



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 09:26 AM JST

PDB ID : 8YGL / pdb_00008ygl
EMDB ID : EMD-39255
Title : Rhodobacter blasticus RC-LH1 monomer
Authors : Liu, L.N.; Zhang, Y.Z.; Wang, P.; Christianson, B.M.; Ugurlar, D.
Deposited on : 2024-02-26
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

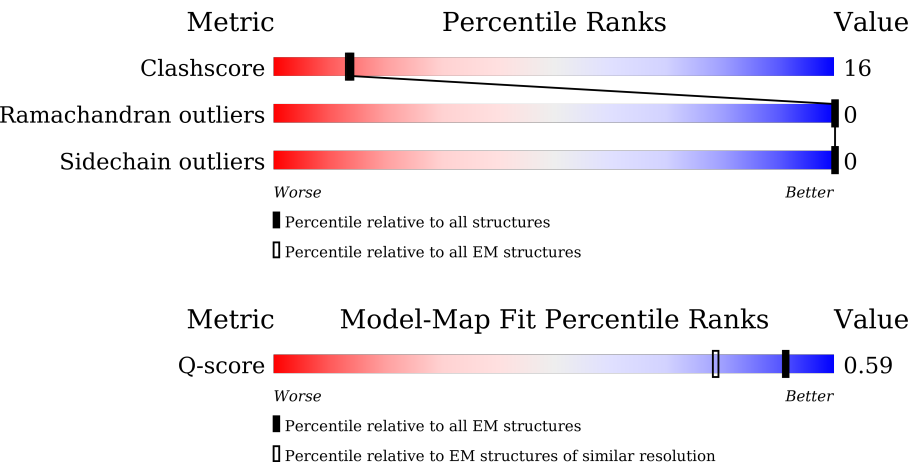
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.60 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	8728 (2.10 - 3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	49	76%14%10%
1	2	49	18% 67%12%20%
1	8	49	63%24%12%
1	B	49	82%6%12%

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Mol	Chain	Length	Quality of chain
1	C	49	
1	E	49	
1	G	49	
1	J	49	
1	N	49	
1	P	49	
1	R	49	
1	T	49	
1	V	49	
1	Z	49	
1	b	49	
2	1	62	
2	3	62	
2	7	62	
2	9	62	
2	A	62	
2	D	62	
2	F	62	
2	I	62	
2	K	62	
2	O	62	
2	Q	62	
2	S	62	
2	U	62	
2	W	62	

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Mol	Chain	Length	Quality of chain
2	a	62	
3	H	256	
4	L	282	
5	M	307	
6	X	75	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CDL	H	301	-	-	X	-
7	BCL	1	101	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 23222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	44	Total	C	N	O	S	0	0
			360	241	56	62	1		
1	2	39	Total	C	N	O	S	0	0
			319	213	51	54	1		
1	8	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	B	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	C	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	E	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	G	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	J	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	N	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	P	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	R	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	T	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	V	43	Total	C	N	O	S	0	0
			352	237	55	59	1		
1	Z	42	Total	C	N	O	S	0	0
			344	231	54	58	1		
1	b	37	Total	C	N	O	S	0	0
			308	207	49	51	1		

- Molecule 2 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	49	Total	C	N	O	S	0	0
			412	283	65	63	1		
2	3	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	7	45	Total	C	N	O	S	0	0
			387	266	61	58	2		
2	9	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	A	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	D	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	F	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	I	53	Total	C	N	O	S	0	0
			446	303	73	68	2		
2	K	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	O	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	Q	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	S	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	U	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	W	52	Total	C	N	O	S	0	0
			438	298	72	67	1		
2	a	49	Total	C	N	O	S	0	0
			412	283	65	63	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	254	Total	C	N	O	S	0	0
			1980	1259	347	366	8		

- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	281	Total	C	N	O	S	0	0
			2231	1503	349	370	9		

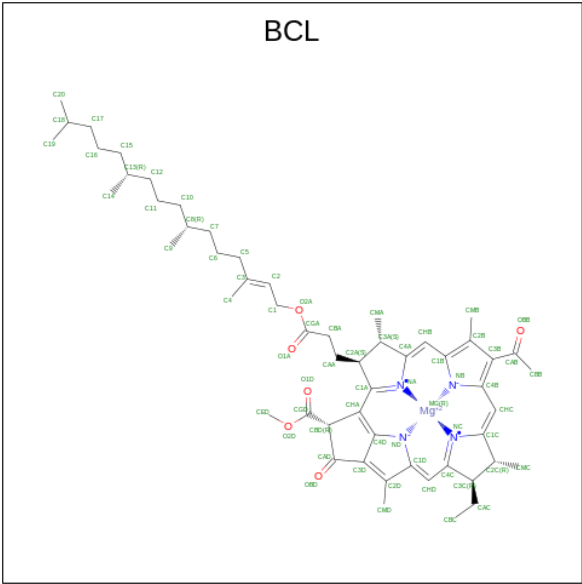
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	304	Total	C	N	O	S	0	0
			2432	1622	394	405	11		

- Molecule 6 is a protein called 1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	51	Total	C	N	O	S	0	0
			379	254	61	62	2		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
7	0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
7	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
7	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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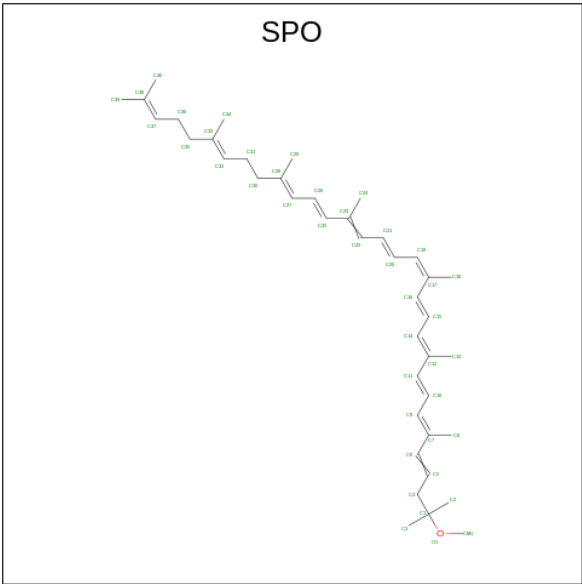
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	C	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 63	C 52	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	U	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
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	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
7	b	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 8 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	0	1	Total	C	O	0
			42	41	1	
8	0	1	Total	C	O	0
			42	41	1	
8	1	1	Total	C	O	0
			42	41	1	
8	2	1	Total	C	O	0
			42	41	1	
8	3	1	Total	C	O	0
			42	41	1	
8	9	1	Total	C	O	0
			42	41	1	

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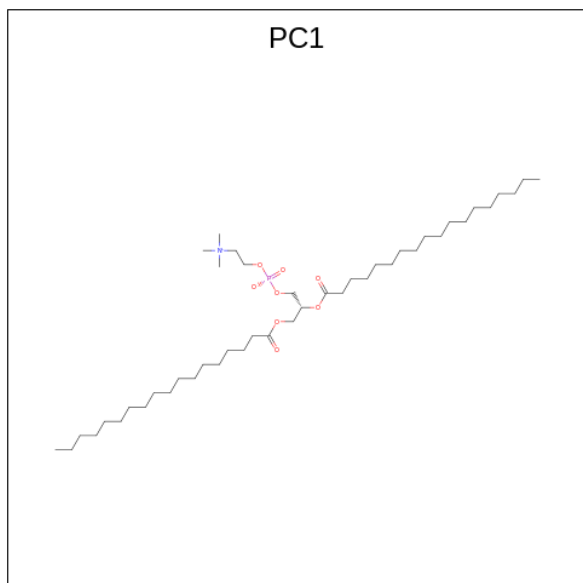
Mol	Chain	Residues	Atoms			AltConf
8	C	1	Total	C	O	0
			42	41	1	
8	D	1	Total	C	O	0
			42	41	1	
8	D	1	Total	C	O	0
			42	41	1	
8	F	1	Total	C	O	0
			42	41	1	
8	F	1	Total	C	O	0
			42	41	1	
8	G	1	Total	C	O	0
			42	41	1	
8	I	1	Total	C	O	0
			42	41	1	
8	J	1	Total	C	O	0
			42	41	1	
8	J	1	Total	C	O	0
			42	41	1	
8	M	1	Total	C	O	0
			42	41	1	
8	N	1	Total	C	O	0
			42	41	1	
8	O	1	Total	C	O	0
			42	41	1	
8	O	1	Total	C	O	0
			42	41	1	
8	P	1	Total	C	O	0
			42	41	1	
8	P	1	Total	C	O	0
			42	41	1	
8	S	1	Total	C	O	0
			42	41	1	
8	T	1	Total	C	O	0
			42	41	1	
8	U	1	Total	C	O	0
			42	41	1	
8	U	1	Total	C	O	0
			42	41	1	
8	V	1	Total	C	O	0
			42	41	1	
8	X	1	Total	C	O	0
			39	38	1	

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Mol	Chain	Residues	Atoms			AltConf
8	Z	1	Total	C	O	0
			42	41	1	
8	b	1	Total	C	O	0
			42	41	1	

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



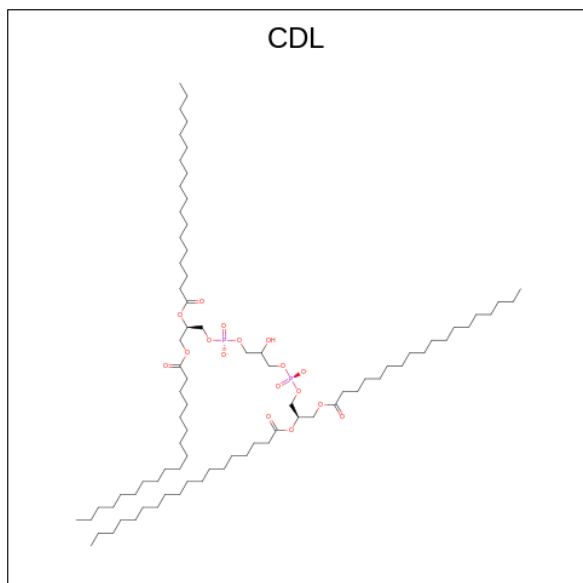
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
9	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
9	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
9	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
9	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
9	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
9	L	1	Total	C	N	O	P	0
			32	22	1	8	1	
9	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
9	M	1	Total	C	N	O	P	0
			47	37	1	8	1	

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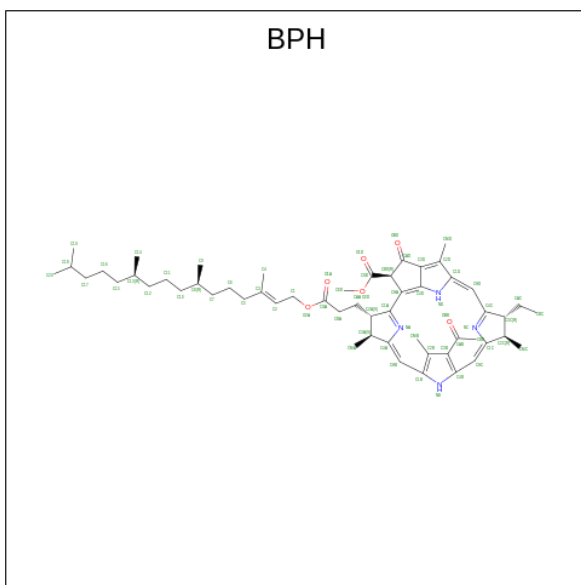
Mol	Chain	Residues	Atoms					AltConf
9	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
9	O	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



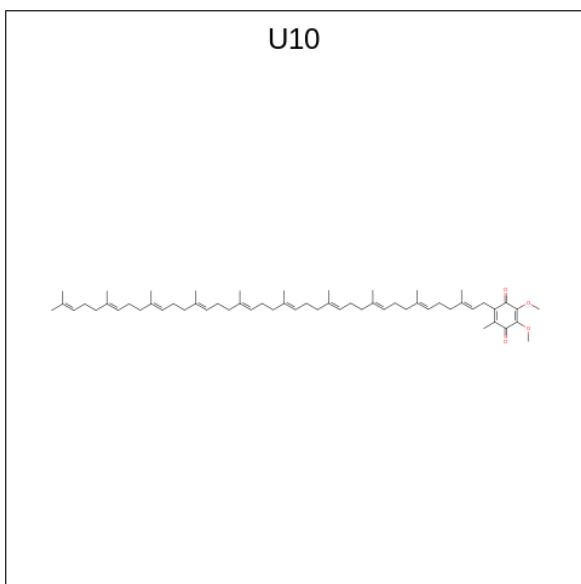
Mol	Chain	Residues	Atoms				AltConf
10	H	1	Total	C	O	P	0
			78	59	17	2	
10	M	1	Total	C	O	P	0
			100	81	17	2	
10	M	1	Total	C	O	P	0
			78	59	17	2	

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



Mol	Chain	Residues	Atoms				AltConf
11	L	1	Total	C	N	O	0
			62	52	4	6	
11	L	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			43	39	4	

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Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			48	44	4	
12	L	1	Total	C	O	0
			19	15	4	
12	L	1	Total	C	O	0
			38	34	4	
12	M	1	Total	C	O	0
			43	39	4	
12	M	1	Total	C	O	0
			48	44	4	
12	X	1	Total	C	O	0
			48	44	4	

- Molecule 13 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

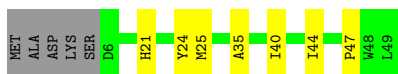
Mol	Chain	Residues	Atoms		AltConf
13	M	1	Total	Fe	0
			1	1	

3 Residue-property plots [i](#)

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

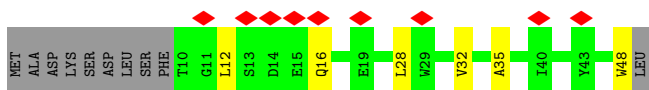
- Molecule 1: Antenna pigment protein beta chain

Chain 0: 



- Molecule 1: Antenna pigment protein beta chain

Chain 2: 



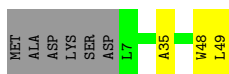
- Molecule 1: Antenna pigment protein beta chain

Chain 8: 



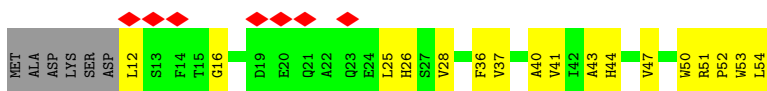
- Molecule 1: Antenna pigment protein beta chain

Chain B: 



- Molecule 1: Antenna pigment protein beta chain

Chain C: 



- Molecule 1: Antenna pigment protein beta chain

Chain E:  65% 22% 12%



- Molecule 1: Antenna pigment protein beta chain

Chain G:  71% 16% 12%



- Molecule 1: Antenna pigment protein beta chain

Chain J:  57% 31% 12%



- Molecule 1: Antenna pigment protein beta chain

Chain N:  71% 16% 12%



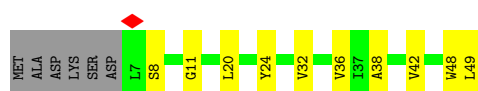
- Molecule 1: Antenna pigment protein beta chain

Chain P:  65% 22% 12%



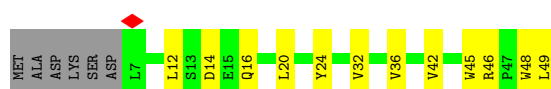
- Molecule 1: Antenna pigment protein beta chain

Chain R:  67% 20% 12%

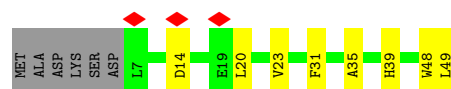
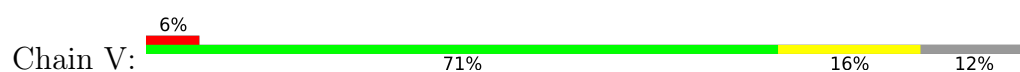


- Molecule 1: Antenna pigment protein beta chain

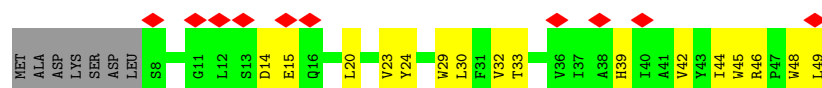
Chain T:  63% 24% 12%



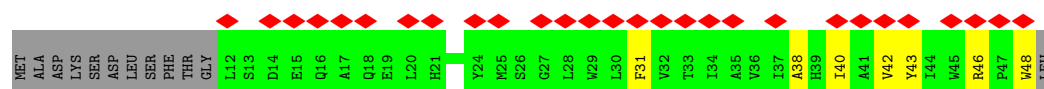
- Molecule 1: Antenna pigment protein beta chain



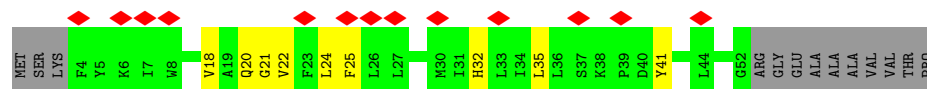
- Molecule 1: Antenna pigment protein beta chain



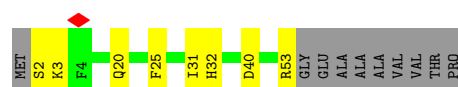
- Molecule 1: Antenna pigment protein beta chain



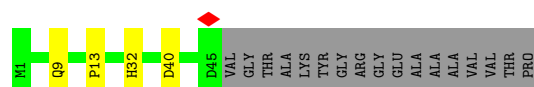
- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain



- Molecule 2: Antenna pigment protein alpha chain

Chain A:  77% 8% 15%



- Molecule 2: Antenna pigment protein alpha chain

Chain D:  61% 24% 15%



- Molecule 2: Antenna pigment protein alpha chain

Chain F:  66% 19% 15%



- Molecule 2: Antenna pigment protein alpha chain

Chain I:  69% 16% 15%



- Molecule 2: Antenna pigment protein alpha chain

Chain K:  71% 13% 16%



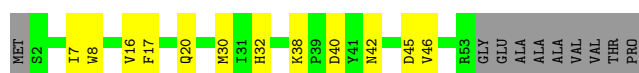
- Molecule 2: Antenna pigment protein alpha chain

Chain O:  68% 16% 16%



- Molecule 2: Antenna pigment protein alpha chain

Chain Q:  65% 19% 16%



- Molecule 2: Antenna pigment protein alpha chain

Chain S:  53% 31% 16%



- Molecule 2: Antenna pigment protein alpha chain

Chain U:  69% 15% 16%



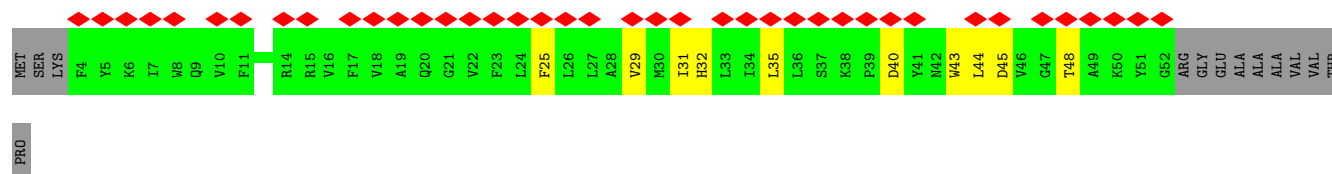
- Molecule 2: Antenna pigment protein alpha chain

Chain W:  63% 21% 16%



- Molecule 2: Antenna pigment protein alpha chain

Chain a:  65% 63% 16% 21%



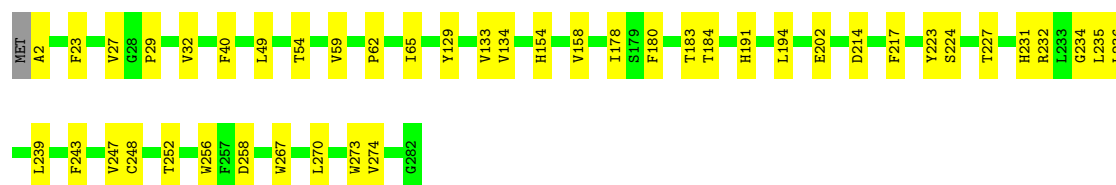
- Molecule 3: Photosynthetic reaction center subunit H

Chain H:  88% 11%



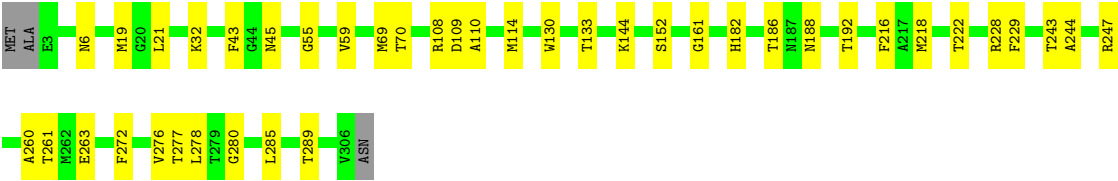
- Molecule 4: Reaction center protein L chain

Chain L:  84% 16%

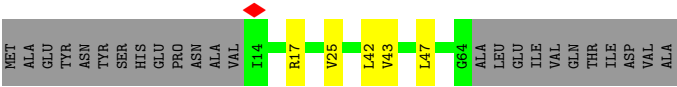


- Molecule 5: Reaction center protein M chain

Chain M:  86% 13%



• Molecule 6: 1-deoxy-D-xylulose-5-phosphate synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45399	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.792	Depositor
Minimum map value	-0.912	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.17	Depositor
Map size ($\text{\AA}$)	297.28, 297.28, 297.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.929, 0.929, 0.929	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, PC1, BPH, CDL, FE2, SPO, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.31	0/372	0.31	0/510
1	2	0.18	0/330	0.28	0/453
1	8	0.27	0/364	0.28	0/499
1	B	0.31	0/364	0.28	0/499
1	C	0.20	0/364	0.31	0/499
1	E	0.30	0/364	0.30	0/499
1	G	0.28	0/364	0.31	0/499
1	J	0.30	0/364	0.34	0/499
1	N	0.27	0/364	0.32	0/499
1	P	0.27	0/364	0.34	0/499
1	R	0.27	0/364	0.32	0/499
1	T	0.27	0/364	0.38	0/499
1	V	0.23	0/364	0.27	0/499
1	Z	0.19	0/356	0.34	0/488
1	b	0.17	0/319	0.38	0/438
2	1	0.19	0/426	0.36	0/579
2	3	0.19	0/452	0.31	0/612
2	7	0.29	0/400	0.32	0/542
2	9	0.31	0/460	0.37	0/622
2	A	0.32	0/460	0.35	0/622
2	D	0.32	0/460	0.39	0/622
2	F	0.31	0/460	0.31	0/622
2	I	0.29	0/460	0.33	0/622
2	K	0.29	0/452	0.34	0/612
2	O	0.28	0/452	0.35	0/612
2	Q	0.34	0/452	0.34	0/612
2	S	0.32	0/452	0.40	0/612
2	U	0.28	0/452	0.37	0/612
2	W	0.23	0/452	0.36	0/612
2	a	0.18	0/426	0.35	0/579
3	H	0.26	0/2030	0.37	0/2757
4	L	0.31	0/2317	0.36	0/3172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	M	0.32	0/2525	0.38	0/3453
6	X	0.30	0/388	0.38	0/532
All	All	0.28	0/19357	0.35	0/26386

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	0	360	0	350	5	0
1	2	319	0	310	8	0
1	8	352	0	346	10	0
1	B	352	0	346	2	0
1	C	352	0	346	15	0
1	E	352	0	346	10	0
1	G	352	0	346	8	0
1	J	352	0	346	14	0
1	N	352	0	346	9	0
1	P	352	0	346	14	0
1	R	352	0	346	7	0
1	T	352	0	346	14	0
1	V	352	0	346	13	0
1	Z	344	0	335	14	0
1	b	308	0	300	9	0
2	1	412	0	420	12	0
2	3	438	0	451	8	0
2	7	387	0	401	4	0
2	9	446	0	463	9	0
2	A	446	0	463	8	0
2	D	446	0	463	16	0
2	F	446	0	463	15	0
2	I	446	0	463	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	438	0	451	8	0
2	O	438	0	451	9	0
2	Q	438	0	451	10	0
2	S	438	0	451	25	0
2	U	438	0	451	11	0
2	W	438	0	451	18	0
2	a	412	0	420	7	0
3	H	1980	0	1952	23	0
4	L	2231	0	2169	36	0
5	M	2432	0	2331	31	0
6	X	379	0	401	6	0
7	0	61	0	61	7	0
7	1	56	0	51	27	0
7	2	61	0	61	11	0
7	3	66	0	74	13	0
7	7	61	0	61	5	0
7	8	66	0	74	5	0
7	9	66	0	74	10	0
7	A	66	0	74	5	0
7	B	66	0	74	7	0
7	C	66	0	74	8	0
7	D	66	0	74	5	0
7	E	66	0	74	20	0
7	F	66	0	74	6	0
7	G	66	0	74	11	0
7	I	66	0	74	14	0
7	J	66	0	74	19	0
7	K	66	0	74	5	0
7	L	129	0	139	13	0
7	M	132	0	148	19	0
7	N	66	0	74	16	0
7	O	66	0	74	10	0
7	P	66	0	74	5	0
7	Q	66	0	74	8	0
7	R	66	0	74	8	0
7	S	66	0	74	14	0
7	T	66	0	74	7	0
7	U	66	0	74	10	0
7	V	66	0	74	6	0
7	W	66	0	74	9	0
7	Z	66	0	74	18	0
7	a	56	0	51	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	b	61	0	61	7	0
8	0	84	0	120	13	0
8	1	42	0	60	16	0
8	2	42	0	60	12	0
8	3	42	0	60	19	0
8	9	42	0	60	5	0
8	C	42	0	60	8	0
8	D	84	0	120	14	0
8	F	84	0	120	4	0
8	G	42	0	60	6	0
8	I	42	0	60	12	0
8	J	84	0	120	39	0
8	M	42	0	60	4	0
8	N	42	0	60	5	0
8	O	84	0	120	14	0
8	P	84	0	120	13	0
8	S	42	0	60	17	0
8	T	42	0	60	7	0
8	U	84	0	120	13	0
8	V	42	0	60	10	0
8	X	39	0	53	5	0
8	Z	42	0	60	8	0
8	b	42	0	60	15	0
9	A	109	0	143	22	0
9	D	37	0	48	3	0
9	L	103	0	128	4	0
9	M	132	0	192	10	0
9	O	32	0	38	0	0
10	H	78	0	106	21	0
10	M	178	0	262	3	0
11	L	117	0	120	8	0
12	L	148	0	182	18	0
12	M	91	0	118	5	0
12	X	48	0	63	10	0
13	M	1	0	0	0	0
All	All	23222	0	24209	754	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 16.

