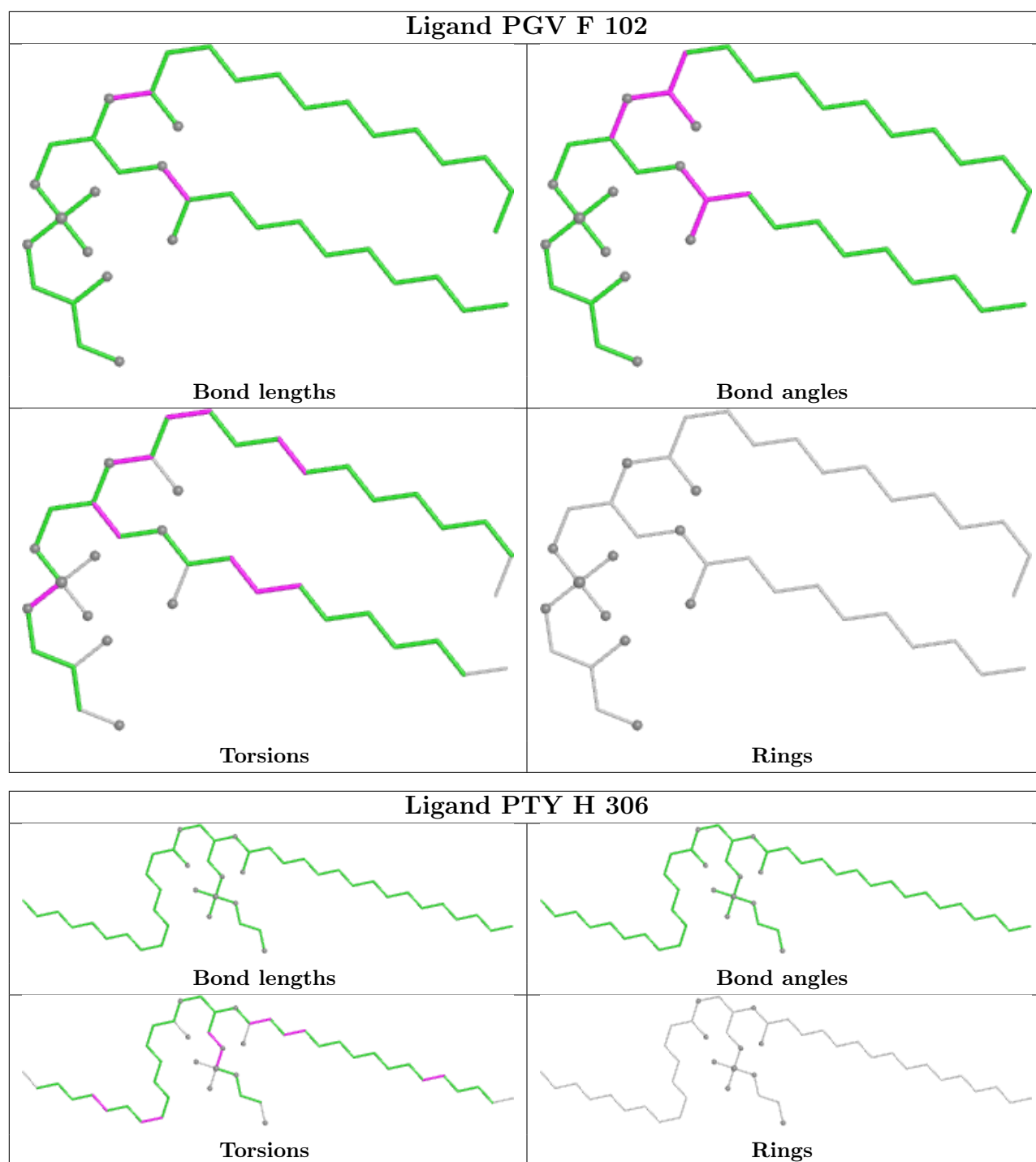












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

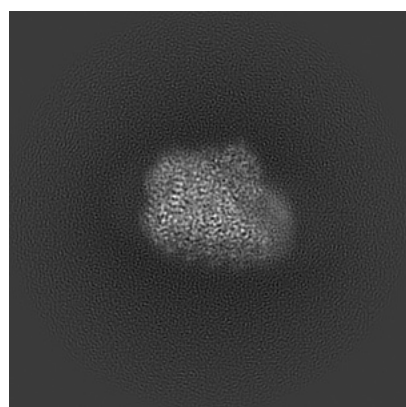
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32193. These allow visual inspection of the internal detail of the map and identification of artifacts.