All (754) 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)
8:0:103:SPO:H9	8:0:103:SPO:H42	1.30	1.06
5:M:152:SER:HG	5:M:277:THR:HG1	0.97	0.97
7:1:101:BCL:HMB2	8:3:102:SPO:H42	1.48	0.95
7:J:101:BCL:H62	8:J:103:SPO:H241	1.49	0.95
8:O:104:SPO:H6	7:S:201:BCL:HMB1	1.49	0.93
1:G:49:LEU:HD13	8:J:102:SPO:H83	1.49	0.92
8:b:101:SPO:H9	8:b:101:SPO:H132	1.51	0.92
8:b:101:SPO:H291	8:b:101:SPO:H32	1.49	0.91
10:H:301:CDL:H331	9:L:304:PC1:H12	1.52	0.91
8:2:102:SPO:H41	8:2:102:SPO:H83	1.53	0.91
7:S:201:BCL:H71	7:S:201:BCL:H41	1.55	0.89
8:J:103:SPO:H83	8:J:103:SPO:H32A	1.52	0.89
8:D:103:SPO:H42	8:D:103:SPO:H83	1.54	0.88
2:O:20:GLN:OE1	1:P:24:TYR:OH	1.90	0.88
8:3:102:SPO:H27	8:3:102:SPO:H241	1.55	0.87
8:D:103:SPO:C18	8:D:103:SPO:H14	2.05	0.85
8:2:102:SPO:H41	8:2:102:SPO:C8	2.06	0.85
8:b:101:SPO:C8	8:b:101:SPO:H42	2.08	0.84
7:L:302:BCL:HMD2	7:M:405:BCL:HBB3	1.57	0.83
3:H:134:LYS:NZ	3:H:174:ASP:OD2	2.11	0.83
8:2:102:SPO:H9	8:2:102:SPO:H132	1.62	0.82
8:J:103:SPO:H14	8:J:103:SPO:C18	2.09	0.82
7:R:101:BCL:HMB1	7:R:101:BCL:HBB2	1.62	0.82
8:0:102:SPO:H131	8:0:102:SPO:H16	1.62	0.82
3:H:210:ASN:O	3:H:252:ARG:NH1	2.14	0.81
2:S:40:ASP:OD1	1:T:46:ARG:NH1	2.13	0.81
8:Z:102:SPO:H14	8:Z:102:SPO:H182	1.62	0.80
8:C:102:SPO:H11	8:C:102:SPO:H81	1.62	0.80
8:J:103:SPO:H14	8:J:103:SPO:H183	1.62	0.80
8:J:102:SPO:C32	8:J:102:SPO:H291	2.12	0.80
7:N:102:BCL:H52	8:P:102:SPO:H293	1.65	0.79
8:0:103:SPO:H182	8:0:103:SPO:H14	1.62	0.79
8:J:103:SPO:C8	8:J:103:SPO:H42	2.13	0.79
7:M:404:BCL:HMB1	7:M:404:BCL:HBB2	1.65	0.79
7:N:102:BCL:HMB1	7:N:102:BCL:HBB2	1.63	0.79
7:1:101:BCL:HED2	7:2:101:BCL:HBD	1.65	0.79
1:O:24:TYR:OH	2:9:20:GLN:OE1	2.01	0.78
8:0:103:SPO:H14	8:0:103:SPO:C18	2.14	0.78
2:S:20:GLN:HE21	8:S:202:SPO:H20	1.47	0.78
2:S:20:GLN:NE2	8:S:202:SPO:H20	1.98	0.78
9:A:102:PC1:H142	3:H:44:MET:SD	2.24	0.78
7:J:101:BCL:HMB1	7:J:101:BCL:HBB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:248:CYS:O	4:L:252:THR:OG1	2.01	0.78
1:b:38:ALA:HB1	8:b:101:SPO:H181	1.66	0.78
7:0:101:BCL:HBB2	7:0:101:BCL:HMB1	1.66	0.77
7:E:101:BCL:H41	8:G:102:SPO:H241	1.66	0.77
7:I:101:BCL:H43	8:J:102:SPO:H292	1.67	0.77
2:K:20:GLN:OE1	1:N:24:TYR:OH	2.01	0.77
8:S:202:SPO:H403	1:T:20:LEU:HD13	1.65	0.77
1:C:51:ARG:NH1	2:W:40:ASP:OD1	2.17	0.77
8:S:202:SPO:H15	8:U:102:SPO:H293	1.66	0.77
2:A:15:ARG:NE	9:A:103:PC1:O12	2.18	0.76
7:C:101:BCL:HBB3	7:C:101:BCL:HMB1	1.68	0.75
8:N:101:SPO:H6	7:O:101:BCL:HMB2	1.68	0.75
2:A:6:LYS:NZ	1:E:19:GLU:OE2	2.19	0.75
8:3:102:SPO:H241	8:3:102:SPO:C27	2.17	0.75
8:0:103:SPO:H352	7:A:101:BCL:H43	1.69	0.75
2:S:20:GLN:NE2	1:T:24:TYR:OH	2.20	0.75
7:O:101:BCL:HBB3	7:O:101:BCL:HMB1	1.69	0.74
2:F:20:GLN:OE1	1:G:24:TYR:OH	2.03	0.74
7:G:101:BCL:H8	7:G:101:BCL:H152	1.69	0.73
7:G:101:BCL:HMB2	8:J:102:SPO:H183	1.70	0.72
8:b:101:SPO:H9	8:b:101:SPO:C13	2.18	0.72
2:F:26:LEU:HD13	10:H:301:CDL:H801	1.71	0.72
7:a:101:BCL:HMB1	7:a:101:BCL:HBB3	1.71	0.72
7:1:101:BCL:CMB	8:3:102:SPO:H42	2.20	0.72
1:C:12:LEU:O	1:C:16:GLY:N	2.23	0.72
7:a:101:BCL:HED1	1:b:31:PHE:CZ	2.24	0.71
7:U:101:BCL:HMB1	7:U:101:BCL:HBB3	1.71	0.71
8:S:202:SPO:HM11	2:U:29:VAL:HG13	1.72	0.71
4:L:256:TRP:NE1	4:L:258:ASP:O	2.23	0.71
8:2:102:SPO:H21	8:2:102:SPO:H181	1.72	0.71
9:D:104:PC1:C37	9:D:104:PC1:H322	2.20	0.71
1:J:31:PHE:CE1	8:J:102:SPO:H27	2.25	0.71
8:D:103:SPO:H14	8:D:103:SPO:H182	1.71	0.71
1:Z:48:TRP:CD1	1:Z:49:LEU:HG	2.26	0.71
7:1:101:BCL:CED	7:2:101:BCL:HBD	2.20	0.71
8:U:103:SPO:H82	8:U:103:SPO:H42	1.73	0.71
7:8:101:BCL:HMB1	7:8:101:BCL:HBB2	1.72	0.70
7:L:302:BCL:HMB1	7:L:302:BCL:HBB2	1.72	0.70
7:R:101:BCL:H8	8:T:102:SPO:H27	1.73	0.70
2:U:35:LEU:HD23	7:U:101:BCL:HBC1	1.74	0.70
7:9:101:BCL:HMB1	7:9:101:BCL:HBB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:101:BCL:H61	8:J:102:SPO:H343	1.74	0.69
7:B:101:BCL:HMB1	7:B:101:BCL:HBB2	1.73	0.69
8:I:102:SPO:H361	1:J:23:VAL:HG11	1.75	0.69
7:V:102:BCL:HMB1	7:V:102:BCL:HBB3	1.74	0.69
7:N:102:BCL:H91	7:N:102:BCL:H13	1.74	0.69
8:J:103:SPO:H11	8:J:103:SPO:H6	1.73	0.69
7:Z:101:BCL:HMB1	7:Z:101:BCL:HBB2	1.74	0.69
7:O:101:BCL:H61	8:O:103:SPO:H241	1.75	0.69
1:E:29:TRP:HH2	7:E:101:BCL:H161	1.58	0.69
12:L:309:U10:H3M1	7:M:404:BCL:H93	1.75	0.69
2:a:25:PHE:O	2:a:29:VAL:HG23	1.92	0.69
1:2:35:ALA:CB	7:2:101:BCL:HBA2	2.24	0.68
8:2:102:SPO:H9	8:2:102:SPO:C13	2.23	0.68
7:M:405:BCL:CBB	7:M:405:BCL:HMB1	2.23	0.68
2:I:17:PHE:CE2	8:I:102:SPO:H342	2.28	0.68
7:3:101:BCL:CBB	7:3:101:BCL:HMB1	2.24	0.68
7:L:301:BCL:CBB	7:L:301:BCL:HMB1	2.23	0.68
7:E:101:BCL:CBB	7:E:101:BCL:HMB1	2.22	0.68
8:J:103:SPO:H83	8:J:103:SPO:H42	1.74	0.68
5:M:280:GLY:HA2	7:M:405:BCL:HED3	1.76	0.68
8:3:102:SPO:H403	2:W:6:LYS:HB3	1.74	0.68
7:L:302:BCL:HBB3	11:L:303:BPH:H141	1.75	0.67
7:V:102:BCL:HMB1	7:V:102:BCL:CBB	2.24	0.67
1:2:35:ALA:HB1	7:2:101:BCL:HBA2	1.76	0.67
2:D:9:GLN:OE1	1:E:8:SER:OG	2.11	0.67
7:N:102:BCL:H91	7:N:102:BCL:C13	2.24	0.67
4:L:267:TRP:CB	12:L:308:U10:H3M3	2.25	0.67
7:9:101:BCL:HMB1	7:9:101:BCL:CBB	2.25	0.67
7:O:101:BCL:H61	8:O:103:SPO:C24	2.26	0.66
7:8:101:BCL:HMB1	7:8:101:BCL:CBB	2.25	0.66
8:O:102:SPO:H361	1:P:23:VAL:HG11	1.77	0.66
7:1:101:BCL:O1D	8:2:102:SPO:H22	1.95	0.66
9:M:411:PC1:H2C2	2:S:29:VAL:HG11	1.75	0.66
7:O:101:BCL:HED1	1:P:31:PHE:CE1	2.31	0.66
1:G:49:LEU:HD13	8:J:102:SPO:C8	2.25	0.66
11:L:310:BPH:HMB1	11:L:310:BPH:HBB3	1.77	0.66
1:C:53:TRP:C	1:C:54:LEU:HD23	2.21	0.66
7:T:101:BCL:CBB	7:T:101:BCL:HMB1	2.25	0.66
7:b:102:BCL:HMB1	7:b:102:BCL:HBB3	1.76	0.65
7:1:101:BCL:HMB2	8:3:102:SPO:C4	2.26	0.65
7:A:101:BCL:HMB1	7:A:101:BCL:HBB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:24:LEU:HD11	8:1:102:SPO:H19	1.77	0.65
8:3:102:SPO:H403	2:W:6:LYS:CB	2.26	0.65
11:L:303:BPH:HBB3	11:L:303:BPH:HMB1	1.78	0.65
8:O:104:SPO:H132	7:S:201:BCL:H42	1.79	0.65
7:U:101:BCL:HMB1	7:U:101:BCL:CBB	2.26	0.65
8:b:101:SPO:H42	8:b:101:SPO:H83	1.78	0.65
7:W:101:BCL:CBB	7:W:101:BCL:HMB1	2.26	0.65
2:K:7:ILE:CD1	7:O:101:BCL:H203	2.27	0.65
7:B:101:BCL:H61	8:D:103:SPO:H241	1.79	0.65
7:K:101:BCL:HMB1	7:K:101:BCL:HBB3	1.78	0.65
2:1:25:PHE:HB2	7:1:101:BCL:H51	1.79	0.64
7:1:101:BCL:HMB1	7:1:101:BCL:HBB3	1.79	0.64
8:J:103:SPO:H83	8:J:103:SPO:C3	2.25	0.64
2:D:15:ARG:NH1	3:H:54:GLY:O	2.30	0.64
8:1:102:SPO:H241	8:1:102:SPO:C27	2.27	0.64
9:A:104:PC1:H143	4:L:29:PRO:HD3	1.78	0.64
7:B:101:BCL:HMB1	7:B:101:BCL:CBB	2.26	0.64
2:S:25:PHE:HB2	7:S:201:BCL:H43	1.80	0.64
8:3:102:SPO:H392	2:W:10:VAL:CG1	2.28	0.64
8:O:104:SPO:H341	1:R:20:LEU:CD1	2.28	0.64
2:S:9:GLN:NE2	1:T:14:ASP:OD1	2.30	0.64
7:a:101:BCL:HMA2	8:b:101:SPO:C24	2.27	0.64
2:1:32:HIS:CE1	7:2:101:BCL:HMD1	2.33	0.64
1:P:25:MET:HE1	7:P:101:BCL:H121	1.78	0.64
10:H:301:CDL:H821	10:H:301:CDL:H781	1.79	0.64
8:b:101:SPO:H42	8:b:101:SPO:H82	1.79	0.64
1:T:48:TRP:CD1	1:T:49:LEU:HG	2.33	0.63
8:3:102:SPO:H393	1:Z:20:LEU:HD12	1.79	0.63
8:C:102:SPO:H81	8:C:102:SPO:C11	2.28	0.63
7:M:405:BCL:HMB1	7:M:405:BCL:HBB2	1.79	0.63
7:I:101:BCL:H43	8:J:102:SPO:C29	2.28	0.63
1:2:48:TRP:CZ2	7:2:101:BCL:HHC	2.33	0.63
2:Q:32:HIS:CE1	7:R:101:BCL:HMD1	2.33	0.63
2:D:26:LEU:HD13	10:H:301:CDL:H452	1.81	0.63
7:O:101:BCL:HMB1	7:O:101:BCL:CBB	2.28	0.63
7:U:101:BCL:HED3	1:V:35:ALA:HB2	1.79	0.63
2:3:32:HIS:CE1	7:Z:101:BCL:HMD1	2.33	0.63
7:T:101:BCL:HMB1	7:T:101:BCL:HBB2	1.81	0.62
8:1:102:SPO:C5	7:a:101:BCL:HMB2	2.29	0.62
7:R:101:BCL:H3A	7:R:101:BCL:H12	1.80	0.62
7:U:101:BCL:HED1	1:V:31:PHE:CZ	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:102:SPO:H25	7:W:101:BCL:HMA2	1.82	0.62
3:H:9:ASP:N	10:H:301:CDL:OB4	2.31	0.62
8:V:101:SPO:H6	7:W:101:BCL:HMB2	1.81	0.62
1:Z:39:HIS:HE1	7:Z:101:BCL:HAA2	1.65	0.62
1:C:53:TRP:O	1:C:54:LEU:HD23	2.00	0.62
2:D:30:MET:HE3	8:F:101:SPO:H32A	1.82	0.62
10:H:301:CDL:H341	10:H:301:CDL:H522	1.82	0.62
7:a:101:BCL:HMA2	8:b:101:SPO:H243	1.80	0.62
1:J:13:SER:OG	1:J:14:ASP:N	2.31	0.62
2:1:24:LEU:HD12	7:1:101:BCL:H42	1.81	0.61
8:J:103:SPO:H6	8:J:103:SPO:C11	2.28	0.61
1:E:32:VAL:HG22	7:E:101:BCL:H11	1.82	0.61
2:a:40:ASP:OD1	1:b:46:ARG:NH2	2.33	0.61
7:1:101:BCL:CHC	7:Z:101:BCL:HBB3	2.30	0.61
7:3:101:BCL:HMB1	7:3:101:BCL:HBB2	1.82	0.61
8:D:103:SPO:H14	8:D:103:SPO:H183	1.80	0.61
12:L:305:U10:H201	12:L:305:U10:H253	1.81	0.61
7:3:101:BCL:CHB	7:C:101:BCL:HMB3	2.30	0.61
7:L:302:BCL:HMB1	7:L:302:BCL:CBB	2.30	0.61
8:0:102:SPO:H131	8:0:102:SPO:C16	2.26	0.61
7:1:101:BCL:HED3	7:2:101:BCL:HAA1	1.83	0.61
7:J:101:BCL:HMB1	7:J:101:BCL:CBB	2.30	0.61
8:S:202:SPO:H361	1:T:20:LEU:CD1	2.30	0.61
7:N:102:BCL:H91	7:N:102:BCL:H142	1.82	0.61
2:U:17:PHE:CE2	8:V:101:SPO:H32	2.36	0.61
2:D:32:HIS:CE1	7:E:101:BCL:HMD1	2.36	0.61
2:I:17:PHE:CZ	8:I:102:SPO:H342	2.36	0.61
8:0:103:SPO:H9	8:0:103:SPO:C4	2.16	0.60
2:I:32:HIS:CE1	7:J:101:BCL:HMD1	2.36	0.60
8:O:104:SPO:H342	2:Q:17:PHE:CE2	2.36	0.60
7:2:101:BCL:CHB	7:a:101:BCL:HMB3	2.31	0.60
1:Z:39:HIS:CE1	7:Z:101:BCL:HAA2	2.36	0.60
8:1:102:SPO:H183	1:2:28:LEU:HD13	1.83	0.60
9:A:102:PC1:H142	3:H:44:MET:CE	2.31	0.60
7:a:101:BCL:H42	1:b:31:PHE:HE2	1.67	0.60
8:S:202:SPO:H15	8:U:102:SPO:C29	2.31	0.60
5:M:218:MET:O	5:M:222:THR:OG1	2.18	0.60
7:N:102:BCL:H91	7:N:102:BCL:C14	2.32	0.60
6:X:25:VAL:CG1	12:X:102:U10:H153	2.32	0.60
8:0:103:SPO:H352	7:A:101:BCL:C4	2.32	0.60
2:S:6:LYS:HB2	8:V:101:SPO:H362	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:301:CDL:H331	9:L:304:PC1:C1	2.29	0.60
7:M:404:BCL:HMB1	7:M:404:BCL:CBB	2.31	0.60
8:O:104:SPO:H6	7:S:201:BCL:CMB	2.28	0.60
2:S:35:LEU:HD21	7:T:101:BCL:HBC3	1.83	0.60
7:F:102:BCL:HMB3	7:F:102:BCL:HBB2	1.83	0.59
7:N:102:BCL:HMB1	7:N:102:BCL:CBB	2.32	0.59
7:2:101:BCL:H41	7:2:101:BCL:HMB2	1.83	0.59
2:S:6:LYS:HD2	8:V:101:SPO:H403	1.84	0.59
8:O:103:SPO:H42	8:O:103:SPO:C9	2.16	0.59
7:C:101:BCL:H92	7:C:101:BCL:H52	1.85	0.59
8:J:102:SPO:H343	8:J:102:SPO:H302	1.85	0.59
2:Q:8:TRP:HZ3	2:Q:16:VAL:HG11	1.68	0.59
2:K:7:ILE:HA	8:O:102:SPO:H342	1.85	0.59
5:M:188:ASN:O	5:M:192:THR:HG23	2.03	0.59
5:M:261:THR:OG1	5:M:263:GLU:O	2.09	0.59
8:P:102:SPO:C4	8:P:102:SPO:H82	2.33	0.59
1:G:48:TRP:CD1	1:G:49:LEU:HG	2.37	0.59
1:J:31:PHE:HE1	8:J:102:SPO:H27	1.67	0.59
1:N:32:VAL:HG21	7:N:102:BCL:H61	1.85	0.59
7:W:101:BCL:HMB1	7:W:101:BCL:HBB2	1.84	0.59
9:A:104:PC1:H2	9:M:401:PC1:H2	1.83	0.58
1:Z:32:VAL:HG21	7:Z:101:BCL:H51	1.85	0.58
8:Z:102:SPO:H14	8:Z:102:SPO:C18	2.33	0.58
7:O:101:BCL:HMB1	7:O:101:BCL:CBB	2.32	0.58
7:O:101:BCL:HMA3	7:O:101:BCL:H12	1.85	0.58
7:E:101:BCL:H203	7:E:101:BCL:H122	1.85	0.58
5:M:114:MET:HE3	9:M:411:PC1:H281	1.85	0.58
8:2:102:SPO:H181	8:2:102:SPO:C21	2.33	0.58
7:L:301:BCL:HMB1	7:L:301:BCL:HBB2	1.85	0.58
1:T:12:LEU:HD12	1:T:16:GLN:OE1	2.03	0.58
10:H:301:CDL:C51	10:H:301:CDL:H312	2.34	0.58
2:9:40:ASP:OD1	2:9:41:TYR:N	2.37	0.58
2:A:15:ARG:HH22	9:A:104:PC1:H142	1.67	0.58
2:S:43:TRP:CZ2	7:S:201:BCL:HBB3	2.38	0.58
2:A:15:ARG:NH2	9:A:102:PC1:H332	2.19	0.58
2:O:17:PHE:HB3	8:P:102:SPO:H401	1.86	0.58
8:S:202:SPO:C8	7:U:101:BCL:HAA1	2.34	0.58
2:D:14:ARG:NH1	3:H:51:PRO:O	2.34	0.57
7:I:101:BCL:H122	8:J:102:SPO:H342	1.86	0.57
8:D:103:SPO:H42	8:D:103:SPO:C8	2.30	0.57
10:H:301:CDL:H541	10:H:301:CDL:H361	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:101:BCL:HHC	7:P:101:BCL:HBB2	1.85	0.57
7:M:404:BCL:HMA1	7:M:404:BCL:C14	2.35	0.57
8:3:102:SPO:H361	1:Z:23:VAL:HG11	1.87	0.57
1:E:29:TRP:CH2	7:E:101:BCL:H161	2.39	0.57
10:H:301:CDL:H312	10:H:301:CDL:H511	1.86	0.57
8:I:102:SPO:H21A	7:K:101:BCL:HBB2	1.87	0.57
7:C:101:BCL:HMD1	2:W:32:HIS:CE1	2.40	0.57
8:C:102:SPO:H25	7:W:101:BCL:CMA	2.35	0.57
7:I:101:BCL:CBB	7:I:101:BCL:HMB3	2.35	0.57
7:F:102:BCL:HED1	1:G:31:PHE:CZ	2.40	0.57
7:C:101:BCL:H162	7:C:101:BCL:H102	1.87	0.57
7:3:101:BCL:H3A	8:U:103:SPO:C9	2.35	0.56
9:A:102:PC1:H131	4:L:2:ALA:HB2	1.88	0.56
12:M:407:U10:H3M3	12:M:407:U10:O2	2.05	0.56
2:7:32:HIS:CE1	7:8:101:BCL:HMD1	2.40	0.56
2:F:42:ASN:O	2:F:46:VAL:HG23	2.05	0.56
7:R:101:BCL:HMB1	7:R:101:BCL:CBB	2.34	0.56
10:H:301:CDL:H541	10:H:301:CDL:C36	2.35	0.56
5:M:152:SER:OG	5:M:277:THR:OG1	1.97	0.56
7:Q:101:BCL:HBB2	7:Q:101:BCL:HMB3	1.87	0.56
12:X:102:U10:H261	12:X:102:U10:H302	1.86	0.56
2:3:20:GLN:NE2	1:Z:24:TYR:OH	2.38	0.56
7:E:101:BCL:H41	8:G:102:SPO:C24	2.35	0.56
7:1:101:BCL:H2A	8:2:102:SPO:H22	1.88	0.56
2:S:32:HIS:CE1	7:T:101:BCL:HMD1	2.41	0.56
2:3:53:ARG:NH1	2:W:40:ASP:OD2	2.38	0.56
1:B:48:TRP:CD1	1:B:49:LEU:HG	2.41	0.56
2:7:9:GLN:NE2	1:8:14:ASP:OD1	2.34	0.56
10:H:301:CDL:H561	10:H:301:CDL:H382	1.88	0.55
7:N:102:BCL:HBB1	7:O:101:BCL:HMC3	1.88	0.55
7:Z:101:BCL:HMB1	7:Z:101:BCL:CBB	2.35	0.55
7:0:101:BCL:HMD1	2:9:32:HIS:CE1	2.42	0.55
7:D:102:BCL:HMB3	7:D:102:BCL:CBB	2.37	0.55
2:U:8:TRP:CD2	1:V:20:LEU:HD23	2.41	0.55
10:H:301:CDL:H522	10:H:301:CDL:C34	2.36	0.55
2:1:24:LEU:HD21	8:1:102:SPO:H19	1.87	0.55
7:G:101:BCL:HMB1	8:J:102:SPO:H131	1.89	0.55
8:S:202:SPO:H131	8:U:102:SPO:H312	1.88	0.55
8:U:103:SPO:H342	2:W:17:PHE:HE2	1.72	0.55
1:V:20:LEU:HD12	8:V:101:SPO:H402	1.87	0.55
2:D:4:PHE:O	2:D:7:ILE:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:SER:O	10:H:301:CDL:H131	2.06	0.55
1:O:35:ALA:HB2	7:9:101:BCL:HED2	1.89	0.55
2:9:40:ASP:OD2	2:A:53:ARG:NH1	2.39	0.55
7:I:101:BCL:HAA2	7:I:101:BCL:HBD	1.89	0.55
7:L:302:BCL:HBB3	11:L:303:BPH:C14	2.38	0.54
1:P:25:MET:HE2	7:Q:101:BCL:H193	1.89	0.54
1:C:47:VAL:HG11	7:C:101:BCL:HBC1	1.90	0.54
3:H:107:ASN:OD1	3:H:110:VAL:HG23	2.08	0.54
8:3:102:SPO:H25	1:Z:24:TYR:CE1	2.42	0.54
9:A:102:PC1:H232	4:L:27:VAL:HG13	1.89	0.54
9:A:104:PC1:H153	9:M:401:PC1:H142	1.89	0.54
4:L:202:GLU:OE2	5:M:144:LYS:NZ	2.34	0.54
4:L:227:THR:O	4:L:231:HIS:ND1	2.40	0.54
8:O:102:SPO:C39	8:O:102:SPO:H341	2.38	0.54
2:a:31:ILE:O	2:a:35:LEU:HD13	2.07	0.54
3:H:36:MET:HE1	3:H:56:PHE:HB2	1.90	0.54
2:S:10:VAL:HG13	8:V:101:SPO:H37	1.89	0.54
2:I:1:MET:SD	7:J:101:BCL:H191	2.48	0.54
7:3:101:BCL:HAA2	7:3:101:BCL:HBD	1.90	0.54
7:9:101:BCL:HMB2	8:X:101:SPO:H6	1.90	0.54
7:I:101:BCL:HED1	1:J:31:PHE:CE1	2.43	0.54
2:U:8:TRP:CG	1:V:20:LEU:HD23	2.43	0.54
7:1:101:BCL:C2B	8:3:102:SPO:H42	2.38	0.54
1:C:36:PHE:CE1	7:W:101:BCL:HED1	2.43	0.54
7:1:101:BCL:H12	8:3:102:SPO:H81	1.90	0.53
2:F:16:VAL:HG11	7:I:101:BCL:H142	1.90	0.53
2:K:40:ASP:O	1:N:46:ARG:NH1	2.41	0.53
2:D:7:ILE:HA	2:D:10:VAL:HG12	1.89	0.53
8:I:102:SPO:H361	1:J:23:VAL:CG1	2.36	0.53
4:L:183:THR:CG2	12:L:305:U10:H151	2.37	0.53
12:L:305:U10:C36	12:L:309:U10:H4M3	2.38	0.53
7:M:405:BCL:HAA2	7:M:405:BCL:HBD	1.90	0.53
7:S:201:BCL:HED1	8:T:102:SPO:C22	2.38	0.53
11:L:310:BPH:C10	7:M:405:BCL:H18	2.39	0.53
2:Q:7:ILE:HB	8:S:202:SPO:H343	1.89	0.53
8:b:101:SPO:H291	8:b:101:SPO:C32	2.22	0.53
2:O:43:TRP:HA	2:O:46:VAL:HG12	1.90	0.53
2:1:25:PHE:N	7:1:101:BCL:H2	2.23	0.53
7:7:101:BCL:HMA1	12:X:102:U10:H303	1.91	0.53
5:M:69:MET:HB3	9:M:411:PC1:H2F1	1.91	0.53
1:P:49:LEU:HD22	8:P:103:SPO:H132	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:9:GLN:NE2	1:P:14:ASP:OD1	2.41	0.53
1:b:42:VAL:HG23	1:b:48:TRP:HH2	1.74	0.53
1:J:8:SER:OG	1:J:10:THR:O	2.23	0.53
7:S:201:BCL:H41	7:S:201:BCL:C7	2.31	0.53
1:T:42:VAL:HA	1:T:45:TRP:CD1	2.43	0.53
8:I:102:SPO:C36	1:J:23:VAL:HG11	2.38	0.53
5:M:70:THR:HG23	9:M:411:PC1:H291	1.91	0.53
1:P:21:HIS:HE1	7:Q:101:BCL:H202	1.74	0.53
8:U:103:SPO:H342	2:W:17:PHE:CE2	2.44	0.53
1:N:23:VAL:HG21	8:N:101:SPO:H352	1.90	0.52
6:X:25:VAL:HG11	12:X:102:U10:H153	1.91	0.52
9:A:102:PC1:H153	3:H:44:MET:CE	2.39	0.52
2:D:1:MET:CE	7:E:101:BCL:H18	2.39	0.52
2:D:40:ASP:OD2	2:F:53:ARG:NH1	2.42	0.52
7:a:101:BCL:HED1	1:b:31:PHE:CE1	2.43	0.52
9:A:102:PC1:O32	9:A:102:PC1:H351	2.09	0.52
2:O:10:VAL:CG2	8:O:104:SPO:H402	2.39	0.52
1:Z:14:ASP:OD1	1:Z:15:GLU:N	2.42	0.52
8:O:102:SPO:H6	7:Q:101:BCL:HMB1	1.91	0.52
7:A:101:BCL:HED2	1:B:35:ALA:HB2	1.91	0.52
1:R:48:TRP:CD1	1:R:49:LEU:HG	2.45	0.52
7:7:101:BCL:H102	1:8:31:PHE:HD1	1.75	0.52
1:R:38:ALA:O	1:R:42:VAL:HG23	2.09	0.52
8:S:202:SPO:H83	7:U:101:BCL:HAA1	1.92	0.52
12:X:102:U10:H1M1	12:X:102:U10:C8	2.40	0.52
2:D:16:VAL:HG21	7:F:102:BCL:H142	1.92	0.51
2:a:43:TRP:CE3	7:a:101:BCL:HBC2	2.44	0.51
1:C:53:TRP:CZ2	7:C:101:BCL:HHC	2.45	0.51
7:L:302:BCL:O1A	7:L:302:BCL:H43	2.10	0.51
6:X:17:ARG:HB3	8:X:101:SPO:H343	1.92	0.51
2:3:40:ASP:O	1:Z:46:ARG:NH1	2.39	0.51
7:E:101:BCL:HMB1	7:E:101:BCL:HBB3	1.90	0.51
8:T:102:SPO:H25	8:T:102:SPO:H292	1.92	0.51
2:a:45:ASP:HA	2:a:48:THR:HG22	1.92	0.51
7:8:101:BCL:CHB	7:9:101:BCL:HMB3	2.41	0.51
7:D:102:BCL:HMB3	7:D:102:BCL:HBB2	1.93	0.51
8:O:104:SPO:H362	1:R:20:LEU:HD13	1.93	0.51
7:1:101:BCL:H3A	8:3:102:SPO:C7	2.41	0.51
2:I:42:ASN:O	2:I:46:VAL:HG23	2.10	0.51
4:L:267:TRP:O	4:L:273:TRP:NE1	2.40	0.51
8:F:103:SPO:H342	8:F:103:SPO:H302	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:270:LEU:O	4:L:274:VAL:HG23	2.10	0.50
7:Q:101:BCL:HMB3	7:Q:101:BCL:CBB	2.41	0.50
7:D:102:BCL:HAA2	7:D:102:BCL:O2D	2.11	0.50
7:S:201:BCL:HHC	7:S:201:BCL:CBB	2.41	0.50
8:F:101:SPO:H6	7:F:102:BCL:HMB1	1.93	0.50
2:O:34:ILE:O	2:O:37:SER:OG	2.26	0.50
2:1:21:GLY:O	7:1:101:BCL:H52	2.12	0.50
2:1:24:LEU:HD11	8:1:102:SPO:C19	2.42	0.50
9:A:102:PC1:H2I1	4:L:40:PHE:HZ	1.77	0.50
7:E:101:BCL:H201	1:G:30:LEU:HD11	1.91	0.50
8:J:103:SPO:H83	8:J:103:SPO:C4	2.42	0.50
12:L:307:U10:H301	12:L:307:U10:H353	1.94	0.50
12:X:102:U10:C8	12:X:102:U10:C1M	2.90	0.50
2:9:30:MET:HE1	4:L:49:LEU:HD23	1.94	0.50
8:D:103:SPO:H83	8:D:103:SPO:C4	2.36	0.50
7:E:101:BCL:H41	8:G:102:SPO:H26	1.93	0.50
8:J:103:SPO:H362	7:K:101:BCL:H41	1.92	0.50
4:L:54:THR:OG1	4:L:59:VAL:O	2.29	0.50
8:S:202:SPO:C6	8:S:202:SPO:H33	2.42	0.50
7:B:101:BCL:H61	8:D:103:SPO:C24	2.42	0.50
3:H:198:THR:OG1	5:M:228:ARG:HA	2.12	0.49
7:N:102:BCL:C5	8:P:102:SPO:H293	2.39	0.49
8:P:102:SPO:H82	8:P:102:SPO:H41	1.94	0.49
7:3:101:BCL:C4	8:Z:102:SPO:H361	2.43	0.49
2:F:33:LEU:HD22	10:H:301:CDL:H532	1.93	0.49
4:L:267:TRP:HB2	12:L:308:U10:H3M3	1.93	0.49
8:I:102:SPO:H341	8:I:102:SPO:C37	2.42	0.49
7:J:101:BCL:H62	8:J:103:SPO:C24	2.33	0.49
2:K:32:HIS:CE1	7:N:102:BCL:HMD1	2.48	0.49
12:X:102:U10:H201	12:X:102:U10:C23	2.41	0.49
8:O:102:SPO:H133	1:8:49:LEU:CD1	2.43	0.49
2:1:35:LEU:HD23	7:1:101:BCL:HBC1	1.95	0.49
1:E:32:VAL:O	1:E:36:VAL:HG23	2.12	0.49
2:S:27:LEU:HD11	8:S:202:SPO:H6	1.94	0.49
4:L:223:TYR:OH	5:M:45:ASN:O	2.24	0.49
7:L:301:BCL:O1A	7:L:301:BCL:HED3	2.13	0.49
7:M:404:BCL:HMA1	7:M:404:BCL:H142	1.94	0.49
10:H:301:CDL:CA6	10:H:301:CDL:H112	2.42	0.49
7:M:404:BCL:H142	7:M:404:BCL:HHB	1.95	0.49
8:O:102:SPO:H341	8:O:102:SPO:H392	1.93	0.49
7:J:101:BCL:HBB1	7:K:101:BCL:HMC3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1:101:BCL:HMB3	7:Z:101:BCL:CHB	2.42	0.48
2:3:2:SER:OG	2:3:3:LYS:N	2.45	0.48
2:3:53:ARG:NH2	1:C:52:PRO:O	2.46	0.48
1:8:35:ALA:CB	7:8:101:BCL:HBA1	2.43	0.48
2:F:20:GLN:HG3	7:I:101:BCL:H91	1.94	0.48
7:Z:101:BCL:H162	7:Z:101:BCL:H101	1.95	0.48
8:1:102:SPO:HM11	7:a:101:BCL:HBB2	1.96	0.48
10:H:301:CDL:H522	10:H:301:CDL:H312	1.95	0.48
7:I:101:BCL:H61	8:J:102:SPO:C34	2.42	0.48
2:U:16:VAL:HG13	7:W:101:BCL:H142	1.94	0.48
4:L:232:ARG:NH2	5:M:6:ASN:OD1	2.43	0.48
1:V:23:VAL:CG2	8:V:101:SPO:H342	2.43	0.48
8:I:102:SPO:C16	7:J:101:BCL:H2	2.44	0.48
8:J:103:SPO:C8	8:J:103:SPO:C4	2.86	0.48
4:L:267:TRP:HB3	12:L:308:U10:H3M3	1.96	0.48
2:S:17:PHE:CE2	8:S:202:SPO:H32	2.48	0.48
2:O:40:ASP:O	1:P:46:ARG:NH2	2.47	0.48
1:V:23:VAL:HG22	8:V:101:SPO:H342	1.95	0.48
8:1:102:SPO:H183	1:2:28:LEU:CD1	2.44	0.48
7:M:404:BCL:H162	8:M:408:SPO:H133	1.96	0.48
7:3:101:BCL:H203	1:C:26:HIS:HE1	1.79	0.48
1:C:50:TRP:HB2	8:C:102:SPO:H10	1.94	0.48
9:D:104:PC1:H142	2:F:14:ARG:HB2	1.95	0.48
12:L:309:U10:H3M2	12:L:309:U10:O2	2.12	0.48
9:L:311:PC1:H332	2:W:33:LEU:HD13	1.95	0.48
5:M:108:ARG:NH2	2:Q:45:ASP:OD2	2.43	0.48
8:2:102:SPO:C29	7:Z:101:BCL:H42	2.43	0.47
7:I:101:BCL:HMB3	7:I:101:BCL:HBB3	1.96	0.47
7:L:301:BCL:HBB3	7:M:404:BCL:HMD2	1.96	0.47
12:X:102:U10:C1M	12:X:102:U10:H8	2.43	0.47
8:1:102:SPO:C8	8:1:102:SPO:C4	2.92	0.47
1:2:12:LEU:HD22	1:2:16:GLN:HB3	1.96	0.47
3:H:235:ASP:OD1	5:M:243:THR:HG22	2.14	0.47
8:3:102:SPO:H27	8:3:102:SPO:C24	2.35	0.47
12:M:407:U10:H4M3	12:M:407:U10:O3	2.14	0.47
2:S:43:TRP:HZ2	7:S:201:BCL:HBB3	1.79	0.47
7:1:101:BCL:C4B	7:Z:101:BCL:HBB3	2.43	0.47
7:E:101:BCL:HMB1	7:E:101:BCL:HBB2	1.93	0.47
2:U:17:PHE:HB3	8:U:102:SPO:H391	1.96	0.47
1:V:20:LEU:HD12	8:V:101:SPO:C38	2.44	0.47
1:0:47:PRO:O	2:A:53:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:31:ILE:HG21	7:Z:101:BCL:C1D	2.44	0.47
1:8:7:LEU:HD23	8:9:102:SPO:H401	1.96	0.47
2:A:15:ARG:NH2	9:A:104:PC1:H133	2.29	0.47
4:L:252:THR:O	4:L:256:TRP:O	2.32	0.47
7:7:101:BCL:H41	7:7:101:BCL:H61	1.37	0.47
1:C:25:LEU:HD23	2:W:8:TRP:CG	2.50	0.47
7:R:101:BCL:HMC3	7:S:201:BCL:HBB1	1.97	0.47
12:X:102:U10:H201	12:X:102:U10:H23	1.96	0.47
9:A:102:PC1:H153	3:H:44:MET:HE1	1.97	0.47
8:C:102:SPO:H341	8:C:102:SPO:C37	2.45	0.47
12:L:307:U10:O5	6:X:42:LEU:HD13	2.14	0.47
7:O:101:BCL:HED1	1:P:31:PHE:CZ	2.50	0.47
9:A:102:PC1:H132	9:A:102:PC1:O14	2.13	0.47
3:H:129:ALA:CB	5:M:21:LEU:HD21	2.44	0.47
4:L:234:GLY:HA3	5:M:216:PHE:CE1	2.50	0.47
2:W:43:TRP:NE1	7:W:101:BCL:OBB	2.48	0.47
7:1:101:BCL:CHA	8:2:102:SPO:H20	2.45	0.46
9:A:104:PC1:O14	9:A:104:PC1:H32	2.15	0.46
2:S:40:ASP:OD2	2:U:53:ARG:HD2	2.16	0.46
1:8:20:LEU:O	1:8:23:VAL:HG22	2.14	0.46
7:E:101:BCL:H203	7:E:101:BCL:C12	2.45	0.46
8:G:102:SPO:H361	8:G:102:SPO:H341	1.67	0.46
2:I:6:LYS:HD3	8:N:101:SPO:H393	1.96	0.46
6:X:17:ARG:CD	8:X:101:SPO:H343	2.45	0.46
2:9:23:PHE:HZ	8:9:102:SPO:H132	1.80	0.46
12:L:308:U10:H3M2	12:L:308:U10:O2	2.15	0.46
5:M:109:ASP:OD1	5:M:110:ALA:N	2.44	0.46
7:0:101:BCL:H12	7:0:101:BCL:CMA	2.44	0.46
7:N:102:BCL:HBA1	7:N:102:BCL:H12	1.36	0.46
8:C:102:SPO:H182	7:V:102:BCL:CBB	2.46	0.46
8:J:103:SPO:H42	8:J:103:SPO:H82	1.92	0.46
5:M:272:PHE:O	5:M:276:VAL:HG23	2.15	0.46
2:S:8:TRP:HZ3	2:S:16:VAL:HG11	1.81	0.46
2:S:40:ASP:OD1	2:S:41:TYR:N	2.49	0.46
7:7:101:BCL:CHD	7:7:101:BCL:HBC2	2.46	0.46
7:A:101:BCL:HMB1	7:A:101:BCL:CBB	2.43	0.46
1:E:21:HIS:O	1:E:25:MET:HG2	2.16	0.46
7:2:101:BCL:HBA1	7:2:101:BCL:H3A	1.57	0.46
7:J:101:BCL:H61	7:J:101:BCL:H41	1.59	0.46
2:K:42:ASN:O	2:K:46:VAL:HG23	2.15	0.46
1:N:11:GLY:C	1:N:12:LEU:HD12	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:102:SPO:H362	8:T:102:SPO:H341	1.73	0.46
7:7:101:BCL:H8	7:7:101:BCL:H122	1.54	0.46
2:A:12:ASP:OD1	2:A:14:ARG:NH1	2.49	0.46
3:H:45:GLU:OE1	3:H:93:ARG:NH2	2.49	0.46
4:L:224:SER:OG	12:L:305:U10:O5	2.21	0.46
7:M:404:BCL:HMA1	7:M:404:BCL:H141	1.97	0.46
8:P:103:SPO:C34	7:Q:101:BCL:H111	2.46	0.46
7:B:101:BCL:H93	7:B:101:BCL:H62	1.82	0.46
2:F:4:PHE:CD1	8:I:102:SPO:H302	2.51	0.46
5:M:55:GLY:O	5:M:59:VAL:HG23	2.15	0.46
8:O:104:SPO:H341	8:O:104:SPO:H362	1.66	0.46
1:T:48:TRP:CZ2	7:T:101:BCL:HHC	2.51	0.46
8:U:102:SPO:H311	8:U:102:SPO:H291	1.70	0.46
7:a:101:BCL:HMA2	8:b:101:SPO:C23	2.46	0.46
8:D:103:SPO:H362	8:D:103:SPO:H341	1.68	0.45
7:I:101:BCL:H102	8:J:102:SPO:H341	1.97	0.45
8:M:408:SPO:H401	2:O:30:MET:SD	2.56	0.45
1:N:23:VAL:CG2	8:N:101:SPO:H352	2.45	0.45
1:b:38:ALA:CB	8:b:101:SPO:H181	2.40	0.45
1:8:28:LEU:C	1:8:28:LEU:HD23	2.41	0.45
4:L:235:LEU:O	4:L:239:LEU:HG	2.17	0.45
8:S:202:SPO:H361	1:T:20:LEU:HD12	1.98	0.45
2:U:32:HIS:CE1	7:V:102:BCL:HMD1	2.51	0.45
8:1:102:SPO:C6	7:a:101:BCL:H3A	2.46	0.45
8:2:102:SPO:H292	7:Z:101:BCL:H42	1.98	0.45
7:9:101:BCL:H162	7:9:101:BCL:H121	1.77	0.45
2:D:8:TRP:HZ3	2:D:16:VAL:HG11	1.81	0.45
8:I:102:SPO:H402	1:J:20:LEU:HA	1.98	0.45
8:P:103:SPO:H291	8:P:103:SPO:H312	1.65	0.45
7:Z:101:BCL:H151	7:Z:101:BCL:H111	1.61	0.45
8:Z:102:SPO:C18	8:Z:102:SPO:C14	2.95	0.45
7:3:101:BCL:H43	8:Z:102:SPO:C32	2.46	0.45
5:M:229:PHE:HB2	5:M:244:ALA:HB2	1.99	0.45
2:1:20:GLN:NE2	8:1:102:SPO:H243	2.31	0.45
7:1:101:BCL:HAA1	8:3:102:SPO:H83	1.98	0.45
8:1:102:SPO:C18	1:2:28:LEU:HD13	2.46	0.45
9:A:102:PC1:C23	4:L:27:VAL:HG13	2.46	0.45
8:J:102:SPO:H26	8:J:102:SPO:H241	1.83	0.45
5:M:130:TRP:O	5:M:133:THR:OG1	2.31	0.45
7:9:101:BCL:H142	12:L:307:U10:H361	1.98	0.45
8:U:103:SPO:H132	2:W:23:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:20:LEU:HD12	8:V:101:SPO:C40	2.46	0.45
2:I:34:ILE:HG23	10:M:410:CDL:H112	1.99	0.45
5:M:19:MET:HE1	5:M:32:LYS:HA	1.98	0.45
8:P:103:SPO:H341	8:P:103:SPO:H362	1.39	0.45
9:A:104:PC1:H121	9:M:401:PC1:O14	2.16	0.45
1:G:7:LEU:HD21	1:G:9:PHE:CE1	2.51	0.45
1:T:42:VAL:HA	1:T:45:TRP:NE1	2.32	0.45
2:W:43:TRP:CG	7:W:101:BCL:HMC2	2.52	0.45
7:E:101:BCL:HMB3	7:F:102:BCL:CHB	2.47	0.45
4:L:194:LEU:HD22	4:L:217:PHE:CD2	2.52	0.45
5:M:260:ALA:N	12:M:407:U10:O5	2.47	0.45
2:Q:38:LYS:HB2	2:Q:40:ASP:O	2.17	0.45
2:W:7:ILE:HA	2:W:10:VAL:HG22	1.99	0.45
8:b:101:SPO:C8	8:b:101:SPO:C4	2.85	0.45
7:1:101:BCL:HAA2	7:1:101:BCL:HBD	1.99	0.44
7:E:101:BCL:H3A	7:E:101:BCL:H2	1.98	0.44
2:F:17:PHE:HB3	8:G:102:SPO:H401	1.98	0.44
11:L:303:BPH:HMB1	11:L:303:BPH:CBB	2.46	0.44
1:P:48:TRP:HE1	7:P:101:BCL:HBB2	1.82	0.44
7:S:201:BCL:HED2	8:T:102:SPO:H293	1.99	0.44
7:a:101:BCL:C1D	7:b:102:BCL:HMD2	2.48	0.44
7:3:101:BCL:HMB2	8:U:103:SPO:C6	2.46	0.44
5:M:186:THR:CG2	7:M:404:BCL:H3C	2.47	0.44
7:N:102:BCL:HBB3	7:O:101:BCL:C1C	2.47	0.44
1:P:32:VAL:O	1:P:36:VAL:HG23	2.18	0.44
2:Q:42:ASN:O	2:Q:46:VAL:HG23	2.17	0.44
2:W:6:LYS:O	2:W:9:GLN:N	2.50	0.44
1:Z:42:VAL:CG1	7:Z:101:BCL:HBC1	2.47	0.44
7:1:101:BCL:HAA2	7:1:101:BCL:CBD	2.47	0.44
8:J:103:SPO:H311	8:J:103:SPO:H291	1.41	0.44
1:N:23:VAL:HG21	8:N:101:SPO:H341	1.99	0.44
2:9:23:PHE:CZ	8:9:102:SPO:H132	2.52	0.44
8:D:101:SPO:H6	7:D:102:BCL:HMB1	2.00	0.44
7:G:101:BCL:H152	7:G:101:BCL:C8	2.44	0.44
3:H:24:LEU:O	3:H:28:ILE:HG12	2.17	0.44
8:J:103:SPO:C18	8:J:103:SPO:C14	2.84	0.44
4:L:154:HIS:O	4:L:158:VAL:HG23	2.18	0.44
4:L:236:LEU:HD12	5:M:43:PHE:CE1	2.52	0.44
7:R:101:BCL:H61	7:R:101:BCL:H41	1.80	0.44
1:Z:29:TRP:HH2	7:Z:101:BCL:H143	1.83	0.44
8:D:103:SPO:C8	8:D:103:SPO:C4	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:BCL:H72	8:J:102:SPO:H20	1.99	0.44
2:I:45:ASP:O	2:I:48:THR:OG1	2.29	0.44
1:P:49:LEU:CD2	8:P:103:SPO:H132	2.47	0.44
6:X:43:VAL:O	6:X:47:LEU:HG	2.17	0.44
7:3:101:BCL:H41	8:Z:102:SPO:H361	1.99	0.44
2:D:34:ILE:O	2:D:37:SER:OG	2.33	0.44
2:F:16:VAL:CG1	7:I:101:BCL:H142	2.48	0.44
4:L:133:VAL:HG23	4:L:134:VAL:HG23	1.98	0.44
12:M:403:U10:H3M2	12:M:403:U10:O2	2.17	0.44
4:L:180:PHE:O	4:L:184:THR:OG1	2.29	0.44
1:N:48:TRP:CD1	1:N:49:LEU:HG	2.53	0.44
8:U:103:SPO:H31	2:W:30:MET:HE3	2.00	0.44
7:B:101:BCL:HMA2	8:D:101:SPO:H11	2.00	0.44
7:J:101:BCL:O1A	7:J:101:BCL:H2A	2.17	0.44
7:B:101:BCL:H13	7:B:101:BCL:H172	1.78	0.43
7:a:101:BCL:HED3	7:a:101:BCL:H2A	2.00	0.43
7:b:102:BCL:HBC2	7:b:102:BCL:H2C	1.63	0.43
1:8:21:HIS:O	1:8:25:MET:HG2	2.18	0.43
8:C:102:SPO:C6	8:C:102:SPO:H21A	2.48	0.43
7:D:102:BCL:HED1	1:E:31:PHE:CZ	2.53	0.43
4:L:191:HIS:ND1	12:L:305:U10:O2	2.34	0.43
7:Z:101:BCL:H61	7:Z:101:BCL:H102	1.83	0.43
2:D:1:MET:HE3	7:E:101:BCL:H18	1.99	0.43
2:F:6:LYS:HB2	8:I:102:SPO:H362	2.00	0.43
3:H:115:PRO:O	5:M:247:ARG:NH1	2.42	0.43
7:N:102:BCL:C4	7:N:102:BCL:H71	2.48	0.43
7:N:102:BCL:O1A	7:N:102:BCL:H2A	2.12	0.43
2:a:32:HIS:NE2	7:b:102:BCL:HMD1	2.33	0.43
2:D:30:MET:HG3	10:H:301:CDL:H381	2.00	0.43
3:H:10:PHE:CE1	10:H:301:CDL:H732	2.54	0.43
3:H:22:GLY:CA	10:H:301:CDL:H811	2.49	0.43
2:K:7:ILE:HD13	7:O:101:BCL:H203	1.99	0.43
7:T:101:BCL:H93	7:T:101:BCL:H61	1.86	0.43
8:1:102:SPO:H5	7:a:101:BCL:HMB2	1.99	0.43
1:C:43:ALA:O	1:C:47:VAL:HG23	2.19	0.43
4:L:32:VAL:HG13	4:L:32:VAL:O	2.18	0.43
1:N:11:GLY:O	1:N:12:LEU:HD12	2.18	0.43
7:R:101:BCL:H8	8:T:102:SPO:C27	2.45	0.43
7:a:101:BCL:HMA1	8:b:101:SPO:C26	2.48	0.43
7:G:101:BCL:OBB	8:J:102:SPO:H133	2.18	0.43
5:M:285:LEU:O	5:M:289:THR:OG1	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:6:LYS:O	2:S:9:GLN:N	2.46	0.43
1:O:21:HIS:O	1:O:25:MET:HG2	2.19	0.43
2:7:13:PRO:CB	1:8:20:LEU:HD21	2.49	0.43
2:F:6:LYS:HD3	8:I:102:SPO:H403	1.98	0.43
7:G:101:BCL:H8	7:G:101:BCL:H121	1.60	0.43
7:G:101:BCL:H2	7:G:101:BCL:H61	1.82	0.43
1:R:8:SER:OG	1:R:11:GLY:N	2.49	0.43
9:M:411:PC1:H2A2	2:Q:30:MET:SD	2.59	0.43
8:O:104:SPO:H342	2:Q:17:PHE:HE2	1.81	0.43
8:1:102:SPO:C27	8:1:102:SPO:C24	2.96	0.43
7:J:101:BCL:H142	7:J:101:BCL:H102	2.01	0.43
8:O:102:SPO:H362	8:O:102:SPO:H341	1.81	0.43
9:D:104:PC1:H261	7:F:102:BCL:H72	2.01	0.43
9:L:311:PC1:H251	2:W:33:LEU:HD21	2.00	0.43
2:9:17:PHE:CE2	8:9:102:SPO:H342	2.54	0.42
9:A:102:PC1:H133	9:A:102:PC1:H111	1.79	0.42
7:J:101:BCL:H41	7:J:101:BCL:H93	2.00	0.42
4:L:23:PHE:O	4:L:32:VAL:O	2.37	0.42
7:C:101:BCL:HMB1	7:C:101:BCL:CBB	2.44	0.42
7:E:101:BCL:H111	1:G:34:ILE:HD13	2.01	0.42
8:F:103:SPO:H5	7:I:101:BCL:HMB1	2.01	0.42
7:G:101:BCL:H3A	7:G:101:BCL:H12	2.01	0.42
7:J:101:BCL:H71	8:J:103:SPO:C24	2.49	0.42
8:P:102:SPO:H341	8:P:102:SPO:H361	1.50	0.42
2:U:6:LYS:NZ	1:V:14:ASP:OD2	2.51	0.42
7:9:101:BCL:H162	7:9:101:BCL:H203	1.79	0.42
1:C:40:ALA:O	1:C:44:HIS:ND1	2.42	0.42
7:J:101:BCL:H151	7:J:101:BCL:H18	1.78	0.42
8:J:103:SPO:H362	7:K:101:BCL:C4	2.49	0.42
12:L:305:U10:H102	12:L:305:U10:H1M2	2.00	0.42
7:a:101:BCL:CHD	7:b:102:BCL:HMD2	2.49	0.42
7:1:101:BCL:HMA3	8:2:102:SPO:C23	2.50	0.42
1:2:32:VAL:HG13	7:2:101:BCL:H2	2.00	0.42
2:I:28:ALA:HB2	7:J:101:BCL:HED2	2.01	0.42
12:L:309:U10:C3M	7:M:404:BCL:H93	2.47	0.42
1:P:25:MET:HE3	7:P:101:BCL:H151	2.02	0.42
7:U:101:BCL:HED1	1:V:31:PHE:CE2	2.54	0.42
1:E:48:TRP:CD1	1:E:49:LEU:HG	2.55	0.42
8:P:102:SPO:C4	8:P:102:SPO:C8	2.96	0.42
8:U:103:SPO:H26	8:U:103:SPO:H241	1.92	0.42
7:3:101:BCL:HMA1	8:Z:102:SPO:C25	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:101:BCL:HBA2	7:9:101:BCL:H3A	1.80	0.42
9:A:102:PC1:H153	3:H:44:MET:HE2	2.02	0.42
7:G:101:BCL:H8	7:G:101:BCL:C15	2.44	0.42
1:J:48:TRP:CZ2	7:J:101:BCL:HHC	2.54	0.42
2:S:10:VAL:HG23	2:S:11:PHE:N	2.34	0.42
1:T:32:VAL:O	1:T:36:VAL:HG23	2.19	0.42
7:V:102:BCL:H122	7:V:102:BCL:H171	2.02	0.42
1:Z:30:LEU:O	1:Z:33:THR:HG22	2.19	0.42
7:1:101:BCL:H3A	8:3:102:SPO:C9	2.50	0.42
2:F:11:PHE:HE2	8:J:102:SPO:H403	1.84	0.42
7:O:101:BCL:HAA2	7:O:101:BCL:HBD	2.02	0.42
8:1:102:SPO:H241	8:1:102:SPO:H27	2.02	0.42
1:R:32:VAL:O	1:R:36:VAL:HG23	2.19	0.42
2:3:25:PHE:HB2	7:3:101:BCL:H51	2.02	0.41
8:T:102:SPO:H25	8:T:102:SPO:C29	2.50	0.41
7:U:101:BCL:HMC2	7:U:101:BCL:HHC	1.91	0.41
2:1:18:VAL:O	2:1:22:VAL:HG23	2.20	0.41
7:E:101:BCL:H142	7:E:101:BCL:H112	1.80	0.41
3:H:175:VAL:HB	3:H:176:PRO:HD3	2.02	0.41
10:M:409:CDL:H722	10:M:409:CDL:HB61	2.02	0.41
2:W:3:LYS:O	2:W:3:LYS:HG3	2.20	0.41
12:X:102:U10:H3M2	12:X:102:U10:O2	2.19	0.41
8:Z:102:SPO:H311	8:Z:102:SPO:H291	1.50	0.41
2:1:41:TYR:CE1	2:a:44:LEU:HD12	2.56	0.41
7:9:101:BCL:H142	7:9:101:BCL:H111	1.93	0.41
8:D:103:SPO:H291	8:D:103:SPO:H311	1.38	0.41
10:H:301:CDL:H541	10:H:301:CDL:H362	2.02	0.41
4:L:214:ASP:OD1	4:L:224:SER:OG	2.38	0.41
7:L:301:BCL:HMB1	7:L:301:BCL:HBB3	2.01	0.41
5:M:278:LEU:HD21	10:M:409:CDL:H631	2.02	0.41
2:S:20:GLN:NE2	8:S:202:SPO:H22	2.34	0.41
7:3:101:BCL:C1D	7:Z:101:BCL:HMD2	2.50	0.41
7:E:101:BCL:H162	7:E:101:BCL:H121	1.63	0.41
12:L:309:U10:H121	12:L:309:U10:H101	1.91	0.41
8:M:408:SPO:H26	8:M:408:SPO:H241	1.93	0.41
7:J:101:BCL:H51	7:J:101:BCL:H12	1.88	0.41
7:L:301:BCL:CBB	7:M:404:BCL:HMD2	2.50	0.41
7:M:404:BCL:H101	7:M:404:BCL:H13	1.75	0.41
7:U:101:BCL:HMD1	1:V:39:HIS:CE1	2.56	0.41
8:b:101:SPO:H26	8:b:101:SPO:H241	1.92	0.41
7:1:101:BCL:HBA2	8:3:102:SPO:C8	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:114:GLY:O	3:H:117:SER:OG	2.27	0.41
4:L:129:TYR:O	4:L:133:VAL:HG22	2.20	0.41
9:M:401:PC1:H341	12:M:407:U10:H201	2.02	0.41
1:C:37:VAL:O	1:C:41:VAL:HG13	2.21	0.41
7:G:101:BCL:H93	8:J:102:SPO:C18	2.51	0.41
1:J:21:HIS:O	1:J:25:MET:HG2	2.20	0.41
4:L:62:PRO:HA	4:L:65:ILE:HD12	2.03	0.41
5:M:161:GLY:HA3	8:M:408:SPO:H292	2.01	0.41
2:Q:20:GLN:NE2	1:R:24:TYR:OH	2.38	0.41
1:Z:44:ILE:HG13	1:Z:45:TRP:N	2.36	0.41
1:b:48:TRP:CD2	7:b:102:BCL:HBC2	2.55	0.41
8:3:102:SPO:H341	8:3:102:SPO:H362	1.64	0.41
1:C:28:VAL:HG12	2:U:3:LYS:HB2	2.03	0.41
3:H:1:MET:SD	3:H:4:VAL:HG11	2.61	0.41
8:J:103:SPO:H241	8:J:103:SPO:H26	1.87	0.41
11:L:310:BPH:HMB1	11:L:310:BPH:CBB	2.50	0.41
2:S:12:ASP:OD2	2:S:14:ARG:HG2	2.20	0.41
1:V:48:TRP:NE1	1:V:49:LEU:HD23	2.36	0.41
8:1:102:SPO:C16	8:1:102:SPO:H131	2.51	0.41
2:7:40:ASP:CG	2:9:53:ARG:HE	2.29	0.41
1:8:40:ILE:O	1:8:44:ILE:HG12	2.21	0.41
8:9:102:SPO:H241	8:9:102:SPO:H26	1.88	0.41
9:A:102:PC1:H2	9:A:102:PC1:H221	1.32	0.41
8:D:103:SPO:H241	8:D:103:SPO:H26	1.79	0.41
1:J:32:VAL:O	1:J:36:VAL:HG23	2.21	0.41
11:L:310:BPH:CHD	11:L:310:BPH:HBC3	2.51	0.41
2:O:20:GLN:HG3	7:Q:101:BCL:H91	2.03	0.41
7:P:101:BCL:H71	8:P:103:SPO:H293	2.02	0.41
7:Q:101:BCL:H161	7:Q:101:BCL:H141	1.69	0.41
2:S:25:PHE:O	2:S:29:VAL:HG23	2.20	0.41
8:X:101:SPO:H361	8:X:101:SPO:H341	1.66	0.41
1:b:40:ILE:HA	1:b:43:TYR:HD2	1.86	0.41
1:0:40:ILE:O	1:0:44:ILE:HG12	2.22	0.40
4:L:243:PHE:O	4:L:247:VAL:HG23	2.21	0.40
12:L:307:U10:O4	12:L:307:U10:C3M	2.69	0.40
5:M:182:HIS:O	5:M:186:THR:HG23	2.21	0.40
2:S:7:ILE:HA	2:S:10:VAL:HG22	2.03	0.40
8:S:202:SPO:H361	1:T:20:LEU:HD13	2.01	0.40
8:X:101:SPO:H311	8:X:101:SPO:H291	1.80	0.40
7:b:102:BCL:HBA1	7:b:102:BCL:H3A	1.89	0.40
1:J:49:LEU:HD22	8:J:103:SPO:C10	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:102:BCL:H152	7:N:102:BCL:H18	1.93	0.40
7:V:102:BCL:H122	7:V:102:BCL:C17	2.51	0.40
7:a:101:BCL:H3A	7:a:101:BCL:HBA1	1.72	0.40
1:E:46:ARG:HH11	2:F:53:ARG:HH11	1.69	0.40
7:J:101:BCL:H61	7:J:101:BCL:H93	1.80	0.40
4:L:178:ILE:HG12	7:L:301:BCL:HMB3	2.03	0.40
9:M:402:PC1:O22	9:M:402:PC1:H12	2.21	0.40
1:T:42:VAL:CG1	7:T:101:BCL:HBC1	2.50	0.40
8:G:102:SPO:H15	8:G:102:SPO:H131	1.97	0.40
7:J:101:BCL:H12	7:J:101:BCL:HBA1	1.80	0.40
2:K:52:GLY:C	2:K:53:ARG:HG3	2.47	0.40
7:S:201:BCL:H141	7:S:201:BCL:H162	1.73	0.40
7:S:201:BCL:HMA1	7:S:201:BCL:HHB	1.77	0.40
7:a:101:BCL:HBC2	7:a:101:BCL:H2C	1.66	0.40
1:J:38:ALA:O	1:J:42:VAL:HG23	2.22	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	0	42/49 (86%)	42 (100%)	0	0	100	100
1	2	37/49 (76%)	37 (100%)	0	0	100	100
1	8	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
1	B	41/49 (84%)	41 (100%)	0	0	100	100
1	C	41/49 (84%)	38 (93%)	3 (7%)	0	100	100
1	E	41/49 (84%)	41 (100%)	0	0	100	100
1	G	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	J	41/49 (84%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
1	P	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
1	R	41/49 (84%)	41 (100%)	0	0	100	100
1	T	41/49 (84%)	41 (100%)	0	0	100	100
1	V	41/49 (84%)	41 (100%)	0	0	100	100
1	Z	40/49 (82%)	40 (100%)	0	0	100	100
1	b	35/49 (71%)	35 (100%)	0	0	100	100
2	1	47/62 (76%)	47 (100%)	0	0	100	100
2	3	50/62 (81%)	49 (98%)	1 (2%)	0	100	100
2	7	43/62 (69%)	42 (98%)	1 (2%)	0	100	100
2	9	51/62 (82%)	50 (98%)	1 (2%)	0	100	100
2	A	51/62 (82%)	51 (100%)	0	0	100	100
2	D	51/62 (82%)	51 (100%)	0	0	100	100
2	F	51/62 (82%)	50 (98%)	1 (2%)	0	100	100
2	I	51/62 (82%)	50 (98%)	1 (2%)	0	100	100
2	K	50/62 (81%)	50 (100%)	0	0	100	100
2	O	50/62 (81%)	50 (100%)	0	0	100	100
2	Q	50/62 (81%)	48 (96%)	2 (4%)	0	100	100
2	S	50/62 (81%)	47 (94%)	3 (6%)	0	100	100
2	U	50/62 (81%)	49 (98%)	1 (2%)	0	100	100
2	W	50/62 (81%)	48 (96%)	2 (4%)	0	100	100
2	a	47/62 (76%)	44 (94%)	3 (6%)	0	100	100
3	H	252/256 (98%)	252 (100%)	0	0	100	100
4	L	279/282 (99%)	274 (98%)	5 (2%)	0	100	100
5	M	302/307 (98%)	301 (100%)	1 (0%)	0	100	100
6	X	49/75 (65%)	49 (100%)	0	0	100	100
All	All	2229/2585 (86%)	2198 (99%)	31 (1%)	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	0	38/42 (90%)	38 (100%)	0	100	100
1	2	33/42 (79%)	33 (100%)	0	100	100
1	8	37/42 (88%)	37 (100%)	0	100	100
1	B	37/42 (88%)	37 (100%)	0	100	100
1	C	37/42 (88%)	37 (100%)	0	100	100
1	E	37/42 (88%)	37 (100%)	0	100	100
1	G	37/42 (88%)	37 (100%)	0	100	100
1	J	37/42 (88%)	37 (100%)	0	100	100
1	N	37/42 (88%)	37 (100%)	0	100	100
1	P	37/42 (88%)	37 (100%)	0	100	100
1	R	37/42 (88%)	37 (100%)	0	100	100
1	T	37/42 (88%)	37 (100%)	0	100	100
1	V	37/42 (88%)	37 (100%)	0	100	100
1	Z	36/42 (86%)	36 (100%)	0	100	100
1	b	32/42 (76%)	32 (100%)	0	100	100
2	1	43/52 (83%)	43 (100%)	0	100	100
2	3	46/52 (88%)	46 (100%)	0	100	100
2	7	42/52 (81%)	42 (100%)	0	100	100
2	9	47/52 (90%)	47 (100%)	0	100	100
2	A	47/52 (90%)	47 (100%)	0	100	100
2	D	47/52 (90%)	47 (100%)	0	100	100
2	F	47/52 (90%)	47 (100%)	0	100	100
2	I	47/52 (90%)	47 (100%)	0	100	100
2	K	46/52 (88%)	46 (100%)	0	100	100
2	O	46/52 (88%)	46 (100%)	0	100	100
2	Q	46/52 (88%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	46/52 (88%)	46 (100%)	0	100	100
2	U	46/52 (88%)	46 (100%)	0	100	100
2	W	46/52 (88%)	46 (100%)	0	100	100
2	a	43/52 (83%)	43 (100%)	0	100	100
3	H	207/208 (100%)	207 (100%)	0	100	100
4	L	223/224 (100%)	223 (100%)	0	100	100
5	M	237/239 (99%)	237 (100%)	0	100	100
6	X	39/59 (66%)	39 (100%)	0	100	100
All	All	1937/2140 (90%)	1937 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	20	GLN
2	3	20	GLN
2	7	20	GLN
1	C	23	GLN
1	C	26	HIS
2	F	9	GLN
2	F	32	HIS
3	H	5	ASN
3	H	130	HIS
3	H	210	ASN
2	I	42	ASN
4	L	212	HIS
4	L	281	ASN
5	M	266	HIS
1	P	21	HIS
2	Q	20	GLN
2	S	20	GLN
1	Z	16	GLN
1	b	21	HIS
1	b	39	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 1 is monoatomic - leaving 86 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	9	101	-	69,74,74	0.84	1 (1%)	83,115,115	1.23	10 (12%)
8	SPO	U	103	-	40,41,41	0.15	0	47,50,50	0.45	0
8	SPO	X	101	-	37,38,41	0.17	0	43,46,50	0.56	1 (2%)
7	BCL	L	301	-	69,74,74	0.84	2 (2%)	83,115,115	1.30	15 (18%)
7	BCL	U	101	-	69,74,74	0.89	2 (2%)	83,115,115	1.25	11 (13%)
11	BPH	L	303	-	56,67,70	1.11	3 (5%)	57,97,101	1.05	5 (8%)
8	SPO	M	408	-	40,41,41	0.18	0	47,50,50	0.63	1 (2%)
12	U10	M	407	-	48,48,63	0.19	0	58,61,79	0.47	1 (1%)
8	SPO	F	103	-	40,41,41	0.17	0	47,50,50	0.59	1 (2%)
12	U10	L	309	-	38,38,63	0.20	0	46,49,79	0.52	1 (2%)
9	PC1	A	103	-	31,31,53	0.36	0	37,39,61	0.36	0
8	SPO	b	101	-	40,41,41	0.14	0	47,50,50	0.46	1 (2%)
7	BCL	P	101	1	69,74,74	0.87	1 (1%)	83,115,115	1.30	13 (15%)
7	BCL	B	101	1	69,74,74	0.89	2 (2%)	83,115,115	1.27	13 (15%)
8	SPO	V	101	-	40,41,41	0.13	0	47,50,50	0.49	0
8	SPO	0	102	-	40,41,41	0.12	0	47,50,50	0.48	1 (2%)
8	SPO	O	102	-	40,41,41	0.19	0	47,50,50	0.56	1 (2%)
8	SPO	D	103	-	40,41,41	0.15	0	47,50,50	0.71	3 (6%)
8	SPO	P	102	-	40,41,41	0.17	0	47,50,50	0.49	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	0	101	1	64,69,74	0.91	2 (3%)	77,109,115	1.34	12 (15%)
7	BCL	K	101	-	69,74,74	0.87	1 (1%)	83,115,115	1.18	10 (12%)
9	PC1	M	401	-	39,39,53	0.34	0	45,47,61	0.31	0
9	PC1	O	103	-	31,31,53	0.36	0	37,39,61	0.32	0
9	PC1	A	104	-	31,31,53	0.36	0	37,39,61	0.30	0
8	SPO	Z	102	-	40,41,41	0.14	0	47,50,50	0.40	0
7	BCL	T	101	1	69,74,74	0.90	3 (4%)	83,115,115	1.27	13 (15%)
9	PC1	M	411	-	44,44,53	0.30	0	50,52,61	0.31	0
7	BCL	L	302	-	66,71,74	0.91	1 (1%)	79,111,115	1.25	13 (16%)
8	SPO	T	102	-	40,41,41	0.30	0	47,50,50	1.06	4 (8%)
9	PC1	L	306	-	35,35,53	0.34	0	41,43,61	0.31	0
7	BCL	I	101	-	69,74,74	0.91	1 (1%)	83,115,115	1.19	9 (10%)
8	SPO	9	102	-	40,41,41	0.13	0	47,50,50	0.37	0
8	SPO	U	102	-	40,41,41	0.13	0	47,50,50	0.48	1 (2%)
7	BCL	7	101	-	64,69,74	0.89	2 (3%)	77,109,115	1.32	14 (18%)
8	SPO	S	202	-	40,41,41	0.16	0	47,50,50	0.56	0
8	SPO	I	102	-	40,41,41	0.14	0	47,50,50	0.39	0
7	BCL	a	101	-	59,64,74	0.85	1 (1%)	71,103,115	1.49	12 (16%)
9	PC1	L	311	-	31,31,53	0.36	0	37,39,61	0.36	0
12	U10	L	307	-	48,48,63	0.20	0	58,61,79	0.57	1 (1%)
7	BCL	M	404	-	69,74,74	0.88	1 (1%)	83,115,115	1.22	11 (13%)
7	BCL	8	101	-	69,74,74	0.88	3 (4%)	83,115,115	1.28	13 (15%)
7	BCL	1	101	-	59,64,74	0.89	2 (3%)	71,103,115	1.29	11 (15%)
7	BCL	N	102	1	69,74,74	0.90	2 (2%)	83,115,115	1.26	13 (15%)
8	SPO	0	103	-	40,41,41	0.18	0	47,50,50	0.65	1 (2%)
9	PC1	A	102	-	44,44,53	0.31	0	50,52,61	0.26	0
7	BCL	3	101	-	69,74,74	0.81	1 (1%)	83,115,115	1.25	12 (14%)
7	BCL	S	201	-	69,74,74	0.86	1 (1%)	83,115,115	1.28	9 (10%)
9	PC1	D	104	-	36,36,53	0.34	0	42,44,61	0.30	0
7	BCL	J	101	1	69,74,74	0.88	2 (2%)	83,115,115	1.30	13 (15%)
9	PC1	L	304	-	34,34,53	0.35	0	40,42,61	0.31	0
7	BCL	Z	101	1	69,74,74	0.84	1 (1%)	83,115,115	1.28	13 (15%)
12	U10	L	308	-	19,19,63	0.29	0	23,26,79	0.66	1 (4%)
8	SPO	O	104	-	40,41,41	0.15	0	47,50,50	0.39	1 (2%)
8	SPO	C	102	-	40,41,41	0.12	0	47,50,50	0.51	1 (2%)
8	SPO	2	102	-	40,41,41	0.14	0	47,50,50	0.65	1 (2%)
7	BCL	G	101	1	69,74,74	0.89	2 (2%)	83,115,115	1.26	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	V	102	1	69,74,74	0.87	1 (1%)	83,115,115	1.23	11 (13%)
10	CDL	M	410	-	77,77,99	0.34	0	83,89,111	0.36	0
8	SPO	P	103	-	40,41,41	0.12	0	47,50,50	0.53	1 (2%)
7	BCL	C	101	1	69,74,74	0.85	2 (2%)	83,115,115	1.27	13 (15%)
8	SPO	1	102	-	40,41,41	0.19	0	47,50,50	0.98	4 (8%)
12	U10	M	403	-	43,43,63	0.21	0	52,55,79	0.51	1 (1%)
10	CDL	M	409	-	99,99,99	0.31	0	105,111,111	0.39	0
8	SPO	G	102	-	40,41,41	0.16	0	47,50,50	0.56	0
7	BCL	W	101	-	69,74,74	0.85	2 (2%)	83,115,115	1.24	12 (14%)
12	U10	X	102	-	48,48,63	0.21	0	58,61,79	0.50	1 (1%)
8	SPO	F	101	-	40,41,41	0.20	0	47,50,50	0.56	1 (2%)
9	PC1	M	402	-	46,46,53	0.31	0	52,54,61	0.30	0
8	SPO	N	101	-	40,41,41	0.15	0	47,50,50	0.40	0
7	BCL	D	102	-	69,74,74	0.88	1 (1%)	83,115,115	1.24	13 (15%)
8	SPO	3	102	-	40,41,41	0.15	0	47,50,50	0.58	1 (2%)
7	BCL	O	101	-	69,74,74	0.87	2 (2%)	83,115,115	1.19	9 (10%)
7	BCL	R	101	1	69,74,74	0.90	1 (1%)	83,115,115	1.27	13 (15%)
11	BPH	L	310	-	49,60,70	1.18	3 (6%)	49,89,101	1.04	4 (8%)
7	BCL	Q	101	2	69,74,74	0.85	2 (2%)	83,115,115	1.21	9 (10%)
7	BCL	2	101	-	64,69,74	0.89	2 (3%)	77,109,115	1.31	12 (15%)
8	SPO	J	102	-	40,41,41	0.14	0	47,50,50	1.00	4 (8%)
7	BCL	M	405	-	69,74,74	0.86	1 (1%)	83,115,115	1.22	12 (14%)
12	U10	L	305	-	43,43,63	0.20	0	52,55,79	0.54	1 (1%)
7	BCL	F	102	-	69,74,74	0.89	1 (1%)	83,115,115	1.23	11 (13%)
7	BCL	E	101	1	69,74,74	0.89	3 (4%)	83,115,115	1.26	13 (15%)
10	CDL	H	301	-	77,77,99	0.32	0	83,89,111	0.31	0
7	BCL	A	101	-	69,74,74	0.87	1 (1%)	83,115,115	1.19	11 (13%)
8	SPO	D	101	-	40,41,41	0.18	0	47,50,50	0.53	1 (2%)
7	BCL	b	102	-	64,69,74	0.85	1 (1%)	77,109,115	1.42	15 (19%)
8	SPO	J	103	-	40,41,41	0.15	0	47,50,50	0.50	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	9	101	-	-	16/41/137/137	-
8	SPO	U	103	-	-	8/47/47/47	-
8	SPO	X	101	-	-	5/44/44/47	-
7	BCL	L	301	-	-	14/41/137/137	-
7	BCL	U	101	-	-	13/41/137/137	-
11	BPH	L	303	-	-	5/34/102/105	0/5/6/6
8	SPO	M	408	-	-	11/47/47/47	-
12	U10	M	407	-	-	6/45/69/87	0/1/1/1
8	SPO	F	103	-	-	11/47/47/47	-
12	U10	L	309	-	-	9/33/57/87	0/1/1/1
9	PC1	A	103	-	-	13/35/35/57	-
8	SPO	b	101	-	-	10/47/47/47	-
7	BCL	P	101	1	-	26/41/137/137	-
7	BCL	B	101	1	-	14/41/137/137	-
8	SPO	V	101	-	-	9/47/47/47	-
8	SPO	0	102	-	-	10/47/47/47	-
8	SPO	O	102	-	-	5/47/47/47	-
8	SPO	D	103	-	-	16/47/47/47	-
8	SPO	P	102	-	-	10/47/47/47	-
7	BCL	0	101	1	-	10/35/131/137	-
7	BCL	K	101	-	-	18/41/137/137	-
9	PC1	M	401	-	-	16/43/43/57	-
9	PC1	O	103	-	-	8/35/35/57	-
9	PC1	A	104	-	-	9/35/35/57	-
8	SPO	Z	102	-	-	15/47/47/47	-
7	BCL	T	101	1	-	19/41/137/137	-
9	PC1	M	411	-	-	12/48/48/57	-
7	BCL	L	302	-	-	5/38/134/137	-
8	SPO	T	102	-	-	9/47/47/47	-
9	PC1	L	306	-	-	7/39/39/57	-
7	BCL	I	101	-	-	16/41/137/137	-
8	SPO	9	102	-	-	6/47/47/47	-
8	SPO	U	102	-	-	7/47/47/47	-
7	BCL	7	101	-	-	22/35/131/137	-
8	SPO	S	202	-	-	17/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SPO	I	102	-	-	7/47/47/47	-
7	BCL	a	101	-	-	12/29/125/137	-
9	PC1	L	311	-	-	16/35/35/57	-
12	U10	L	307	-	-	11/45/69/87	0/1/1/1
7	BCL	M	404	-	-	13/41/137/137	-
7	BCL	8	101	-	-	14/41/137/137	-
7	BCL	1	101	-	-	10/29/125/137	-
7	BCL	N	102	1	-	17/41/137/137	-
8	SPO	0	103	-	-	11/47/47/47	-
9	PC1	A	102	-	-	20/48/48/57	-
7	BCL	3	101	-	-	10/41/137/137	-
7	BCL	S	201	-	-	14/41/137/137	-
9	PC1	D	104	-	-	14/40/40/57	-
7	BCL	J	101	1	-	18/41/137/137	-
9	PC1	L	304	-	-	10/38/38/57	-
7	BCL	Z	101	1	-	21/41/137/137	-
12	U10	L	308	-	-	4/11/35/87	0/1/1/1
8	SPO	O	104	-	-	9/47/47/47	-
8	SPO	C	102	-	-	7/47/47/47	-
8	SPO	2	102	-	-	10/47/47/47	-
7	BCL	G	101	1	-	27/41/137/137	-
7	BCL	V	102	1	-	17/41/137/137	-
10	CDL	M	410	-	-	28/88/88/110	-
8	SPO	P	103	-	-	14/47/47/47	-
7	BCL	C	101	1	-	19/41/137/137	-
8	SPO	1	102	-	-	11/47/47/47	-
12	U10	M	403	-	-	11/39/63/87	0/1/1/1
10	CDL	M	409	-	-	51/110/110/110	-
8	SPO	G	102	-	-	10/47/47/47	-
7	BCL	W	101	-	-	13/41/137/137	-
12	U10	X	102	-	-	16/45/69/87	0/1/1/1
8	SPO	F	101	-	-	6/47/47/47	-
9	PC1	M	402	-	-	17/50/50/57	-
8	SPO	N	101	-	-	8/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	D	102	-	-	21/41/137/137	-
8	SPO	3	102	-	-	11/47/47/47	-
7	BCL	O	101	-	-	17/41/137/137	-
7	BCL	R	101	1	-	24/41/137/137	-
11	BPH	L	310	-	-	6/25/93/105	0/5/6/6
7	BCL	Q	101	2	-	15/41/137/137	-
7	BCL	2	101	-	-	21/35/131/137	-
8	SPO	J	102	-	-	8/47/47/47	-
7	BCL	M	405	-	-	11/41/137/137	-
12	U10	L	305	-	-	9/39/63/87	0/1/1/1
7	BCL	F	102	-	-	19/41/137/137	-
7	BCL	E	101	1	-	23/41/137/137	-
10	CDL	H	301	-	-	29/88/88/110	-
7	BCL	A	101	-	-	16/41/137/137	-
8	SPO	D	101	-	-	3/47/47/47	-
7	BCL	b	102	-	-	20/35/131/137	-
8	SPO	J	103	-	-	8/47/47/47	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	303	BPH	C1D-C2D	6.31	1.46	1.39
11	L	310	BPH	C1D-C2D	6.17	1.46	1.39
7	L	302	BCL	C4D-ND	-6.05	1.29	1.37
7	I	101	BCL	C4D-ND	-5.96	1.29	1.37
7	F	102	BCL	C4D-ND	-5.89	1.29	1.37
7	B	101	BCL	C4D-ND	-5.87	1.29	1.37
7	N	102	BCL	C4D-ND	-5.83	1.29	1.37
7	M	405	BCL	C4D-ND	-5.83	1.29	1.37
7	V	102	BCL	C4D-ND	-5.83	1.29	1.37
7	M	404	BCL	C4D-ND	-5.82	1.29	1.37
7	D	102	BCL	C4D-ND	-5.81	1.29	1.37
7	G	101	BCL	C4D-ND	-5.79	1.29	1.37
7	R	101	BCL	C4D-ND	-5.78	1.29	1.37
7	0	101	BCL	C4D-ND	-5.76	1.29	1.37
7	E	101	BCL	C4D-ND	-5.73	1.29	1.37
7	T	101	BCL	C4D-ND	-5.69	1.29	1.37
7	P	101	BCL	C4D-ND	-5.66	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	8	101	BCL	C4D-ND	-5.60	1.30	1.37
7	U	101	BCL	C4D-ND	-5.60	1.30	1.37
7	J	101	BCL	C4D-ND	-5.55	1.30	1.37
7	S	201	BCL	C4D-ND	-5.53	1.30	1.37
7	A	101	BCL	C4D-ND	-5.46	1.30	1.37
7	9	101	BCL	C4D-ND	-5.45	1.30	1.37
7	7	101	BCL	C4D-ND	-5.44	1.30	1.37
7	2	101	BCL	C4D-ND	-5.43	1.30	1.37
7	Z	101	BCL	C4D-ND	-5.43	1.30	1.37
7	O	101	BCL	C4D-ND	-5.43	1.30	1.37
7	K	101	BCL	C4D-ND	-5.40	1.30	1.37
7	Q	101	BCL	C4D-ND	-5.36	1.30	1.37
7	C	101	BCL	C4D-ND	-5.36	1.30	1.37
7	W	101	BCL	C4D-ND	-5.22	1.30	1.37
7	1	101	BCL	C4D-ND	-5.15	1.30	1.37
7	L	301	BCL	C4D-ND	-5.11	1.30	1.37
7	b	102	BCL	C4D-ND	-5.07	1.30	1.37
7	3	101	BCL	C4D-ND	-5.03	1.30	1.37
7	a	101	BCL	C4D-ND	-5.00	1.30	1.37
11	L	303	BPH	C3B-C2B	2.51	1.43	1.39
11	L	310	BPH	C3B-C2B	2.49	1.43	1.39
7	L	301	BCL	C1D-C2D	-2.33	1.40	1.45
7	G	101	BCL	C1D-C2D	-2.26	1.40	1.45
7	J	101	BCL	C1D-C2D	-2.21	1.41	1.45
11	L	303	BPH	C3B-C4B	-2.15	1.37	1.41
7	E	101	BCL	C1D-C2D	-2.12	1.41	1.45
7	O	101	BCL	C1D-C2D	-2.11	1.41	1.45
7	1	101	BCL	C3C-C4C	2.09	1.54	1.51
7	T	101	BCL	C1D-C2D	-2.09	1.41	1.45
7	C	101	BCL	C1D-C2D	-2.09	1.41	1.45
7	2	101	BCL	C1D-C2D	-2.09	1.41	1.45
7	8	101	BCL	MG-NA	-2.08	2.01	2.06
7	0	101	BCL	C1D-C2D	-2.06	1.41	1.45
7	U	101	BCL	C1D-C2D	-2.06	1.41	1.45
7	W	101	BCL	C1D-C2D	-2.04	1.41	1.45
7	N	102	BCL	MG-NA	-2.04	2.01	2.06
7	8	101	BCL	C1D-C2D	-2.03	1.41	1.45
11	L	310	BPH	C3B-C4B	-2.03	1.38	1.41
7	B	101	BCL	C1D-C2D	-2.02	1.41	1.45
7	T	101	BCL	C3C-C4C	2.02	1.54	1.51
7	7	101	BCL	C1D-C2D	-2.02	1.41	1.45
7	E	101	BCL	MG-NA	-2.02	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	101	BCL	C1D-C2D	-2.00	1.41	1.45