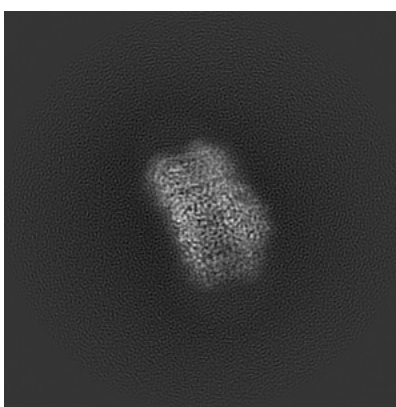
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

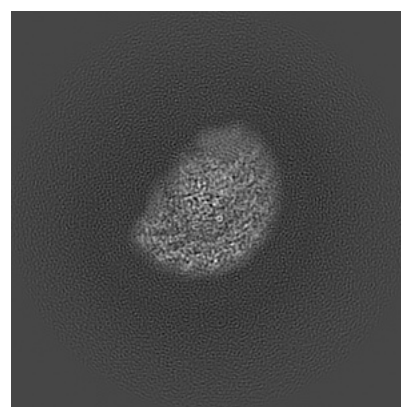
6.1.1 Primary map



X



Y

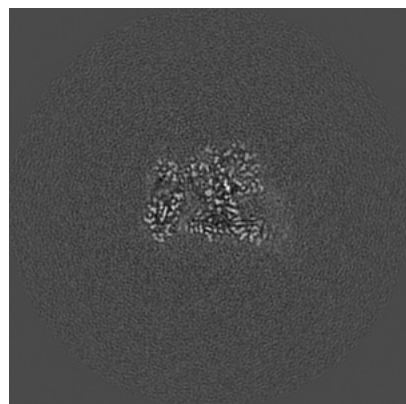


Z

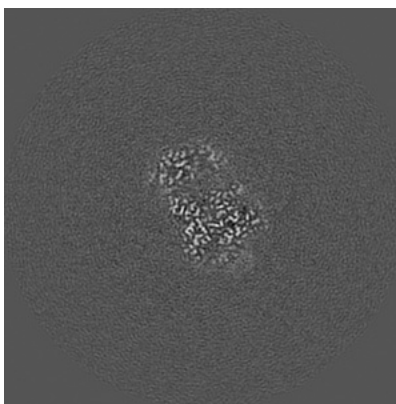
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

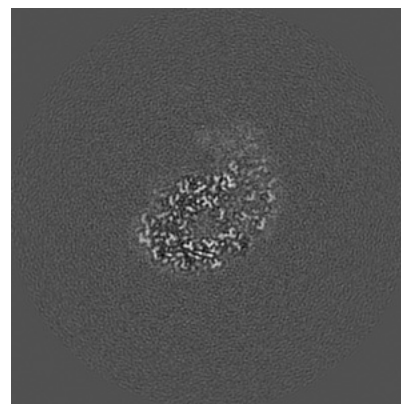
6.2.1 Primary map



X Index: 180



Y Index: 180

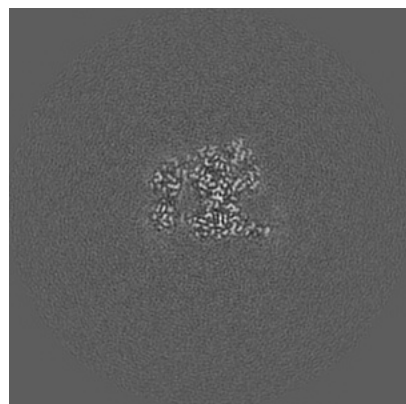


Z Index: 180

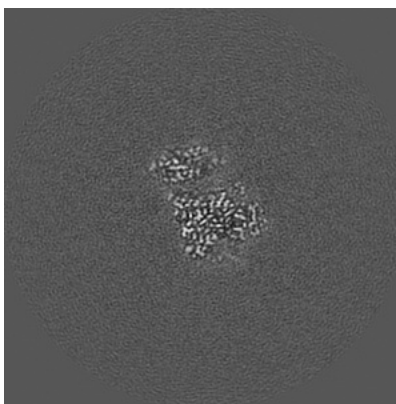
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

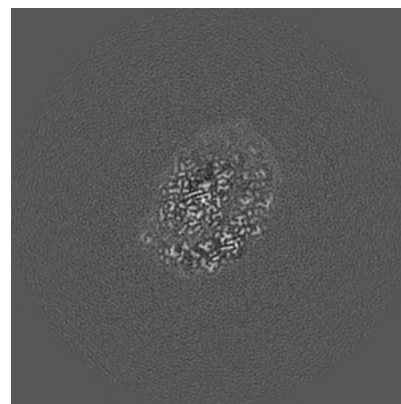
6.3.1 Primary map



X Index: 169



Y Index: 185

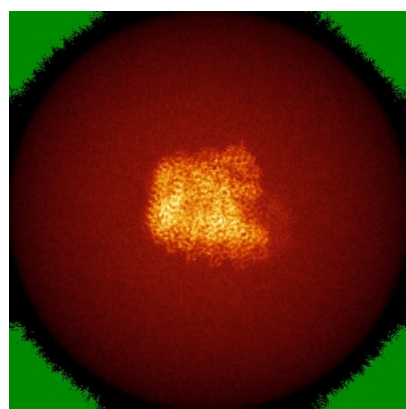


Z Index: 168

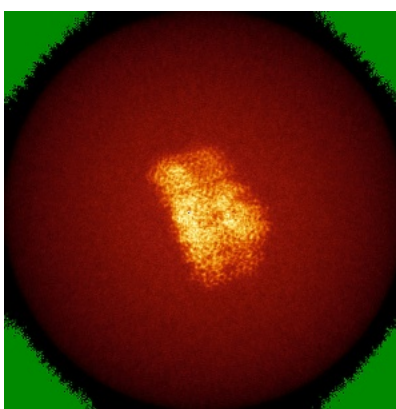
The images above show the largest variance slices of the map in three orthogonal directions.