All (454) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	101	BCL	CAC-C3C-C2C	-4.91	101.99	114.26
7	1	101	BCL	CAC-C3C-C2C	-4.87	102.10	114.26
7	a	101	BCL	CAC-C3C-C2C	-4.77	102.34	114.26
7	N	102	BCL	CAC-C3C-C2C	-4.77	102.35	114.26
7	T	101	BCL	CAC-C3C-C2C	-4.75	102.39	114.26
7	2	101	BCL	CAC-C3C-C2C	-4.74	102.43	114.26
7	Z	101	BCL	CAC-C3C-C2C	-4.71	102.49	114.26
7	R	101	BCL	CAC-C3C-C2C	-4.70	102.51	114.26
7	0	101	BCL	CAC-C3C-C2C	-4.68	102.56	114.26
7	Q	101	BCL	CAC-C3C-C2C	-4.68	102.57	114.26
7	W	101	BCL	CAC-C3C-C2C	-4.67	102.58	114.26
7	P	101	BCL	CAC-C3C-C2C	-4.67	102.58	114.26
7	I	101	BCL	CAC-C3C-C2C	-4.62	102.72	114.26
7	D	102	BCL	CAC-C3C-C2C	-4.60	102.76	114.26
7	C	101	BCL	CAC-C3C-C2C	-4.60	102.77	114.26
7	A	101	BCL	CAC-C3C-C2C	-4.60	102.78	114.26
7	b	102	BCL	CAC-C3C-C2C	-4.59	102.79	114.26
7	V	102	BCL	CAC-C3C-C2C	-4.59	102.80	114.26
7	K	101	BCL	CAC-C3C-C2C	-4.58	102.82	114.26
7	3	101	BCL	CAC-C3C-C2C	-4.57	102.84	114.26
7	8	101	BCL	CAC-C3C-C2C	-4.53	102.95	114.26
7	G	101	BCL	CAC-C3C-C2C	-4.52	102.97	114.26
7	E	101	BCL	CAC-C3C-C2C	-4.51	102.98	114.26
7	S	201	BCL	CAC-C3C-C2C	-4.49	103.03	114.26
7	J	101	BCL	CAC-C3C-C2C	-4.49	103.04	114.26
7	F	102	BCL	CAC-C3C-C2C	-4.49	103.04	114.26
7	9	101	BCL	CAC-C3C-C2C	-4.49	103.04	114.26
7	O	101	BCL	CAC-C3C-C2C	-4.46	103.12	114.26
7	L	302	BCL	CAC-C3C-C2C	-4.42	103.22	114.26
7	B	101	BCL	CAC-C3C-C2C	-4.41	103.24	114.26
7	L	301	BCL	CAC-C3C-C2C	-4.40	103.27	114.26
7	3	101	BCL	CHC-C4B-NB	-4.38	119.61	124.26
7	M	405	BCL	CAC-C3C-C2C	-4.30	103.50	114.26
7	M	404	BCL	CAC-C3C-C2C	-4.29	103.55	114.26
7	7	101	BCL	CAC-C3C-C2C	-4.24	103.66	114.26
7	b	102	BCL	CHC-C4B-NB	-4.22	119.78	124.26
7	J	101	BCL	CHC-C4B-NB	-4.18	119.83	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	101	BCL	CHC-C4B-NB	-4.15	119.86	124.26
7	1	101	BCL	CHC-C4B-NB	-4.14	119.88	124.26
7	W	101	BCL	CHC-C4B-NB	-4.13	119.88	124.26
7	8	101	BCL	CHC-C4B-NB	-4.13	119.89	124.26
7	N	102	BCL	CHC-C4B-NB	-4.12	119.89	124.26
7	E	101	BCL	CHC-C4B-NB	-4.12	119.89	124.26
7	a	101	BCL	CHC-C4B-NB	-4.09	119.93	124.26
7	L	301	BCL	CHC-C4B-NB	-4.08	119.94	124.26
7	0	101	BCL	CHC-C4B-NB	-4.08	119.94	124.26
7	T	101	BCL	CHC-C4B-NB	-4.08	119.94	124.26
7	G	101	BCL	CHC-C4B-NB	-4.06	119.95	124.26
7	R	101	BCL	CHC-C4B-NB	-4.06	119.95	124.26
7	7	101	BCL	CHC-C4B-NB	-4.06	119.96	124.26
7	L	302	BCL	CHC-C4B-NB	-4.04	119.98	124.26
7	M	404	BCL	CHC-C4B-NB	-4.04	119.98	124.26
7	B	101	BCL	CHC-C4B-NB	-4.02	120.01	124.26
7	V	102	BCL	CHC-C4B-NB	-4.00	120.03	124.26
7	M	405	BCL	CHC-C4B-NB	-3.99	120.03	124.26
7	2	101	BCL	CHC-C4B-NB	-3.99	120.04	124.26
11	L	303	BPH	C1C-C2C-C3C	-3.98	99.05	102.84
7	U	101	BCL	CHC-C4B-NB	-3.98	120.04	124.26
7	9	101	BCL	CHC-C4B-NB	-3.97	120.05	124.26
7	P	101	BCL	CHC-C4B-NB	-3.97	120.06	124.26
7	S	201	BCL	CHC-C4B-NB	-3.96	120.06	124.26
7	Z	101	BCL	CHC-C4B-NB	-3.94	120.08	124.26
7	F	102	BCL	CHC-C4B-NB	-3.89	120.14	124.26
7	K	101	BCL	CHC-C4B-NB	-3.89	120.14	124.26
7	D	102	BCL	CHC-C4B-NB	-3.88	120.15	124.26
7	Q	101	BCL	CHC-C4B-NB	-3.87	120.16	124.26
7	O	101	BCL	CHC-C4B-NB	-3.87	120.16	124.26
7	I	101	BCL	CHC-C4B-NB	-3.83	120.20	124.26
7	A	101	BCL	CHC-C4B-NB	-3.76	120.28	124.26
7	b	102	BCL	C3D-C4D-ND	-3.65	104.32	110.24
7	a	101	BCL	CHB-C1B-NB	-3.59	120.46	124.26
7	L	301	BCL	C3D-C4D-ND	-3.57	104.46	110.24
7	S	201	BCL	CHC-C1C-NC	3.44	129.26	124.51
7	a	101	BCL	CHC-C1C-NC	3.41	129.23	124.51
7	3	101	BCL	CHB-C1B-NB	-3.39	120.67	124.26
7	B	101	BCL	C2A-C3A-C4A	-3.35	96.46	101.87
8	M	408	SPO	C3-C1-C4	-3.34	105.72	110.86
7	P	101	BCL	C2A-C3A-C4A	-3.33	96.48	101.87
7	a	101	BCL	C3D-C4D-ND	-3.33	104.85	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	101	BCL	C2A-C3A-C4A	-3.31	96.52	101.87
7	A	101	BCL	CHC-C1C-NC	3.30	129.07	124.51
7	2	101	BCL	CHB-C1B-NB	-3.27	120.80	124.26
7	3	101	BCL	C4D-CHA-C1A	3.25	125.20	121.25
7	F	102	BCL	CHB-C1B-NB	-3.23	120.83	124.26
7	O	101	BCL	CHC-C1C-NC	3.22	128.97	124.51
7	F	102	BCL	CHC-C1C-NC	3.21	128.96	124.51
7	Z	101	BCL	CHB-C1B-NB	-3.21	120.86	124.26
7	0	101	BCL	CHB-C1B-NB	-3.20	120.86	124.26
7	M	404	BCL	CHC-C1C-NC	3.20	128.94	124.51
7	b	102	BCL	CHB-C1B-NB	-3.20	120.87	124.26
7	D	102	BCL	CHC-C1C-NC	3.16	128.89	124.51
7	7	101	BCL	CHB-C1B-NB	-3.15	120.93	124.26
7	S	201	BCL	CHB-C1B-NB	-3.14	120.93	124.26
7	C	101	BCL	CHB-C1B-NB	-3.14	120.93	124.26
7	9	101	BCL	CHC-C1C-NC	3.14	128.85	124.51
7	M	405	BCL	C4D-CHA-C1A	3.14	125.07	121.25
11	L	310	BPH	C4D-CHA-CBD	3.13	109.93	108.52
7	T	101	BCL	CHB-C1B-NB	-3.13	120.94	124.26
7	7	101	BCL	CHC-C1C-NC	3.13	128.84	124.51
7	2	101	BCL	CHC-C1C-NC	3.12	128.83	124.51
7	D	102	BCL	C4D-CHA-C1A	3.11	125.04	121.25
7	I	101	BCL	CHC-C1C-NC	3.11	128.81	124.51
7	U	101	BCL	CHC-C1C-NC	3.10	128.81	124.51
8	1	102	SPO	C21-C20-C19	3.10	129.83	123.47
8	T	102	SPO	C20-C21-C22	3.09	129.81	123.47
7	P	101	BCL	CHC-C1C-NC	3.09	128.78	124.51
7	E	101	BCL	C2A-C3A-C4A	-3.09	96.89	101.87
11	L	303	BPH	C2D-C1D-ND	-3.06	107.41	109.53
7	T	101	BCL	C4D-CHA-C1A	3.06	124.97	121.25
7	Q	101	BCL	CHC-C1C-NC	3.06	128.74	124.51
7	a	101	BCL	C4D-CHA-C1A	3.05	124.96	121.25
11	L	310	BPH	C2D-C1D-ND	-3.05	107.42	109.53
7	Q	101	BCL	CHB-C1B-NB	-3.05	121.03	124.26
7	B	101	BCL	CHB-C1B-NB	-3.05	121.03	124.26
7	P	101	BCL	CHB-C1B-NB	-3.04	121.03	124.26
8	1	102	SPO	C3-C1-C4	-3.04	106.19	110.86
7	1	101	BCL	CHB-C1B-NB	-3.04	121.04	124.26
7	Z	101	BCL	CHC-C1C-NC	3.04	128.71	124.51
7	L	302	BCL	CHB-C1B-NB	-3.04	121.04	124.26
7	N	102	BCL	CHB-C1B-NB	-3.02	121.06	124.26
8	J	102	SPO	C21-C20-C19	3.02	129.65	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	101	BCL	CHB-C1B-NB	-3.01	121.07	124.26
7	M	404	BCL	CHB-C1B-NB	-3.01	121.07	124.26
7	S	201	BCL	C4D-CHA-C1A	3.01	124.91	121.25
7	b	102	BCL	C2A-C3A-C4A	-2.99	97.04	101.87
7	8	101	BCL	C2A-C3A-C4A	-2.99	97.04	101.87
7	R	101	BCL	C2A-C3A-C4A	-2.98	97.05	101.87
7	U	101	BCL	CHB-C1B-NB	-2.98	121.10	124.26
7	8	101	BCL	CHB-C1B-NB	-2.98	121.10	124.26
7	9	101	BCL	CHB-C1B-NB	-2.97	121.11	124.26
7	V	102	BCL	CHB-C1B-NB	-2.97	121.11	124.26
7	D	102	BCL	CHB-C1B-NB	-2.96	121.12	124.26
7	G	101	BCL	CHB-C1B-NB	-2.96	121.12	124.26
7	J	101	BCL	CHB-C1B-NB	-2.96	121.12	124.26
7	0	101	BCL	C4D-CHA-C1A	2.95	124.84	121.25
7	N	102	BCL	C2A-C3A-C4A	-2.93	97.14	101.87
7	R	101	BCL	CHB-C1B-NB	-2.93	121.16	124.26
7	G	101	BCL	C2A-C3A-C4A	-2.92	97.16	101.87
7	C	101	BCL	C4D-CHA-C1A	2.91	124.79	121.25
7	L	301	BCL	CHB-C1B-NB	-2.91	121.17	124.26
7	9	101	BCL	C4D-CHA-C1A	2.90	124.78	121.25
7	0	101	BCL	CMA-C3A-C4A	-2.90	103.98	111.77
7	M	405	BCL	CHC-C1C-NC	2.90	128.52	124.51
7	O	101	BCL	CHB-C1B-NB	-2.89	121.20	124.26
7	W	101	BCL	CHB-C1B-NB	-2.89	121.20	124.26
7	A	101	BCL	C4D-CHA-C1A	2.89	124.76	121.25
7	M	405	BCL	CHB-C1B-NB	-2.88	121.21	124.26
7	E	101	BCL	C4D-CHA-C1A	2.87	124.74	121.25
7	S	201	BCL	CMA-C3A-C4A	-2.86	104.08	111.77
7	V	102	BCL	CHC-C1C-NC	2.86	128.47	124.51
7	G	101	BCL	C4D-CHA-C1A	2.85	124.72	121.25
7	J	101	BCL	C4D-CHA-C1A	2.85	124.72	121.25
7	L	302	BCL	CHC-C1C-NC	2.84	128.44	124.51
7	K	101	BCL	C4D-CHA-C1A	2.84	124.70	121.25
7	W	101	BCL	C4D-CHA-C1A	2.83	124.70	121.25
7	F	102	BCL	C4D-CHA-C1A	2.83	124.69	121.25
11	L	303	BPH	C2B-C1B-NB	-2.81	107.59	109.53
11	L	310	BPH	C2B-C1B-NB	-2.79	107.60	109.53
7	K	101	BCL	CHB-C1B-NB	-2.79	121.30	124.26
7	1	101	BCL	C4D-CHA-C1A	2.79	124.64	121.25
7	J	101	BCL	C3D-C4D-ND	-2.79	105.73	110.24
7	Q	101	BCL	C4D-CHA-C1A	2.79	124.64	121.25
7	8	101	BCL	C4D-CHA-C1A	2.78	124.64	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	301	BCL	CHC-C1C-NC	2.78	128.36	124.51
7	I	101	BCL	C4D-CHA-C1A	2.78	124.64	121.25
7	C	101	BCL	CMA-C3A-C4A	-2.77	104.32	111.77
7	R	101	BCL	C4D-CHA-C1A	2.77	124.62	121.25
7	V	102	BCL	C4D-CHA-C1A	2.77	124.62	121.25
7	I	101	BCL	CHB-C1B-NB	-2.76	121.33	124.26
7	8	101	BCL	C3D-C4D-ND	-2.76	105.76	110.24
7	2	101	BCL	C4D-CHA-C1A	2.76	124.60	121.25
7	N	102	BCL	C4D-CHA-C1A	2.75	124.60	121.25
7	3	101	BCL	C1D-ND-C4D	2.74	108.28	106.33
8	T	102	SPO	C14-C15-C16	2.74	131.76	123.22
7	K	101	BCL	CHC-C1C-NC	2.74	128.30	124.51
7	A	101	BCL	CHB-C1B-NB	-2.73	121.36	124.26
7	a	101	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
7	L	301	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
7	I	101	BCL	CMA-C3A-C4A	-2.71	104.49	111.77
7	O	101	BCL	C4D-CHA-C1A	2.71	124.55	121.25
8	1	102	SPO	C20-C21-C22	2.71	129.02	123.47
7	R	101	BCL	CMA-C3A-C4A	-2.71	104.50	111.77
7	0	101	BCL	CHC-C1C-NC	2.70	128.25	124.51
7	P	101	BCL	C4D-CHA-C1A	2.70	124.53	121.25
7	Z	101	BCL	CMA-C3A-C4A	-2.70	104.52	111.77
7	b	102	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
7	N	102	BCL	CHC-C1C-NC	2.69	128.23	124.51
7	B	101	BCL	C4D-CHA-C1A	2.69	124.52	121.25
12	X	102	U10	C7-C6-C5	-2.68	115.25	118.48
7	T	101	BCL	C2A-C3A-C4A	-2.67	97.56	101.87
7	R	101	BCL	CHC-C1C-NC	2.66	128.19	124.51
7	V	102	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
7	8	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
7	1	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
7	T	101	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
7	C	101	BCL	CHC-C1C-NC	2.65	128.17	124.51
7	M	404	BCL	CMA-C3A-C4A	-2.64	104.67	111.77
7	7	101	BCL	C4D-CHA-C1A	2.64	124.46	121.25
8	P	102	SPO	C3-C1-C4	-2.64	106.81	110.86
7	b	102	BCL	CHC-C1C-NC	2.63	128.16	124.51
7	Z	101	BCL	C3D-C4D-ND	-2.63	105.98	110.24
7	F	102	BCL	CMA-C3A-C4A	-2.63	104.70	111.77
7	U	101	BCL	CMA-C3A-C4A	-2.63	104.71	111.77
7	T	101	BCL	C3D-C4D-ND	-2.63	105.99	110.24
7	G	101	BCL	CHC-C1C-NC	2.62	128.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	102	BCL	CMA-C3A-C4A	-2.62	104.74	111.77
12	M	403	U10	C7-C6-C5	-2.60	115.35	118.48
7	7	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
7	L	301	BCL	C4D-CHA-C1A	2.59	124.41	121.25
7	U	101	BCL	C4D-CHA-C1A	2.59	124.40	121.25
7	3	101	BCL	CMA-C3A-C4A	-2.58	104.83	111.77
7	a	101	BCL	CMD-C2D-C1D	2.58	129.25	124.71
7	C	101	BCL	C2A-C3A-C4A	-2.58	97.71	101.87
7	B	101	BCL	CMA-C3A-C4A	-2.57	104.87	111.77
7	J	101	BCL	CHC-C1C-NC	2.56	128.06	124.51
7	E	101	BCL	CHC-C1C-NC	2.56	128.05	124.51
7	K	101	BCL	CMA-C3A-C4A	-2.56	104.90	111.77
7	N	102	BCL	CMA-C3A-C4A	-2.56	104.90	111.77
7	7	101	BCL	C2A-C3A-C4A	-2.55	97.75	101.87
7	b	102	BCL	C1D-CHD-C4C	-2.55	120.47	126.62
7	P	101	BCL	CMA-C3A-C4A	-2.55	104.92	111.77
7	W	101	BCL	CHC-C1C-NC	2.53	128.02	124.51
7	0	101	BCL	C3D-C4D-ND	-2.53	106.15	110.24
7	7	101	BCL	C1D-CHD-C4C	-2.52	120.53	126.62
7	Z	101	BCL	C4D-CHA-C1A	2.52	124.32	121.25
7	Z	101	BCL	C3D-C2D-C1D	-2.51	102.40	105.83
7	L	301	BCL	C3D-C2D-C1D	-2.51	102.41	105.83
7	Q	101	BCL	CMA-C3A-C4A	-2.50	105.05	111.77
8	D	101	SPO	C3-C1-C4	-2.50	107.02	110.86
7	8	101	BCL	CHC-C1C-NC	2.50	127.96	124.51
7	W	101	BCL	CMA-C3A-C4A	-2.50	105.06	111.77
7	b	102	BCL	CMA-C3A-C4A	-2.49	105.08	111.77
7	T	101	BCL	C3D-C2D-C1D	-2.49	102.44	105.83
8	J	102	SPO	C20-C21-C22	2.49	128.57	123.47
7	0	101	BCL	CHA-C1A-NA	-2.49	120.70	126.40
8	O	102	SPO	C3-C1-C4	-2.49	107.04	110.86
7	D	102	BCL	C3D-C2D-C1D	-2.48	102.45	105.83
7	E	101	BCL	CMA-C3A-C4A	-2.48	105.11	111.77
12	L	305	U10	C7-C6-C5	-2.48	115.50	118.48
7	b	102	BCL	CMD-C2D-C1D	2.47	129.06	124.71
7	8	101	BCL	C3D-C2D-C1D	-2.46	102.47	105.83
8	F	103	SPO	C2-C1-C4	-2.46	107.08	110.86
8	J	102	SPO	C3-C1-C4	-2.45	107.09	110.86
7	b	102	BCL	C4D-CHA-C1A	2.45	124.24	121.25
7	2	101	BCL	CMA-C3A-C4A	-2.45	105.18	111.77
7	1	101	BCL	CHC-C1C-NC	2.45	127.90	124.51
7	M	405	BCL	CMA-C3A-C4A	-2.45	105.18	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	101	BCL	CHC-C1C-NC	2.44	127.89	124.51
7	2	101	BCL	C2B-C1B-NB	-2.44	108.60	110.23
7	O	101	BCL	CMA-C3A-C4A	-2.43	105.23	111.77
7	0	101	BCL	C3D-C2D-C1D	-2.43	102.51	105.83
7	L	301	BCL	CMD-C2D-C1D	2.43	129.00	124.71
7	9	101	BCL	CMA-C3A-C4A	-2.43	105.24	111.77
7	D	102	BCL	CMD-C2D-C1D	2.43	128.99	124.71
7	a	101	BCL	CHA-C1A-NA	-2.41	120.88	126.40
7	E	101	BCL	C3D-C2D-C1D	-2.41	102.55	105.83
7	G	101	BCL	C3D-C4D-ND	-2.40	106.35	110.24
8	D	103	SPO	C3-C1-C4	-2.40	107.17	110.86
7	A	101	BCL	C3C-C4C-CHD	-2.40	118.26	123.39
7	M	404	BCL	C2A-C3A-C4A	-2.40	97.99	101.87
8	T	102	SPO	C21-C20-C19	-2.40	118.56	123.47
7	L	302	BCL	C2B-C1B-NB	-2.39	108.63	110.23
7	C	101	BCL	C3D-C4D-ND	-2.39	106.37	110.24
7	O	101	BCL	C3C-C4C-CHD	-2.39	118.29	123.39
7	M	404	BCL	C4D-CHA-C1A	2.39	124.15	121.25
7	b	102	BCL	C2B-C1B-NB	-2.39	108.63	110.23
8	J	102	SPO	C14-C15-C16	2.38	130.65	123.22
7	R	101	BCL	C3D-C4D-ND	-2.38	106.39	110.24
7	7	101	BCL	CHA-C1A-NA	-2.38	120.96	126.40
7	B	101	BCL	C1D-CHD-C4C	-2.37	120.89	126.62
7	J	101	BCL	CMA-C3A-C4A	-2.37	105.39	111.77
7	Z	101	BCL	CHA-C1A-NA	-2.37	120.97	126.40
7	L	301	BCL	CHA-C1A-NA	-2.37	120.97	126.40
7	R	101	BCL	C3D-C2D-C1D	-2.37	102.60	105.83
7	8	101	BCL	CMD-C2D-C1D	2.37	128.88	124.71
7	P	101	BCL	C3D-C2D-C1D	-2.36	102.61	105.83
7	B	101	BCL	C3D-C2D-C1D	-2.36	102.61	105.83
12	L	307	U10	C7-C6-C5	-2.36	115.64	118.48
7	2	101	BCL	C4B-C3B-C2B	-2.36	104.56	108.36
12	L	308	U10	C7-C6-C5	-2.36	115.64	118.48
7	3	101	BCL	CHC-C1C-NC	2.36	127.77	124.51
7	L	302	BCL	C4D-CHA-C1A	2.36	124.12	121.25
12	M	407	U10	C7-C6-C5	-2.34	115.67	118.48
7	Z	101	BCL	C2A-C3A-C4A	-2.33	98.10	101.87
7	J	101	BCL	C3D-C2D-C1D	-2.33	102.65	105.83
7	T	101	BCL	CMD-C2D-C1D	2.33	128.82	124.71
7	Z	101	BCL	CMD-C2D-C1D	2.33	128.82	124.71
7	0	101	BCL	CMD-C2D-C1D	2.33	128.81	124.71
7	P	101	BCL	CMD-C2D-C1D	2.32	128.81	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	101	BCL	C2B-C1B-NB	-2.32	108.68	110.23
7	b	102	BCL	C4B-C3B-C2B	-2.32	104.63	108.36
8	U	102	SPO	C3-C1-C4	-2.32	107.30	110.86
7	J	101	BCL	C2B-C1B-NB	-2.32	108.68	110.23
7	U	101	BCL	C3C-C4C-CHD	-2.31	118.45	123.39
7	7	101	BCL	C2C-C3C-C4C	-2.31	97.88	101.34
7	W	101	BCL	CHA-C1A-NA	-2.31	121.10	126.40
7	E	101	BCL	C1D-CHD-C4C	-2.31	121.05	126.62
7	N	102	BCL	C3D-C2D-C1D	-2.31	102.68	105.83
7	L	302	BCL	CMA-C3A-C4A	-2.31	105.57	111.77
7	b	102	BCL	CHA-C1A-NA	-2.31	121.11	126.40
7	S	201	BCL	CHA-C1A-NA	-2.30	121.12	126.40
7	8	101	BCL	C2B-C1B-NB	-2.30	108.69	110.23
7	N	102	BCL	C2B-C1B-NB	-2.30	108.69	110.23
7	U	101	BCL	C2A-C3A-C4A	-2.30	98.15	101.87
7	T	101	BCL	C2B-C1B-NB	-2.30	108.69	110.23
7	M	404	BCL	C2B-C1B-NB	-2.30	108.69	110.23
7	F	102	BCL	C3C-C4C-CHD	-2.29	118.49	123.39
7	E	101	BCL	C2B-C1B-NB	-2.29	108.69	110.23
7	U	101	BCL	CHA-C1A-NA	-2.29	121.15	126.40
8	b	101	SPO	C3-C1-C4	-2.29	107.34	110.86
7	L	302	BCL	CHA-C1A-NA	-2.29	121.16	126.40
7	7	101	BCL	C3D-C4D-ND	-2.29	106.54	110.24
7	T	101	BCL	CHC-C1C-NC	2.28	127.67	124.51
7	G	101	BCL	C2B-C1B-NB	-2.28	108.70	110.23
7	U	101	BCL	C2B-C1B-NB	-2.28	108.70	110.23
8	0	103	SPO	C3-C1-C4	-2.28	107.36	110.86
7	I	101	BCL	C3C-C4C-CHD	-2.28	118.52	123.39
7	M	404	BCL	CHA-C1A-NA	-2.28	121.18	126.40
7	P	101	BCL	CHA-C1A-NA	-2.28	121.18	126.40
7	V	102	BCL	C1D-CHD-C4C	-2.28	121.13	126.62
7	R	101	BCL	CMD-C2D-C1D	2.28	128.72	124.71
7	W	101	BCL	C3D-C4D-ND	-2.27	106.57	110.24
7	L	301	BCL	C1D-ND-C4D	2.27	107.95	106.33
7	9	101	BCL	CHA-C1A-NA	-2.27	121.20	126.40
7	C	101	BCL	C3D-C2D-C1D	-2.27	102.74	105.83
11	L	303	BPH	C4D-CHA-CBD	2.26	109.54	108.52
7	b	102	BCL	C2C-C3C-C4C	-2.26	97.95	101.34
7	9	101	BCL	C3C-C4C-CHD	-2.26	118.56	123.39
7	7	101	BCL	C3D-C2D-C1D	-2.26	102.75	105.83
7	F	102	BCL	CHA-C1A-NA	-2.26	121.23	126.40
7	B	101	BCL	C2B-C1B-NB	-2.26	108.72	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	101	BCL	CMA-C3A-C4A	-2.26	105.71	111.77
7	E	101	BCL	C3D-C4D-ND	-2.25	106.59	110.24
7	8	101	BCL	C1D-CHD-C4C	-2.25	121.19	126.62
7	a	101	BCL	CMA-C3A-C4A	-2.25	105.73	111.77
7	G	101	BCL	C3D-C2D-C1D	-2.25	102.76	105.83
7	7	101	BCL	C2B-C1B-NB	-2.25	108.73	110.23
7	W	101	BCL	C3C-C4C-CHD	-2.25	118.59	123.39
7	N	102	BCL	CMD-C2D-C1D	2.24	128.67	124.71
7	L	302	BCL	C2A-C3A-C4A	-2.24	98.25	101.87
7	P	101	BCL	C2B-C1B-NB	-2.24	108.73	110.23
7	E	101	BCL	CMD-C2D-C1D	2.24	128.66	124.71
7	D	102	BCL	CHA-C1A-NA	-2.24	121.28	126.40
7	Z	101	BCL	C1D-CHD-C4C	-2.24	121.23	126.62
7	A	101	BCL	CMA-C3A-C4A	-2.23	105.77	111.77
7	3	101	BCL	C2B-C1B-NB	-2.23	108.73	110.23
7	Q	101	BCL	CHA-C1A-NA	-2.23	121.29	126.40
7	R	101	BCL	C2B-C1B-NB	-2.23	108.74	110.23
7	a	101	BCL	C2B-C1B-NB	-2.23	108.74	110.23
7	P	101	BCL	C3D-C4D-ND	-2.23	106.64	110.24
7	9	101	BCL	C2B-C1B-NB	-2.22	108.74	110.23
7	V	102	BCL	C2B-C1B-NB	-2.22	108.74	110.23
8	0	102	SPO	C3-C1-C4	-2.22	107.45	110.86
7	C	101	BCL	CMD-C2D-C1D	2.22	128.62	124.71
7	B	101	BCL	CHA-C1A-NA	-2.22	121.32	126.40
7	2	101	BCL	CHA-C1A-NA	-2.22	121.32	126.40
7	V	102	BCL	CMD-C2D-C1D	2.22	128.62	124.71
11	L	303	BPH	CMD-C2D-C3D	2.21	128.82	124.68
7	L	301	BCL	C2B-C1B-NB	-2.21	108.75	110.23
7	M	404	BCL	CMD-C2D-C1D	2.21	128.61	124.71
7	0	101	BCL	C1D-CHD-C4C	-2.21	121.28	126.62
8	P	103	SPO	C3-C1-C4	-2.21	107.46	110.86
7	1	101	BCL	CMD-C2D-C1D	2.21	128.61	124.71
7	N	102	BCL	C3D-C4D-ND	-2.21	106.66	110.24
7	M	405	BCL	C2B-C1B-NB	-2.21	108.75	110.23
7	V	102	BCL	CHA-C1A-NA	-2.21	121.34	126.40
7	V	102	BCL	C3D-C2D-C1D	-2.21	102.82	105.83
7	J	101	BCL	CMD-C2D-C1D	2.21	128.61	124.71
12	L	309	U10	C7-C6-C5	-2.21	115.82	118.48
7	2	101	BCL	C3D-C2D-C1D	-2.21	102.82	105.83
7	3	101	BCL	CMD-C2D-C1D	2.20	128.60	124.71
7	Q	101	BCL	C3C-C4C-CHD	-2.20	118.69	123.39
7	B	101	BCL	CMD-C2D-C1D	2.20	128.59	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	101	BCL	CHA-C1A-NA	-2.20	121.36	126.40
7	G	101	BCL	C1D-CHD-C4C	-2.20	121.32	126.62
7	1	101	BCL	C3D-C2D-C1D	-2.20	102.83	105.83
7	K	101	BCL	C2B-C1B-NB	-2.20	108.76	110.23
7	T	101	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
7	3	101	BCL	C3C-C4C-CHD	-2.19	118.71	123.39
7	M	405	BCL	C1D-ND-C4D	2.19	107.89	106.33
11	L	310	BPH	CMD-C2D-C3D	2.19	128.77	124.68
7	L	301	BCL	C2A-C3A-C4A	-2.18	98.34	101.87
7	W	101	BCL	CMD-C2D-C1D	2.18	128.56	124.71
7	W	101	BCL	C2B-C1B-NB	-2.18	108.77	110.23
7	G	101	BCL	CHA-C1A-NA	-2.18	121.40	126.40
7	M	405	BCL	CMD-C2D-C1D	2.18	128.55	124.71
7	7	101	BCL	CMD-C2D-C1D	2.18	128.55	124.71
7	M	405	BCL	CHA-C1A-NA	-2.18	121.42	126.40
7	R	101	BCL	C1D-CHD-C4C	-2.18	121.37	126.62
8	D	103	SPO	C20-C21-C22	2.17	127.92	123.47
7	0	101	BCL	C2B-C1B-NB	-2.17	108.78	110.23
8	C	102	SPO	C3-C1-C4	-2.17	107.53	110.86
7	O	101	BCL	C2B-C1B-NB	-2.16	108.78	110.23
8	F	101	SPO	C2-C1-C4	-2.16	107.54	110.86
7	W	101	BCL	C3D-C2D-C1D	-2.15	102.89	105.83
7	R	101	BCL	CHA-C1A-NA	-2.15	121.47	126.40
7	C	101	BCL	CHA-C1A-NA	-2.15	121.47	126.40
7	D	102	BCL	C1D-CHD-C4C	-2.15	121.44	126.62
7	A	101	BCL	C2B-C1B-NB	-2.15	108.79	110.23
7	L	302	BCL	C2C-C3C-C4C	-2.15	98.12	101.34
7	J	101	BCL	CHA-C1A-NA	-2.14	121.49	126.40
7	T	101	BCL	CHA-C1A-NA	-2.14	121.49	126.40
7	S	201	BCL	C3C-C4C-CHD	-2.14	118.83	123.39
7	F	102	BCL	CMD-C2D-C1D	2.13	128.47	124.71
8	D	103	SPO	C21-C20-C19	2.13	127.84	123.47
7	S	201	BCL	C2B-C1B-NB	-2.13	108.80	110.23
8	T	102	SPO	C15-C16-C17	2.13	132.39	126.42
7	F	102	BCL	C2B-C1B-NB	-2.13	108.81	110.23
7	P	101	BCL	C1D-CHD-C4C	-2.12	121.50	126.62
7	D	102	BCL	C3D-C4D-ND	-2.12	106.80	110.24
7	3	101	BCL	CHA-C1A-NA	-2.12	121.54	126.40
7	K	101	BCL	CHA-C1A-NA	-2.12	121.54	126.40
7	Q	101	BCL	C2B-C1B-NB	-2.12	108.81	110.23
7	D	102	BCL	C2B-C1B-NB	-2.11	108.82	110.23
7	L	302	BCL	CMD-C2D-C1D	2.11	128.43	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	102	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
8	3	102	SPO	C3-C1-C4	-2.11	107.62	110.86
7	2	101	BCL	C1D-CHD-C4C	-2.11	121.54	126.62
7	O	101	BCL	CHA-C1A-NA	-2.10	121.58	126.40
7	C	101	BCL	C1D-CHD-C4C	-2.10	121.55	126.62
7	8	101	BCL	CHA-C1A-NA	-2.10	121.60	126.40
7	L	301	BCL	C1D-CHD-C4C	-2.10	121.56	126.62
7	1	101	BCL	C2B-C1B-NB	-2.09	108.83	110.23
7	I	101	BCL	C2B-C1B-NB	-2.09	108.83	110.23
7	J	101	BCL	C1D-CHD-C4C	-2.09	121.58	126.62
7	A	101	BCL	CHA-C1A-NA	-2.09	121.61	126.40
7	1	101	BCL	CHA-C1A-NA	-2.09	121.61	126.40
7	a	101	BCL	CHB-C4A-NA	-2.09	121.62	124.51
8	2	102	SPO	C3-C1-C4	-2.09	107.65	110.86
7	G	101	BCL	CMD-C2D-C1D	2.08	128.38	124.71
7	9	101	BCL	C1D-ND-C4D	2.08	107.81	106.33
8	X	101	SPO	C3-C1-C4	-2.08	107.67	110.86
7	M	405	BCL	C3D-C2D-C1D	-2.08	103.00	105.83
7	2	101	BCL	CMD-C2D-C1D	2.07	128.37	124.71
7	M	405	BCL	C2C-C3C-C4C	-2.07	98.24	101.34
7	Z	101	BCL	C2B-C1B-NB	-2.07	108.84	110.23
7	L	302	BCL	C1D-ND-C4D	2.07	107.80	106.33
7	D	102	BCL	C3C-C4C-CHD	-2.05	119.01	123.39
7	L	301	BCL	C3C-C4C-CHD	-2.05	119.02	123.39
7	M	404	BCL	C3C-C4C-CHD	-2.04	119.02	123.39
7	B	101	BCL	C3D-C4D-ND	-2.04	106.94	110.24
7	E	101	BCL	CHA-C1A-NA	-2.04	121.74	126.40
7	U	101	BCL	C1D-ND-C4D	2.02	107.77	106.33
7	L	302	BCL	C1D-CHD-C4C	-2.02	121.75	126.62
7	1	101	BCL	C1D-CHD-C4C	-2.02	121.76	126.62
7	A	101	BCL	CMD-C2D-C1D	2.02	128.26	124.71
7	F	102	BCL	C3D-C2D-C1D	-2.02	103.08	105.83
7	K	101	BCL	CMD-C2D-C1D	2.01	128.26	124.71
8	1	102	SPO	C5-C6-C7	2.01	128.93	125.89
7	K	101	BCL	C3C-C4C-CHD	-2.01	119.10	123.39
7	N	102	BCL	CHA-C1A-NA	-2.01	121.80	126.40
7	3	101	BCL	C3D-C2D-C1D	-2.01	103.09	105.83
8	O	104	SPO	C3-C1-C4	-2.01	107.78	110.86
7	A	101	BCL	C3D-C2D-C1D	-2.00	103.10	105.83

There are no chirality outliers.