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

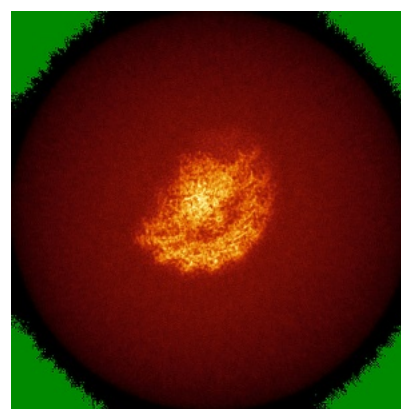
6.4.1 Primary map



X



Y

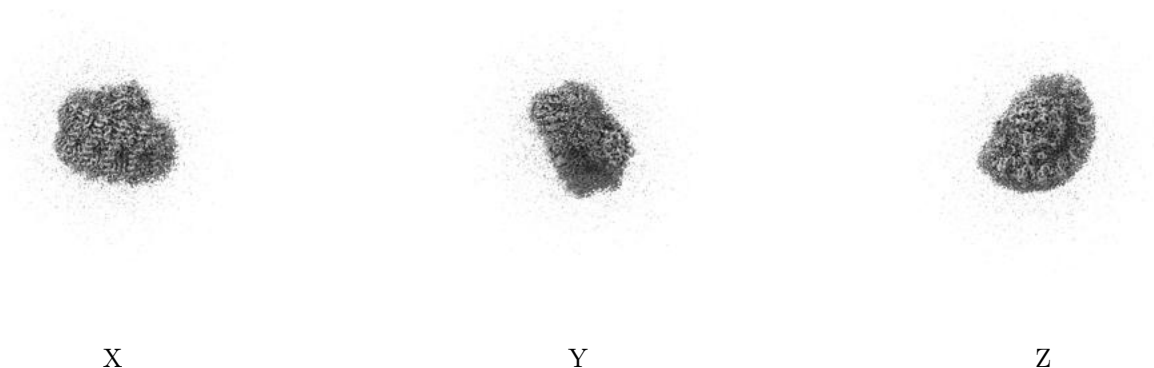


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