All (1164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	0	101	BCL	C2C-C3C-CAC-CBC
7	1	101	BCL	CBD-CGD-O2D-CED
7	1	101	BCL	O1D-CGD-O2D-CED
7	1	101	BCL	C1-C2-C3-C4
7	1	101	BCL	C1-C2-C3-C5
7	2	101	BCL	C1A-C2A-CAA-CBA
7	2	101	BCL	C3A-C2A-CAA-CBA
7	2	101	BCL	C1-C2-C3-C4
7	2	101	BCL	C1-C2-C3-C5
7	3	101	BCL	C2C-C3C-CAC-CBC
7	3	101	BCL	C1-C2-C3-C4
7	3	101	BCL	C1-C2-C3-C5
7	7	101	BCL	C1A-C2A-CAA-CBA
7	7	101	BCL	C3A-C2A-CAA-CBA
7	7	101	BCL	C4C-C3C-CAC-CBC
7	7	101	BCL	O2A-C1-C2-C3
7	7	101	BCL	C1-C2-C3-C4
7	7	101	BCL	C1-C2-C3-C5
7	8	101	BCL	C1A-C2A-CAA-CBA
7	8	101	BCL	C1-C2-C3-C4
7	8	101	BCL	C1-C2-C3-C5
7	8	101	BCL	C2-C3-C5-C6
7	8	101	BCL	C4-C3-C5-C6
7	9	101	BCL	C2C-C3C-CAC-CBC
7	A	101	BCL	C2C-C3C-CAC-CBC
7	B	101	BCL	C1A-C2A-CAA-CBA
7	C	101	BCL	C2C-C3C-CAC-CBC
7	C	101	BCL	C4C-C3C-CAC-CBC
7	C	101	BCL	O2A-C1-C2-C3
7	D	102	BCL	C2C-C3C-CAC-CBC
7	D	102	BCL	C4C-C3C-CAC-CBC
7	D	102	BCL	CBD-CGD-O2D-CED
7	E	101	BCL	C1A-C2A-CAA-CBA
7	E	101	BCL	C3A-C2A-CAA-CBA
7	E	101	BCL	C2-C1-O2A-CGA
7	E	101	BCL	C2C-C3C-CAC-CBC
7	E	101	BCL	C4C-C3C-CAC-CBC
7	E	101	BCL	C1-C2-C3-C4
7	E	101	BCL	C1-C2-C3-C5
7	F	102	BCL	C2C-C3C-CAC-CBC
7	F	102	BCL	C4C-C3C-CAC-CBC
7	G	101	BCL	C2C-C3C-CAC-CBC
7	I	101	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	I	101	BCL	C4C-C3C-CAC-CBC
7	J	101	BCL	C2C-C3C-CAC-CBC
7	K	101	BCL	C2C-C3C-CAC-CBC
7	K	101	BCL	C4C-C3C-CAC-CBC
7	L	302	BCL	C4C-C3C-CAC-CBC
7	M	404	BCL	C4C-C3C-CAC-CBC
7	M	404	BCL	C1-C2-C3-C4
7	N	102	BCL	C1A-C2A-CAA-CBA
7	N	102	BCL	C3A-C2A-CAA-CBA
7	N	102	BCL	CBA-CGA-O2A-C1
7	N	102	BCL	O1A-CGA-O2A-C1
7	N	102	BCL	C2C-C3C-CAC-CBC
7	N	102	BCL	C4C-C3C-CAC-CBC
7	O	101	BCL	CHA-CBD-CGD-O1D
7	O	101	BCL	C1-C2-C3-C4
7	O	101	BCL	C1-C2-C3-C5
7	P	101	BCL	C1A-C2A-CAA-CBA
7	P	101	BCL	C2C-C3C-CAC-CBC
7	P	101	BCL	C4C-C3C-CAC-CBC
7	Q	101	BCL	C1A-C2A-CAA-CBA
7	Q	101	BCL	C3A-C2A-CAA-CBA
7	Q	101	BCL	C2C-C3C-CAC-CBC
7	Q	101	BCL	C4C-C3C-CAC-CBC
7	R	101	BCL	O2A-C1-C2-C3
7	R	101	BCL	C1-C2-C3-C4
7	R	101	BCL	C2-C3-C5-C6
7	R	101	BCL	C4-C3-C5-C6
7	R	101	BCL	C11-C10-C8-C9
7	T	101	BCL	C1A-C2A-CAA-CBA
7	T	101	BCL	C3A-C2A-CAA-CBA
7	T	101	BCL	C2C-C3C-CAC-CBC
7	T	101	BCL	C4C-C3C-CAC-CBC
7	U	101	BCL	C1A-C2A-CAA-CBA
7	U	101	BCL	C3A-C2A-CAA-CBA
7	U	101	BCL	CBD-CGD-O2D-CED
7	U	101	BCL	C1-C2-C3-C4
7	U	101	BCL	C1-C2-C3-C5
7	Z	101	BCL	C1A-C2A-CAA-CBA
7	Z	101	BCL	C3A-C2A-CAA-CBA
7	Z	101	BCL	C2C-C3C-CAC-CBC
7	Z	101	BCL	C1-C2-C3-C4
7	Z	101	BCL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
7	a	101	BCL	C1-C2-C3-C4
7	a	101	BCL	C1-C2-C3-C5
7	a	101	BCL	C4-C3-C5-C6
7	b	102	BCL	C1A-C2A-CAA-CBA
7	b	102	BCL	C3A-C2A-CAA-CBA
7	b	102	BCL	C4C-C3C-CAC-CBC
8	0	102	SPO	C1-C4-C5-C6
8	0	102	SPO	C5-C6-C7-C8
8	0	102	SPO	C5-C6-C7-C9
8	0	102	SPO	C32-C33-C35-C36
8	0	102	SPO	C34-C33-C35-C36
8	0	103	SPO	C10-C11-C12-C14
8	0	103	SPO	C33-C35-C36-C37
8	1	102	SPO	C1-C4-C5-C6
8	1	102	SPO	C17-C19-C20-C21
8	1	102	SPO	C24-C23-C25-C26
8	1	102	SPO	C34-C33-C35-C36
8	2	102	SPO	C3-C1-O1-CM1
8	2	102	SPO	C4-C1-O1-CM1
8	2	102	SPO	C33-C35-C36-C37
8	3	102	SPO	C5-C6-C7-C8
8	3	102	SPO	C5-C6-C7-C9
8	C	102	SPO	C4-C1-O1-CM1
8	C	102	SPO	C1-C4-C5-C6
8	C	102	SPO	C28-C30-C31-C32
8	D	103	SPO	C2-C1-O1-CM1
8	D	103	SPO	C4-C1-O1-CM1
8	D	103	SPO	C10-C11-C12-C13
8	D	103	SPO	C10-C11-C12-C14
8	D	103	SPO	C29-C28-C30-C31
8	D	103	SPO	C34-C33-C35-C36
8	F	101	SPO	C33-C35-C36-C37
8	F	103	SPO	C1-C4-C5-C6
8	G	102	SPO	C3-C1-O1-CM1
8	G	102	SPO	C4-C1-O1-CM1
8	G	102	SPO	C10-C11-C12-C13
8	G	102	SPO	C10-C11-C12-C14
8	G	102	SPO	C34-C33-C35-C36
8	I	102	SPO	C2-C1-O1-CM1
8	J	103	SPO	C27-C28-C30-C31
8	J	103	SPO	C29-C28-C30-C31
8	M	408	SPO	C4-C1-O1-CM1

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Mol	Chain	Res	Type	Atoms
8	M	408	SPO	O1-C1-C4-C5
8	M	408	SPO	C2-C1-C4-C5
8	M	408	SPO	C3-C1-C4-C5
8	N	101	SPO	C30-C31-C32-C33
8	O	104	SPO	C4-C1-O1-CM1
8	O	104	SPO	O1-C1-C4-C5
8	O	104	SPO	C2-C1-C4-C5
8	O	104	SPO	C3-C1-C4-C5
8	P	102	SPO	C5-C6-C7-C8
8	P	102	SPO	C5-C6-C7-C9
8	P	102	SPO	C10-C11-C12-C13
8	P	102	SPO	C10-C11-C12-C14
8	P	103	SPO	C4-C1-O1-CM1
8	P	103	SPO	C5-C6-C7-C8
8	P	103	SPO	C5-C6-C7-C9
8	P	103	SPO	C10-C11-C12-C14
8	P	103	SPO	C27-C28-C30-C31
8	P	103	SPO	C29-C28-C30-C31
8	P	103	SPO	C34-C33-C35-C36
8	S	202	SPO	C1-C4-C5-C6
8	S	202	SPO	C15-C16-C17-C18
8	S	202	SPO	C30-C31-C32-C33
8	T	102	SPO	C1-C4-C5-C6
8	T	102	SPO	C20-C21-C22-C23
8	T	102	SPO	C28-C30-C31-C32
8	U	102	SPO	C1-C4-C5-C6
8	U	102	SPO	C27-C28-C30-C31
8	U	102	SPO	C29-C28-C30-C31
8	U	103	SPO	C5-C6-C7-C8
8	U	103	SPO	C33-C35-C36-C37
8	V	101	SPO	C2-C1-O1-CM1
8	V	101	SPO	C30-C31-C32-C33
8	V	101	SPO	C32-C33-C35-C36
8	V	101	SPO	C34-C33-C35-C36
8	X	101	SPO	C2-C1-O1-CM1
8	X	101	SPO	C32-C33-C35-C36
8	X	101	SPO	C34-C33-C35-C36
8	Z	102	SPO	C3-C1-O1-CM1
8	Z	102	SPO	C4-C1-O1-CM1
8	Z	102	SPO	C27-C28-C30-C31
8	Z	102	SPO	C29-C28-C30-C31
8	Z	102	SPO	C28-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
8	b	101	SPO	C2-C1-O1-CM1
8	b	101	SPO	C4-C1-O1-CM1
9	A	102	PC1	C11-O13-P-O14
9	A	102	PC1	C2-C1-O11-P
9	A	102	PC1	O22-C21-O21-C2
9	A	102	PC1	C22-C21-O21-C2
9	A	104	PC1	C1-O11-P-O14
9	D	104	PC1	C11-O13-P-O14
9	D	104	PC1	C1-O11-P-O12
9	L	304	PC1	C11-O13-P-O14
9	L	304	PC1	C11-O13-P-O11
9	L	304	PC1	C1-O11-P-O14
9	L	304	PC1	C12-C11-O13-P
9	L	304	PC1	O13-C11-C12-N
9	L	306	PC1	C1-O11-P-O14
9	L	306	PC1	O21-C2-C3-O31
9	L	311	PC1	C11-O13-P-O11
9	L	311	PC1	C1-O11-P-O12
9	L	311	PC1	C1-O11-P-O14
9	L	311	PC1	C12-C11-O13-P
9	M	401	PC1	C11-O13-P-O14
9	M	401	PC1	C1-O11-P-O12
9	M	401	PC1	C1-O11-P-O14
9	M	401	PC1	C1-O11-P-O13
9	M	401	PC1	O32-C31-O31-C3
9	M	401	PC1	C32-C31-O31-C3
9	M	402	PC1	C11-O13-P-O12
9	M	402	PC1	C1-O11-P-O12
9	M	402	PC1	C1-O11-P-O14
9	M	402	PC1	C1-O11-P-O13
9	M	411	PC1	C11-O13-P-O14
9	M	411	PC1	C1-O11-P-O14
9	O	103	PC1	C11-O13-P-O12
9	O	103	PC1	C1-O11-P-O12
9	O	103	PC1	C1-O11-P-O14
10	H	301	CDL	O1-C1-CA2-OA2
10	H	301	CDL	CA2-OA2-PA1-OA3
10	H	301	CDL	CA2-OA2-PA1-OA4
10	H	301	CDL	CA2-OA2-PA1-OA5
10	H	301	CDL	CA3-OA5-PA1-OA3
10	H	301	CDL	CA3-OA5-PA1-OA4
10	H	301	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
10	H	301	CDL	OA7-CA5-OA6-CA4
10	H	301	CDL	C11-CA5-OA6-CA4
10	M	409	CDL	CA2-OA2-PA1-OA5
10	M	409	CDL	CA3-OA5-PA1-OA3
10	M	409	CDL	CA3-OA5-PA1-OA4
10	M	409	CDL	OA7-CA5-OA6-CA4
10	M	409	CDL	C11-CA5-OA6-CA4
10	M	409	CDL	CB3-OB5-PB2-OB4
10	M	409	CDL	OB9-CB7-OB8-CB6
10	M	409	CDL	C71-CB7-OB8-CB6
10	M	410	CDL	O1-C1-CB2-OB2
10	M	410	CDL	CA2-OA2-PA1-OA3
10	M	410	CDL	CA2-OA2-PA1-OA4
10	M	410	CDL	OB7-CB5-OB6-CB4
10	M	410	CDL	C51-CB5-OB6-CB4
12	L	305	U10	C29-C31-C32-C33
12	L	307	U10	C14-C16-C17-C18
12	L	309	U10	C12-C11-C9-C8
12	L	309	U10	C12-C11-C9-C10
12	L	309	U10	C14-C16-C17-C18
12	L	309	U10	C20-C19-C21-C22
12	L	309	U10	C24-C26-C27-C28
12	M	403	U10	C18-C19-C21-C22
12	M	403	U10	C20-C19-C21-C22
12	M	403	U10	C24-C26-C27-C28
12	M	407	U10	C34-C36-C37-C38
12	X	102	U10	C1-C6-C7-C8
12	X	102	U10	C5-C6-C7-C8
12	X	102	U10	C14-C16-C17-C18
12	X	102	U10	C18-C19-C21-C22
12	X	102	U10	C20-C19-C21-C22
12	X	102	U10	C24-C26-C27-C28
12	X	102	U10	C29-C31-C32-C33
12	X	102	U10	C34-C36-C37-C38
7	F	102	BCL	O1D-CGD-O2D-CED
7	U	101	BCL	O1D-CGD-O2D-CED
7	M	404	BCL	C10-C11-C12-C13
7	D	102	BCL	O1D-CGD-O2D-CED
7	O	101	BCL	O1D-CGD-O2D-CED
7	9	101	BCL	CBD-CGD-O2D-CED
7	A	101	BCL	CBD-CGD-O2D-CED
7	F	102	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
7	M	405	BCL	CBD-CGD-O2D-CED
7	O	101	BCL	CBD-CGD-O2D-CED
7	2	101	BCL	O1A-CGA-O2A-C1
7	J	101	BCL	O1A-CGA-O2A-C1
7	G	101	BCL	C8-C10-C11-C12
7	Z	101	BCL	C8-C10-C11-C12
7	J	101	BCL	CBA-CGA-O2A-C1
7	W	101	BCL	CBD-CGD-O2D-CED
7	b	102	BCL	O1A-CGA-O2A-C1
7	C	101	BCL	C5-C6-C7-C8
7	7	101	BCL	CBD-CGD-O2D-CED
7	a	101	BCL	CBD-CGD-O2D-CED
7	7	101	BCL	C3-C5-C6-C7
7	B	101	BCL	C3-C5-C6-C7
7	K	101	BCL	C3-C5-C6-C7
7	L	301	BCL	C3-C5-C6-C7
7	U	101	BCL	C3-C5-C6-C7
7	2	101	BCL	CBA-CGA-O2A-C1
7	N	102	BCL	C15-C16-C17-C18
12	X	102	U10	C26-C27-C28-C29
7	A	101	BCL	O1D-CGD-O2D-CED
7	R	101	BCL	CBD-CGD-O2D-CED
7	J	101	BCL	C4-C3-C5-C6
7	K	101	BCL	C4-C3-C5-C6
8	3	102	SPO	C34-C33-C35-C36
7	J	101	BCL	C2-C3-C5-C6
7	K	101	BCL	C2-C3-C5-C6
8	1	102	SPO	C32-C33-C35-C36
8	D	103	SPO	C32-C33-C35-C36
8	P	103	SPO	C32-C33-C35-C36
12	L	309	U10	C18-C19-C21-C22
7	N	102	BCL	C2A-CAA-CBA-CGA
7	R	101	BCL	C2A-CAA-CBA-CGA
7	a	101	BCL	C2A-CAA-CBA-CGA
7	1	101	BCL	CBA-CGA-O2A-C1
7	b	102	BCL	CBA-CGA-O2A-C1
7	M	405	BCL	O1D-CGD-O2D-CED
7	1	101	BCL	O1A-CGA-O2A-C1
7	7	101	BCL	C8-C10-C11-C12
7	I	101	BCL	CBD-CGD-O2D-CED
7	K	101	BCL	CBD-CGD-O2D-CED
10	M	410	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
9	M	401	PC1	C2-C1-O11-P
7	J	101	BCL	C15-C16-C17-C18
7	7	101	BCL	C4-C3-C5-C6
7	Z	101	BCL	C4-C3-C5-C6
8	0	102	SPO	C29-C28-C30-C31
8	0	103	SPO	C29-C28-C30-C31
8	G	102	SPO	C29-C28-C30-C31
8	P	102	SPO	C34-C33-C35-C36
8	T	102	SPO	C34-C33-C35-C36
12	L	305	U10	C12-C11-C9-C10
12	X	102	U10	C15-C14-C16-C17
7	7	101	BCL	C2-C3-C5-C6
7	Z	101	BCL	C2-C3-C5-C6
7	a	101	BCL	C2-C3-C5-C6
8	0	102	SPO	C27-C28-C30-C31
8	0	103	SPO	C27-C28-C30-C31
8	D	103	SPO	C27-C28-C30-C31
8	G	102	SPO	C27-C28-C30-C31
8	G	102	SPO	C32-C33-C35-C36
8	P	102	SPO	C32-C33-C35-C36
8	T	102	SPO	C32-C33-C35-C36
12	L	305	U10	C12-C11-C9-C8
12	X	102	U10	C13-C14-C16-C17
7	P	101	BCL	CBD-CGD-O2D-CED
9	M	401	PC1	C21-C22-C23-C24
7	V	102	BCL	C2A-CAA-CBA-CGA
8	9	102	SPO	C33-C35-C36-C37
8	D	103	SPO	C28-C30-C31-C32
8	D	103	SPO	C33-C35-C36-C37
8	F	101	SPO	C28-C30-C31-C32
8	J	103	SPO	C28-C30-C31-C32
8	N	101	SPO	C28-C30-C31-C32
8	O	102	SPO	C28-C30-C31-C32
8	P	102	SPO	C33-C35-C36-C37
8	P	103	SPO	C28-C30-C31-C32
8	P	103	SPO	C33-C35-C36-C37
8	S	202	SPO	C33-C35-C36-C37
8	Z	102	SPO	C33-C35-C36-C37
12	L	307	U10	C29-C31-C32-C33
12	M	403	U10	C9-C11-C12-C13
7	9	101	BCL	O1D-CGD-O2D-CED
7	M	404	BCL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
10	H	301	CDL	CB2-C1-CA2-OA2
10	M	410	CDL	CA2-C1-CB2-OB2
7	E	101	BCL	CBA-CGA-O2A-C1
7	Z	101	BCL	CBA-CGA-O2A-C1
7	J	101	BCL	CBD-CGD-O2D-CED
8	1	102	SPO	C12-C14-C15-C16
7	R	101	BCL	C13-C15-C16-C17
7	8	101	BCL	C5-C6-C7-C8
7	N	102	BCL	C5-C6-C7-C8
7	T	101	BCL	C8-C10-C11-C12
7	U	101	BCL	C10-C11-C12-C13
7	b	102	BCL	C10-C11-C12-C13
8	3	102	SPO	C32-C33-C35-C36
8	F	101	SPO	C32-C33-C35-C36
7	3	101	BCL	C14-C13-C15-C16
7	8	101	BCL	C11-C10-C8-C9
7	A	101	BCL	C14-C13-C15-C16
7	B	101	BCL	C6-C7-C8-C9
7	D	102	BCL	C11-C12-C13-C14
7	E	101	BCL	C11-C12-C13-C14
7	J	101	BCL	C11-C10-C8-C9
7	K	101	BCL	C11-C10-C8-C9
7	O	101	BCL	C14-C13-C15-C16
7	P	101	BCL	C11-C10-C8-C9
7	P	101	BCL	C14-C13-C15-C16
7	Q	101	BCL	C14-C13-C15-C16
7	S	201	BCL	C14-C13-C15-C16
7	T	101	BCL	C6-C7-C8-C9
7	W	101	BCL	O1D-CGD-O2D-CED
8	0	102	SPO	C10-C11-C12-C13
8	0	103	SPO	C5-C6-C7-C8
8	D	103	SPO	C5-C6-C7-C8
8	F	103	SPO	C5-C6-C7-C8
8	P	103	SPO	C10-C11-C12-C13
8	0	102	SPO	C10-C11-C12-C14
8	0	103	SPO	C5-C6-C7-C9
8	F	103	SPO	C5-C6-C7-C9
8	U	103	SPO	C5-C6-C7-C9
9	M	402	PC1	C21-C22-C23-C24
7	E	101	BCL	O1A-CGA-O2A-C1
7	Z	101	BCL	O1A-CGA-O2A-C1
7	7	101	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	B	101	BCL	C10-C11-C12-C13
7	E	101	BCL	C10-C11-C12-C13
7	F	102	BCL	C5-C6-C7-C8
7	M	404	BCL	C13-C15-C16-C17
7	P	101	BCL	C15-C16-C17-C18
7	V	102	BCL	C8-C10-C11-C12
7	L	302	BCL	C13-C15-C16-C17
7	9	101	BCL	C8-C10-C11-C12
7	B	101	BCL	C5-C6-C7-C8
7	E	101	BCL	C13-C15-C16-C17
7	B	101	BCL	C8-C10-C11-C12
7	B	101	BCL	C13-C15-C16-C17
7	P	101	BCL	C8-C10-C11-C12
7	Q	101	BCL	C13-C15-C16-C17
7	Z	101	BCL	C10-C11-C12-C13
7	b	102	BCL	C8-C10-C11-C12
7	J	101	BCL	C5-C6-C7-C8
7	M	405	BCL	C10-C11-C12-C13
7	D	102	BCL	C11-C12-C13-C15
7	E	101	BCL	C12-C13-C15-C16
7	G	101	BCL	C6-C7-C8-C10
7	Z	101	BCL	C6-C7-C8-C10
7	Z	101	BCL	C11-C12-C13-C15
10	M	409	CDL	CB5-C51-C52-C53
7	F	102	BCL	C2A-CAA-CBA-CGA
7	A	101	BCL	C13-C15-C16-C17
7	T	101	BCL	C13-C15-C16-C17
7	b	102	BCL	C5-C6-C7-C8
7	a	101	BCL	O1D-CGD-O2D-CED
8	J	103	SPO	C33-C35-C36-C37
8	M	408	SPO	C33-C35-C36-C37
8	N	101	SPO	C33-C35-C36-C37
8	O	102	SPO	C33-C35-C36-C37
8	U	102	SPO	C33-C35-C36-C37
12	L	305	U10	C14-C16-C17-C18
12	L	305	U10	C19-C21-C22-C23
12	L	305	U10	C24-C26-C27-C28
12	L	307	U10	C9-C11-C12-C13
12	L	307	U10	C24-C26-C27-C28
12	L	309	U10	C19-C21-C22-C23
9	M	411	PC1	C27-C28-C29-C2A
7	A	101	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	C	101	BCL	C10-C11-C12-C13
7	I	101	BCL	C13-C15-C16-C17
7	7	101	BCL	O1D-CGD-O2D-CED
7	3	101	BCL	C15-C16-C17-C18
7	F	102	BCL	C15-C16-C17-C18
7	K	101	BCL	C15-C16-C17-C18
7	S	201	BCL	C15-C16-C17-C18
7	V	102	BCL	C10-C11-C12-C13
9	A	102	PC1	C11-O13-P-O11
9	A	103	PC1	C1-O11-P-O13
9	D	104	PC1	C11-O13-P-O11
9	D	104	PC1	C1-O11-P-O13
9	L	311	PC1	C1-O11-P-O13
9	M	402	PC1	C11-O13-P-O11
9	O	103	PC1	C1-O11-P-O13
10	H	301	CDL	CA3-OA5-PA1-OA2
10	H	301	CDL	CB2-OB2-PB2-OB5
10	H	301	CDL	CB3-OB5-PB2-OB2
10	M	409	CDL	CA3-OA5-PA1-OA2
10	M	409	CDL	CB2-OB2-PB2-OB5
10	M	409	CDL	CB3-OB5-PB2-OB2
10	M	410	CDL	CA2-OA2-PA1-OA5
10	M	410	CDL	CB3-OB5-PB2-OB2
7	1	101	BCL	C3-C5-C6-C7
7	G	101	BCL	C3-C5-C6-C7
7	M	404	BCL	C3-C5-C6-C7
7	G	101	BCL	C10-C11-C12-C13
7	R	101	BCL	O1D-CGD-O2D-CED
10	M	410	CDL	CB2-C1-CA2-OA2
8	F	101	SPO	C34-C33-C35-C36
8	O	104	SPO	C34-C33-C35-C36
9	L	311	PC1	C11-C12-N-C13
9	L	311	PC1	C11-C12-N-C14
9	L	311	PC1	C11-C12-N-C15
7	0	101	BCL	C2A-CAA-CBA-CGA
7	R	101	BCL	CBA-CGA-O2A-C1
7	L	301	BCL	CBD-CGD-O2D-CED
7	G	101	BCL	C15-C16-C17-C18
10	M	409	CDL	C54-C55-C56-C57
10	M	410	CDL	C71-C72-C73-C74
7	I	101	BCL	C16-C17-C18-C19
7	J	101	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
10	M	410	CDL	C83-C84-C85-C86
8	1	102	SPO	C16-C17-C19-C20
8	S	202	SPO	C11-C12-C14-C15
8	S	202	SPO	C16-C17-C19-C20
7	M	405	BCL	C16-C17-C18-C20
7	Q	101	BCL	C16-C17-C18-C19
7	P	101	BCL	C4B-C3B-CAB-OBB
7	P	101	BCL	C4B-C3B-CAB-CBB
8	M	408	SPO	C34-C33-C35-C36
12	L	307	U10	C20-C19-C21-C22
7	E	101	BCL	C6-C7-C8-C9
7	I	101	BCL	C11-C12-C13-C14
7	K	101	BCL	C11-C12-C13-C14
7	L	302	BCL	C14-C13-C15-C16
7	M	405	BCL	C11-C10-C8-C9
7	R	101	BCL	C6-C7-C8-C9
7	Z	101	BCL	C11-C10-C8-C9
7	Z	101	BCL	C11-C12-C13-C14
10	M	410	CDL	C75-C76-C77-C78
8	S	202	SPO	C15-C16-C17-C19
10	M	410	CDL	C51-C52-C53-C54
8	J	102	SPO	C30-C31-C32-C33
9	A	103	PC1	C21-C22-C23-C24
10	M	409	CDL	CA5-C11-C12-C13
10	M	409	CDL	C72-C73-C74-C75
9	M	411	PC1	C11-C12-N-C15
7	E	101	BCL	C16-C17-C18-C19
7	P	101	BCL	C16-C17-C18-C19
7	Z	101	BCL	C16-C17-C18-C19
10	M	409	CDL	C35-C36-C37-C38
10	M	410	CDL	C36-C37-C38-C39
7	K	101	BCL	O1D-CGD-O2D-CED
7	8	101	BCL	C3A-C2A-CAA-CBA
7	B	101	BCL	C3A-C2A-CAA-CBA
7	P	101	BCL	C3A-C2A-CAA-CBA
7	R	101	BCL	C3A-C2A-CAA-CBA
7	N	102	BCL	C10-C11-C12-C13
8	2	102	SPO	C17-C19-C20-C21
10	M	409	CDL	C71-C72-C73-C74
7	1	101	BCL	C6-C7-C8-C10
7	Z	101	BCL	C16-C17-C18-C20
10	M	409	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
9	A	102	PC1	C1-C2-C3-O31
7	b	102	BCL	C3-C5-C6-C7
7	9	101	BCL	C4-C3-C5-C6
7	C	101	BCL	C4-C3-C5-C6
7	9	101	BCL	C2-C3-C5-C6
7	C	101	BCL	C2-C3-C5-C6
8	M	408	SPO	C32-C33-C35-C36
12	L	307	U10	C18-C19-C21-C22
12	L	305	U10	C31-C32-C33-C34
7	R	101	BCL	C1-C2-C3-C5
7	I	101	BCL	O1D-CGD-O2D-CED
10	M	409	CDL	C59-C60-C61-C62
7	R	101	BCL	O1A-CGA-O2A-C1
10	M	409	CDL	C83-C84-C85-C86
7	b	102	BCL	C2-C1-O2A-CGA
7	S	201	BCL	C13-C15-C16-C17
11	L	310	BPH	C6-C7-C8-C9
7	7	101	BCL	C5-C6-C7-C8
7	J	101	BCL	C13-C15-C16-C17
7	F	102	BCL	C4-C3-C5-C6
8	I	102	SPO	C34-C33-C35-C36
7	7	101	BCL	C11-C10-C8-C7
7	8	101	BCL	C6-C7-C8-C10
7	9	101	BCL	C11-C10-C8-C7
7	E	101	BCL	C11-C10-C8-C7
7	F	102	BCL	C2-C3-C5-C6
7	G	101	BCL	C12-C13-C15-C16
7	V	102	BCL	C2-C3-C5-C6
7	C	101	BCL	C8-C10-C11-C12
7	R	101	BCL	C8-C10-C11-C12
10	M	409	CDL	C41-C42-C43-C44
7	B	101	BCL	C16-C17-C18-C20
9	M	401	PC1	O11-C1-C2-O21
8	S	202	SPO	C14-C15-C16-C17
7	3	101	BCL	C8-C10-C11-C12
9	L	311	PC1	O21-C2-C3-O31
10	M	409	CDL	C31-C32-C33-C34
7	M	405	BCL	C16-C17-C18-C19
7	Q	101	BCL	C16-C17-C18-C20
7	9	101	BCL	C5-C6-C7-C8
7	9	101	BCL	C15-C16-C17-C18
7	G	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	V	102	BCL	C4-C3-C5-C6
8	2	102	SPO	C34-C33-C35-C36
8	O	104	SPO	C32-C33-C35-C36
7	7	101	BCL	C11-C10-C8-C9
7	8	101	BCL	C6-C7-C8-C9
7	9	101	BCL	C11-C10-C8-C9
7	D	102	BCL	C11-C10-C8-C9
7	E	101	BCL	C11-C10-C8-C9
7	G	101	BCL	C14-C13-C15-C16
7	W	101	BCL	C6-C7-C8-C9
7	Z	101	BCL	C6-C7-C8-C9
11	L	303	BPH	C11-C10-C8-C9
7	7	101	BCL	C2A-CAA-CBA-CGA
7	L	302	BCL	C1A-C2A-CAA-CBA
7	J	101	BCL	C16-C17-C18-C20
10	M	409	CDL	C21-C22-C23-C24
8	0	102	SPO	C12-C14-C15-C16
8	C	102	SPO	C11-C10-C9-C7
7	P	101	BCL	O1D-CGD-O2D-CED
9	O	103	PC1	C11-O13-P-O11
10	M	410	CDL	CA3-OA5-PA1-OA2
10	M	409	CDL	C1-CA2-OA2-PA1
7	2	101	BCL	C8-C10-C11-C12
9	L	304	PC1	O11-C1-C2-C3
9	L	311	PC1	O11-C1-C2-C3
9	M	401	PC1	O11-C1-C2-C3
10	M	409	CDL	OB5-CB3-CB4-CB6
7	J	101	BCL	O1D-CGD-O2D-CED
7	M	404	BCL	C15-C16-C17-C18
7	N	102	BCL	C16-C17-C18-C19
7	L	301	BCL	C8-C10-C11-C12
8	P	102	SPO	C1-C4-C5-C6
8	P	103	SPO	C1-C4-C5-C6
12	X	102	U10	C30-C29-C31-C32
7	L	301	BCL	C2C-C3C-CAC-CBC
7	P	101	BCL	C2-C3-C5-C6
7	S	201	BCL	C10-C11-C12-C13
10	M	409	CDL	C78-C79-C80-C81
10	M	409	CDL	C58-C59-C60-C61
7	T	101	BCL	C5-C6-C7-C8
7	K	101	BCL	C16-C17-C18-C19
9	M	402	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
10	H	301	CDL	CA3-CA4-CA6-OA8
10	M	409	CDL	CA3-CA4-CA6-OA8
7	T	101	BCL	C10-C11-C12-C13
7	W	101	BCL	C10-C11-C12-C13
7	J	101	BCL	C3-C5-C6-C7
7	P	101	BCL	C16-C17-C18-C20
8	O	103	SPO	C4-C1-O1-CM1
8	J	102	SPO	C4-C1-O1-CM1
8	U	102	SPO	C4-C1-O1-CM1
9	M	402	PC1	C2C-C2D-C2E-C2F
7	A	101	BCL	C15-C16-C17-C18
7	2	101	BCL	C4-C3-C5-C6
7	P	101	BCL	C4-C3-C5-C6
8	O	102	SPO	C29-C28-C30-C31
8	S	202	SPO	C29-C28-C30-C31
7	2	101	BCL	C2-C3-C5-C6
8	I	102	SPO	C32-C33-C35-C36
8	S	202	SPO	C27-C28-C30-C31
12	L	307	U10	C5-C6-C7-C8
12	L	309	U10	C5-C6-C7-C8
7	O	101	BCL	C10-C11-C12-C13
7	A	101	BCL	CBA-CGA-O2A-C1
10	M	410	CDL	OB5-CB3-CB4-OB6
9	M	411	PC1	C11-C12-N-C14
10	M	410	CDL	C32-C33-C34-C35
7	A	101	BCL	C8-C10-C11-C12
7	K	101	BCL	C10-C11-C12-C13
7	Q	101	BCL	C8-C10-C11-C12
8	O	103	SPO	C2-C1-O1-CM1
8	2	102	SPO	C2-C1-O1-CM1
8	3	102	SPO	C2-C1-O1-CM1
8	3	102	SPO	C3-C1-O1-CM1
8	9	102	SPO	C2-C1-O1-CM1
8	9	102	SPO	C3-C1-O1-CM1
8	D	103	SPO	C3-C1-O1-CM1
8	F	103	SPO	C3-C1-O1-CM1
8	G	102	SPO	C2-C1-O1-CM1
8	J	102	SPO	C2-C1-O1-CM1
8	M	408	SPO	C3-C1-O1-CM1
8	N	101	SPO	C3-C1-O1-CM1
8	O	104	SPO	C3-C1-O1-CM1
8	P	102	SPO	C3-C1-O1-CM1

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Mol	Chain	Res	Type	Atoms
8	P	103	SPO	C2-C1-O1-CM1
8	U	102	SPO	C2-C1-O1-CM1
8	U	102	SPO	C3-C1-O1-CM1
8	V	101	SPO	C3-C1-O1-CM1
8	Z	102	SPO	C2-C1-O1-CM1
8	b	101	SPO	C3-C1-O1-CM1
9	M	402	PC1	O21-C2-C3-O31
10	M	409	CDL	OA6-CA4-CA6-OA8
7	2	101	BCL	C4B-C3B-CAB-CBB
7	7	101	BCL	C4B-C3B-CAB-OB
8	3	102	SPO	C2-C1-C4-C5
8	3	102	SPO	C3-C1-C4-C5
8	N	101	SPO	C2-C1-C4-C5
8	N	101	SPO	C3-C1-C4-C5
8	U	103	SPO	C3-C1-C4-C5
7	B	101	BCL	C4-C3-C5-C6
12	M	403	U10	C15-C14-C16-C17
7	0	101	BCL	C11-C10-C8-C7
7	8	101	BCL	C11-C12-C13-C15
7	A	101	BCL	C11-C12-C13-C15
7	B	101	BCL	C6-C7-C8-C10
7	D	102	BCL	C11-C10-C8-C7
7	E	101	BCL	C6-C7-C8-C10
7	L	301	BCL	C11-C12-C13-C15
7	M	404	BCL	C11-C12-C13-C15
7	N	102	BCL	C12-C13-C15-C16
7	S	201	BCL	C11-C10-C8-C7
7	T	101	BCL	C6-C7-C8-C10
7	T	101	BCL	C11-C12-C13-C15
7	W	101	BCL	C6-C7-C8-C10
7	b	102	BCL	C6-C7-C8-C10
8	O	102	SPO	C27-C28-C30-C31
11	L	303	BPH	C11-C10-C8-C7
12	X	102	U10	C28-C29-C31-C32
7	9	101	BCL	C3-C5-C6-C7
7	0	101	BCL	C11-C10-C8-C9
7	A	101	BCL	C11-C12-C13-C14
7	F	102	BCL	C6-C7-C8-C9
7	G	101	BCL	C6-C7-C8-C9
7	S	201	BCL	C11-C10-C8-C9
7	T	101	BCL	C11-C12-C13-C14
7	V	102	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	b	102	BCL	C6-C7-C8-C9
8	T	102	SPO	C25-C26-C27-C28
8	0	103	SPO	C10-C11-C12-C13
7	2	101	BCL	C11-C12-C13-C15
10	M	409	CDL	C62-C63-C64-C65
7	L	301	BCL	O1D-CGD-O2D-CED
7	I	101	BCL	C15-C16-C17-C18
7	P	101	BCL	C10-C11-C12-C13
7	I	101	BCL	C8-C10-C11-C12
7	b	102	BCL	CBD-CGD-O2D-CED
10	M	410	CDL	OB5-CB3-CB4-CB6
7	Q	101	BCL	C3-C5-C6-C7
8	C	102	SPO	C33-C35-C36-C37
8	I	102	SPO	C33-C35-C36-C37
12	M	407	U10	C14-C16-C17-C18
12	X	102	U10	C19-C21-C22-C23
7	E	101	BCL	C15-C16-C17-C18
8	J	102	SPO	C29-C28-C30-C31
7	B	101	BCL	C2-C3-C5-C6
7	G	101	BCL	C2-C3-C5-C6
12	M	403	U10	C13-C14-C16-C17
7	C	101	BCL	CBA-CGA-O2A-C1
10	H	301	CDL	C1-CA2-OA2-PA1
7	A	101	BCL	O1A-CGA-O2A-C1
7	D	102	BCL	C3A-C2A-CAA-CBA
7	a	101	BCL	C3A-C2A-CAA-CBA
7	P	101	BCL	C2B-C3B-CAB-OBB
7	P	101	BCL	C2B-C3B-CAB-CBB
7	F	102	BCL	C16-C17-C18-C20
9	L	306	PC1	C1-C2-C3-O31
10	M	410	CDL	CA3-CA4-CA6-OA8
11	L	303	BPH	O2A-C1-C2-C3
11	L	310	BPH	O2A-C1-C2-C3
8	T	102	SPO	C29-C28-C30-C31
7	N	102	BCL	C16-C17-C18-C20
7	V	102	BCL	C16-C17-C18-C20
8	S	202	SPO	C35-C36-C37-C38
7	J	101	BCL	C10-C11-C12-C13
7	R	101	BCL	C5-C6-C7-C8
10	M	409	CDL	OB5-CB3-CB4-OB6
7	9	101	BCL	C16-C17-C18-C20
7	I	101	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
7	K	101	BCL	C16-C17-C18-C20
10	M	409	CDL	C13-C14-C15-C16
9	A	102	PC1	O21-C2-C3-O31
8	J	103	SPO	C11-C10-C9-C7
7	1	101	BCL	C6-C7-C8-C9
7	A	101	BCL	C16-C17-C18-C20
7	E	101	BCL	C16-C17-C18-C20
7	Q	101	BCL	C15-C16-C17-C18
8	M	408	SPO	C28-C30-C31-C32
8	U	103	SPO	C28-C30-C31-C32
12	M	403	U10	C19-C21-C22-C23
7	E	101	BCL	C3-C5-C6-C7
7	9	101	BCL	C2-C1-O2A-CGA
7	D	102	BCL	C2-C1-O2A-CGA
7	Z	101	BCL	C2-C1-O2A-CGA
7	O	101	BCL	C15-C16-C17-C18
7	2	101	BCL	C11-C10-C8-C9
7	L	301	BCL	C11-C10-C8-C9
7	M	404	BCL	C6-C7-C8-C9
7	K	101	BCL	C5-C6-C7-C8
9	A	104	PC1	C2-C1-O11-P
9	O	103	PC1	C2-C1-O11-P
7	F	102	BCL	C16-C17-C18-C19
7	R	101	BCL	C16-C17-C18-C19
7	G	101	BCL	C4C-C3C-CAC-CBC
7	a	101	BCL	C4C-C3C-CAC-CBC
8	J	102	SPO	C10-C11-C12-C14
8	S	202	SPO	C22-C23-C25-C26
9	A	102	PC1	C29-C2A-C2B-C2C
7	B	101	BCL	C16-C17-C18-C19
11	L	310	BPH	C6-C7-C8-C10
10	M	409	CDL	C16-C17-C18-C19
9	A	103	PC1	O11-C1-C2-C3
7	2	101	BCL	C11-C10-C8-C7
7	3	101	BCL	C12-C13-C15-C16
7	7	101	BCL	C6-C7-C8-C10
7	8	101	BCL	C11-C10-C8-C7
7	D	102	BCL	C12-C13-C15-C16
7	E	101	BCL	C11-C12-C13-C15
7	F	102	BCL	C6-C7-C8-C10
7	G	101	BCL	C11-C10-C8-C7
7	I	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
7	J	101	BCL	C11-C10-C8-C7
7	M	404	BCL	C6-C7-C8-C10
7	O	101	BCL	C6-C7-C8-C10
7	P	101	BCL	C11-C10-C8-C7
7	P	101	BCL	C12-C13-C15-C16
7	S	201	BCL	C12-C13-C15-C16
7	T	101	BCL	C11-C10-C8-C7
7	V	102	BCL	C6-C7-C8-C10
7	W	101	BCL	C11-C10-C8-C7
7	T	101	BCL	CBD-CGD-O2D-CED
7	U	101	BCL	C2A-CAA-CBA-CGA
9	M	411	PC1	C11-C12-N-C13
7	G	101	BCL	CBA-CGA-O2A-C1
7	a	101	BCL	C5-C6-C7-C8
7	M	404	BCL	CAD-CBD-CGD-O2D
7	C	101	BCL	C13-C15-C16-C17
7	W	101	BCL	C13-C15-C16-C17
7	F	102	BCL	CBA-CGA-O2A-C1
8	D	101	SPO	C29-C28-C30-C31
8	U	103	SPO	C34-C33-C35-C36
12	M	403	U10	C5-C4-O4-C4M
10	M	409	CDL	CB3-CB4-CB6-OB8
9	L	311	PC1	O11-C1-C2-O21
9	M	411	PC1	O11-C1-C2-O21
8	F	103	SPO	C30-C31-C32-C33
7	P	101	BCL	CBA-CGA-O2A-C1
7	M	405	BCL	CHA-CBD-CGD-O1D
7	M	405	BCL	CHA-CBD-CGD-O2D
7	O	101	BCL	CHA-CBD-CGD-O2D
7	C	101	BCL	O1A-CGA-O2A-C1
7	9	101	BCL	C10-C11-C12-C13
9	A	103	PC1	O21-C2-C3-O31
10	H	301	CDL	C32-C31-CA7-OA8
9	M	402	PC1	C2-C3-O31-C31
7	2	101	BCL	C4B-C3B-CAB-OB8
7	7	101	BCL	C4B-C3B-CAB-CBB
7	G	101	BCL	O1A-CGA-O2A-C1
7	7	101	BCL	C6-C7-C8-C9
7	D	102	BCL	C14-C13-C15-C16
7	N	102	BCL	C11-C10-C8-C9
7	O	101	BCL	C6-C7-C8-C9
7	V	102	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	b	102	BCL	O1D-CGD-O2D-CED
7	Z	101	BCL	C15-C16-C17-C18
10	M	409	CDL	C81-C82-C83-C84
8	D	103	SPO	C5-C6-C7-C9
8	b	101	SPO	C10-C11-C12-C14
7	D	102	BCL	C1A-C2A-CAA-CBA
9	A	102	PC1	C31-C32-C33-C34
9	L	304	PC1	C1-O11-P-O13
9	M	401	PC1	C11-O13-P-O11
9	M	411	PC1	C11-O13-P-O11
9	A	102	PC1	C11-O13-P-O12
9	A	103	PC1	C1-O11-P-O12
9	D	104	PC1	C11-O13-P-O12
9	L	311	PC1	C11-O13-P-O12
9	M	402	PC1	C11-O13-P-O14
9	O	103	PC1	C11-O13-P-O14
10	H	301	CDL	CB2-OB2-PB2-OB3
10	H	301	CDL	CB3-OB5-PB2-OB3
10	H	301	CDL	CB3-OB5-PB2-OB4
10	M	409	CDL	CA2-OA2-PA1-OA4
10	M	409	CDL	CB2-OB2-PB2-OB3
10	M	409	CDL	CB2-OB2-PB2-OB4
10	M	410	CDL	CA3-OA5-PA1-OA3
10	M	410	CDL	CB3-OB5-PB2-OB3
12	L	307	U10	C6-C7-C8-C9
7	9	101	BCL	C16-C17-C18-C19
7	D	102	BCL	C10-C11-C12-C13
8	2	102	SPO	C28-C30-C31-C32
8	3	102	SPO	C28-C30-C31-C32
7	V	102	BCL	C16-C17-C18-C19
7	M	405	BCL	CAD-CBD-CGD-O1D
9	M	402	PC1	C12-C11-O13-P
12	L	308	U10	C12-C11-C9-C8
10	H	301	CDL	C81-C82-C83-C84
7	F	102	BCL	O1A-CGA-O2A-C1
8	Z	102	SPO	C1-C4-C5-C6
10	M	409	CDL	C20-C21-C22-C23
7	A	101	BCL	C12-C13-C15-C16
7	I	101	BCL	C11-C10-C8-C7
7	O	101	BCL	C2C-C3C-CAC-CBC
7	R	101	BCL	C11-C10-C8-C7
7	W	101	BCL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	b	102	BCL	C11-C10-C8-C7
8	2	102	SPO	C32-C33-C35-C36
9	A	103	PC1	O11-C1-C2-O21
9	L	304	PC1	O11-C1-C2-O21
9	L	306	PC1	C31-C32-C33-C34
7	P	101	BCL	O1A-CGA-O2A-C1
7	2	101	BCL	C2B-C3B-CAB-OBB
7	2	101	BCL	C2B-C3B-CAB-CBB
7	G	101	BCL	C2B-C3B-CAB-OBB
7	G	101	BCL	C2B-C3B-CAB-CBB
7	O	101	BCL	C5-C6-C7-C8
9	D	104	PC1	C11-C12-N-C15
7	2	101	BCL	C11-C12-C13-C14
7	a	101	BCL	C6-C7-C8-C10
9	A	102	PC1	O13-C11-C12-N
9	A	103	PC1	O13-C11-C12-N
9	A	104	PC1	O13-C11-C12-N
9	D	104	PC1	O13-C11-C12-N
9	L	311	PC1	O13-C11-C12-N
9	L	311	PC1	C1-C2-C3-O31
9	M	401	PC1	O13-C11-C12-N
9	M	402	PC1	O13-C11-C12-N
10	M	409	CDL	C51-C52-C53-C54
10	M	409	CDL	OB6-CB4-CB6-OB8
10	M	410	CDL	OA6-CA4-CA6-OA8
12	L	307	U10	C1-C6-C7-C8
8	F	101	SPO	C29-C28-C30-C31
8	V	101	SPO	C29-C28-C30-C31
7	3	101	BCL	C11-C10-C8-C9
7	G	101	BCL	C11-C10-C8-C9
7	I	101	BCL	C6-C7-C8-C9
7	L	301	BCL	C11-C12-C13-C14
7	T	101	BCL	C11-C10-C8-C9
8	N	101	SPO	C4-C1-O1-CM1
9	A	103	PC1	C31-C32-C33-C34
8	0	103	SPO	C14-C15-C16-C17
8	1	102	SPO	C23-C25-C26-C27
8	2	102	SPO	C9-C10-C11-C12
8	3	102	SPO	C23-C25-C26-C27
8	D	103	SPO	C14-C15-C16-C17
8	J	103	SPO	C14-C15-C16-C17
8	T	102	SPO	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	Z	102	SPO	C14-C15-C16-C17
8	b	101	SPO	C9-C10-C11-C12
7	T	101	BCL	C16-C17-C18-C19
7	C	101	BCL	C15-C16-C17-C18
12	L	308	U10	C5-C4-O4-C4M
12	L	309	U10	C5-C4-O4-C4M
10	M	410	CDL	C43-C44-C45-C46
8	T	102	SPO	C27-C28-C30-C31
7	D	102	BCL	C8-C10-C11-C12
10	H	301	CDL	CA7-C31-C32-C33
7	O	101	BCL	C3-C5-C6-C7
7	W	101	BCL	C15-C16-C17-C18
7	L	301	BCL	C2A-CAA-CBA-CGA
7	C	101	BCL	C2-C1-O2A-CGA
7	R	101	BCL	C16-C17-C18-C20
7	S	201	BCL	C3-C5-C6-C7
8	D	101	SPO	C27-C28-C30-C31
8	J	102	SPO	C27-C28-C30-C31
9	M	402	PC1	C24-C25-C26-C27
8	0	103	SPO	C3-C1-O1-CM1
8	C	102	SPO	C2-C1-O1-CM1
8	D	101	SPO	C28-C30-C31-C32
8	F	103	SPO	C2-C1-O1-CM1
8	I	102	SPO	C3-C1-O1-CM1
8	J	102	SPO	C3-C1-O1-CM1
8	M	408	SPO	C2-C1-O1-CM1
8	N	101	SPO	C2-C1-O1-CM1
8	O	104	SPO	C2-C1-O1-CM1
8	P	102	SPO	C2-C1-O1-CM1
8	P	103	SPO	C3-C1-O1-CM1
8	S	202	SPO	C2-C1-O1-CM1
8	S	202	SPO	C28-C30-C31-C32
8	X	101	SPO	C3-C1-O1-CM1
9	A	102	PC1	C1-O11-P-O13
9	A	104	PC1	C11-O13-P-O11
9	A	104	PC1	C1-O11-P-O13
7	G	101	BCL	C4B-C3B-CAB-OB
7	G	101	BCL	C4B-C3B-CAB-CB
8	9	102	SPO	C2-C1-C4-C5
8	9	102	SPO	C3-C1-C4-C5
8	I	102	SPO	C3-C1-C4-C5
10	H	301	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
9	A	103	PC1	C1-C2-C3-O31
8	F	103	SPO	C29-C28-C30-C31
7	K	101	BCL	C11-C10-C8-C7
7	K	101	BCL	C11-C12-C13-C15
7	L	302	BCL	C12-C13-C15-C16
7	Q	101	BCL	C6-C7-C8-C10
7	Z	101	BCL	C11-C10-C8-C7
7	8	101	BCL	C11-C12-C13-C14
7	M	404	BCL	C11-C12-C13-C14
7	W	101	BCL	C11-C10-C8-C9
7	0	101	BCL	C8-C10-C11-C12
10	M	410	CDL	CB5-C51-C52-C53
7	S	201	BCL	CBA-CGA-O2A-C1
12	L	305	U10	C5-C4-O4-C4M
8	3	102	SPO	O1-C1-C4-C5
8	b	101	SPO	C10-C11-C12-C13
7	Q	101	BCL	CBA-CGA-O2A-C1
10	M	409	CDL	CB4-CB3-OB5-PB2
10	M	410	CDL	C1-CB2-OB2-PB2
11	L	310	BPH	C4-C3-C5-C6
8	U	103	SPO	C32-C33-C35-C36
7	Q	101	BCL	O1A-CGA-O2A-C1
9	D	104	PC1	C11-C12-N-C13
7	S	201	BCL	O1A-CGA-O2A-C1
8	O	102	SPO	C35-C36-C37-C38
12	M	403	U10	C12-C11-C9-C10
8	V	101	SPO	C27-C28-C30-C31
11	L	303	BPH	C2-C3-C5-C6
7	L	301	BCL	C2-C1-O2A-CGA
7	P	101	BCL	C2-C1-O2A-CGA
7	A	101	BCL	C16-C17-C18-C19
7	R	101	BCL	C10-C11-C12-C13
7	2	101	BCL	C2A-CAA-CBA-CGA
7	D	102	BCL	CBA-CGA-O2A-C1
9	D	104	PC1	C21-C22-C23-C24
9	L	306	PC1	C2-C1-O11-P
10	M	409	CDL	C34-C35-C36-C37
7	M	405	BCL	CAA-CBA-CGA-O2A
8	F	101	SPO	C27-C28-C30-C31
7	U	101	BCL	C6-C7-C8-C9
7	V	102	BCL	C11-C10-C8-C9
7	V	102	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
8	D	103	SPO	C8-C7-C9-C10
8	J	103	SPO	C8-C7-C9-C10
8	Z	102	SPO	C8-C7-C9-C10
8	Z	102	SPO	C13-C12-C14-C15
8	Z	102	SPO	C18-C17-C19-C20
8	b	101	SPO	C8-C7-C9-C10
8	b	101	SPO	C13-C12-C14-C15
7	T	101	BCL	O1D-CGD-O2D-CED
8	1	102	SPO	C22-C23-C25-C26
9	A	104	PC1	C1-C2-O21-C21
9	L	311	PC1	C1-C2-O21-C21
9	L	311	PC1	C3-C2-O21-C21
9	M	411	PC1	C1-C2-O21-C21
11	L	303	BPH	C4-C3-C5-C6
7	G	101	BCL	C1A-C2A-CAA-CBA
7	R	101	BCL	C1A-C2A-CAA-CBA
7	a	101	BCL	C1A-C2A-CAA-CBA
7	C	101	BCL	C6-C7-C8-C10
7	F	102	BCL	C11-C12-C13-C15
7	I	101	BCL	C11-C12-C13-C15
7	L	301	BCL	C6-C7-C8-C10
7	O	101	BCL	C11-C12-C13-C15
7	O	101	BCL	C12-C13-C15-C16
7	R	101	BCL	C6-C7-C8-C10
7	D	102	BCL	C3-C5-C6-C7
9	D	104	PC1	C32-C33-C34-C35
12	L	308	U10	C3-C4-O4-C4M
12	M	407	U10	C4-C3-O3-C3M
9	D	104	PC1	C34-C35-C36-C37
7	D	102	BCL	O1A-CGA-O2A-C1
7	K	101	BCL	C13-C15-C16-C17
10	M	409	CDL	C53-C54-C55-C56
8	M	408	SPO	C29-C28-C30-C31
11	L	310	BPH	C2-C3-C5-C6
12	M	407	U10	C5-C4-O4-C4M
8	D	103	SPO	C6-C7-C9-C10
8	J	103	SPO	C6-C7-C9-C10
8	S	202	SPO	C21-C22-C23-C25
8	Z	102	SPO	C6-C7-C9-C10
8	Z	102	SPO	C11-C12-C14-C15
8	Z	102	SPO	C16-C17-C19-C20
8	b	101	SPO	C6-C7-C9-C10

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Mol	Chain	Res	Type	Atoms
8	b	101	SPO	C11-C12-C14-C15
9	D	104	PC1	O21-C2-C3-O31
7	1	101	BCL	C2-C1-O2A-CGA
7	2	101	BCL	C2-C1-O2A-CGA
7	I	101	BCL	C2-C1-O2A-CGA
7	W	101	BCL	C2-C1-O2A-CGA
8	F	103	SPO	C27-C28-C30-C31
12	L	308	U10	C12-C11-C9-C10
7	D	102	BCL	C2A-CAA-CBA-CGA
9	A	103	PC1	O31-C31-C32-C33
9	M	401	PC1	C29-C2A-C2B-C2C
8	S	202	SPO	C12-C14-C15-C16
7	O	101	BCL	C4-C3-C5-C6
7	U	101	BCL	C4-C3-C5-C6
7	A	101	BCL	C4C-C3C-CAC-CBC
10	M	410	CDL	CA7-C31-C32-C33
7	P	101	BCL	C5-C6-C7-C8
10	H	301	CDL	OB5-CB3-CB4-OB6
9	A	102	PC1	C11-C12-N-C13
9	D	104	PC1	C11-C12-N-C14
8	F	103	SPO	C4-C1-O1-CM1
8	V	101	SPO	C28-C30-C31-C32
7	0	101	BCL	C2-C3-C5-C6
7	3	101	BCL	C11-C10-C8-C7
7	C	101	BCL	C12-C13-C15-C16
7	L	301	BCL	C11-C10-C8-C7
7	M	405	BCL	C12-C13-C15-C16
7	O	101	BCL	C2-C3-C5-C6
7	V	102	BCL	C11-C12-C13-C15
7	0	101	BCL	C1-C2-C3-C4
7	C	101	BCL	C1-C2-C3-C4
7	G	101	BCL	C1-C2-C3-C4
7	b	102	BCL	C1-C2-C3-C4
7	W	101	BCL	C5-C6-C7-C8
7	b	102	BCL	CAA-CBA-CGA-O2A
9	A	102	PC1	C28-C29-C2A-C2B
7	W	101	BCL	C16-C17-C18-C19
10	M	409	CDL	C52-C53-C54-C55
8	C	102	SPO	C29-C28-C30-C31
8	F	103	SPO	C34-C33-C35-C36
8	X	101	SPO	C29-C28-C30-C31
7	I	101	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
7	N	102	BCL	C14-C13-C15-C16
7	b	102	BCL	C11-C10-C8-C9
9	A	103	PC1	C23-C24-C25-C26
7	G	101	BCL	C3A-C2A-CAA-CBA
7	S	201	BCL	C3A-C2A-CAA-CBA
7	L	301	BCL	CAD-CBD-CGD-O2D
7	b	102	BCL	CAD-CBD-CGD-O2D
9	A	103	PC1	C1-C2-O21-C21
9	M	402	PC1	C3-C2-O21-C21
9	M	411	PC1	C3-C2-O21-C21
11	L	310	BPH	CAD-CBD-CGD-O2D
7	T	101	BCL	C16-C17-C18-C20
8	1	102	SPO	C25-C26-C27-C28
7	7	101	BCL	C2B-C3B-CAB-OBB
10	M	409	CDL	C82-C83-C84-C85
8	J	102	SPO	C34-C33-C35-C36
12	M	407	U10	C35-C34-C36-C37
12	X	102	U10	C25-C24-C26-C27
12	M	407	U10	C33-C34-C36-C37
7	N	102	BCL	CAA-CBA-CGA-O2A
12	L	307	U10	C2-C3-O3-C3M
10	H	301	CDL	CB3-CB4-CB6-OB8
10	H	301	CDL	OA5-CA3-CA4-OA6
9	A	102	PC1	O21-C21-C22-C23
9	M	401	PC1	O21-C21-C22-C23
9	M	401	PC1	C11-C12-N-C15
9	M	402	PC1	C11-C12-N-C14
7	G	101	BCL	O2A-C1-C2-C3
7	M	404	BCL	O2A-C1-C2-C3
7	R	101	BCL	CAA-CBA-CGA-O2A
7	D	102	BCL	CHA-CBD-CGD-O2D
7	F	102	BCL	CHA-CBD-CGD-O1D
7	F	102	BCL	CHA-CBD-CGD-O2D
7	S	201	BCL	CHA-CBD-CGD-O2D
7	U	101	BCL	C2-C3-C5-C6
12	X	102	U10	C23-C24-C26-C27
8	S	202	SPO	C3-C1-O1-CM1
9	L	304	PC1	O21-C2-C3-O31
7	V	102	BCL	CAA-CBA-CGA-O2A
7	G	101	BCL	C2A-CAA-CBA-CGA
8	1	102	SPO	C2-C1-C4-C5
8	I	102	SPO	C2-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
8	U	103	SPO	C2-C1-C4-C5
8	V	101	SPO	C3-C1-C4-C5
10	M	409	CDL	C18-C19-C20-C21
8	F	103	SPO	C32-C33-C35-C36
7	C	101	BCL	C6-C7-C8-C9
7	S	201	BCL	C6-C7-C8-C9
7	b	102	BCL	CAA-CBA-CGA-O1A
12	L	305	U10	C3-C4-O4-C4M
10	M	409	CDL	C19-C20-C21-C22
10	H	301	CDL	C31-C32-C33-C34
7	3	101	BCL	C2A-CAA-CBA-CGA
7	Q	101	BCL	C2A-CAA-CBA-CGA
7	0	101	BCL	C1A-C2A-CAA-CBA
7	C	101	BCL	C1A-C2A-CAA-CBA
7	F	102	BCL	C1A-C2A-CAA-CBA
7	S	201	BCL	C1A-C2A-CAA-CBA
7	V	102	BCL	C1A-C2A-CAA-CBA
9	A	102	PC1	O22-C21-C22-C23
8	O	104	SPO	C35-C36-C37-C38
7	R	101	BCL	CAA-CBA-CGA-O1A
9	M	401	PC1	O22-C21-C22-C23
9	D	104	PC1	C1-C2-C3-O31
10	M	410	CDL	C31-C32-C33-C34
7	J	101	BCL	C2A-CAA-CBA-CGA
9	L	306	PC1	C1-O11-P-O13
9	L	304	PC1	C27-C28-C29-C2A
7	8	101	BCL	C10-C11-C12-C13
7	0	101	BCL	C4-C3-C5-C6
10	M	409	CDL	C72-C71-CB7-OB8
7	2	101	BCL	C10-C11-C12-C13
9	L	306	PC1	C1-O11-P-O12
9	M	411	PC1	C2C-C2D-C2E-C2F
7	V	102	BCL	CAA-CBA-CGA-O1A
7	N	102	BCL	CAA-CBA-CGA-O1A
7	G	101	BCL	CAA-CBA-CGA-O2A
12	L	307	U10	C35-C34-C36-C37
8	2	102	SPO	C35-C36-C37-C38
7	D	102	BCL	CAD-CBD-CGD-O1D
7	T	101	BCL	CAD-CBD-CGD-O1D
9	A	102	PC1	C12-C11-O13-P
9	A	103	PC1	C3-C2-O21-C21
9	A	104	PC1	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
9	M	402	PC1	C1-C2-O21-C21
10	H	301	CDL	CB3-CB4-OB6-CB5
7	9	101	BCL	C11-C12-C13-C14
7	E	101	BCL	C14-C13-C15-C16
7	L	301	BCL	C6-C7-C8-C9
10	M	409	CDL	C36-C37-C38-C39
9	A	104	PC1	C11-C12-N-C14
7	G	101	BCL	C16-C17-C18-C19
9	A	104	PC1	O21-C21-C22-C23
8	G	102	SPO	C1-C4-C5-C6
7	J	101	BCL	C8-C10-C11-C12
9	A	102	PC1	O31-C31-C32-C33
9	M	411	PC1	O31-C31-C32-C33
10	H	301	CDL	C72-C71-CB7-OB8
7	U	101	BCL	C8-C10-C11-C12
7	2	101	BCL	C2C-C3C-CAC-CBC
7	B	101	BCL	C2C-C3C-CAC-CBC
7	K	101	BCL	C6-C7-C8-C10
7	P	101	BCL	C6-C7-C8-C10
7	V	102	BCL	C12-C13-C15-C16
12	M	403	U10	C12-C11-C9-C8
8	9	102	SPO	C15-C16-C17-C19
10	H	301	CDL	C72-C71-CB7-OB9
9	A	102	PC1	O32-C31-C32-C33
10	M	409	CDL	C72-C71-CB7-OB9
12	M	403	U10	C29-C31-C32-C33
9	O	103	PC1	O21-C21-C22-C23
9	A	102	PC1	C11-C12-N-C14
7	C	101	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