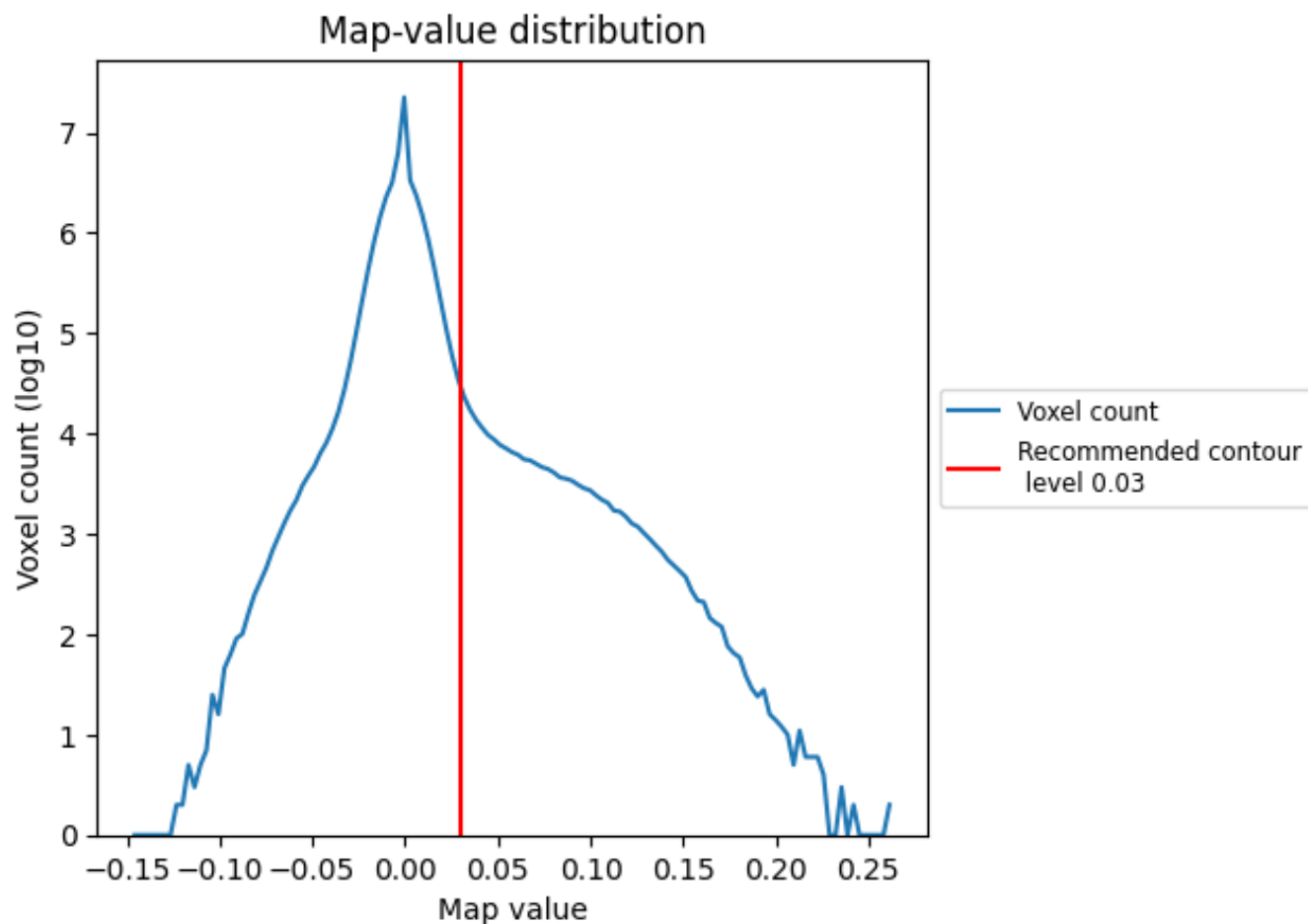
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

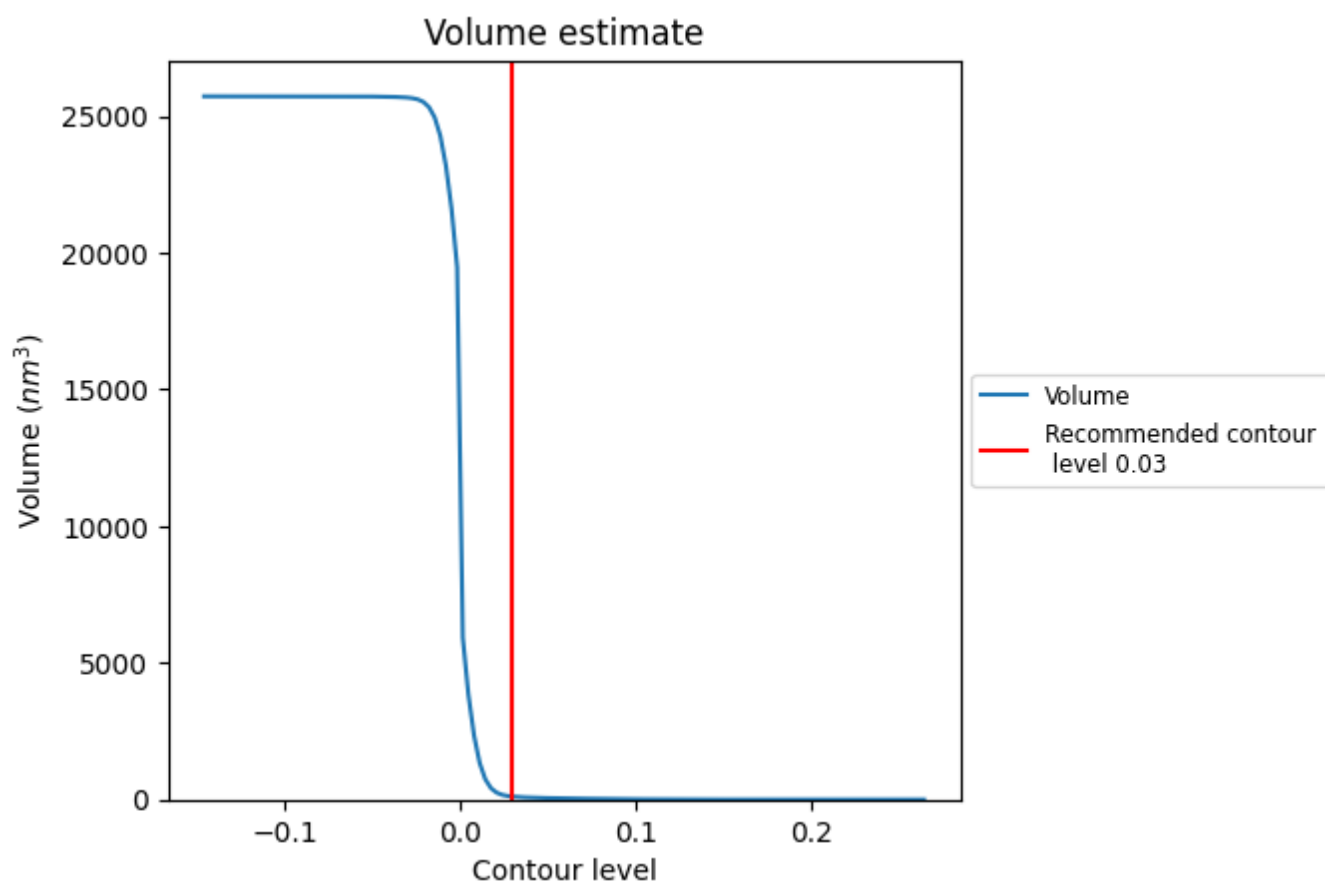
This section contains the results of statistical analysis of the map.

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.

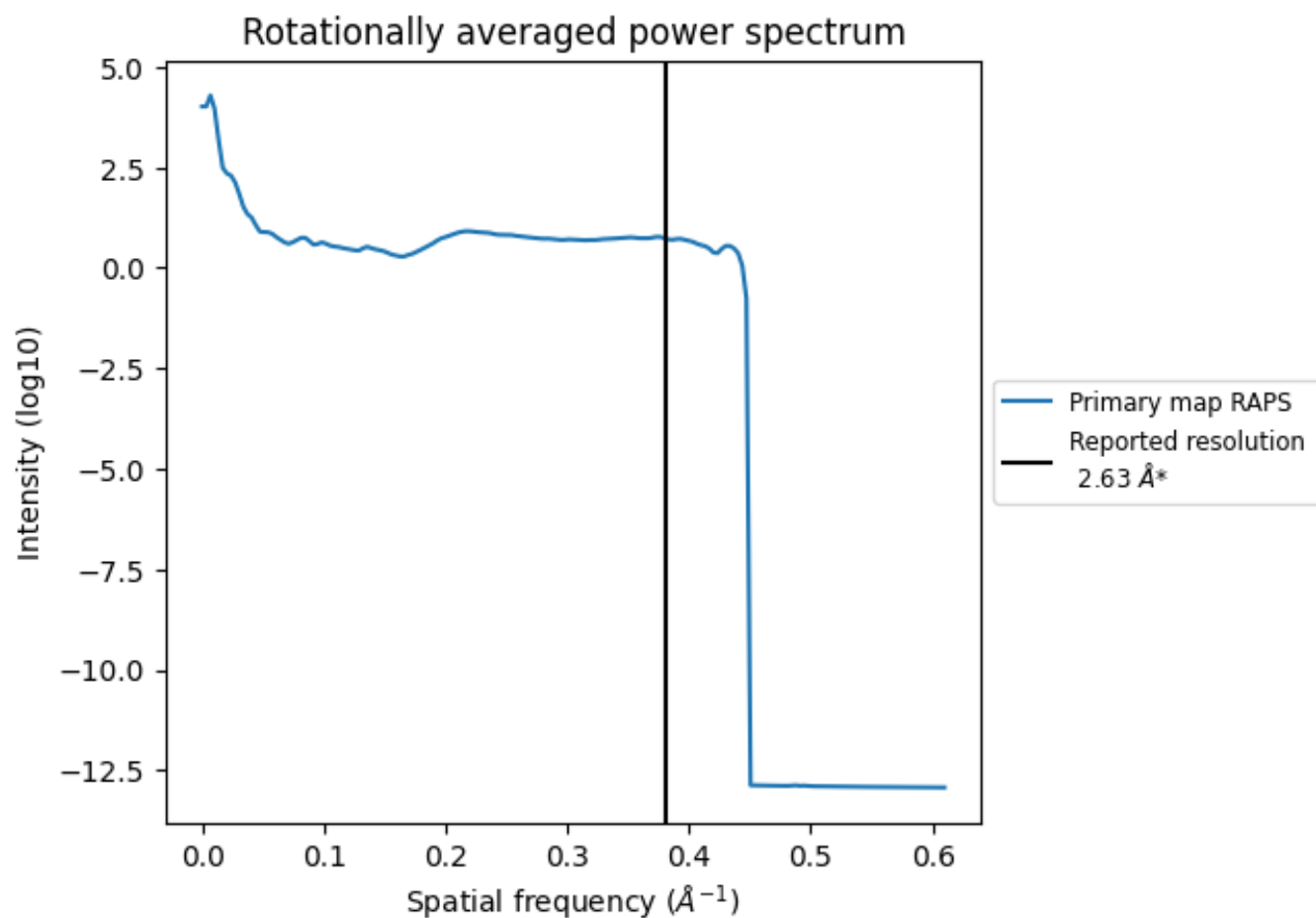
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm^3 ; this corresponds to an approximate mass of 100 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 ⓘ