84 monomers are involved in 592 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	9	101	BCL	10	0
8	U	103	SPO	8	0
8	X	101	SPO	5	0
7	L	301	BCL	7	0
7	U	101	BCL	10	0
11	L	303	BPH	4	0
8	M	408	SPO	4	0
12	M	407	U10	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	103	SPO	2	0
12	L	309	U10	5	0
9	A	103	PC1	1	0
8	b	101	SPO	15	0
7	P	101	BCL	5	0
7	B	101	BCL	7	0
8	V	101	SPO	10	0
8	0	102	SPO	4	0
8	O	102	SPO	5	0
8	D	103	SPO	12	0
8	P	102	SPO	7	0
7	0	101	BCL	7	0
7	K	101	BCL	5	0
9	M	401	PC1	4	0
9	A	104	PC1	7	0
8	Z	102	SPO	8	0
7	T	101	BCL	7	0
9	M	411	PC1	5	0
7	L	302	BCL	6	0
8	T	102	SPO	7	0
7	I	101	BCL	14	0
8	9	102	SPO	5	0
8	U	102	SPO	5	0
7	7	101	BCL	5	0
8	S	202	SPO	17	0
8	I	102	SPO	12	0
7	a	101	BCL	19	0
9	L	311	PC1	2	0
12	L	307	U10	4	0
7	M	404	BCL	13	0
7	8	101	BCL	5	0
7	1	101	BCL	27	0
7	N	102	BCL	16	0
8	0	103	SPO	9	0
9	A	102	PC1	14	0
7	3	101	BCL	13	0
7	S	201	BCL	14	0
9	D	104	PC1	3	0
7	J	101	BCL	19	0
9	L	304	PC1	2	0
7	Z	101	BCL	18	0
12	L	308	U10	4	0

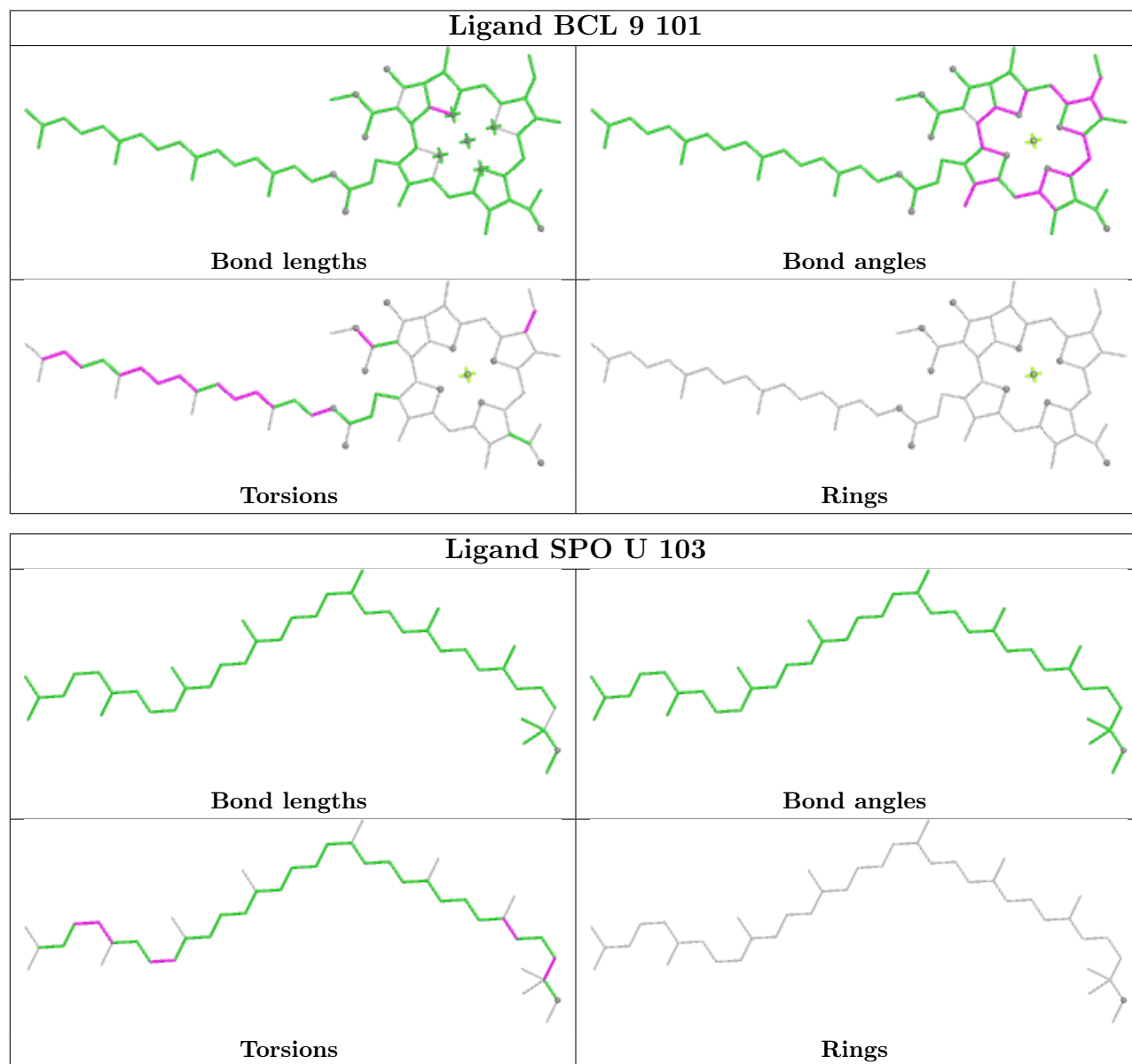
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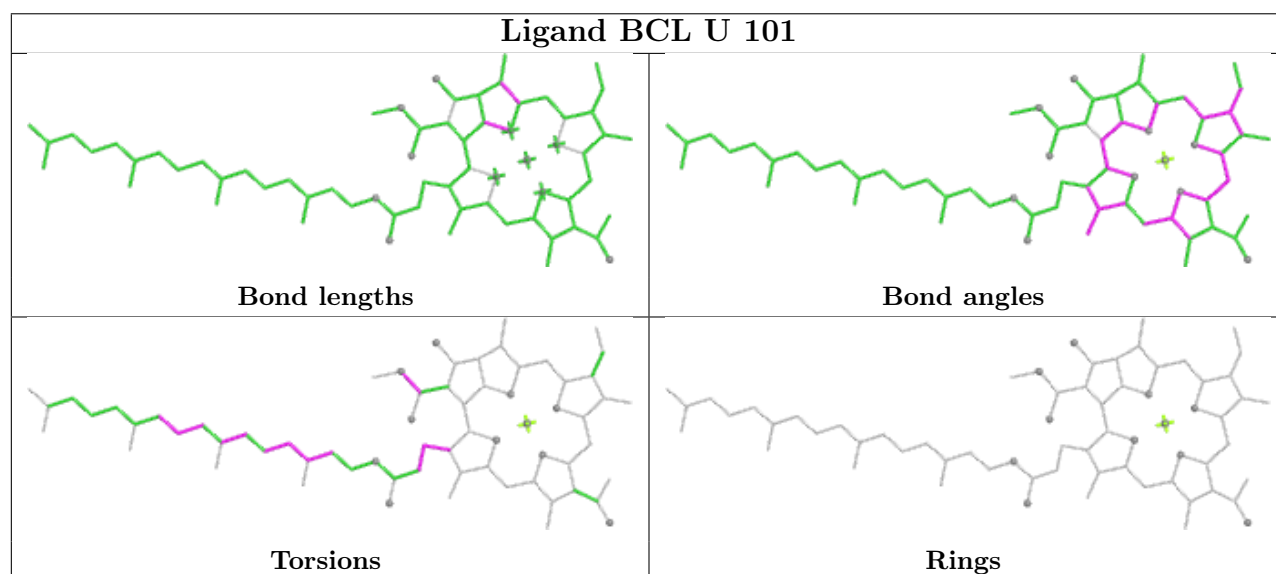
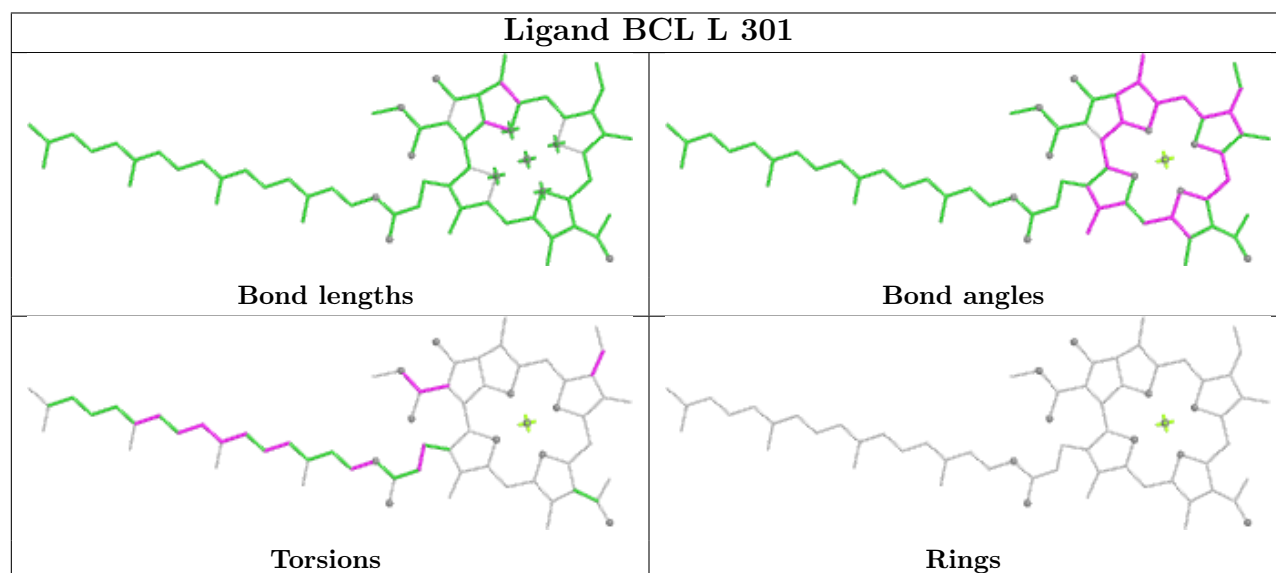
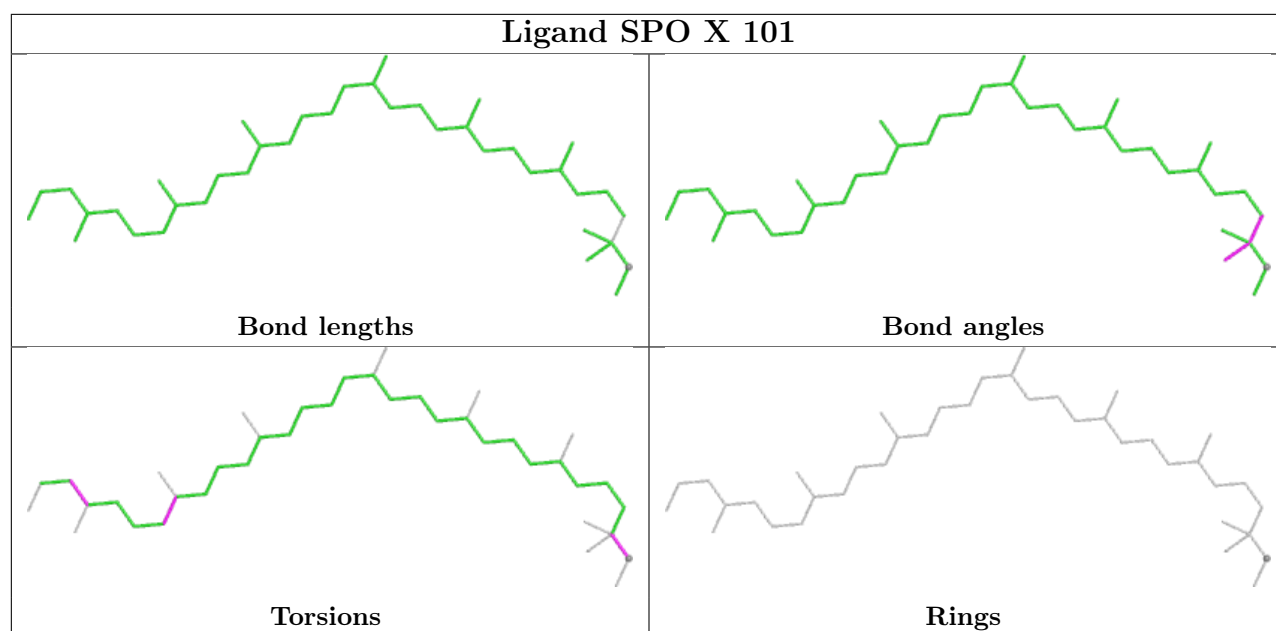
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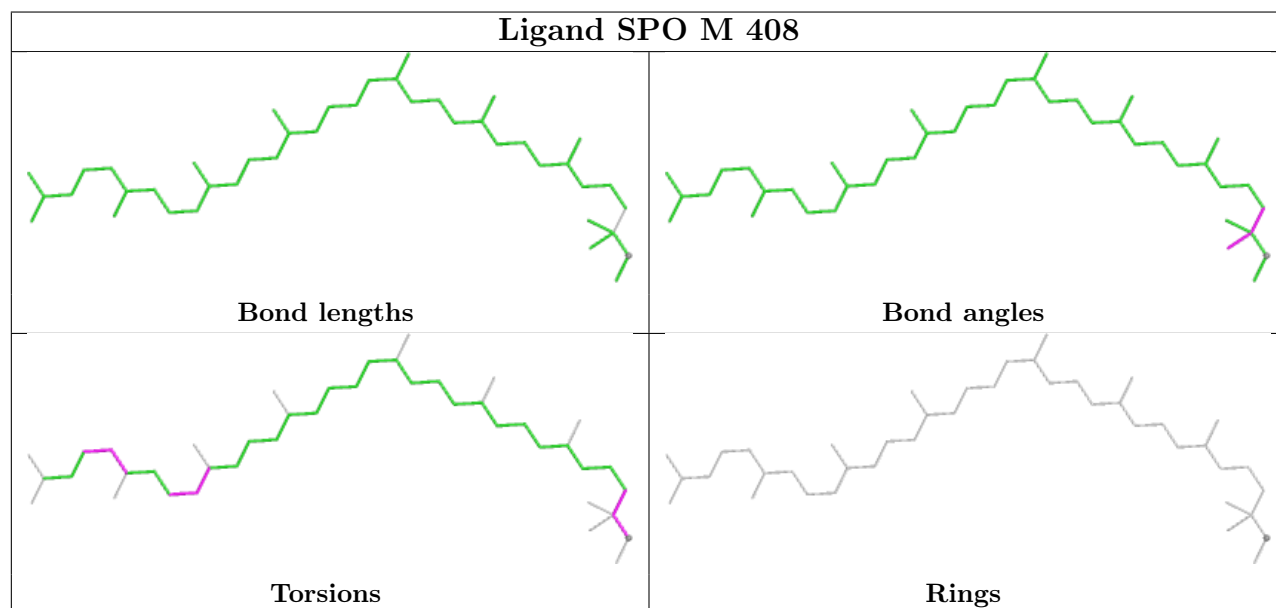
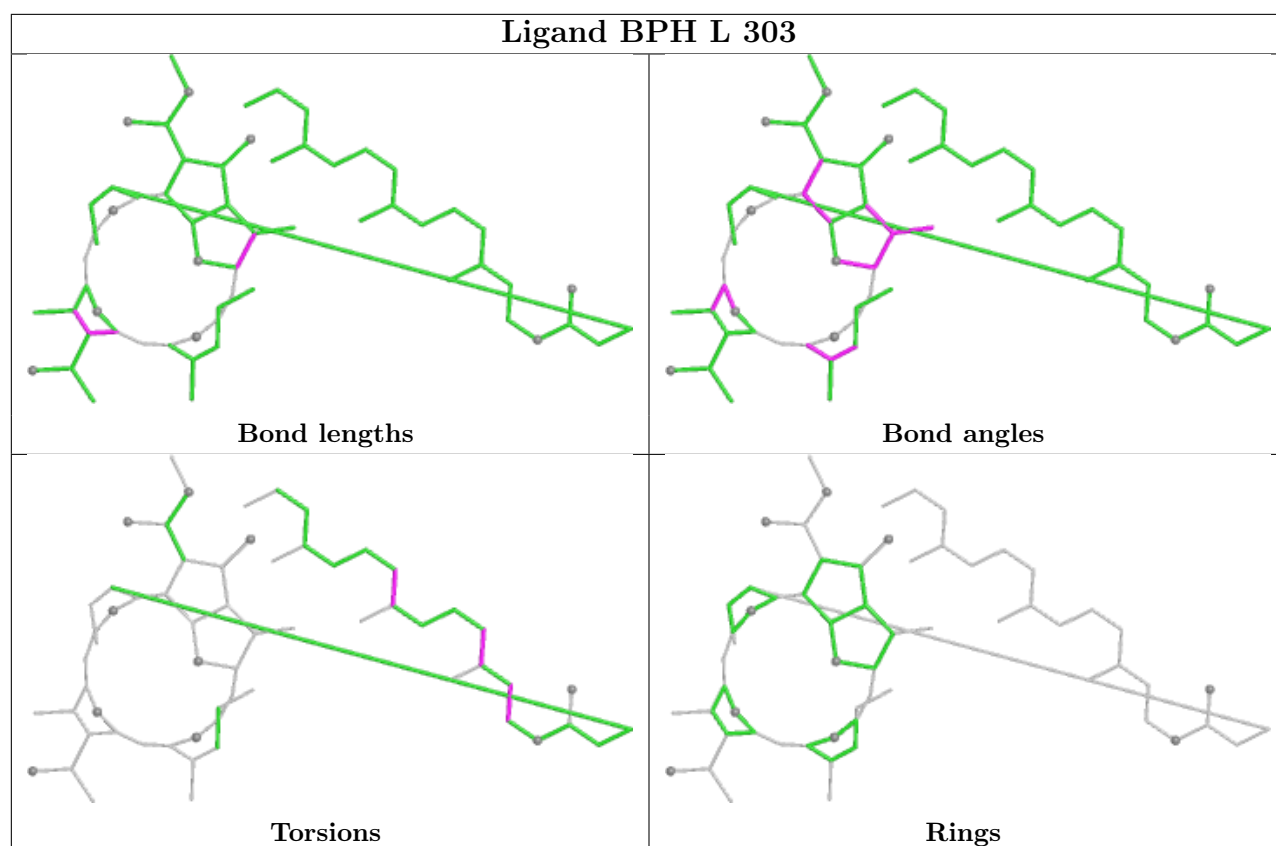
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	O	104	SPO	9	0
8	C	102	SPO	8	0
8	2	102	SPO	12	0
7	G	101	BCL	11	0
7	V	102	BCL	6	0
10	M	410	CDL	1	0
8	P	103	SPO	6	0
7	C	101	BCL	8	0
8	1	102	SPO	16	0
12	M	403	U10	1	0
10	M	409	CDL	2	0
8	G	102	SPO	6	0
7	W	101	BCL	9	0
12	X	102	U10	10	0
8	F	101	SPO	2	0
9	M	402	PC1	1	0
8	N	101	SPO	5	0
7	D	102	BCL	5	0
8	3	102	SPO	19	0
7	O	101	BCL	10	0
7	R	101	BCL	8	0
11	L	310	BPH	4	0
7	Q	101	BCL	8	0
7	2	101	BCL	11	0
8	J	102	SPO	19	0
7	M	405	BCL	6	0
12	L	305	U10	6	0
7	F	102	BCL	6	0
7	E	101	BCL	20	0
10	H	301	CDL	21	0
7	A	101	BCL	5	0
8	D	101	SPO	2	0
7	b	102	BCL	7	0
8	J	103	SPO	20	0

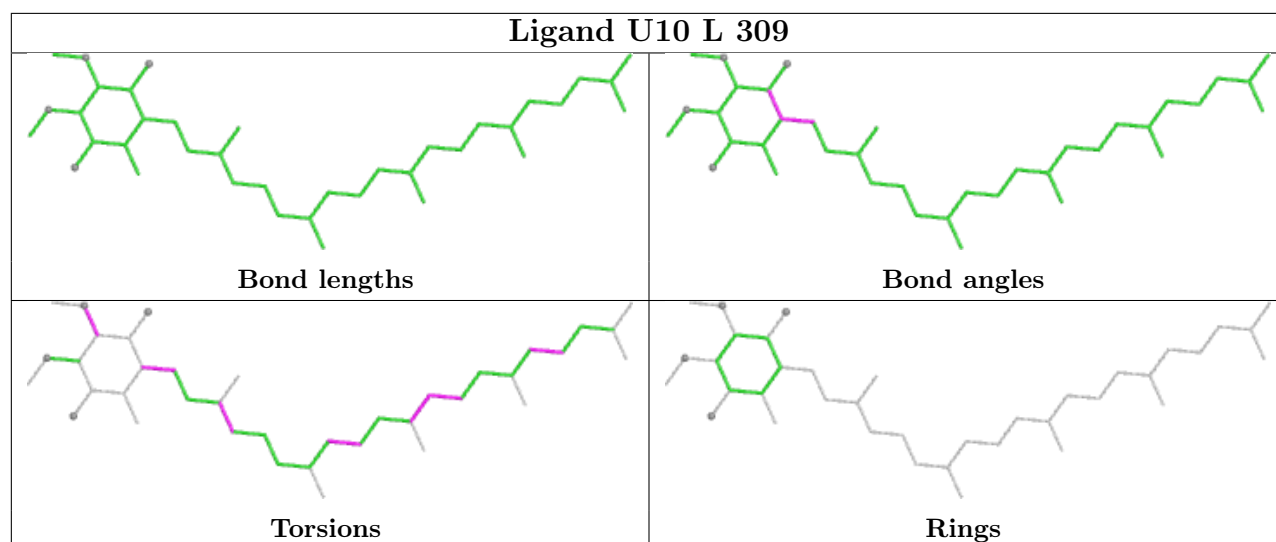
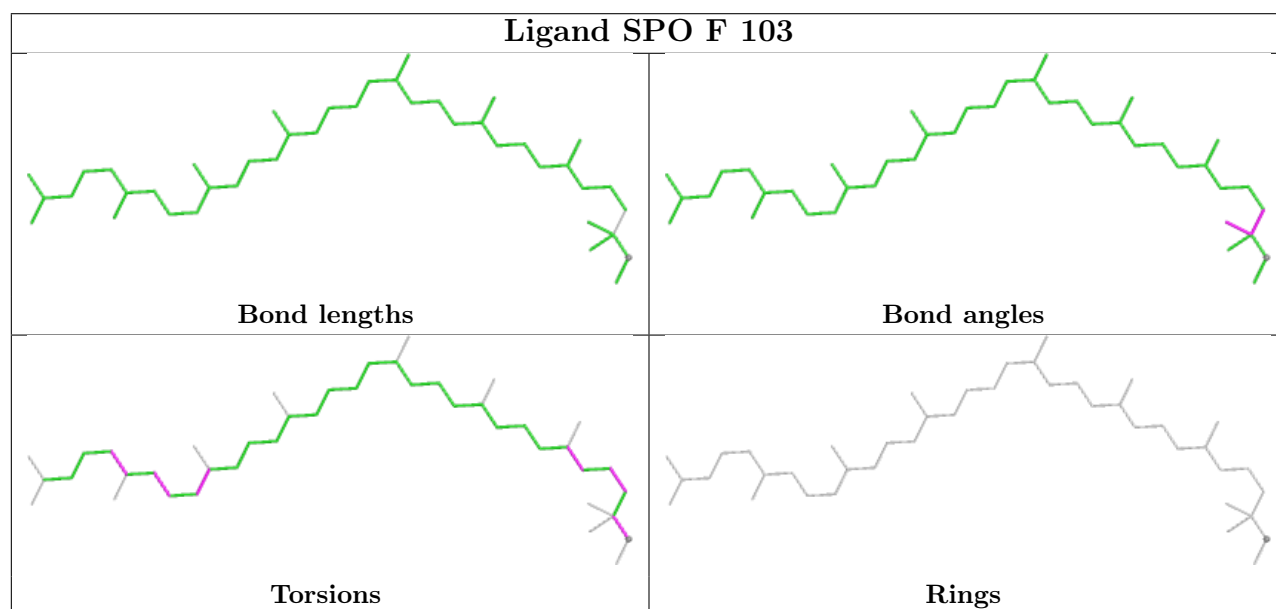
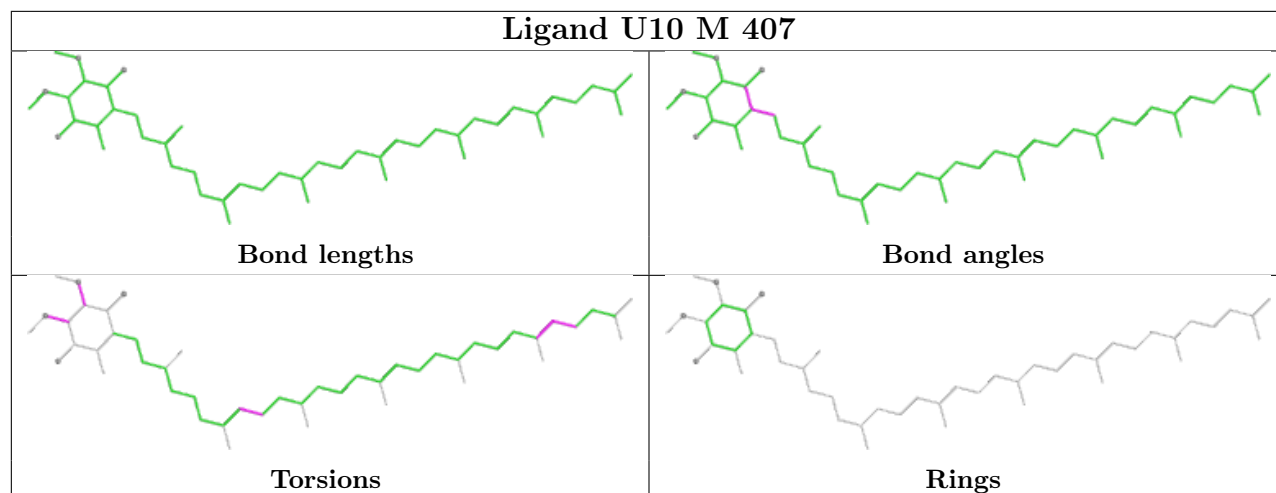
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

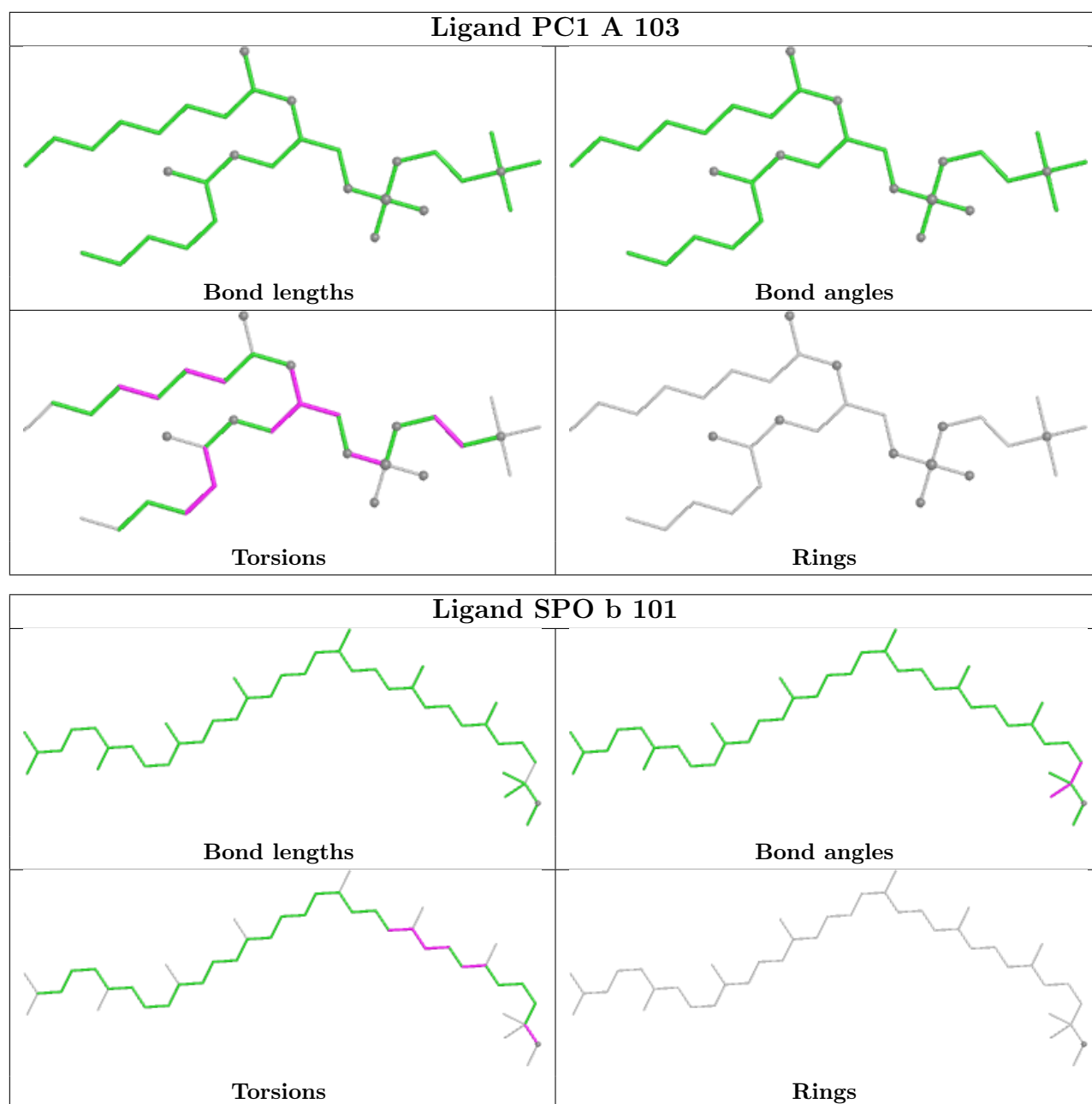
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

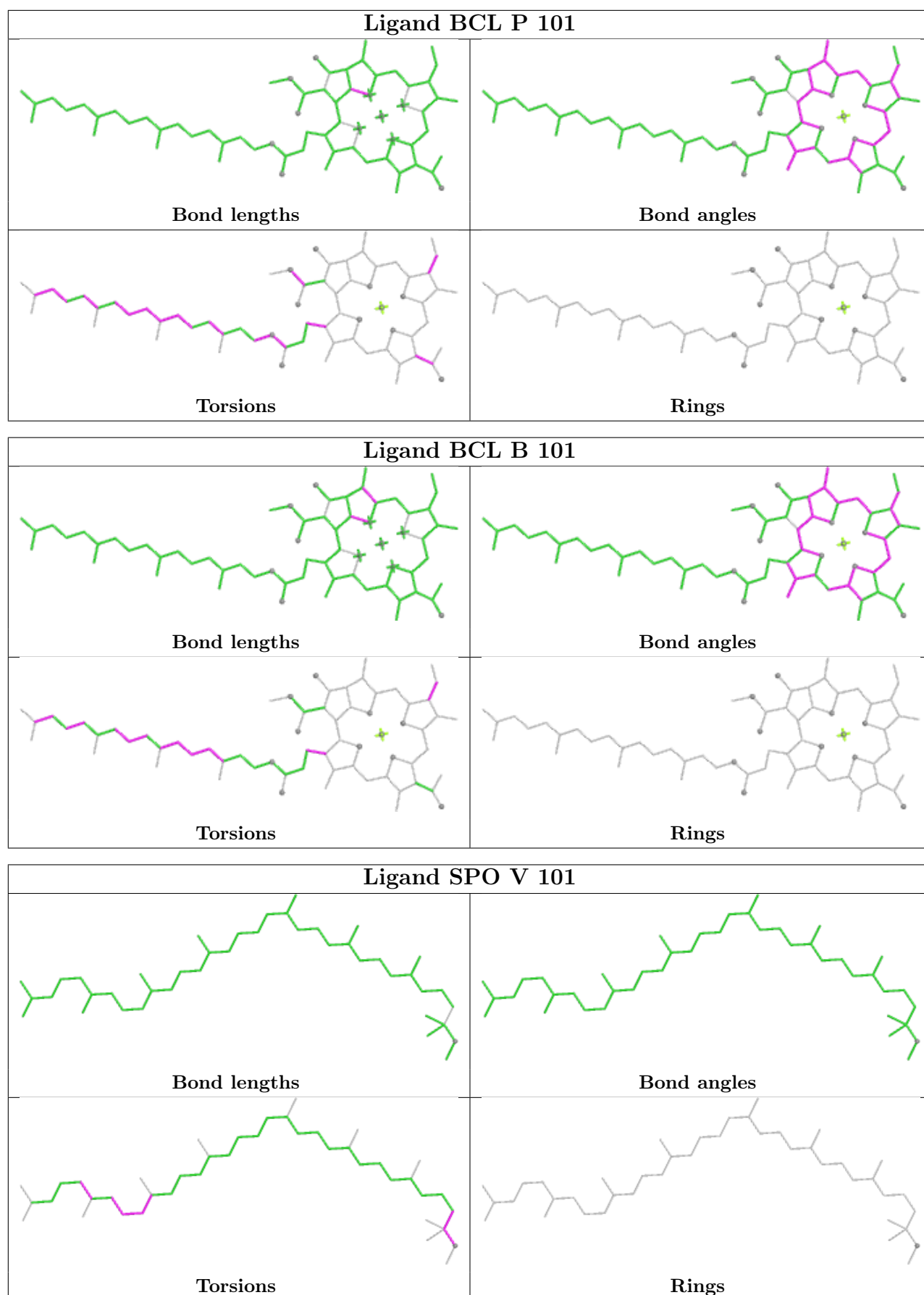


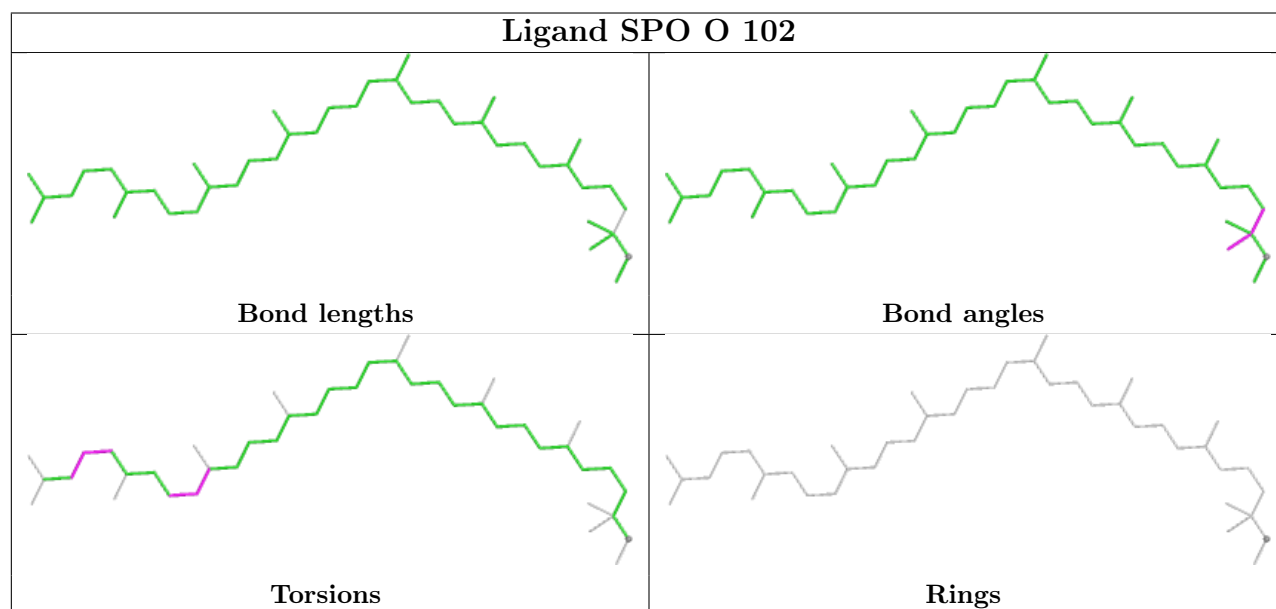
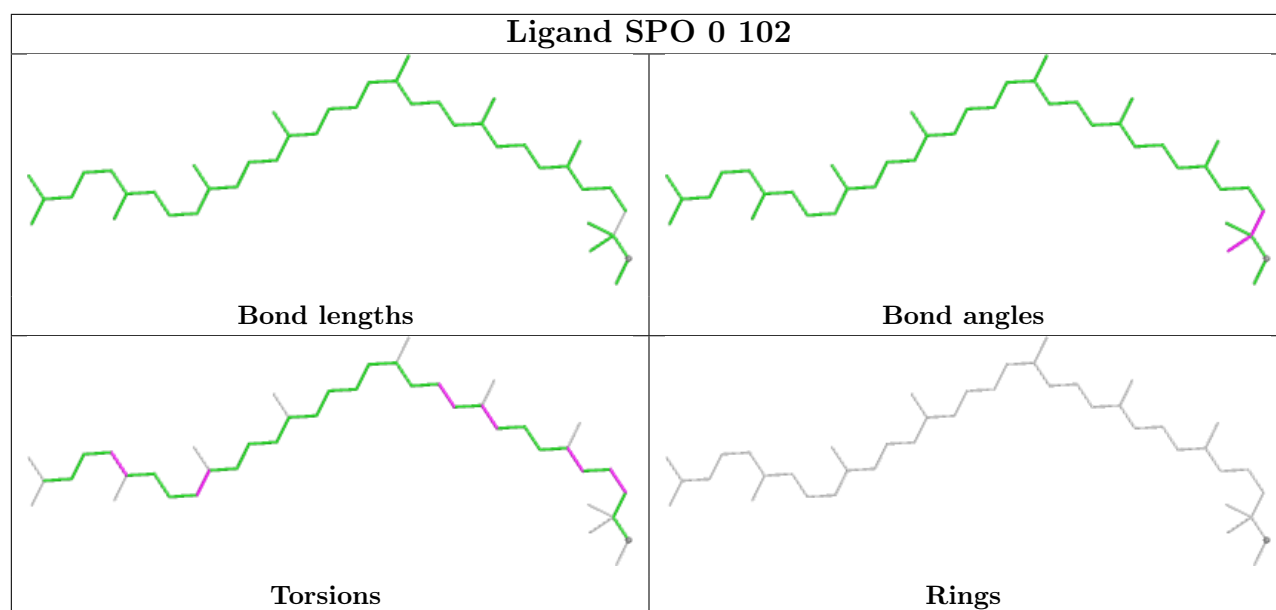