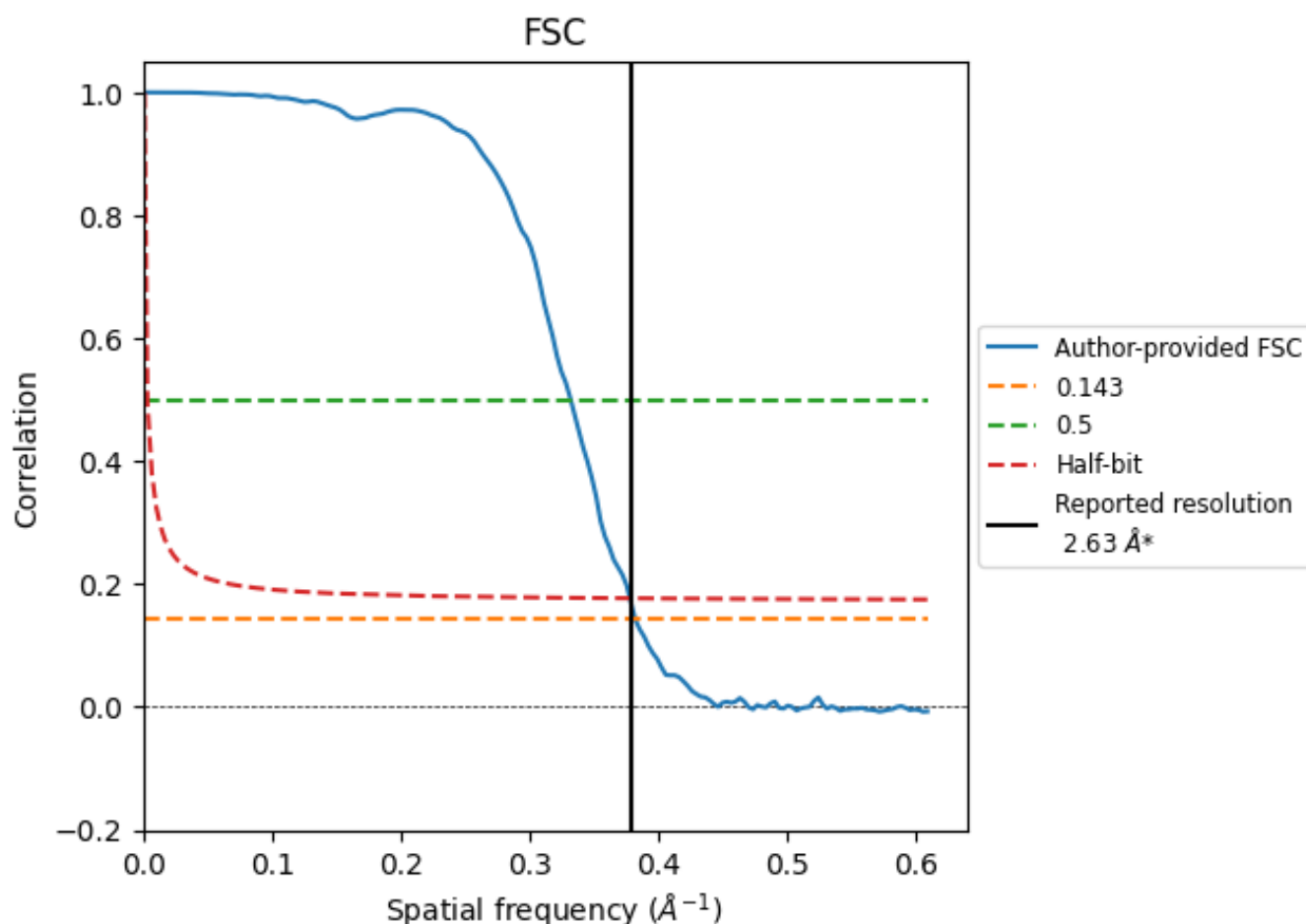


*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

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 0.380 Å⁻¹

8.2 Resolution estimates [i](#)

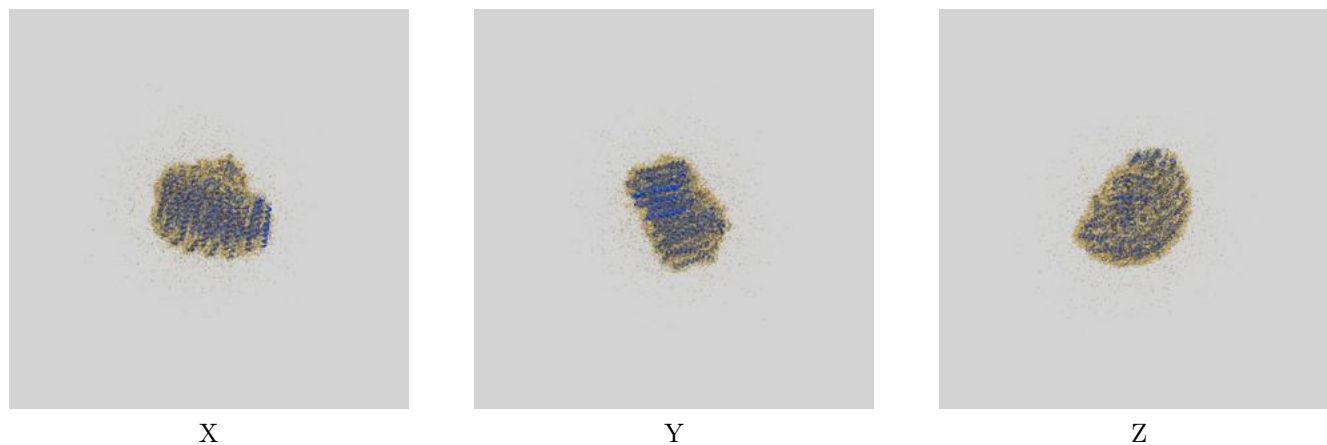
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.61	3.01	2.64
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

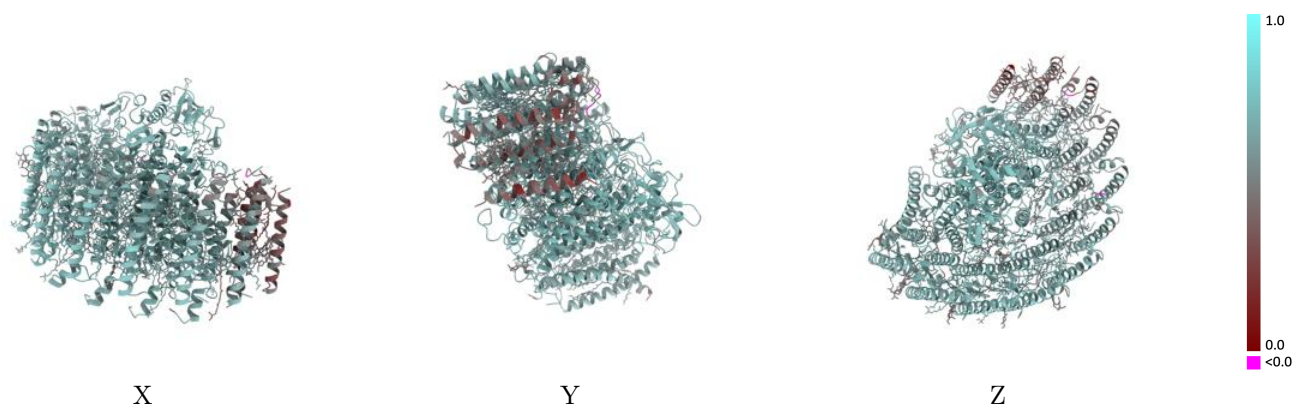
This section contains information regarding the fit between EMDB map EMD-32193 and PDB model 7VY3. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



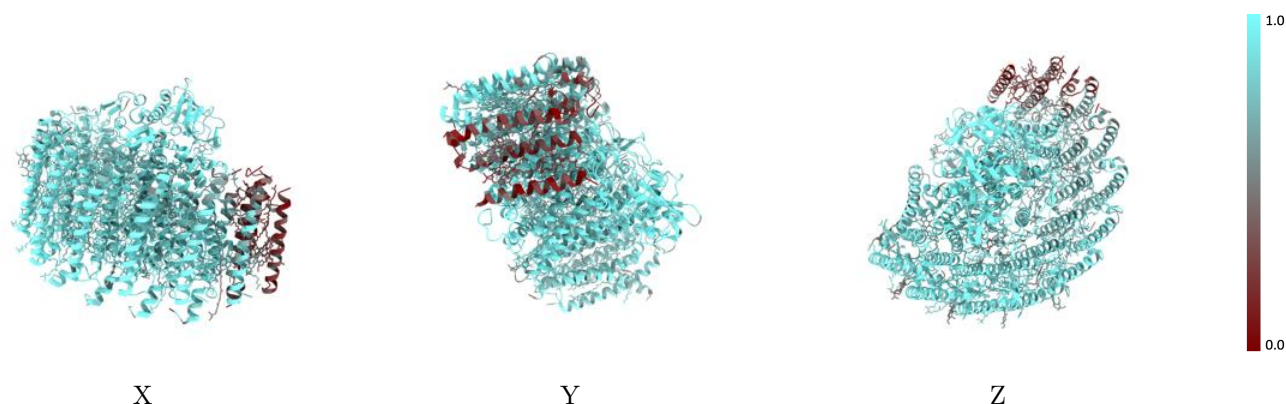
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