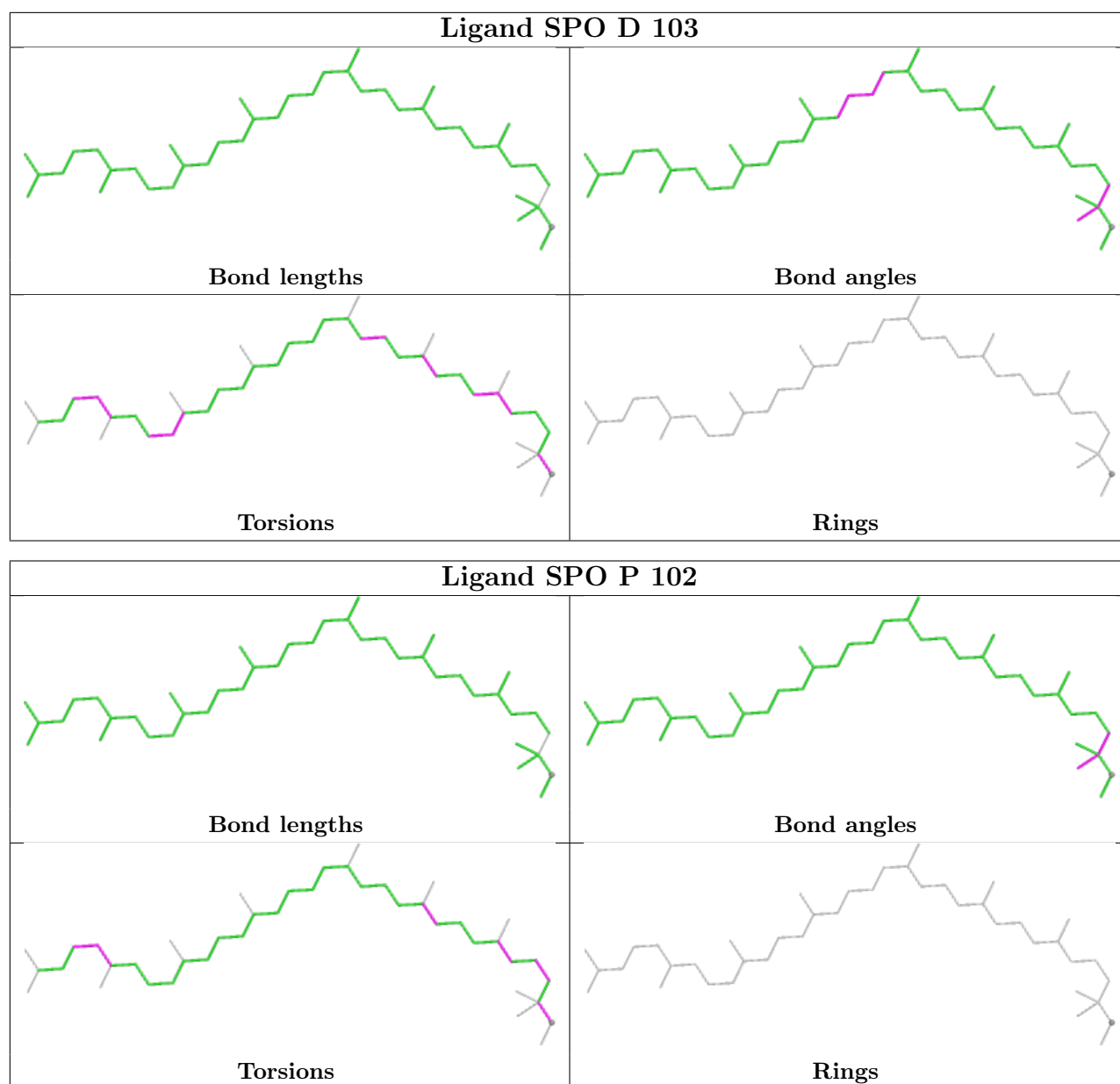


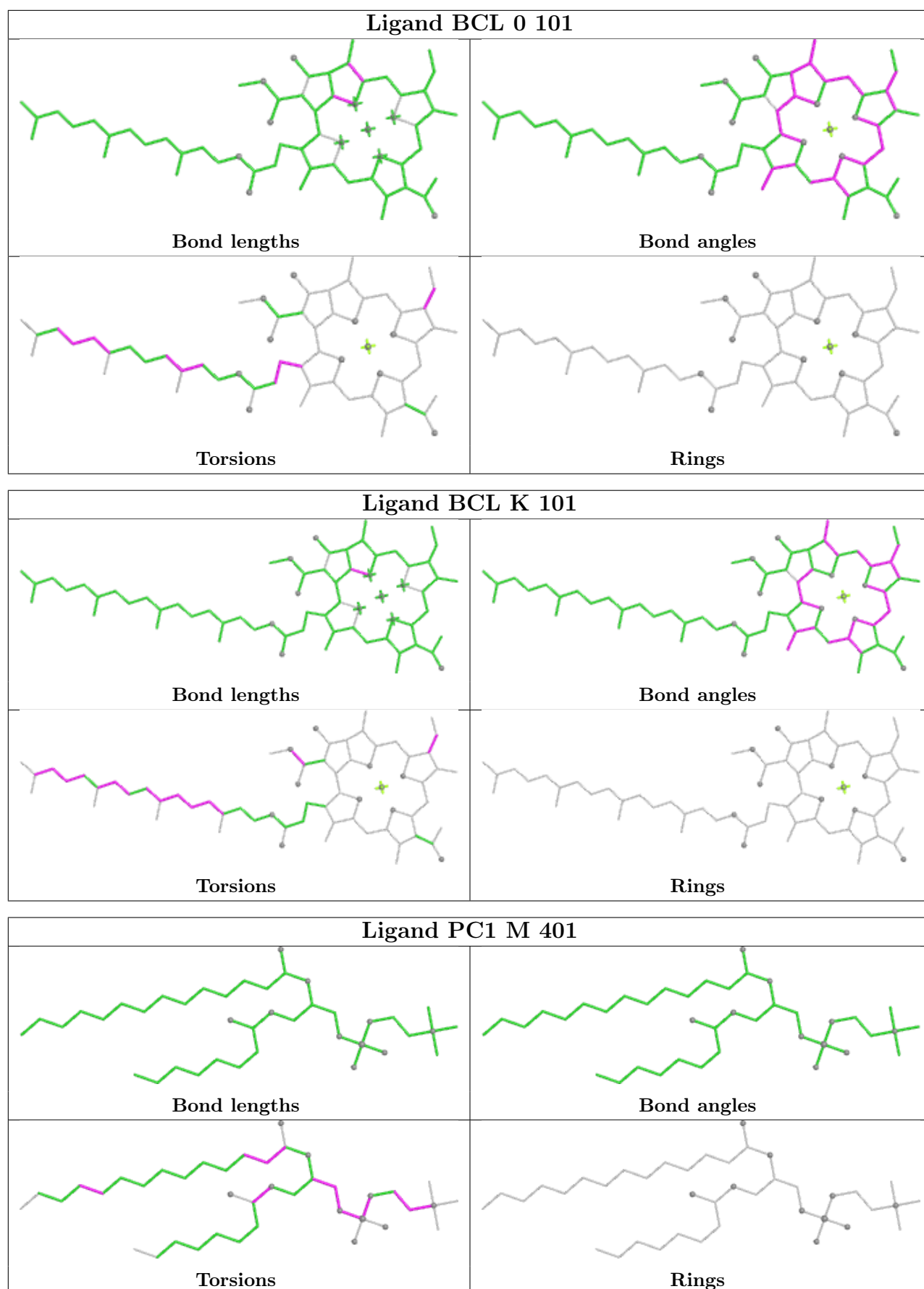




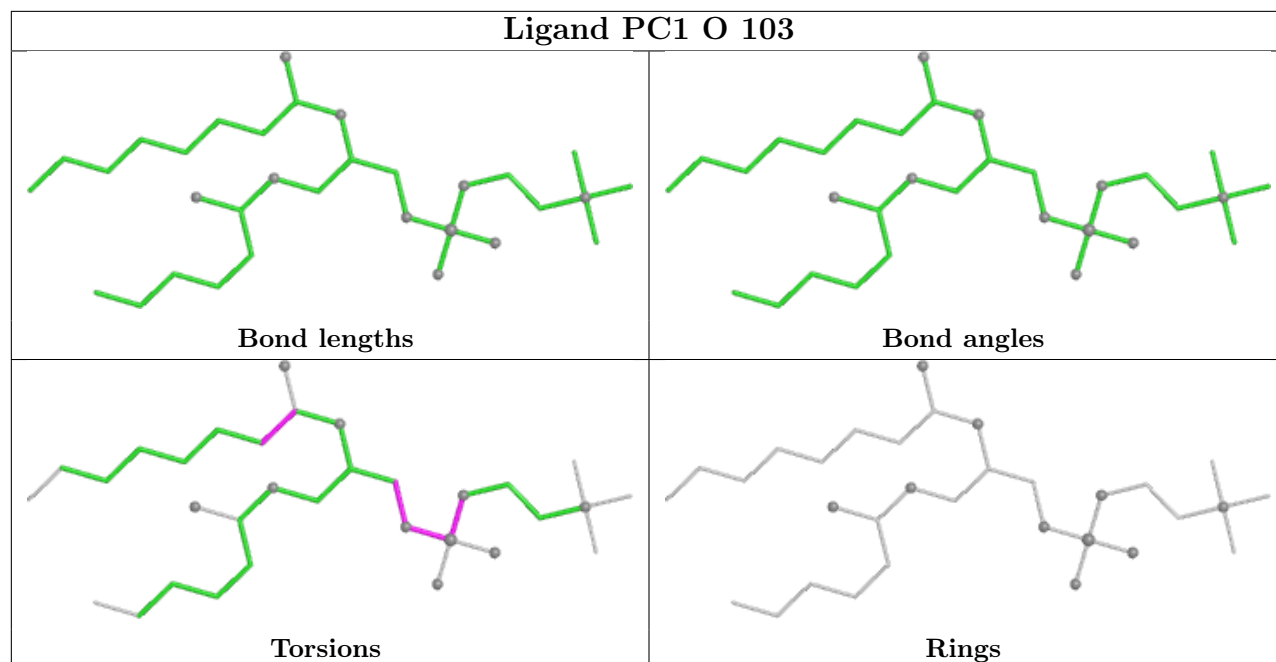




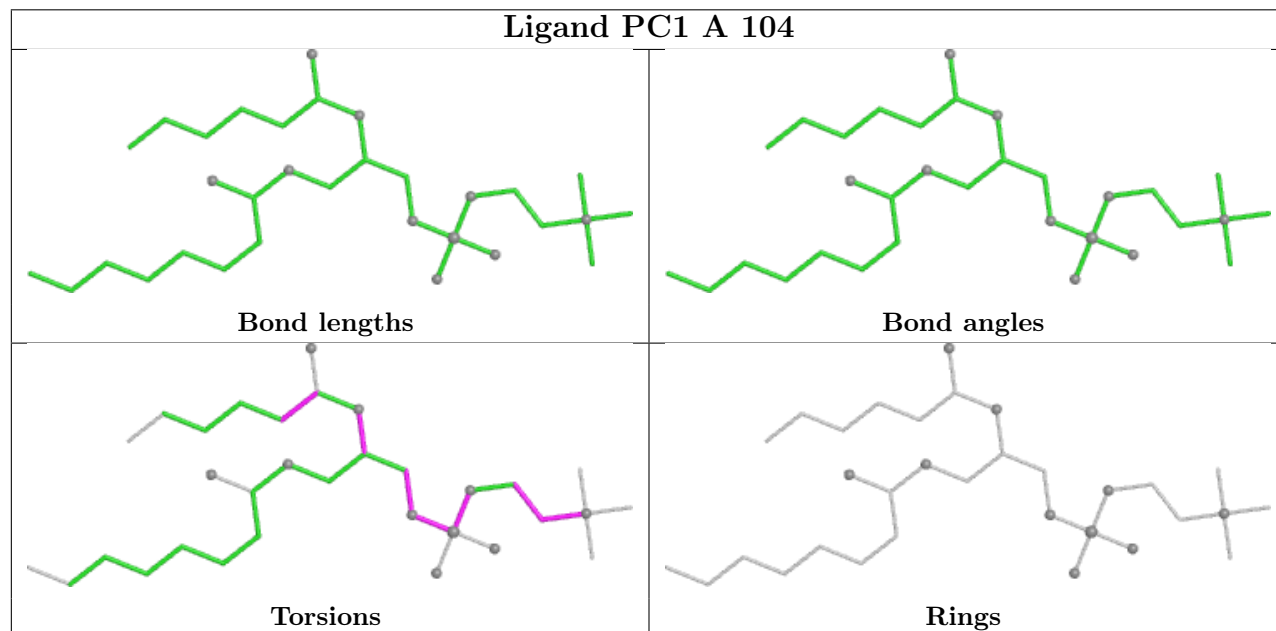


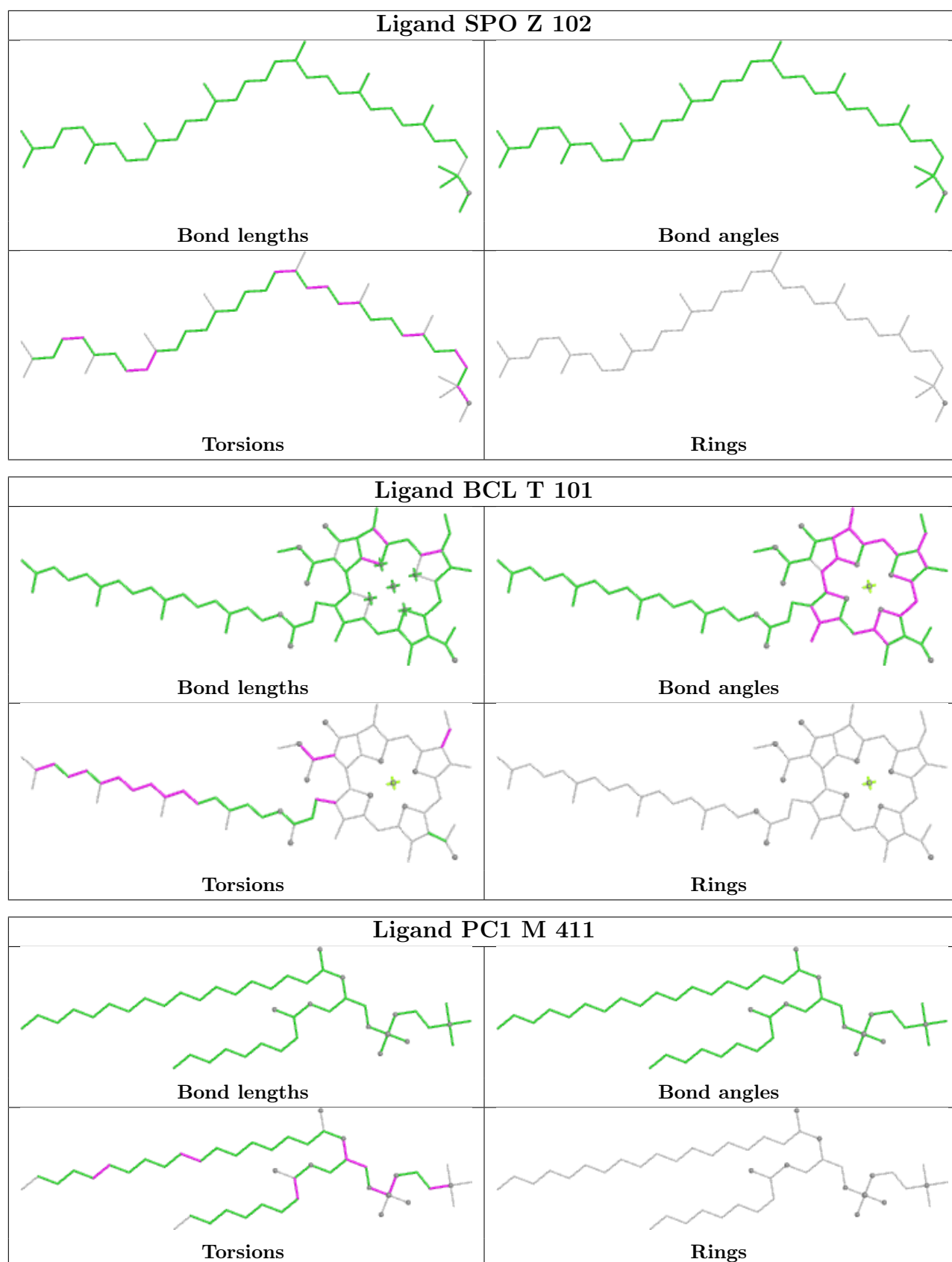


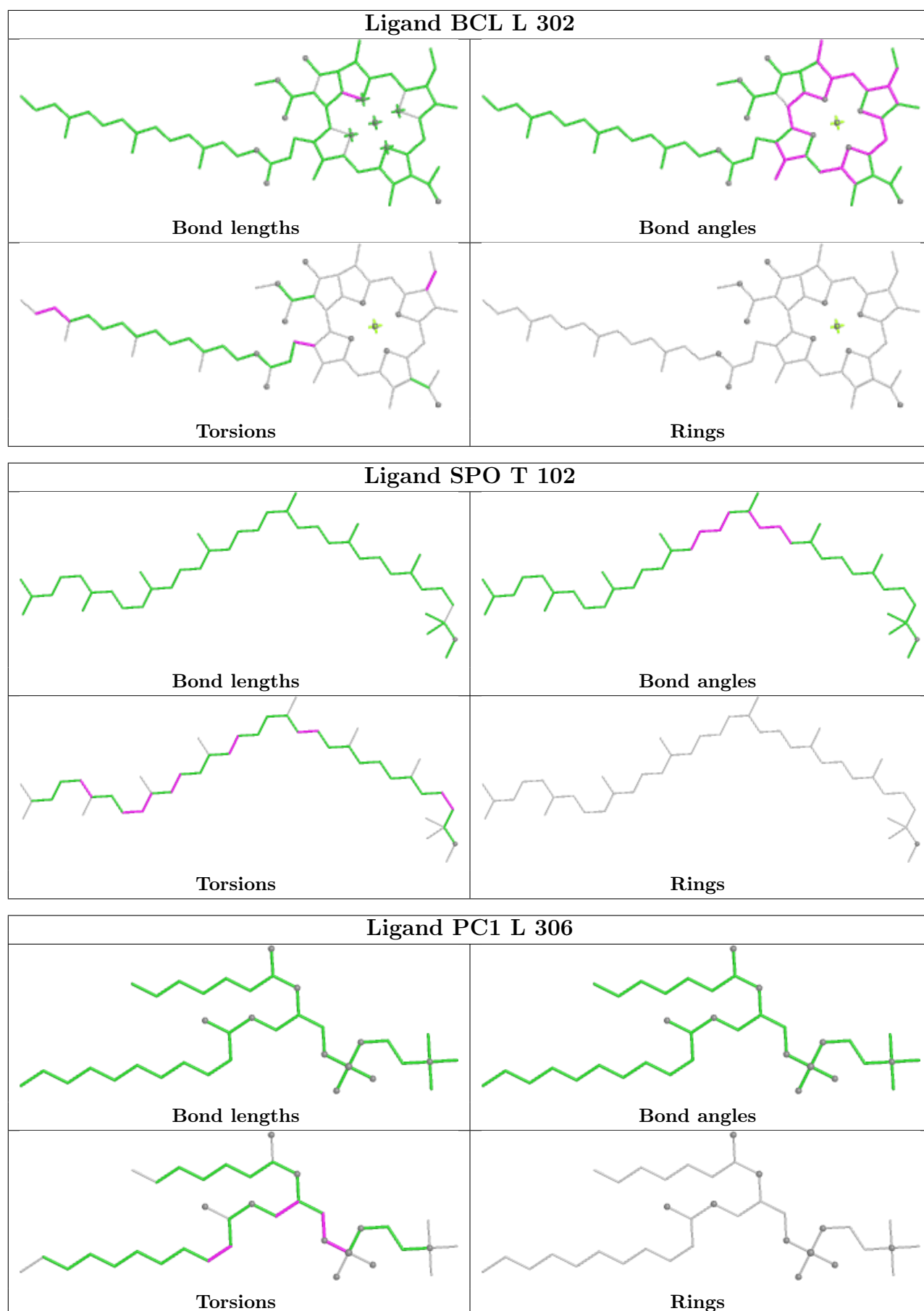
Ligand PC1 O 103

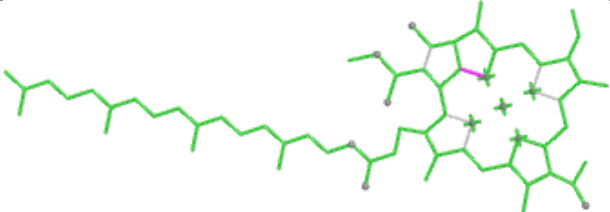
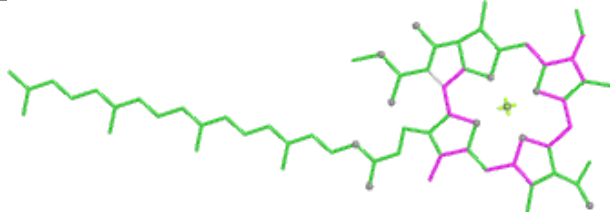
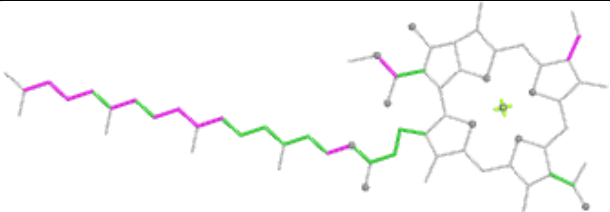
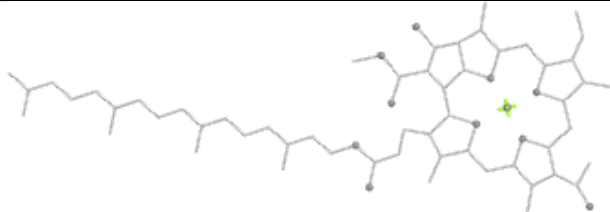
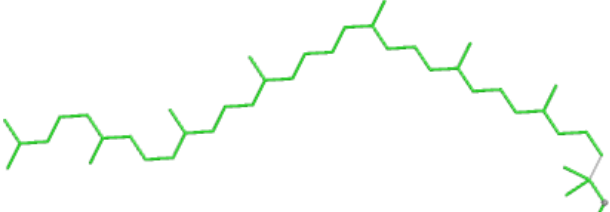
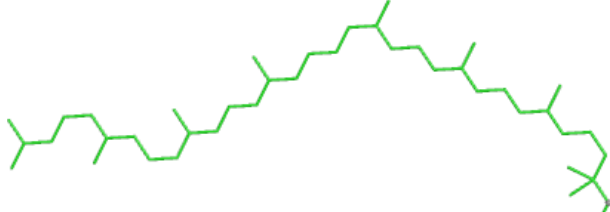
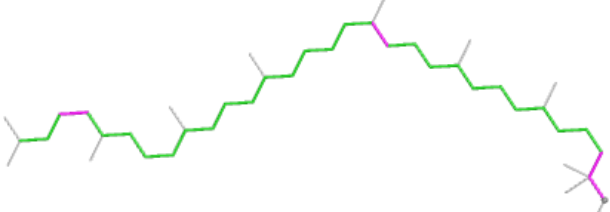
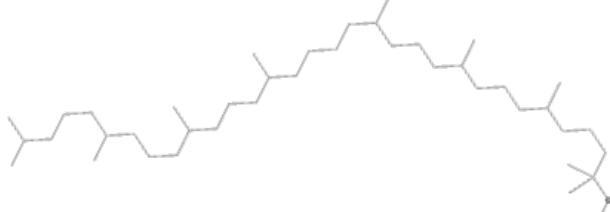


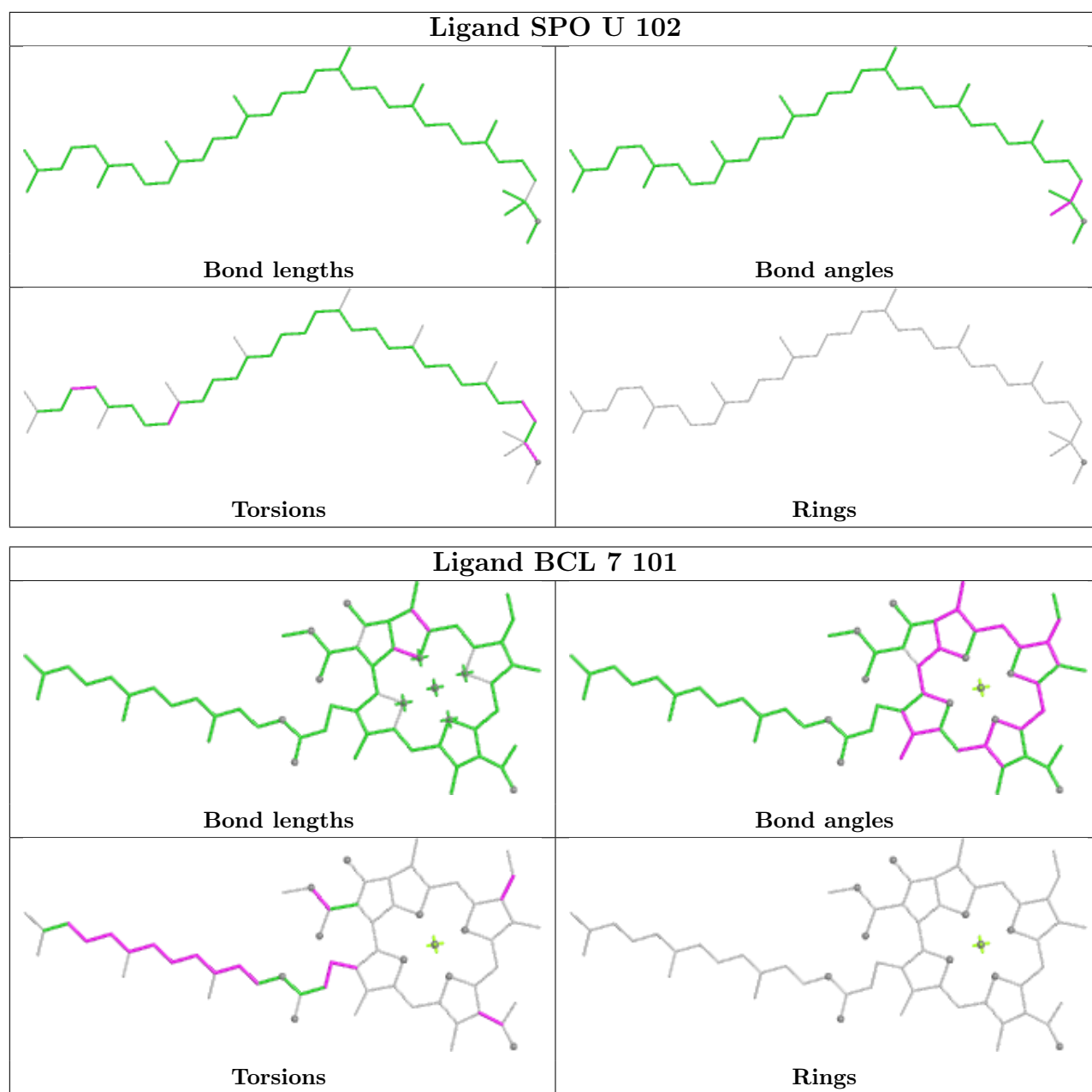
Ligand PC1 A 104

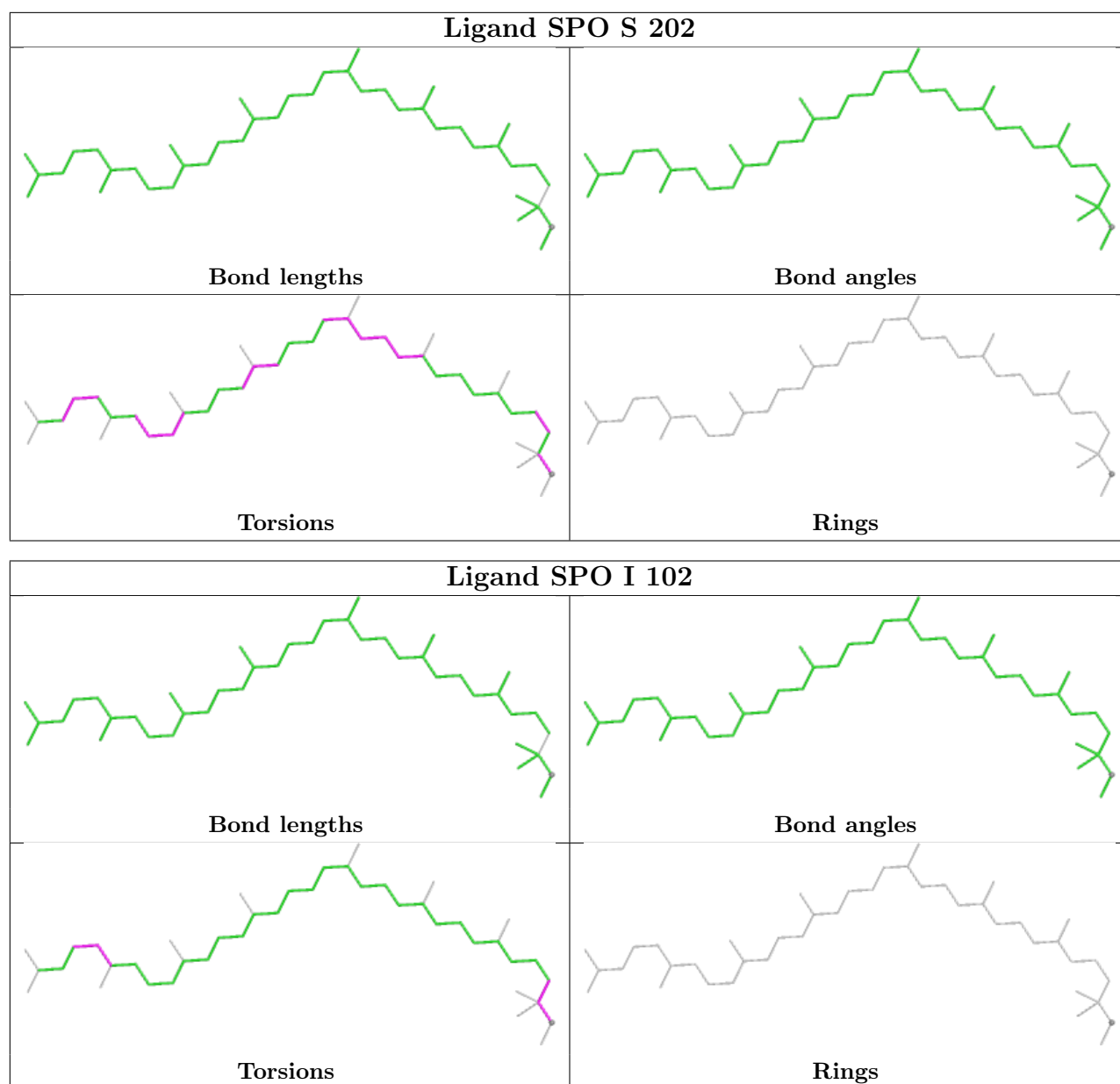


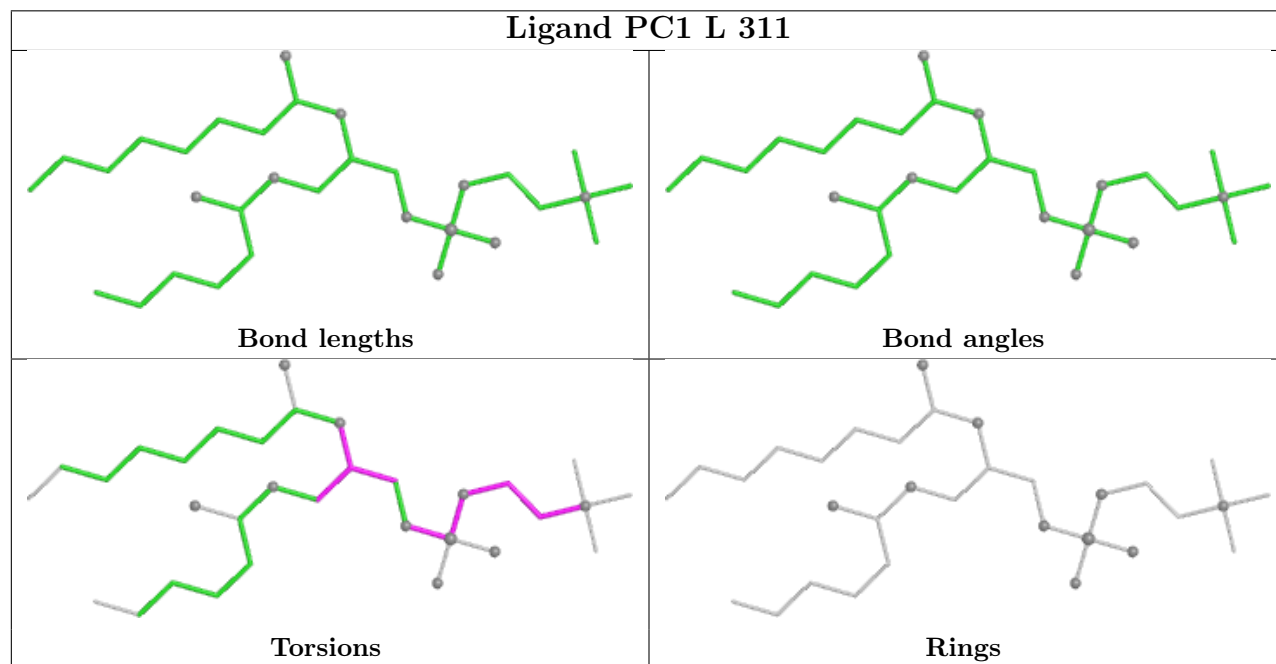
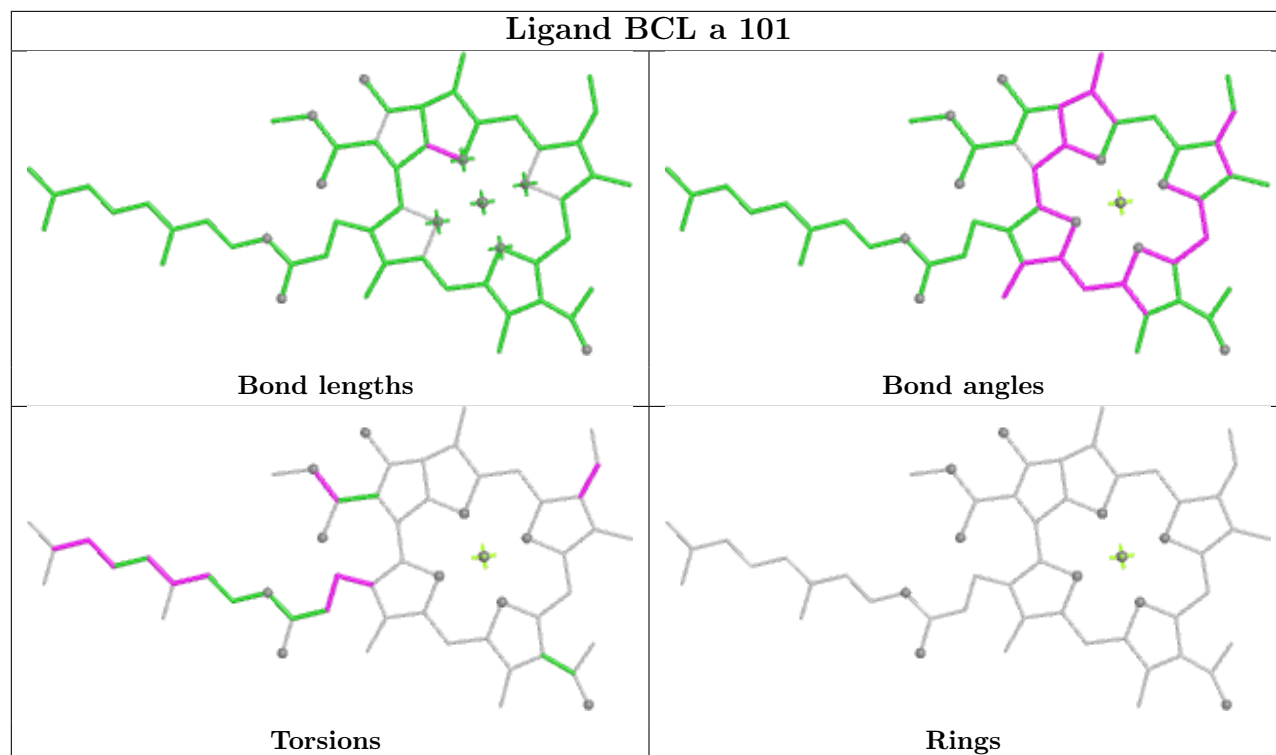


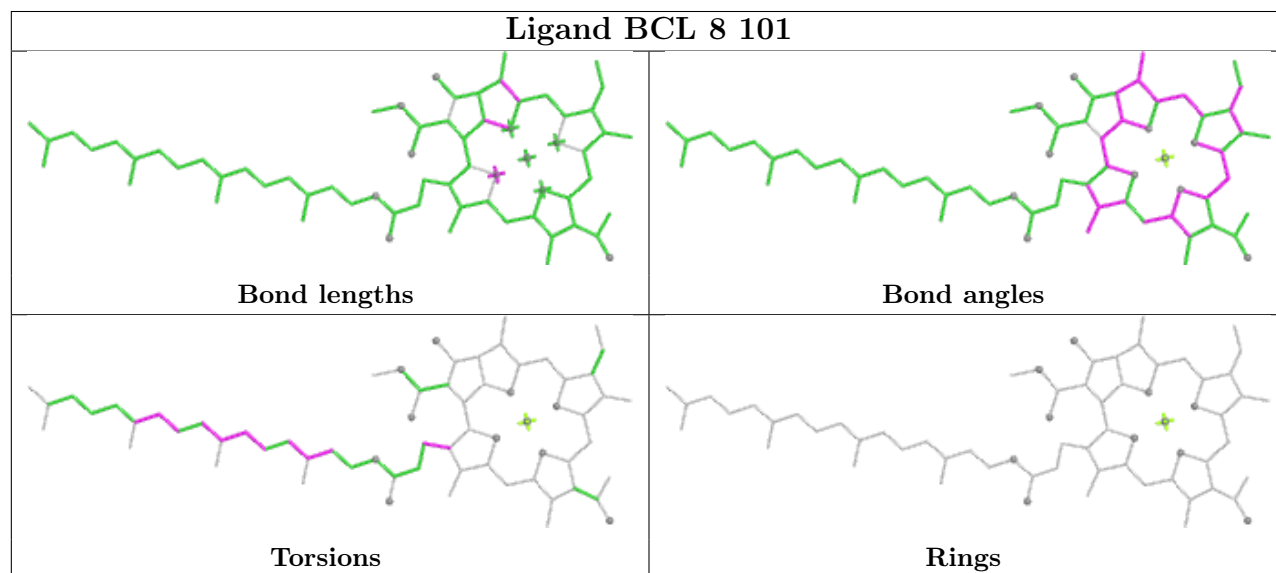
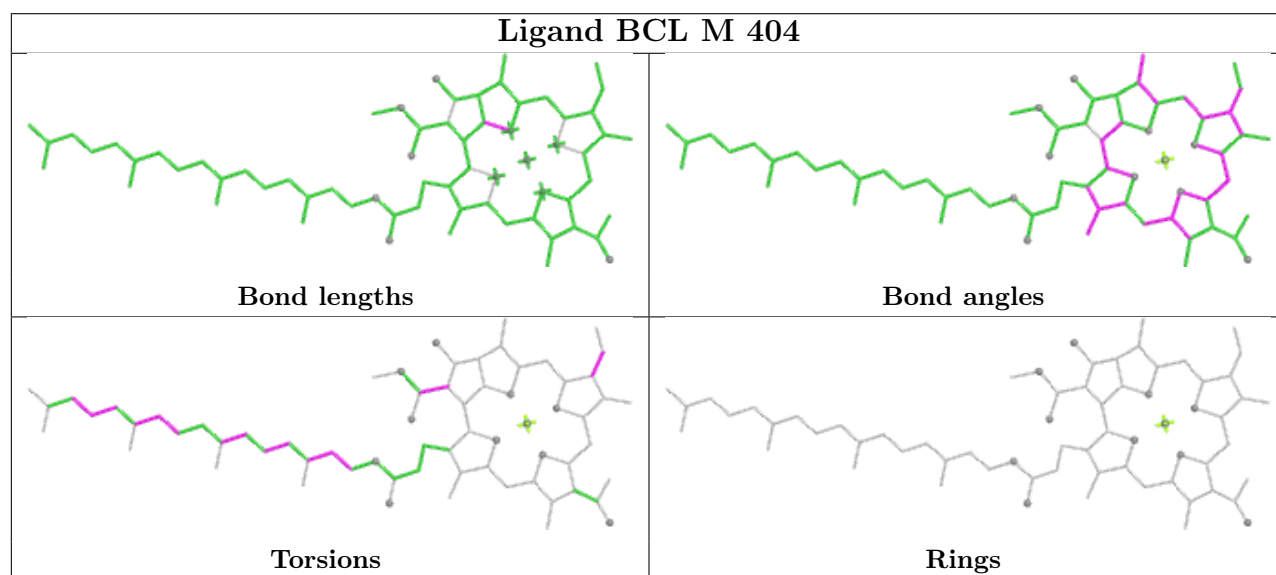
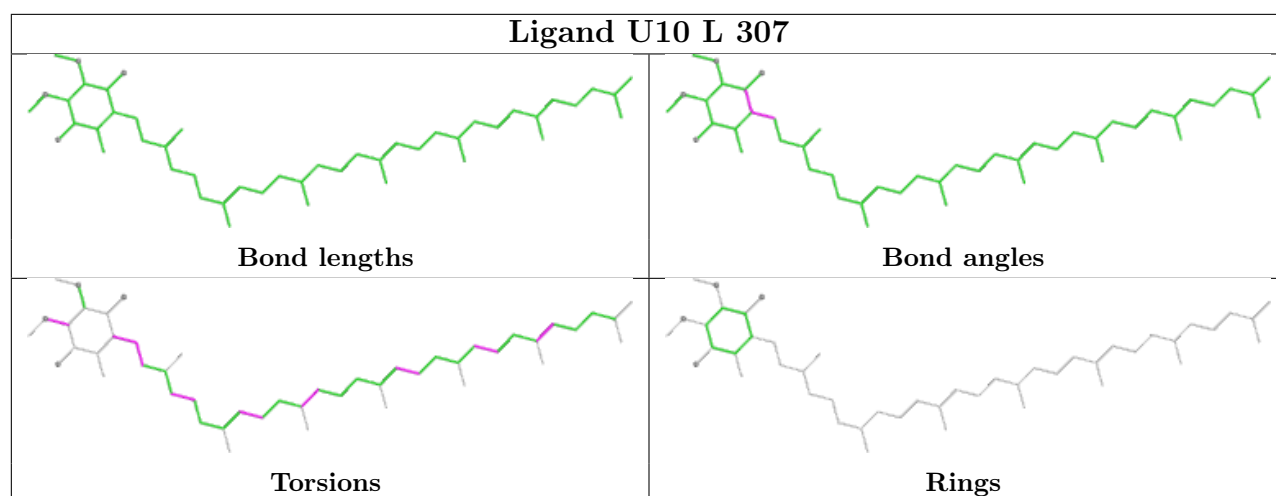


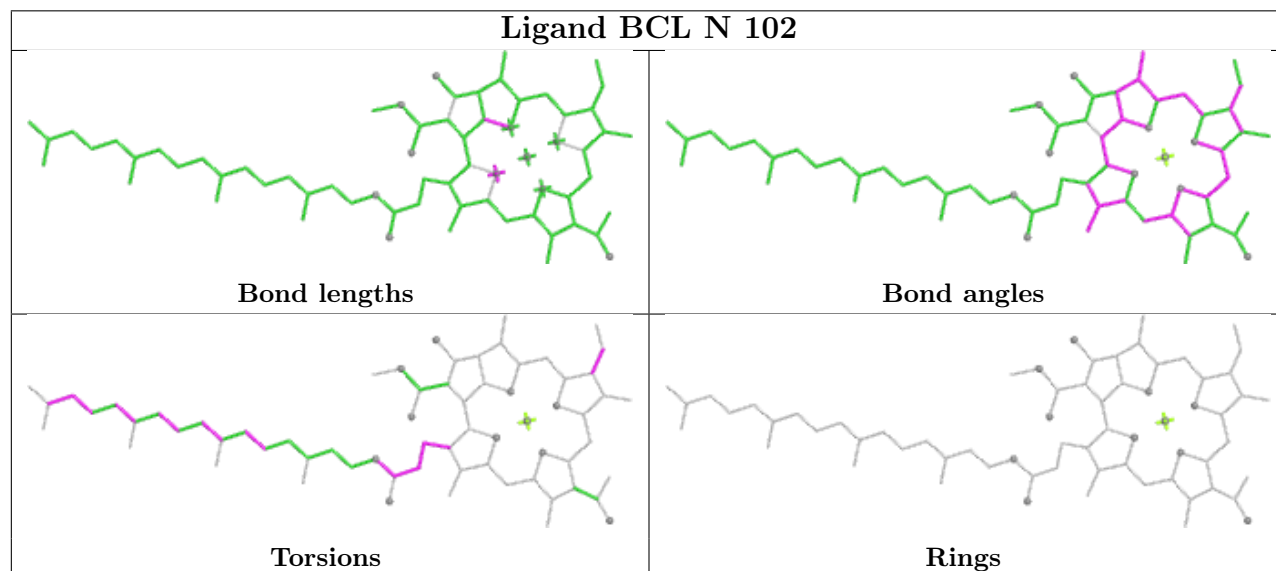
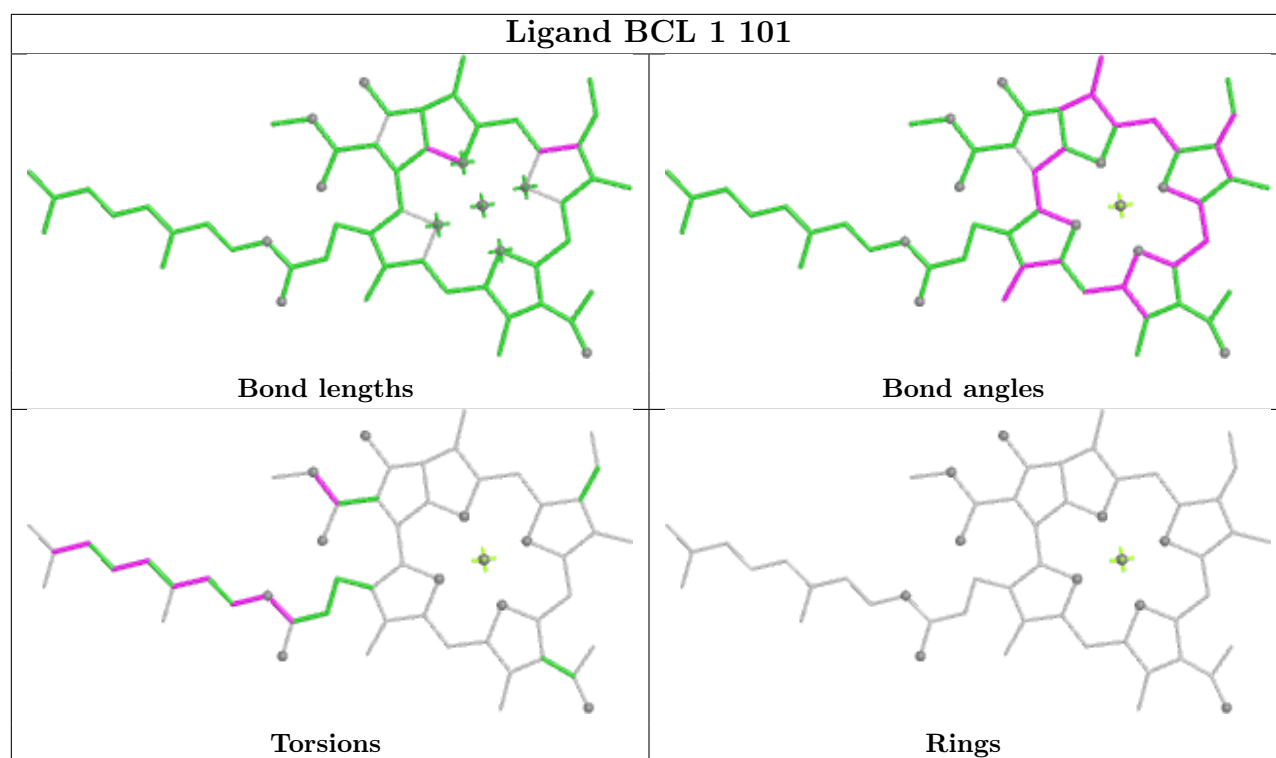
Ligand BCL I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO 9 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

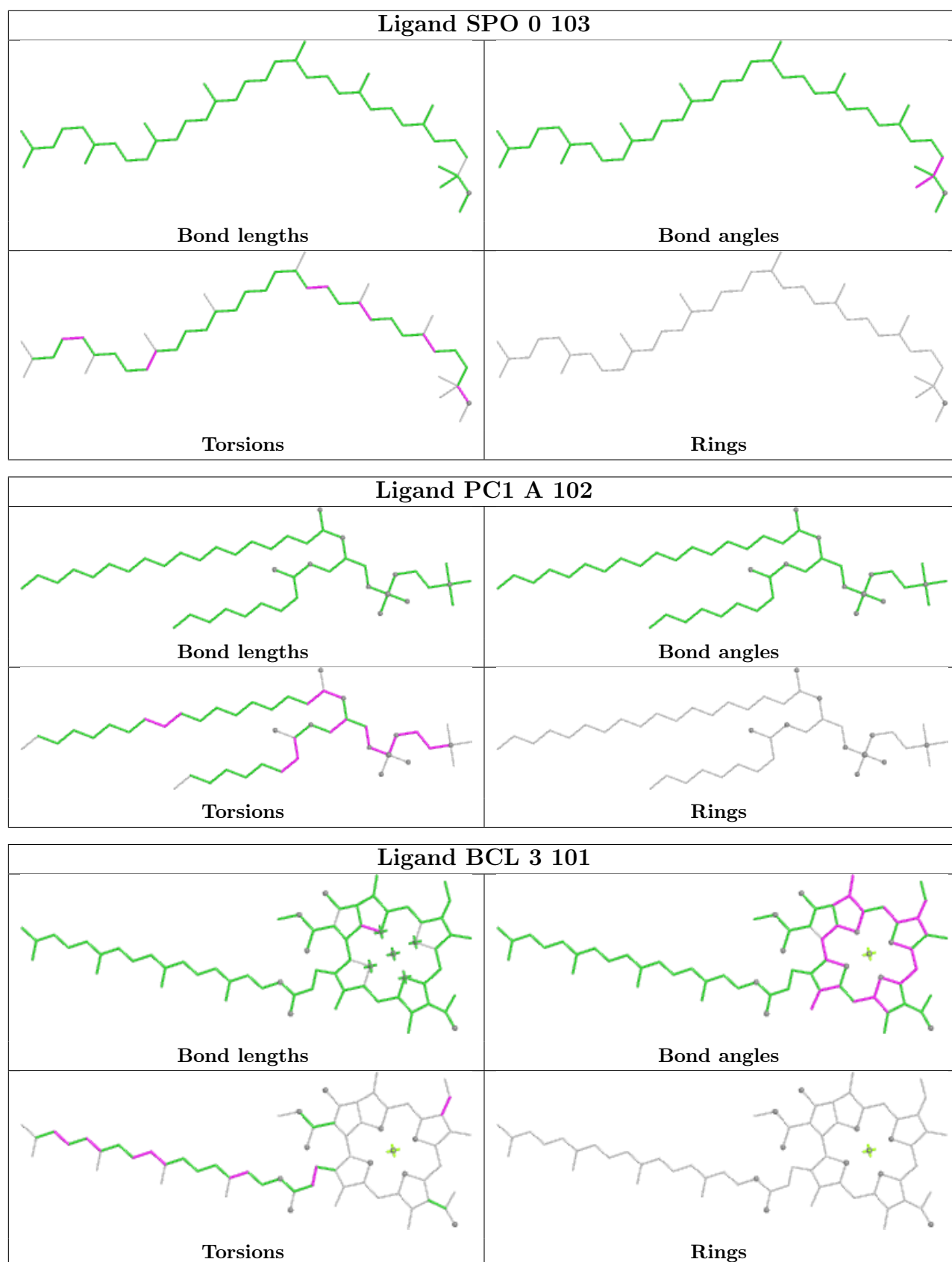


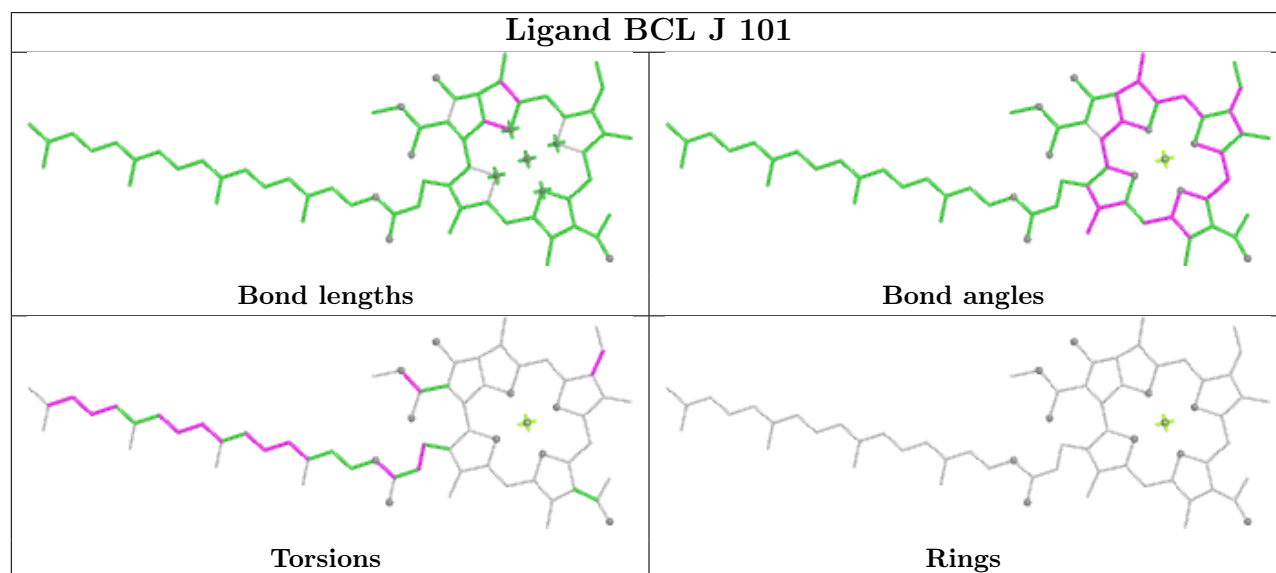
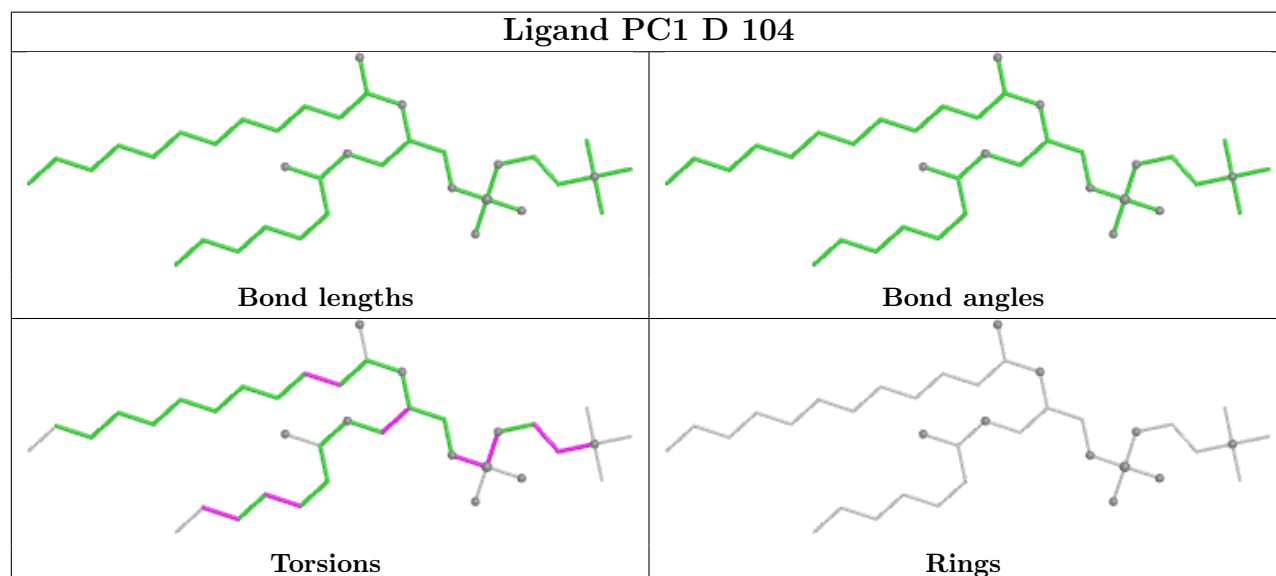
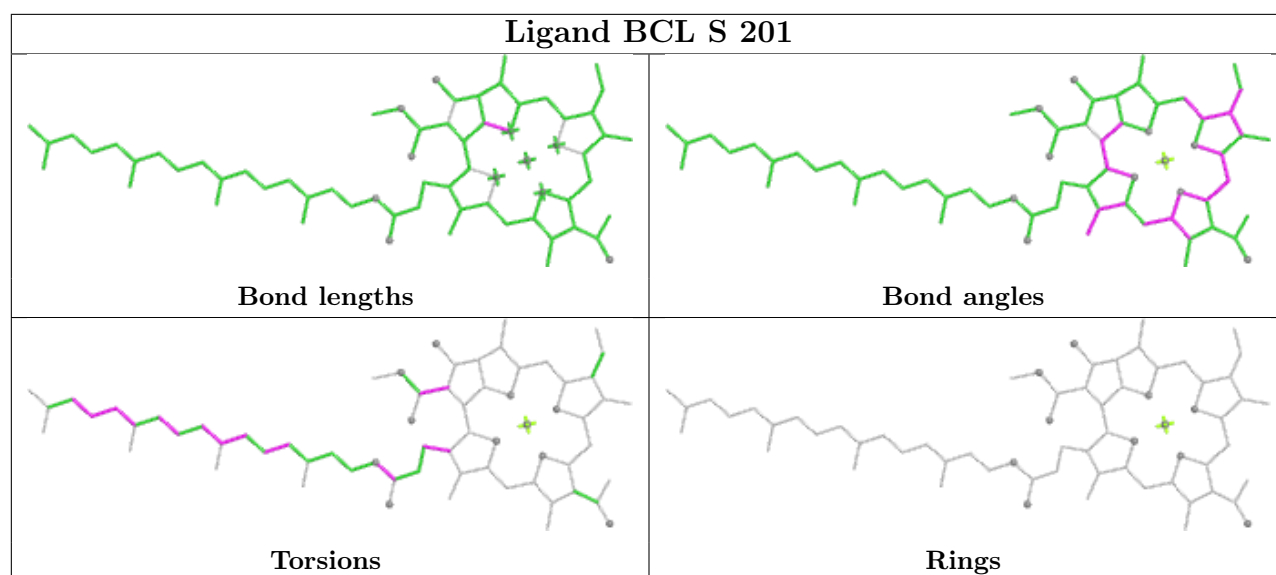


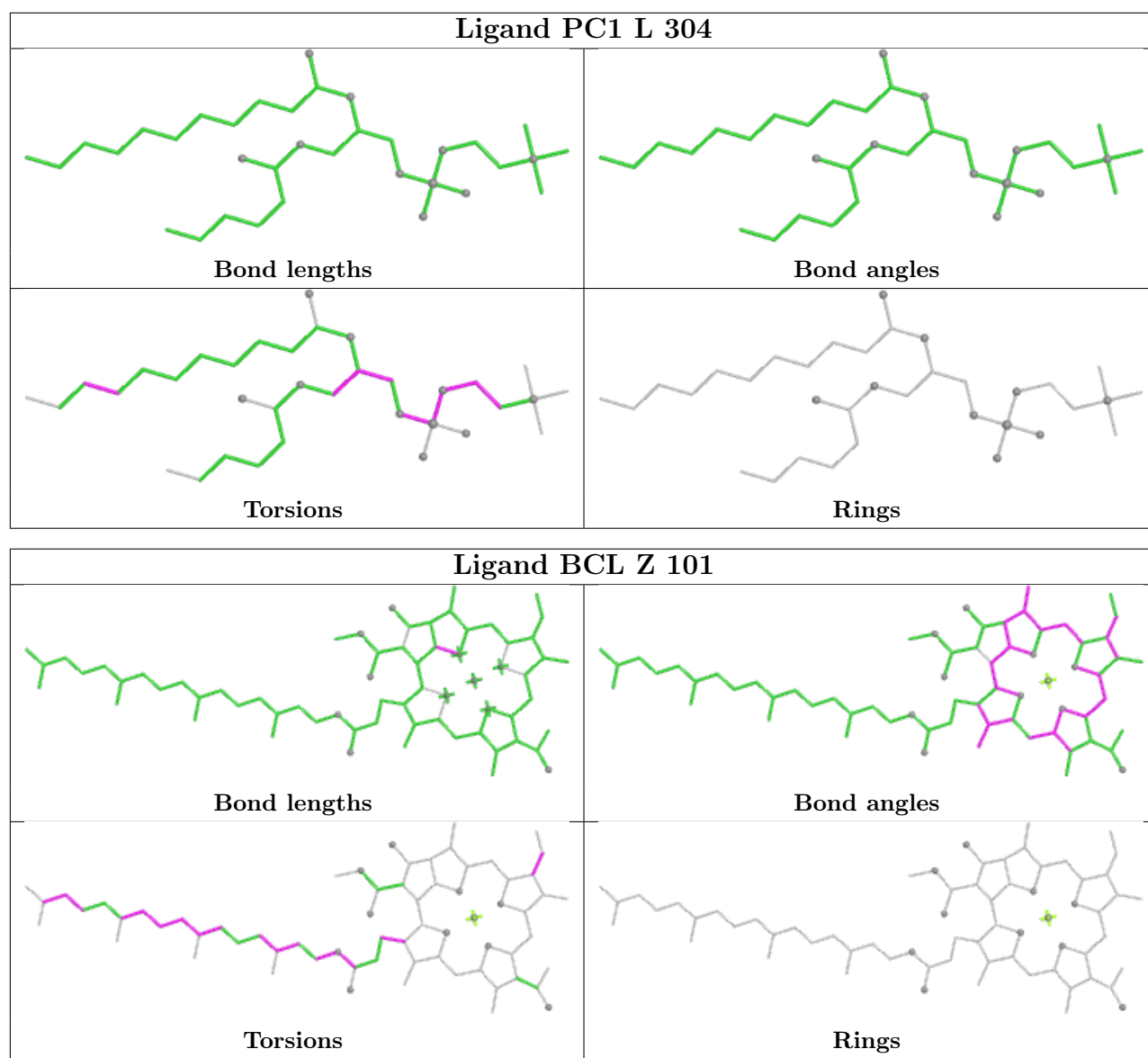


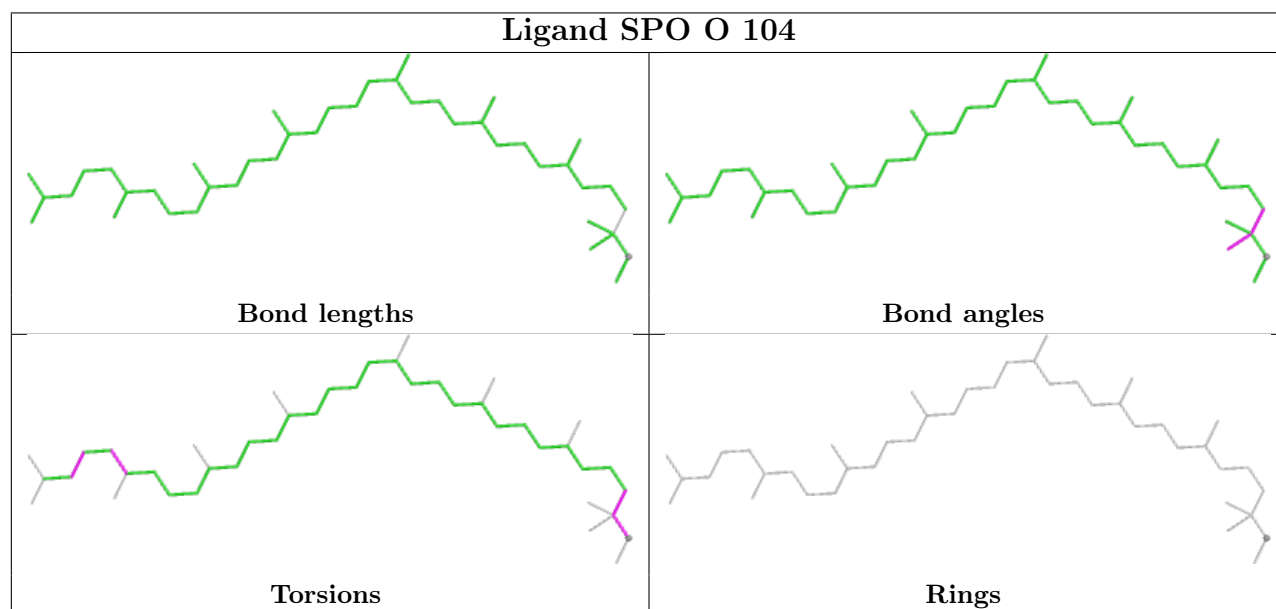
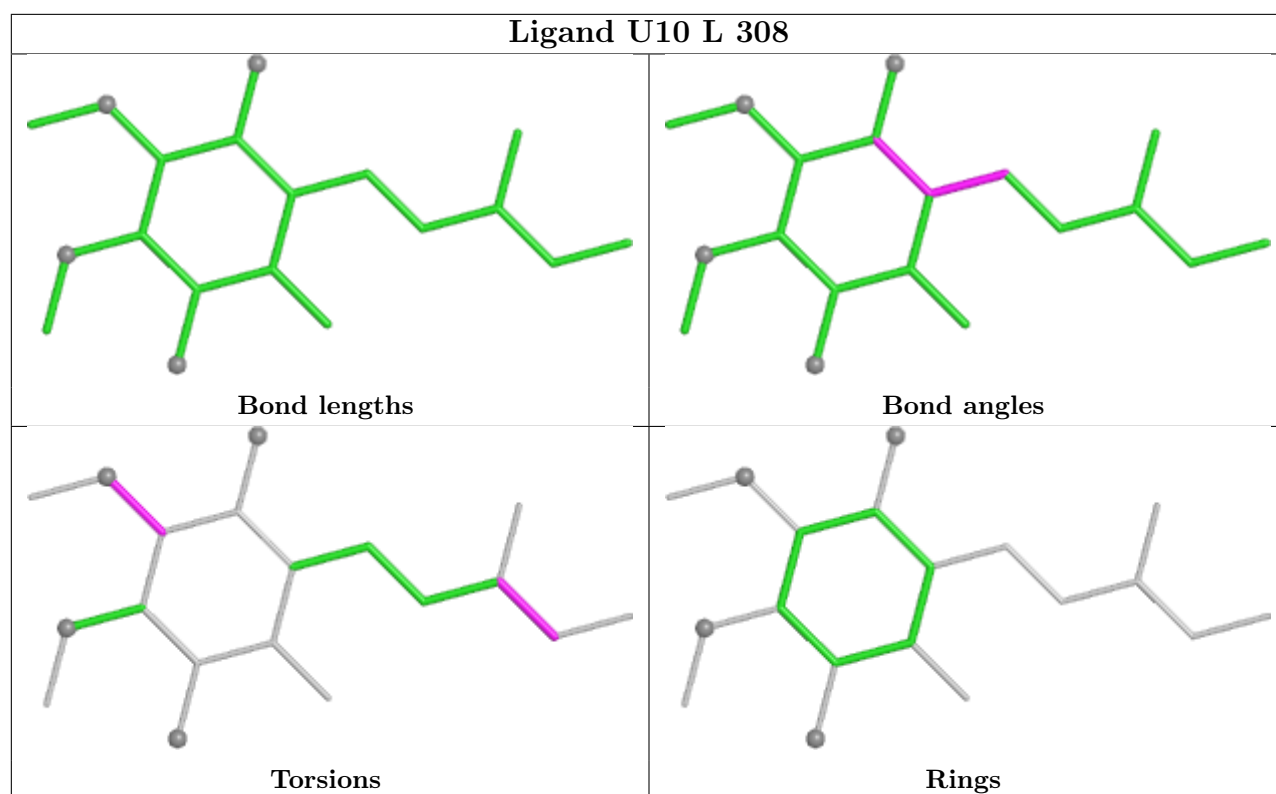


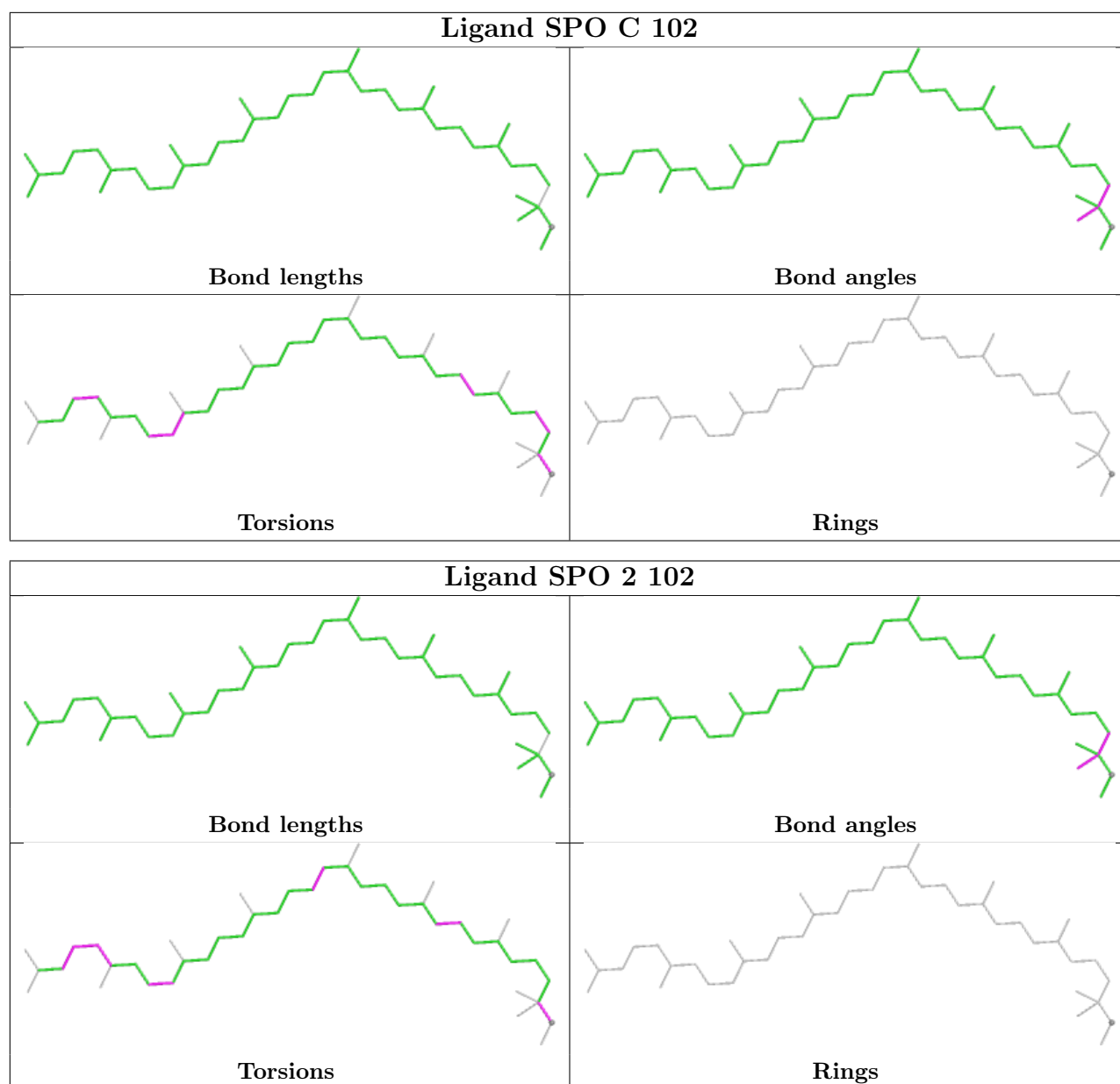


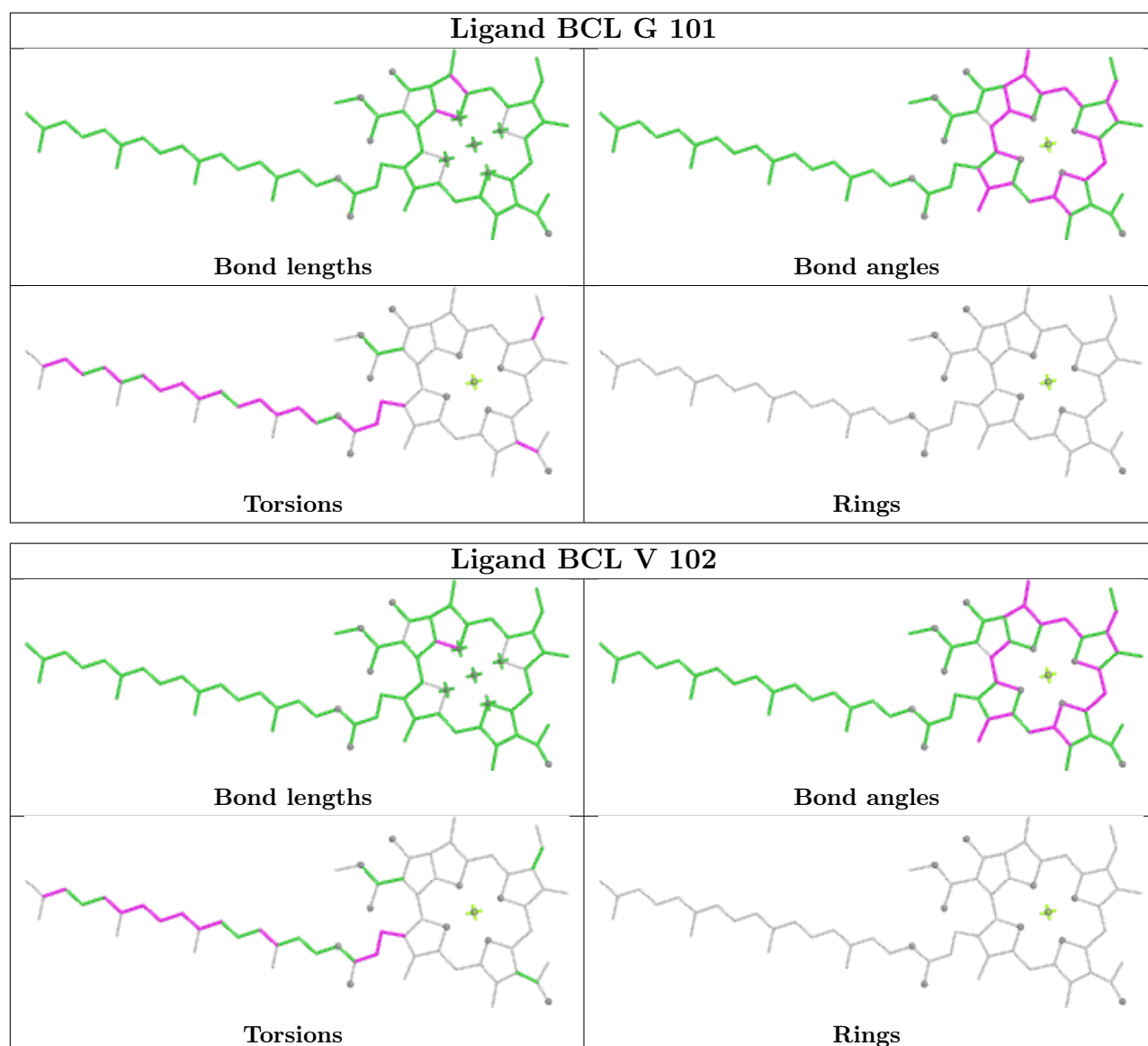


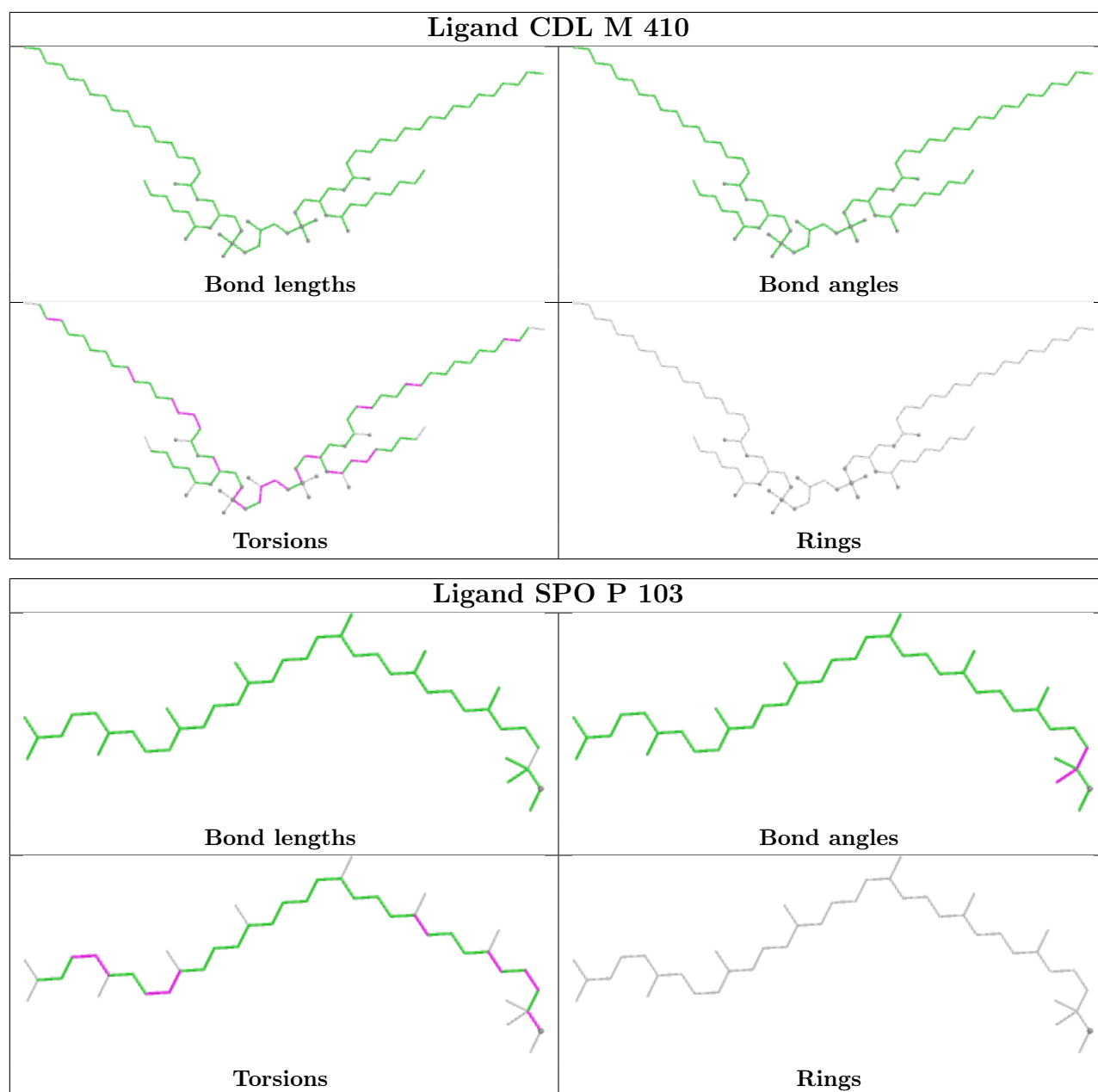


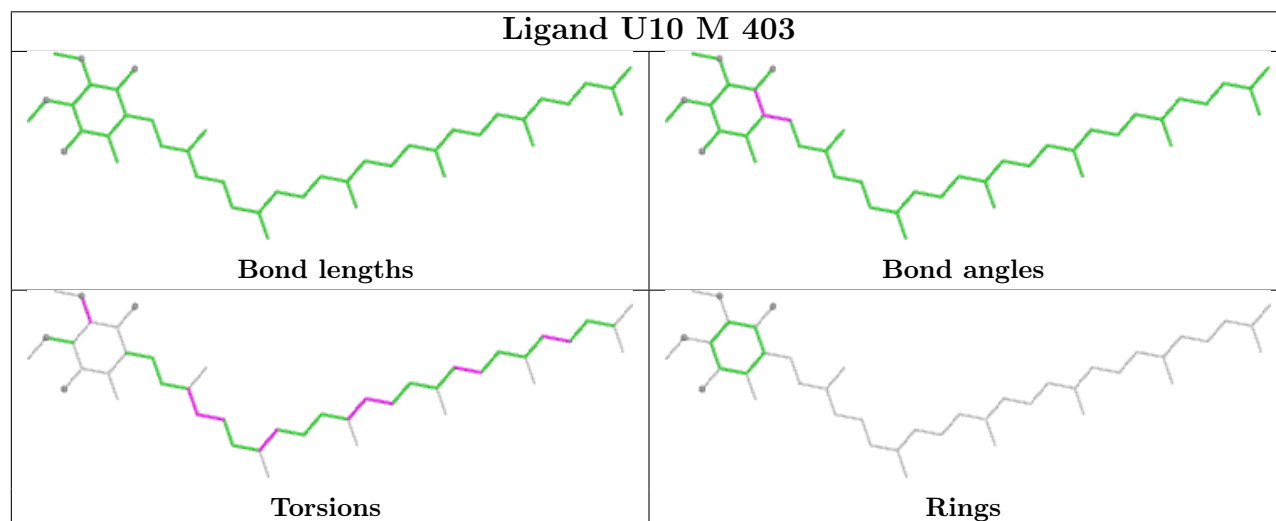
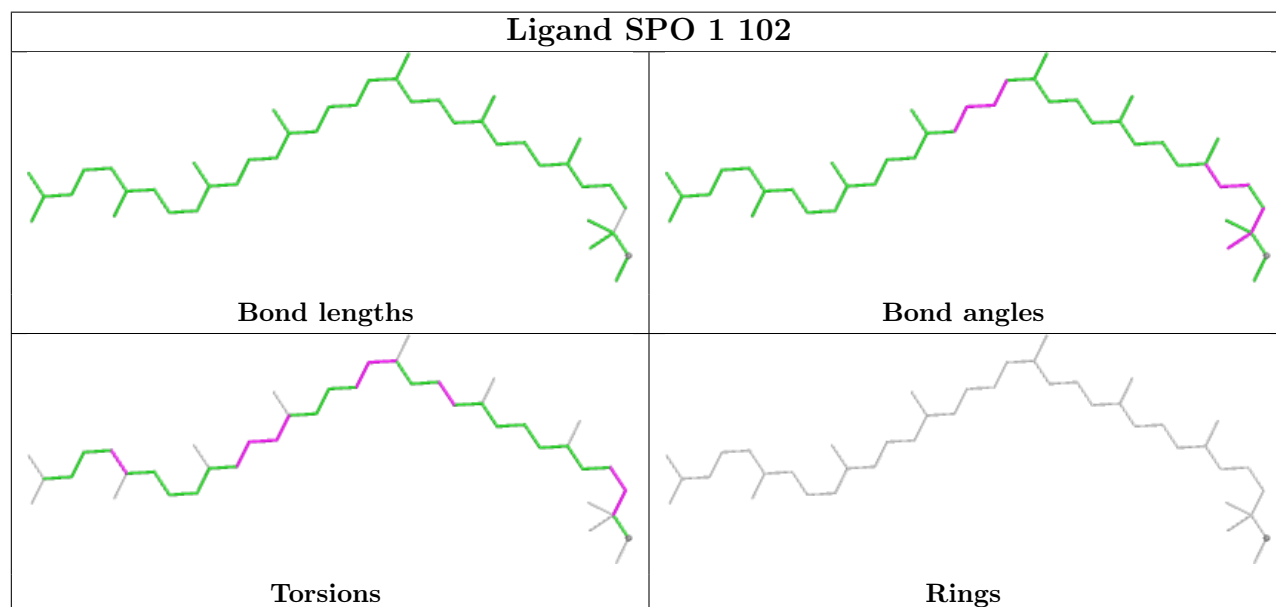
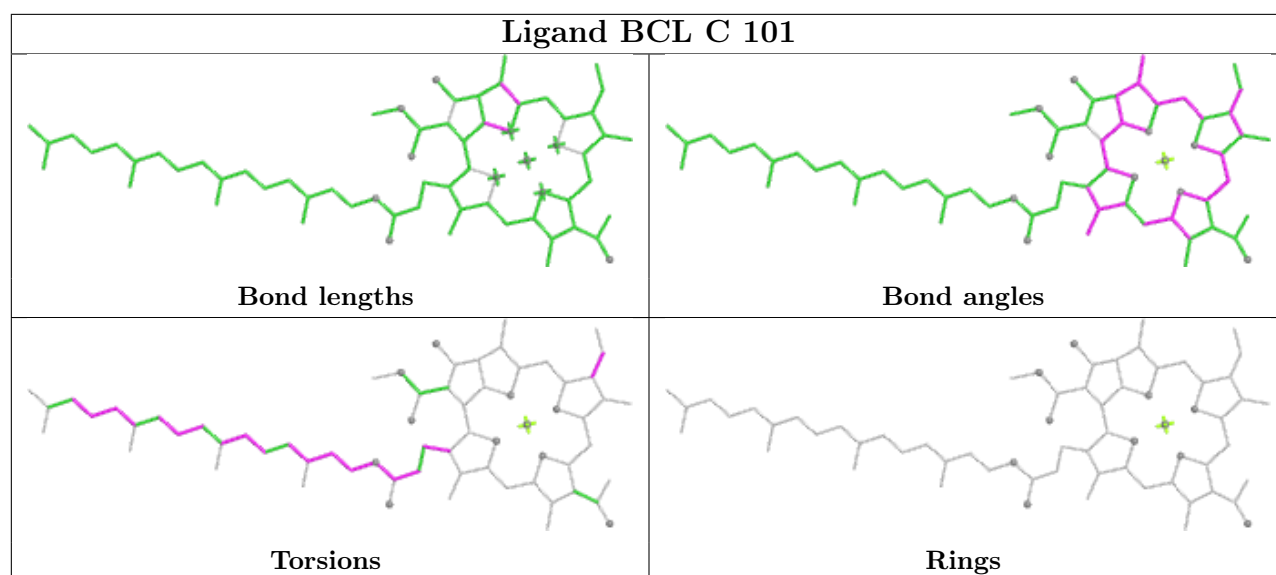


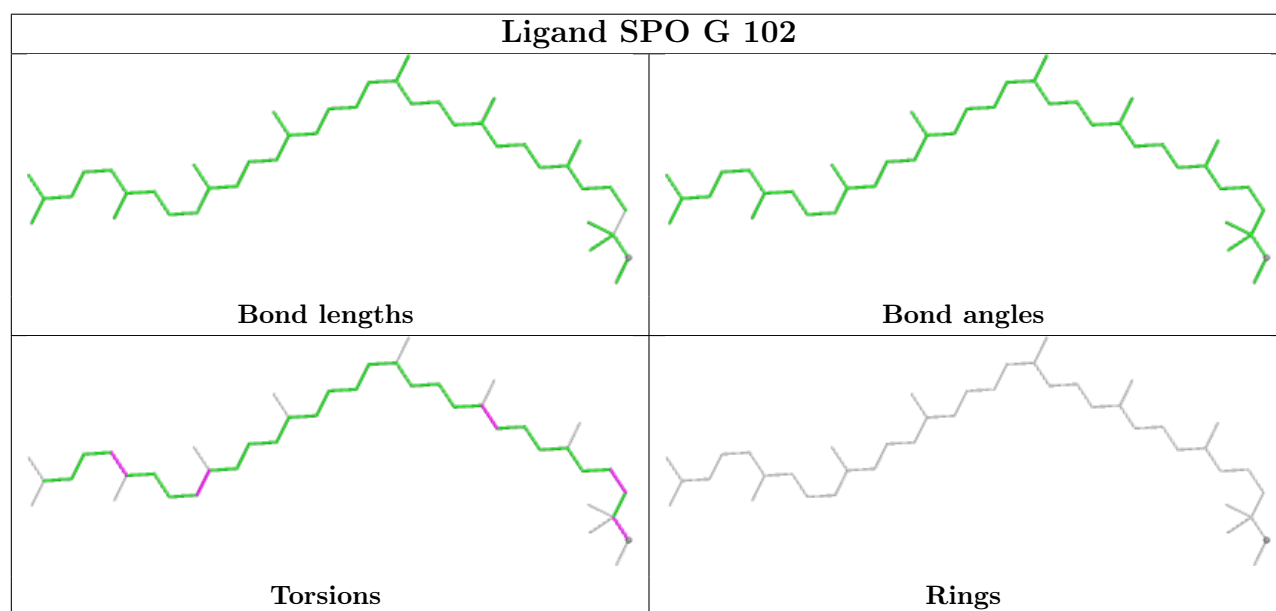
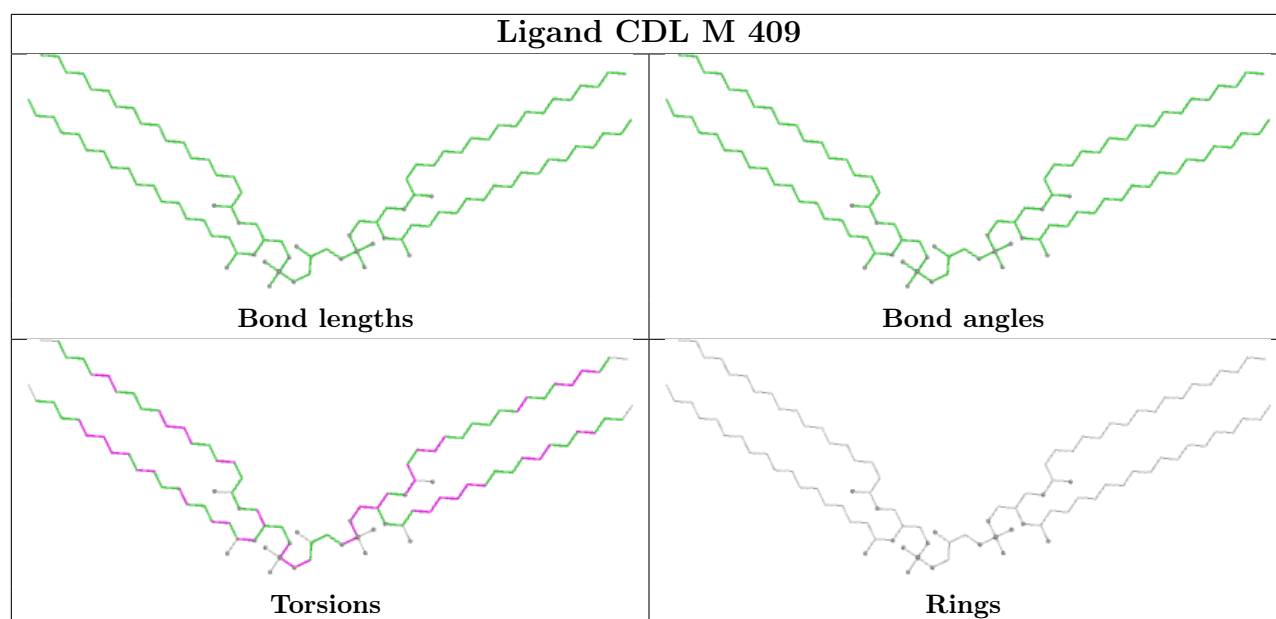


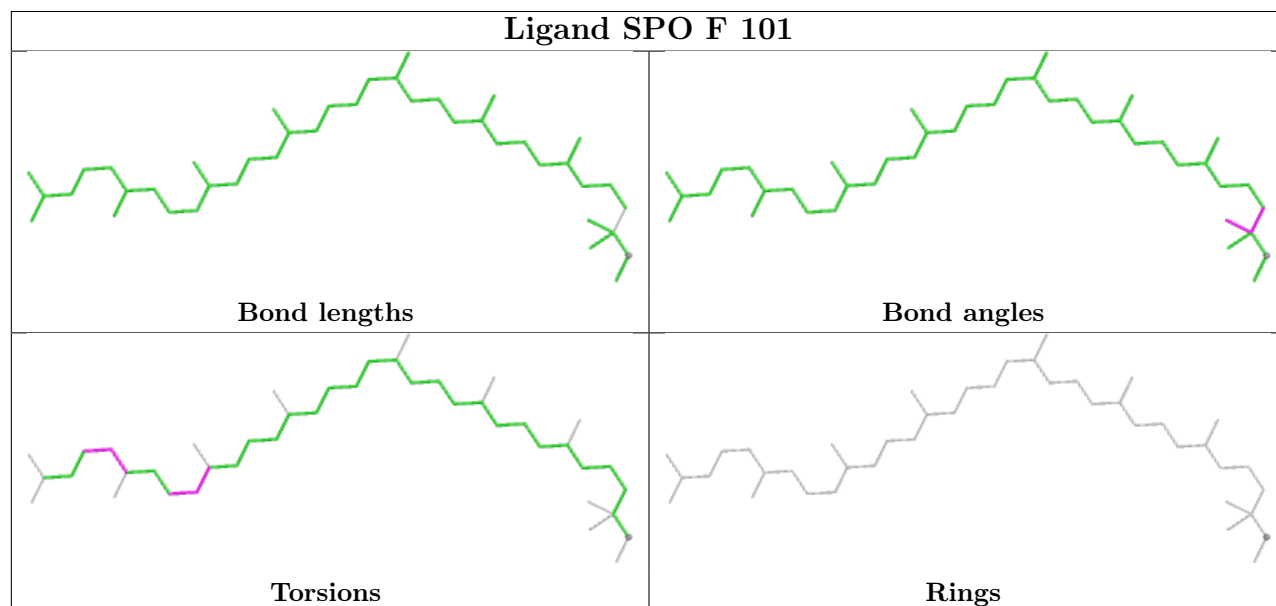
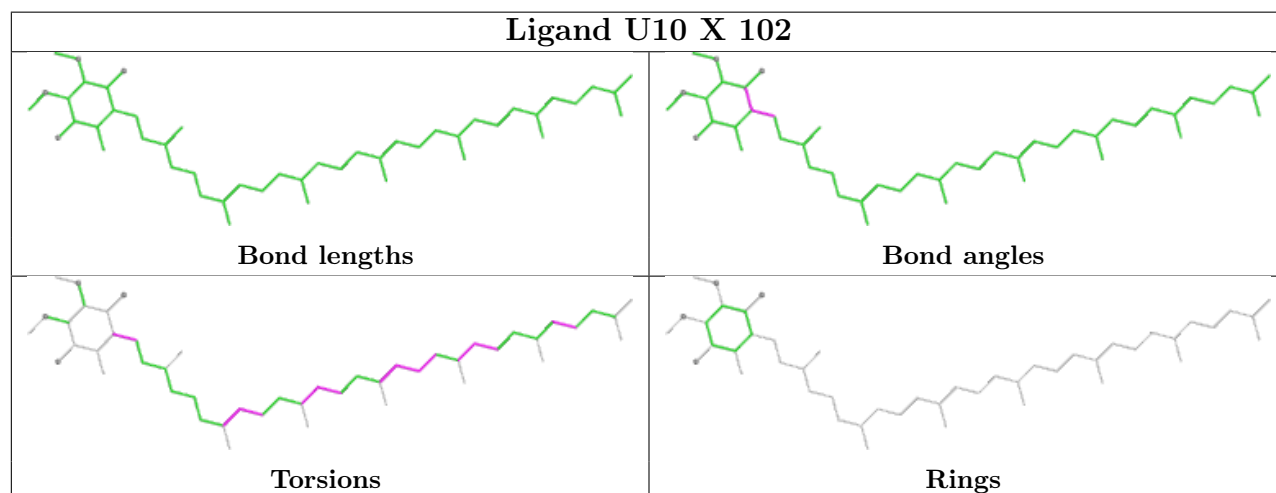
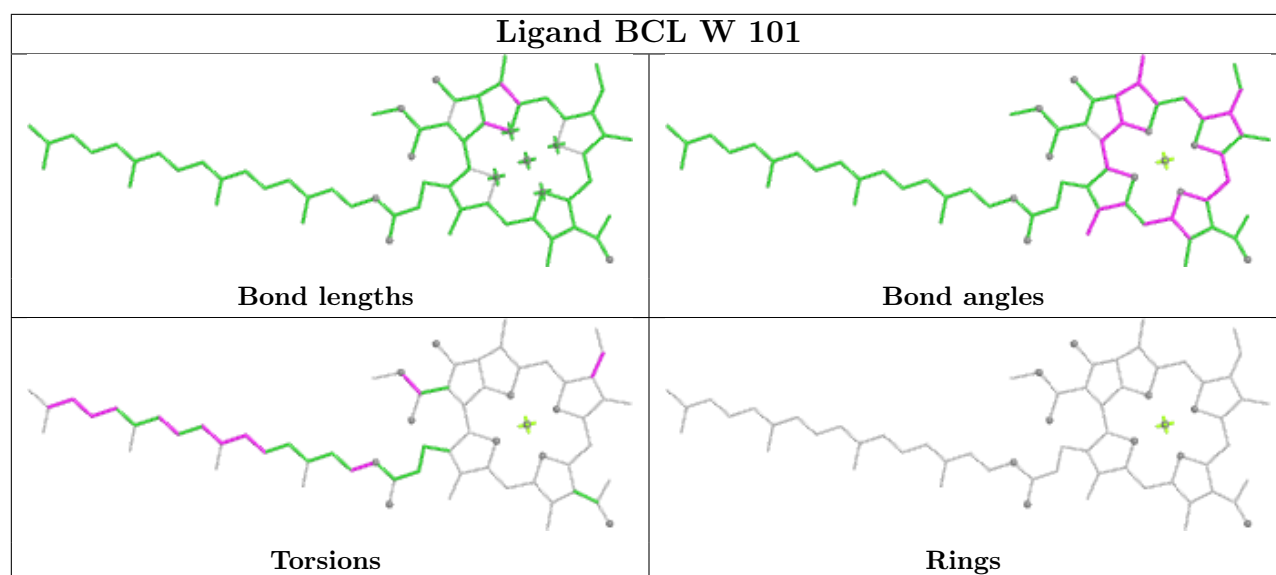