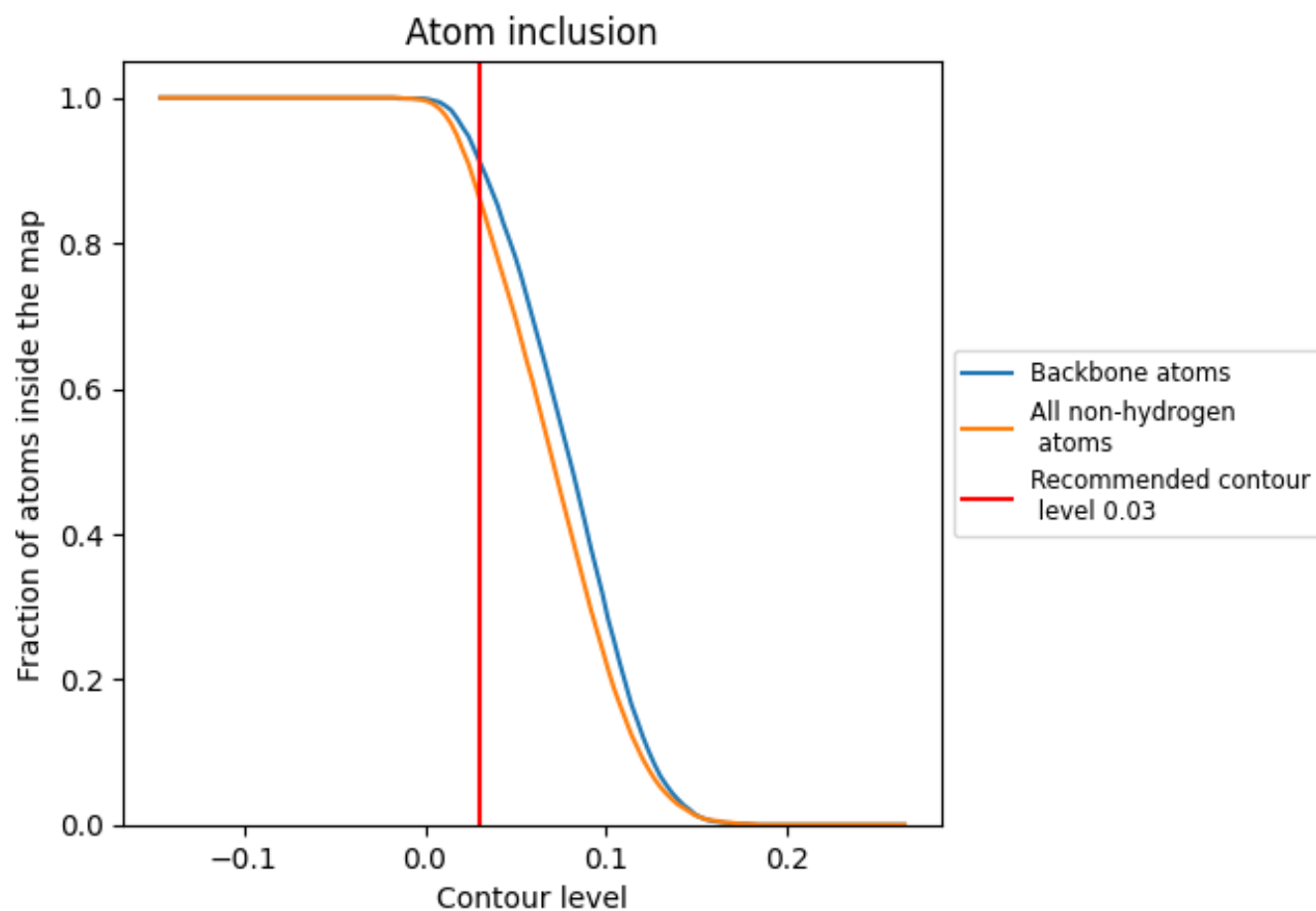
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.6280
1	 0.2040	 0.3620
A	 0.9210	 0.6360
B	 0.8550	 0.6120
D	 0.9070	 0.6430
E	 0.9330	 0.6520
F	 0.9070	 0.6460
G	 0.9140	 0.6500
H	 0.9030	 0.6430
I	 0.9270	 0.6470
J	 0.9280	 0.6550
K	 0.9070	 0.6410
L	 0.9560	 0.6780
M	 0.9550	 0.6760
N	 0.9260	 0.6500
O	 0.9190	 0.6440
P	 0.8730	 0.6150
Q	 0.8430	 0.6100
R	 0.8790	 0.6260
S	 0.8460	 0.6120
T	 0.8020	 0.5860
V	 0.6940	 0.5490
W	 0.6740	 0.5360
X	 0.7780	 0.6000
Y	 0.3450	 0.4390
Z	 0.2350	 0.3920