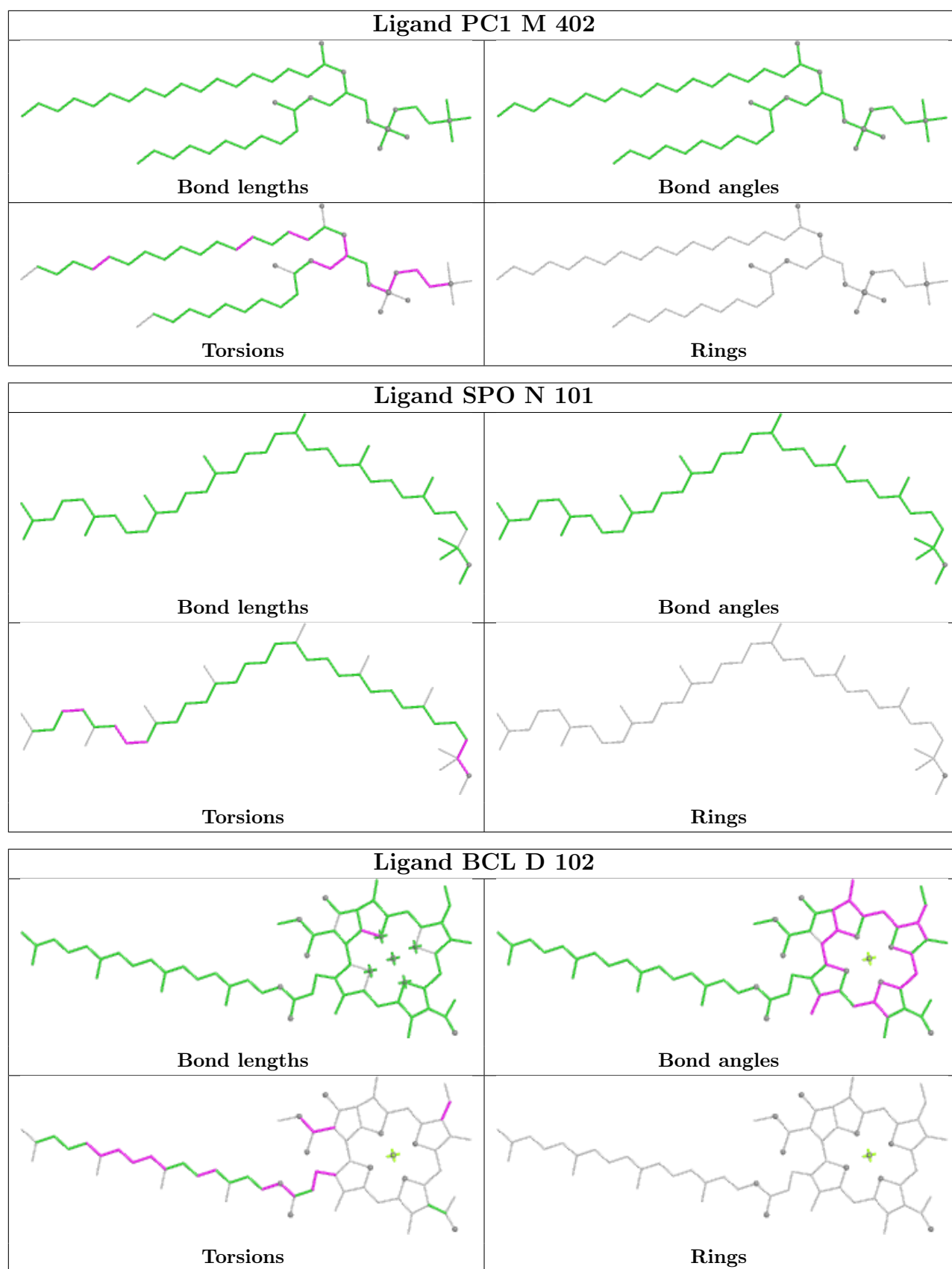


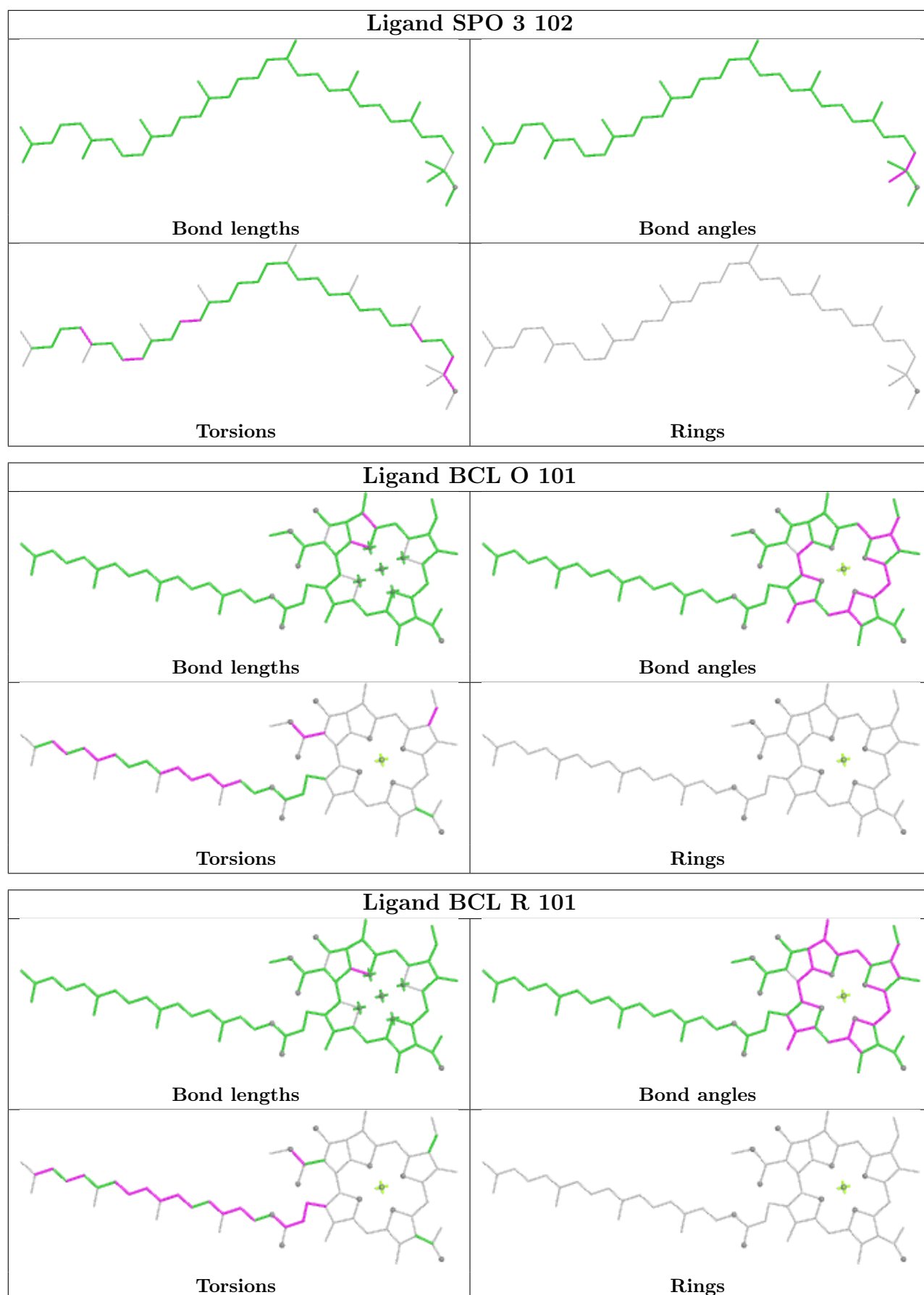




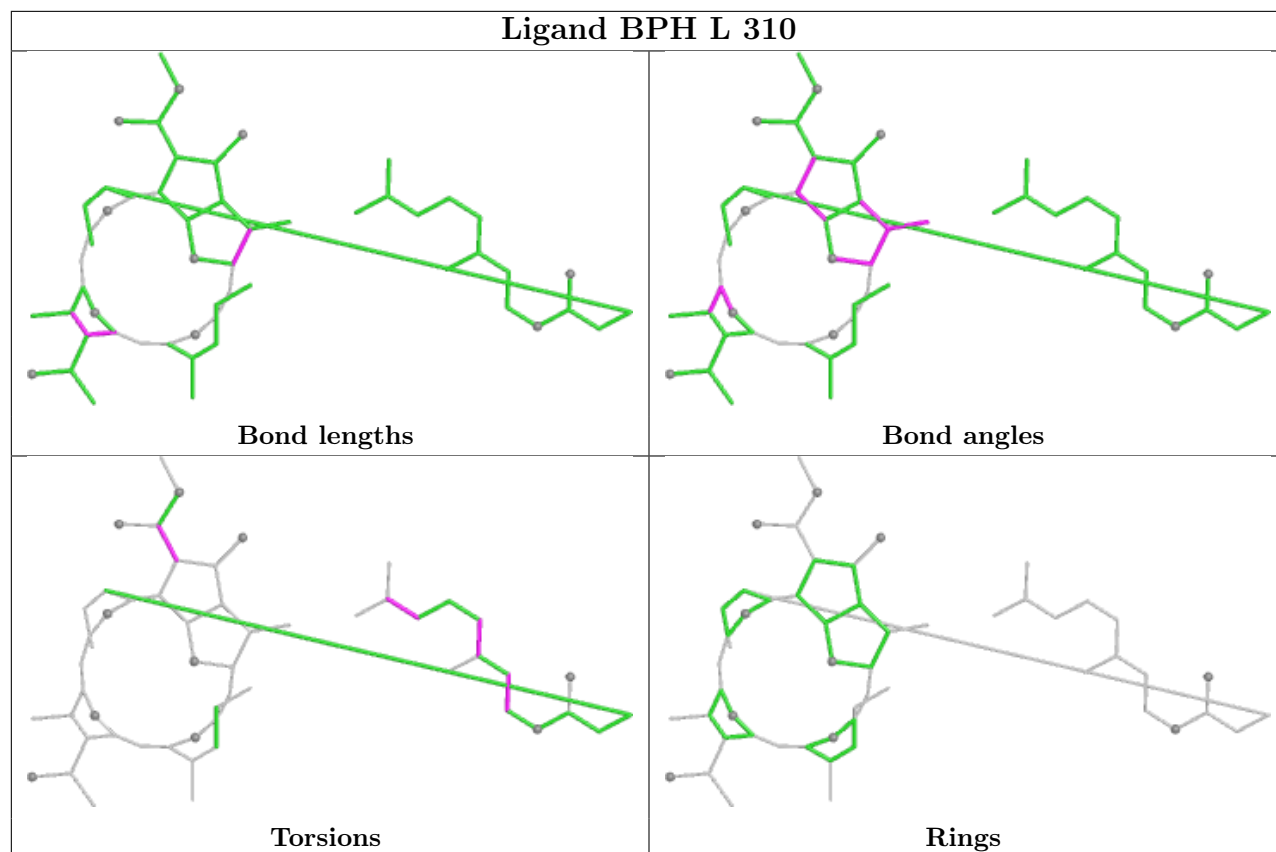




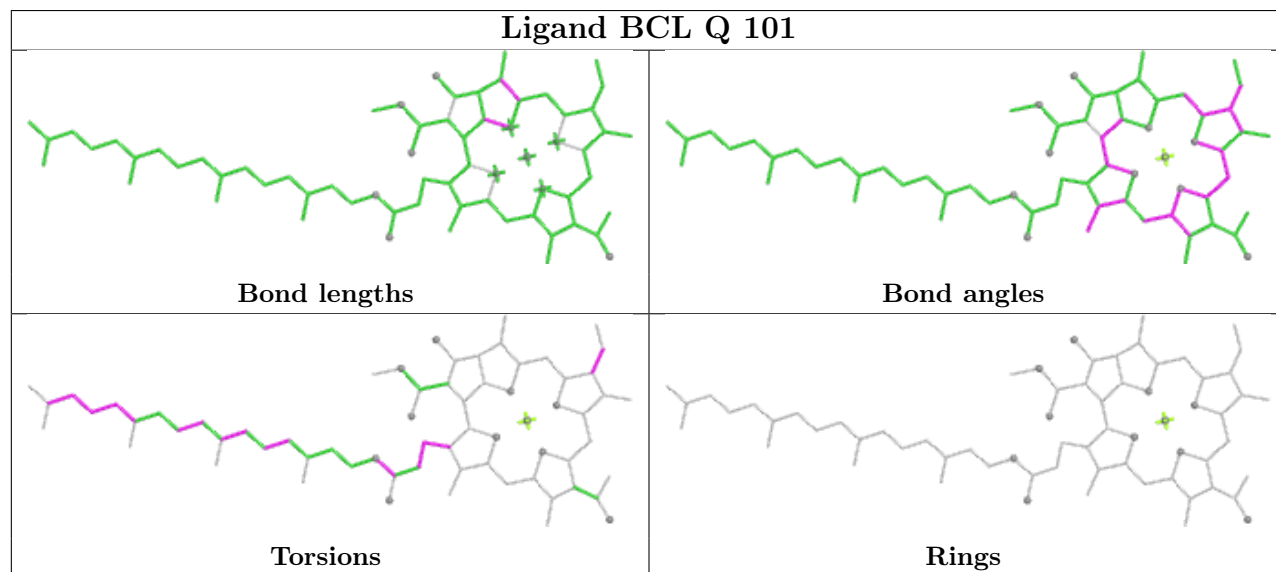


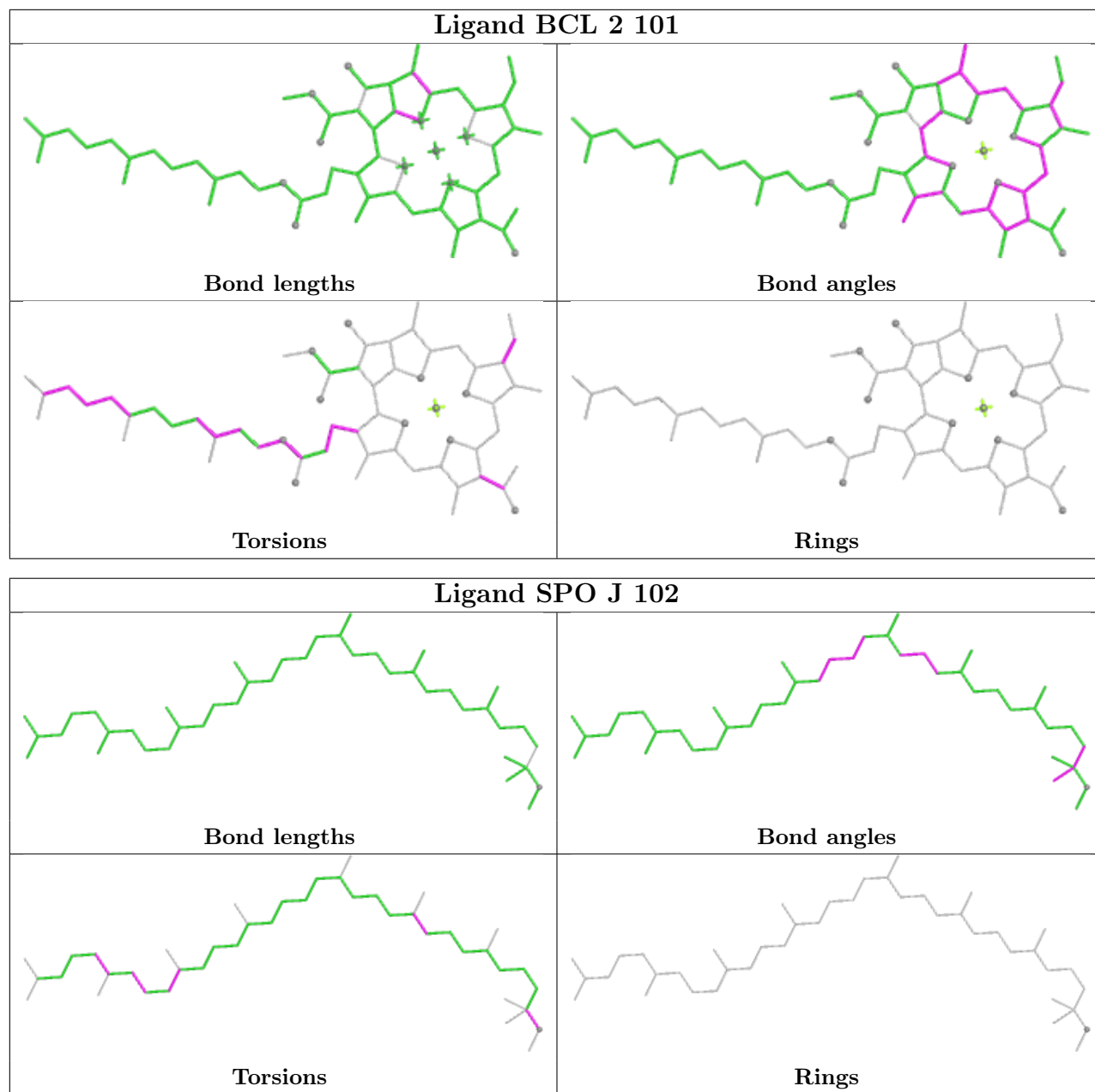


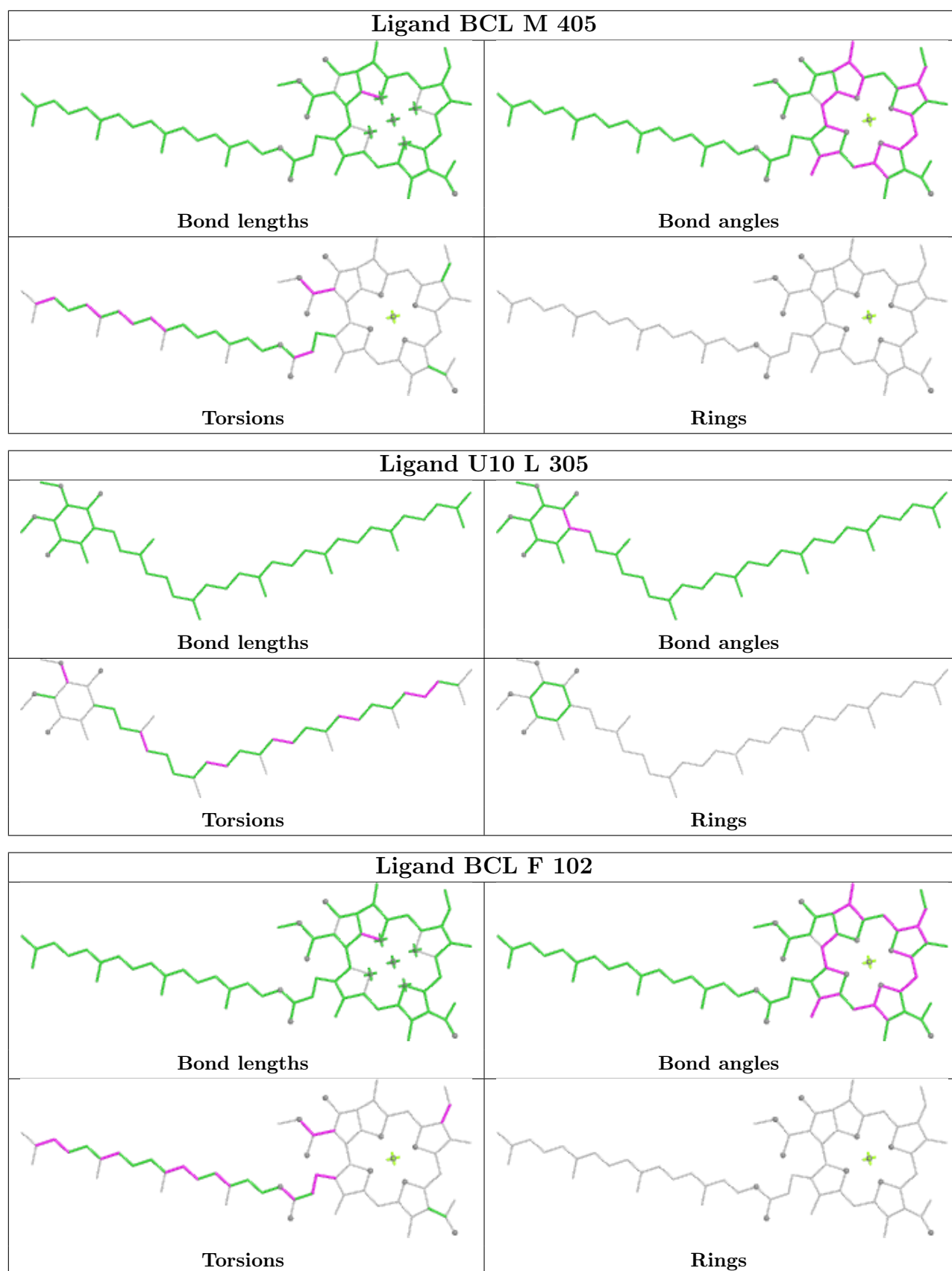
Ligand BPH L 310

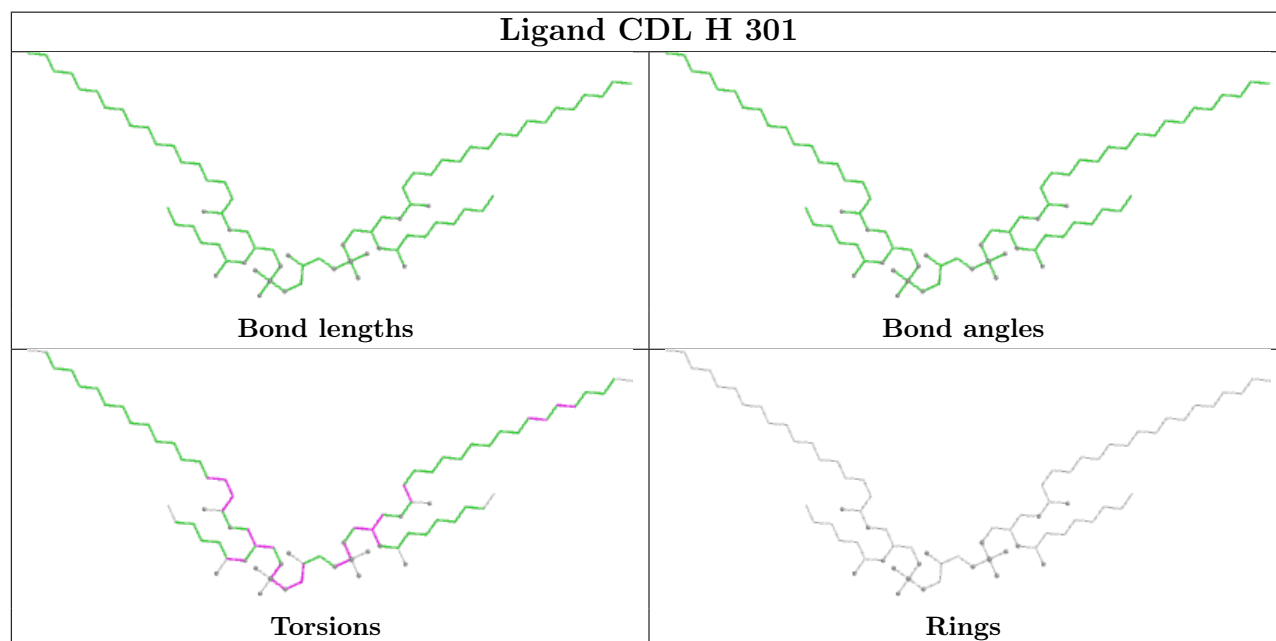
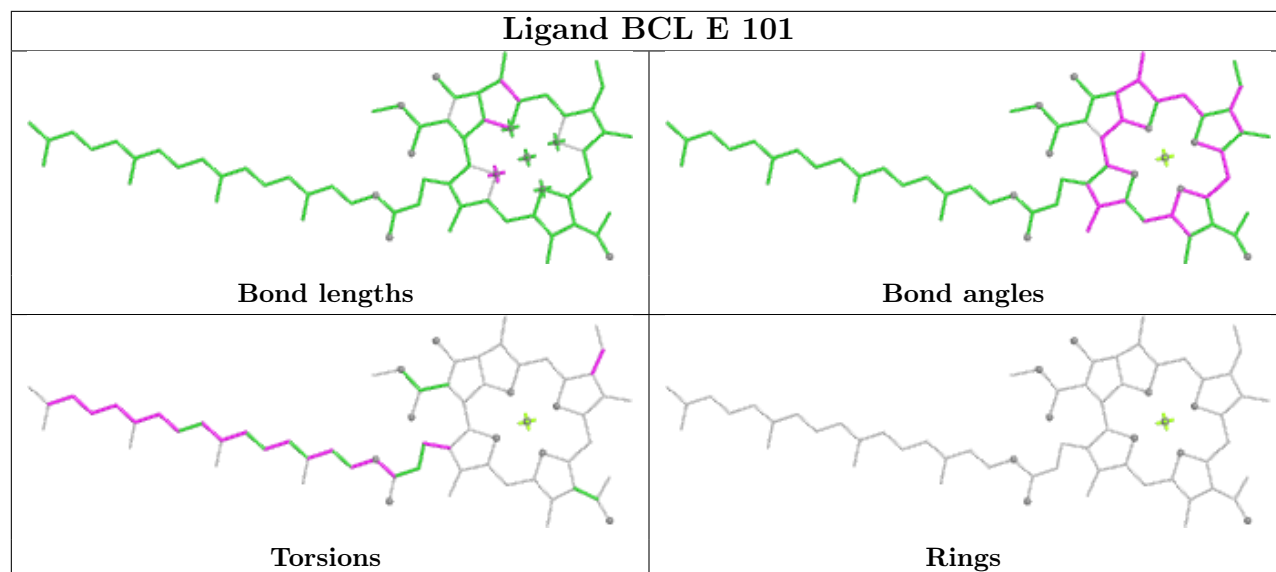


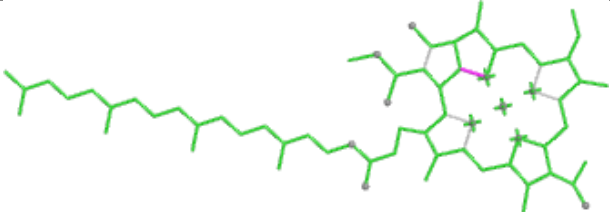
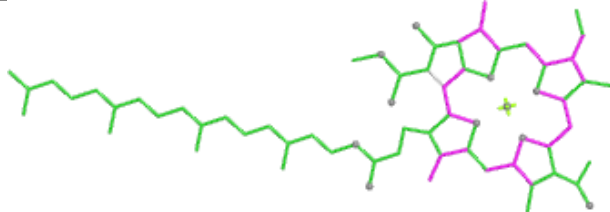
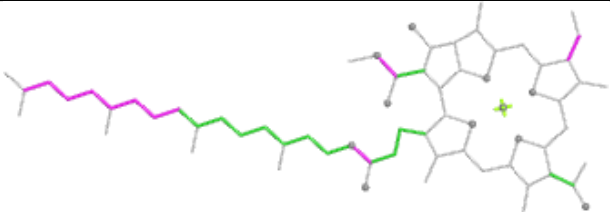
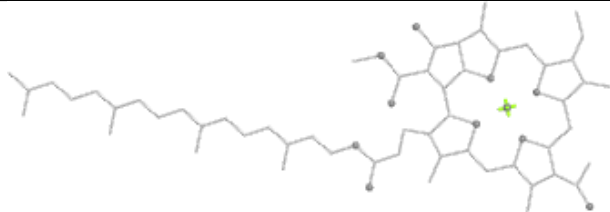
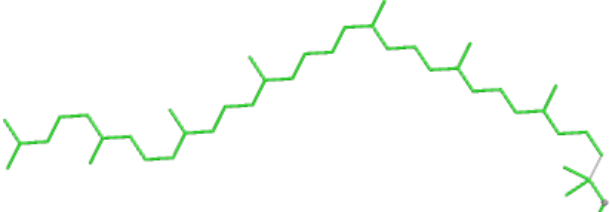
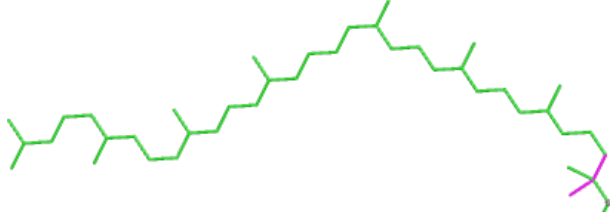
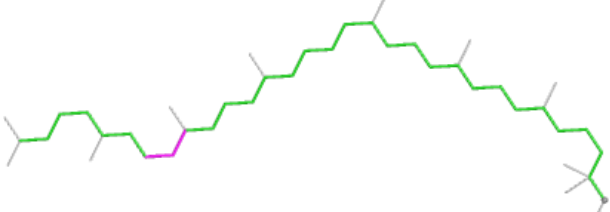
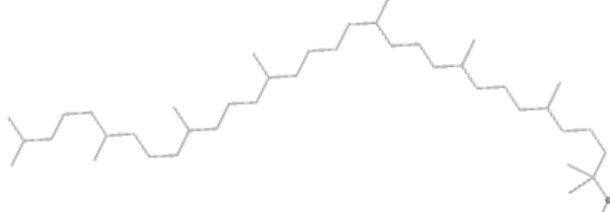
Ligand BCL Q 101

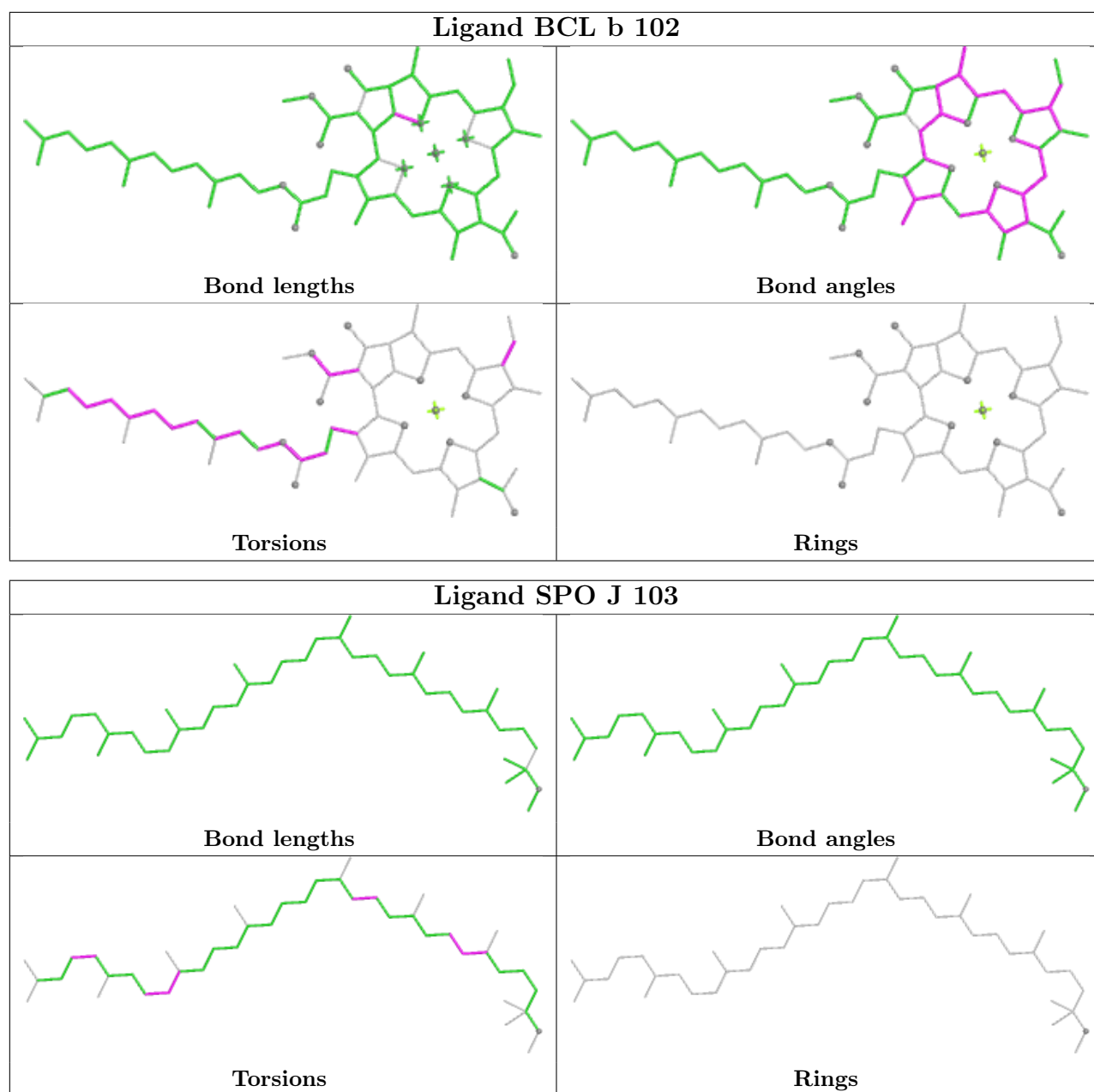








Ligand BCL A 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO D 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

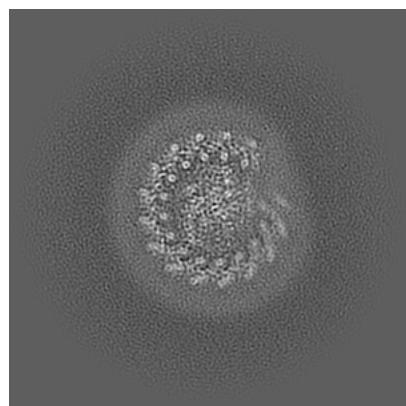
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39255. These allow visual inspection of the internal detail of the map and identification of artifacts.

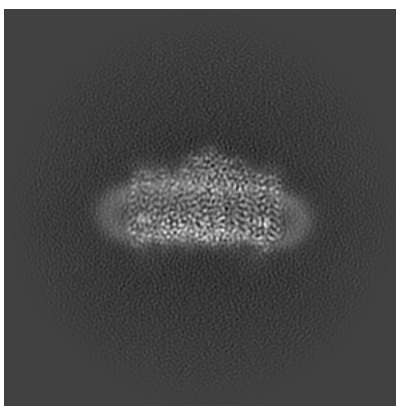
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

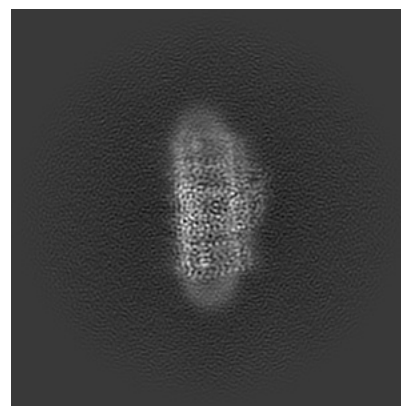
6.1.1 Primary map



X

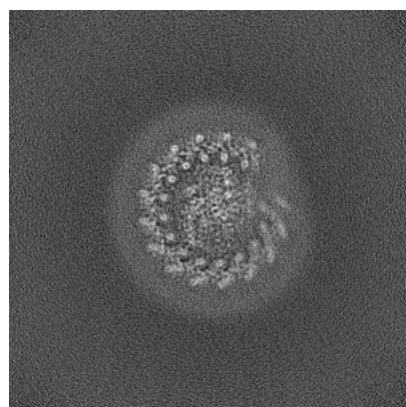


Y

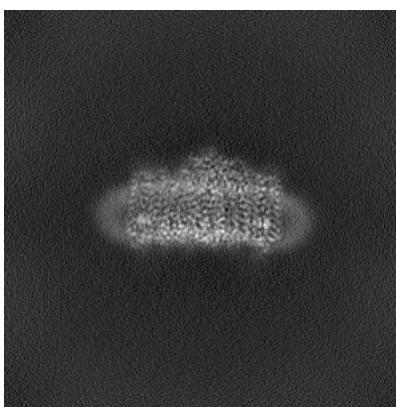


Z

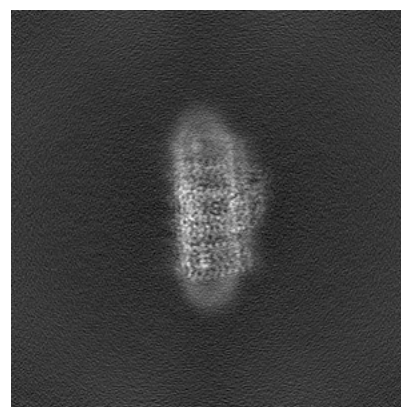
6.1.2 Raw map



X



Y

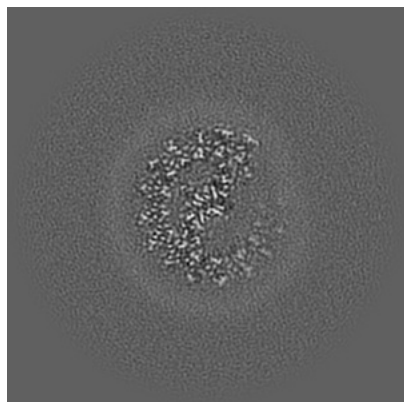


Z

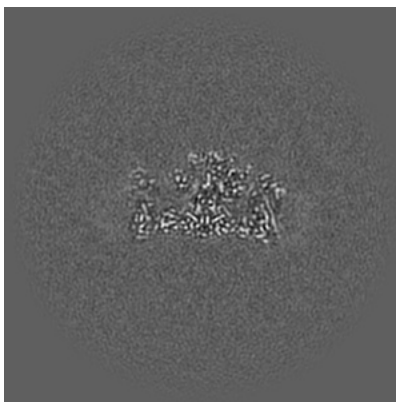
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

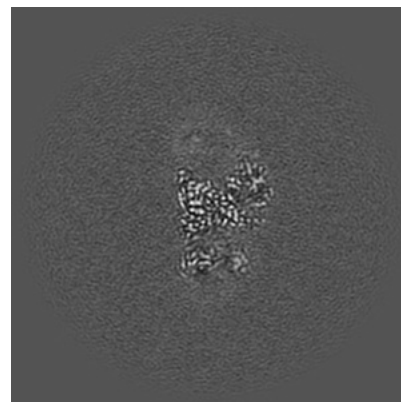
6.2.1 Primary map



X Index: 160

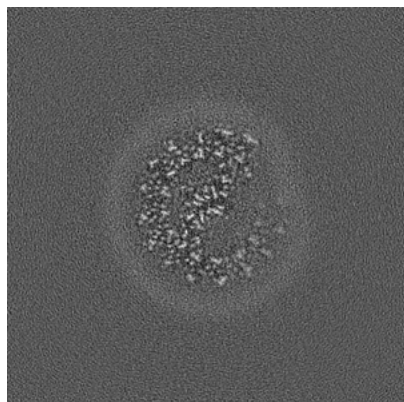


Y Index: 160

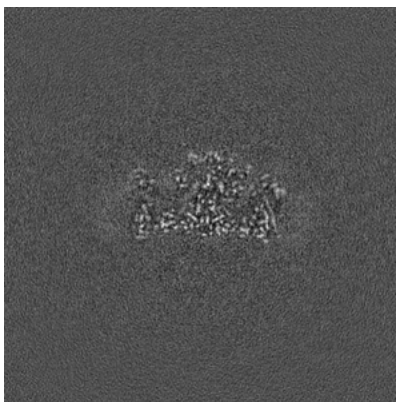


Z Index: 160

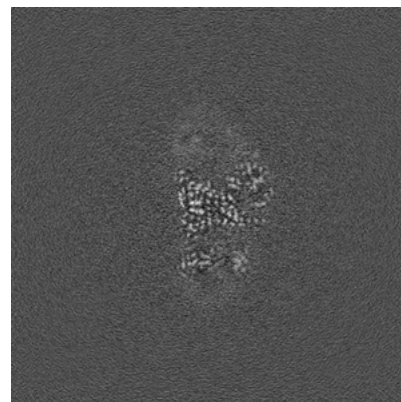
6.2.2 Raw map



X Index: 160



Y Index: 160

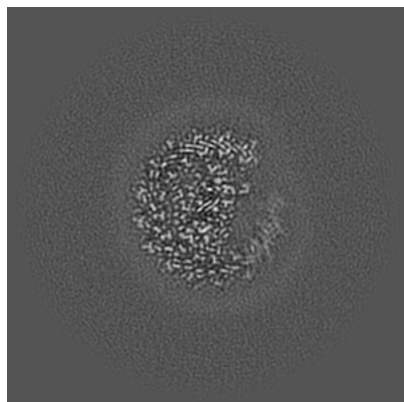


Z Index: 160

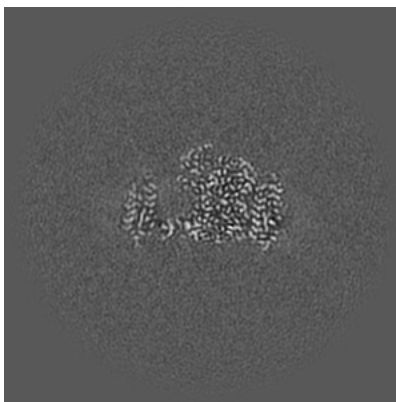
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

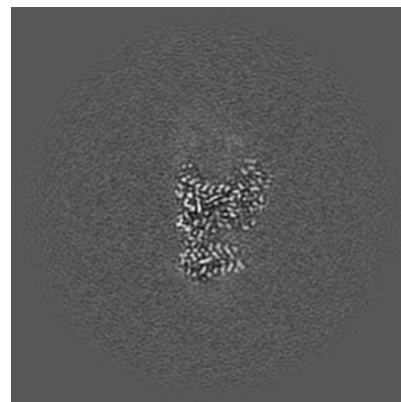
6.3.1 Primary map



X Index: 147

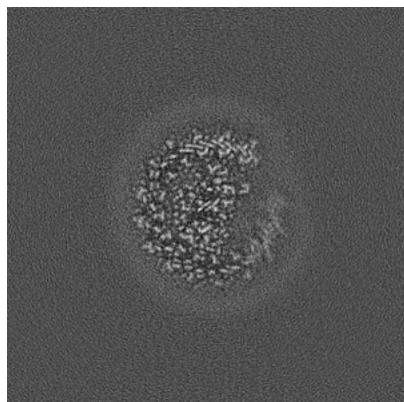


Y Index: 171

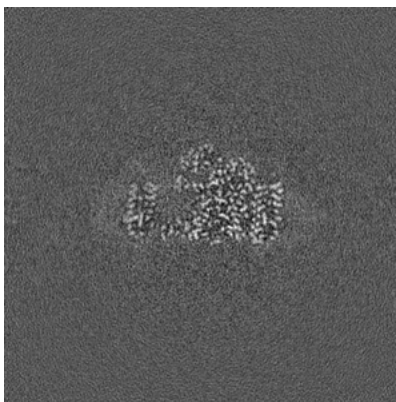


Z Index: 170

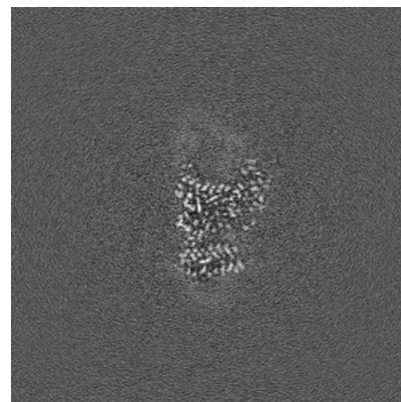
6.3.2 Raw map



X Index: 147



Y Index: 172

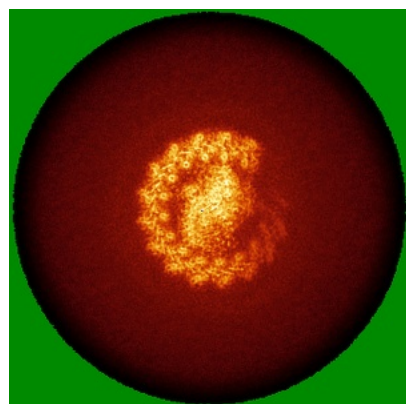


Z Index: 170

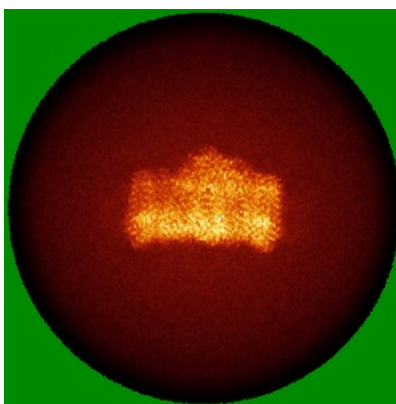
The images above show the largest variance slices of the map in three orthogonal directions.

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

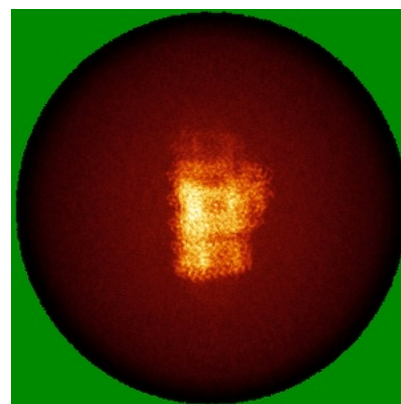
6.4.1 Primary map



X

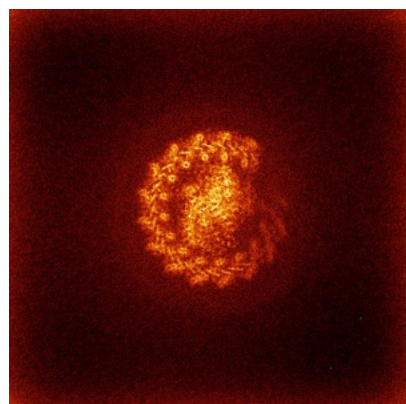


Y

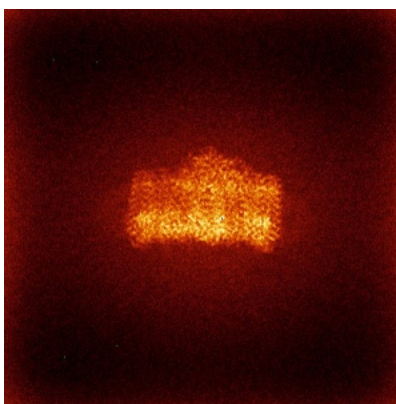


Z

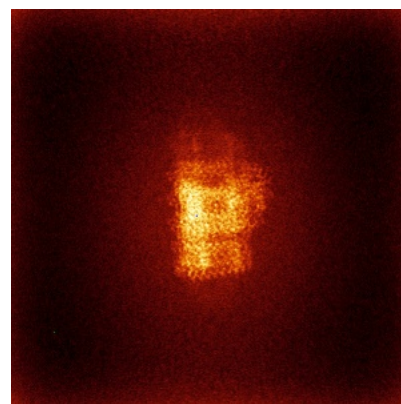
6.4.2 Raw map



X



Y

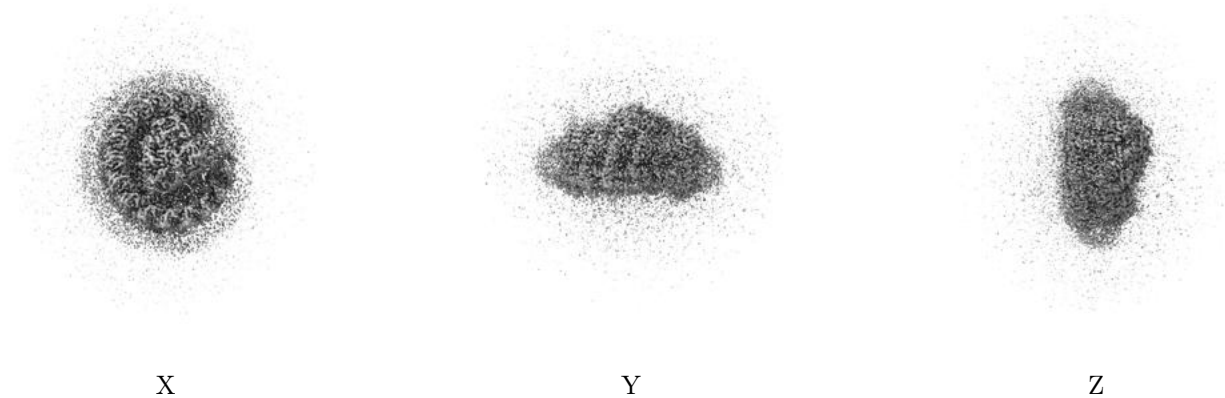


Z

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

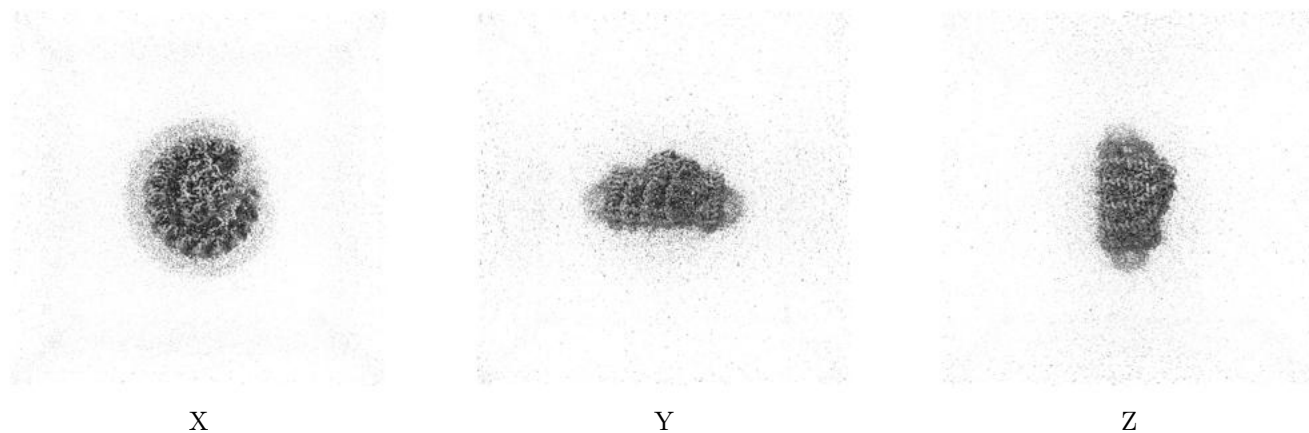
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

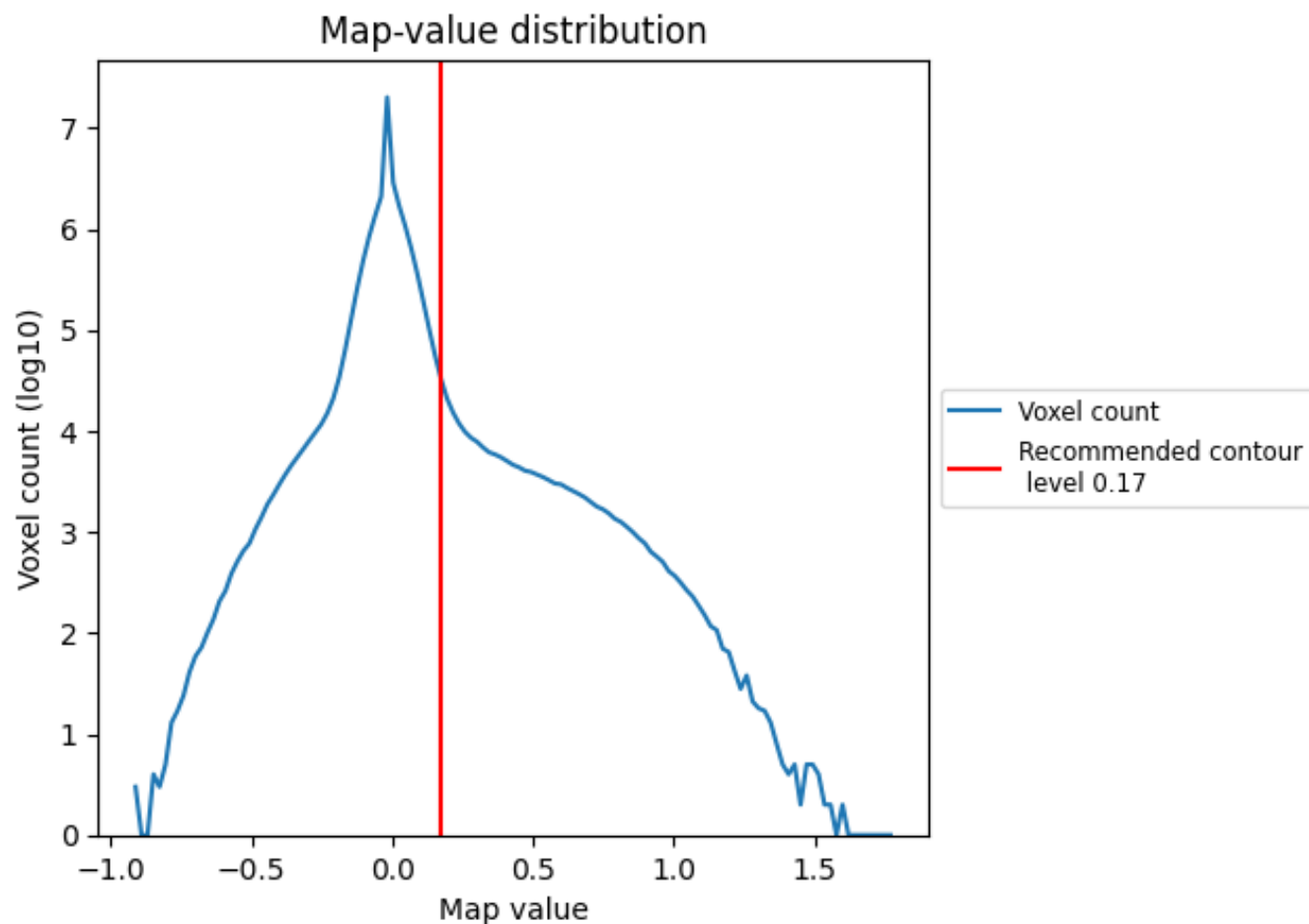
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

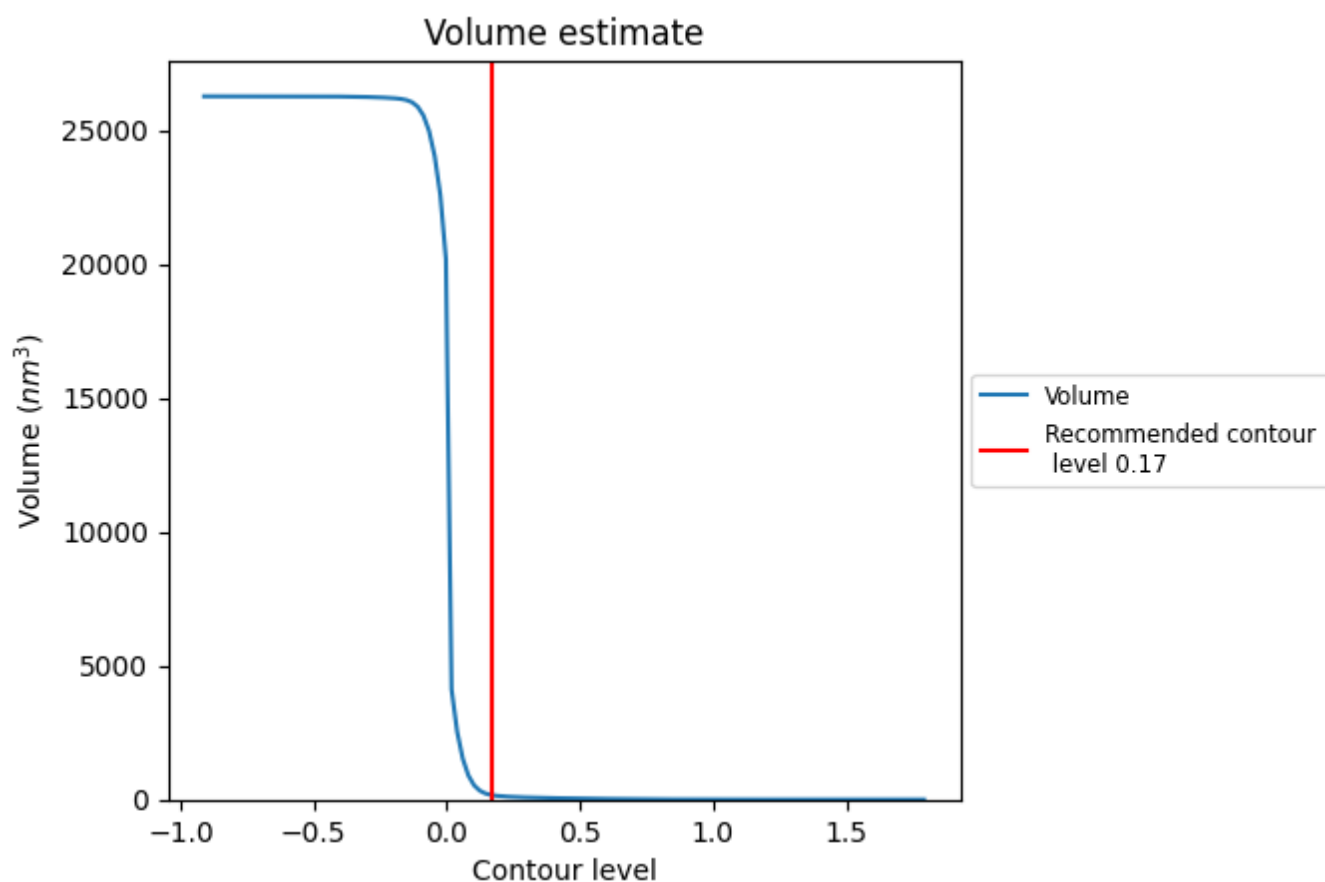
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

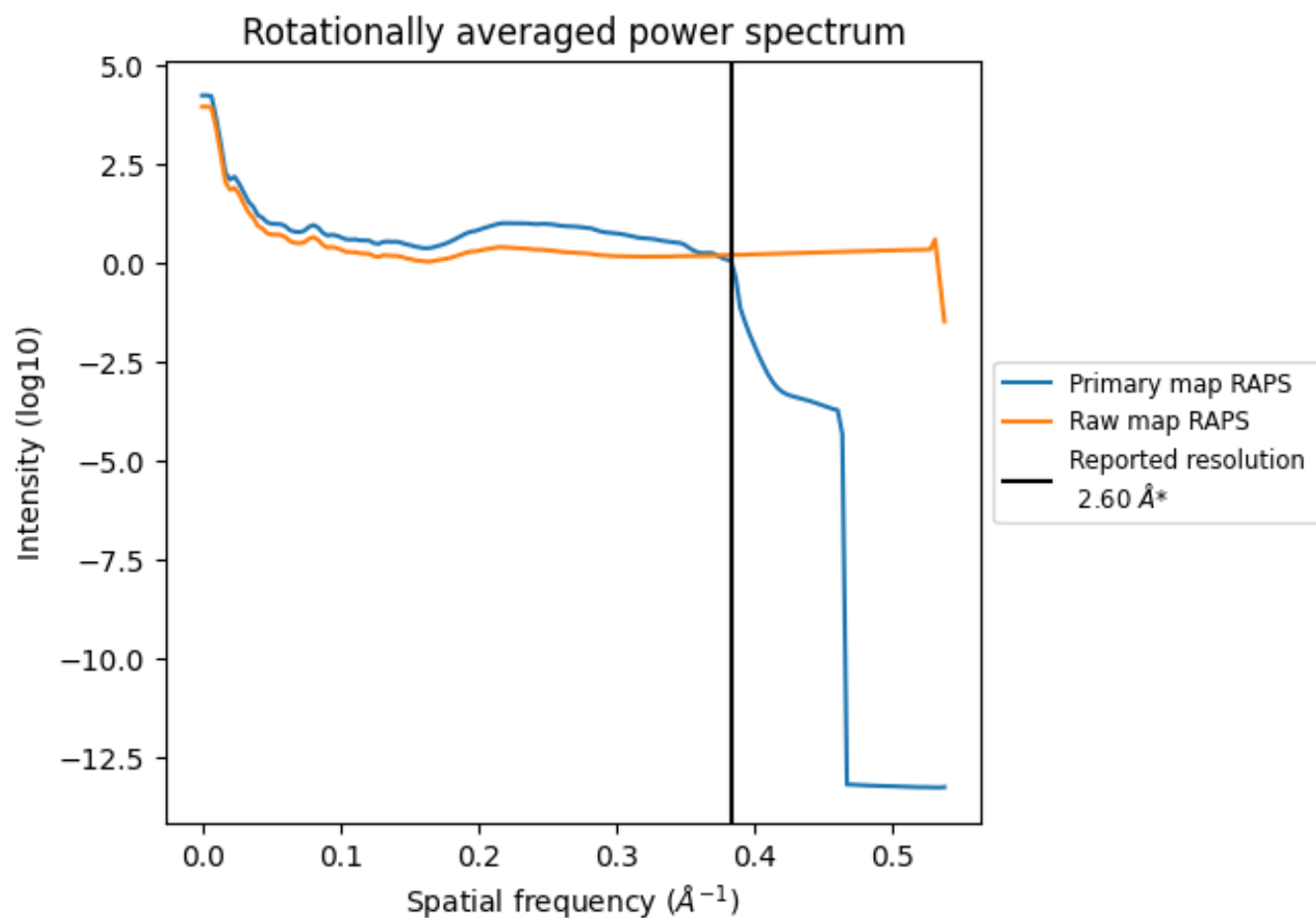
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm³; this corresponds to an approximate mass of 150 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 ⓘ

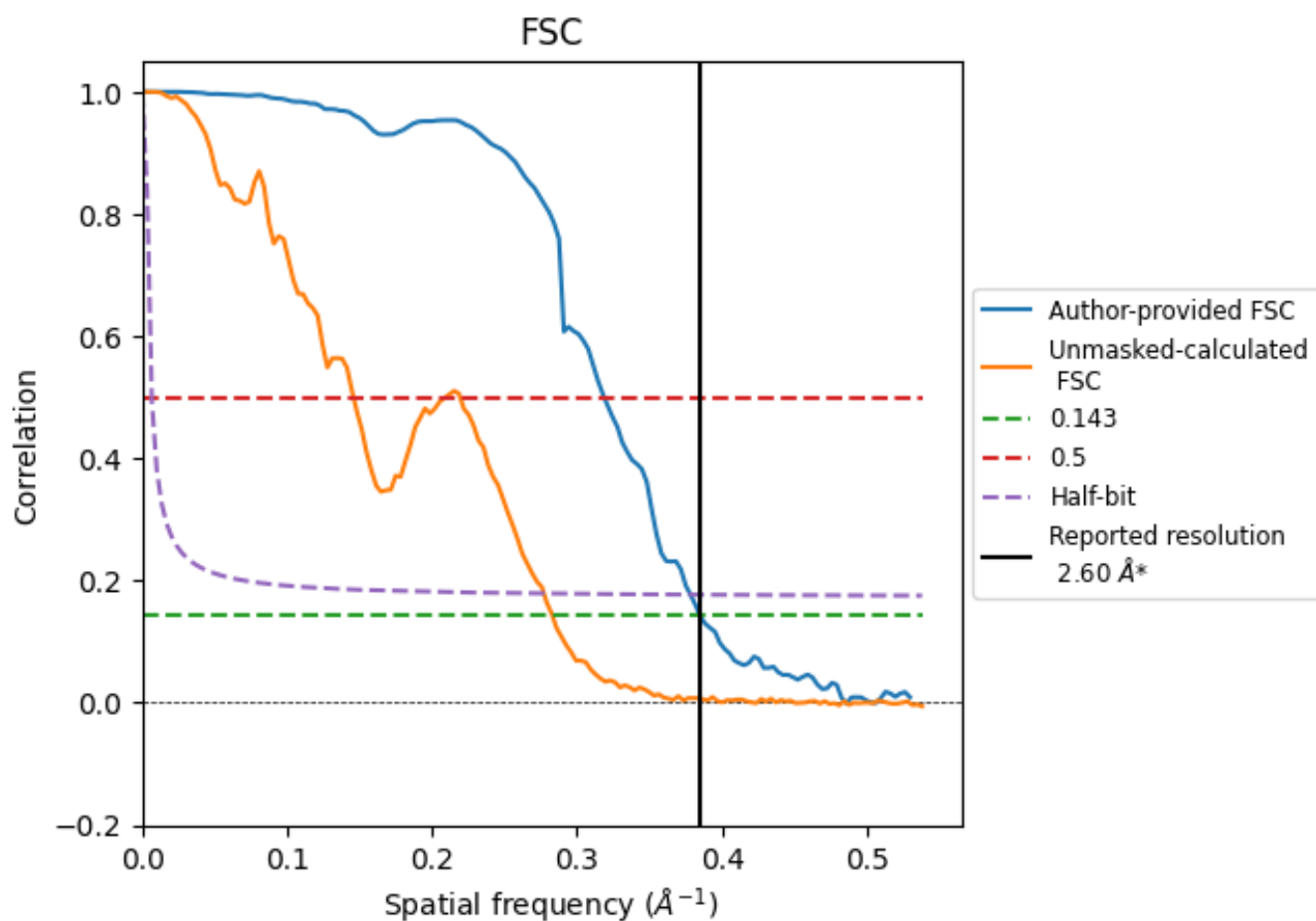


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

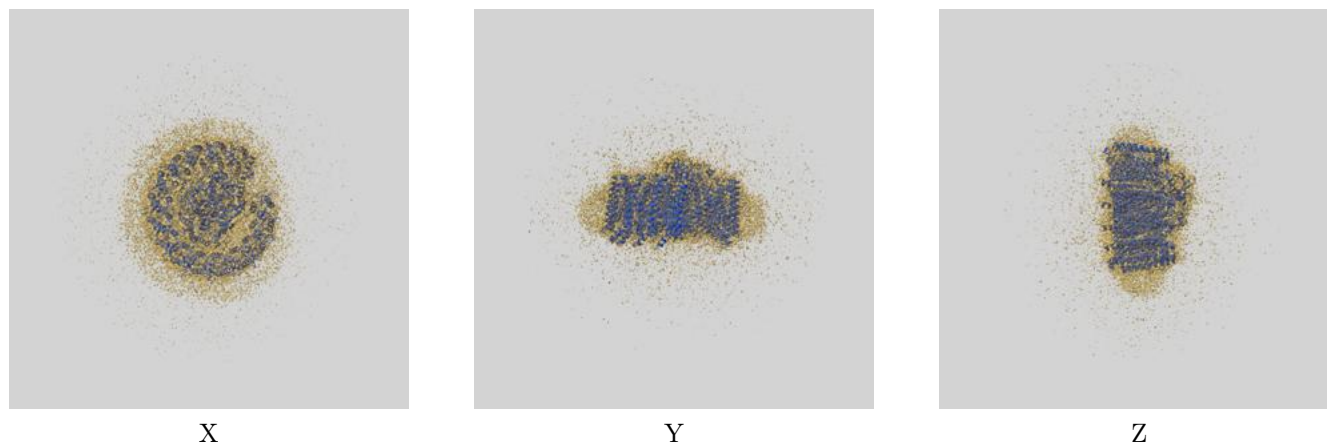
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.14	2.64
Unmasked-calculated*	3.53	6.86	3.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

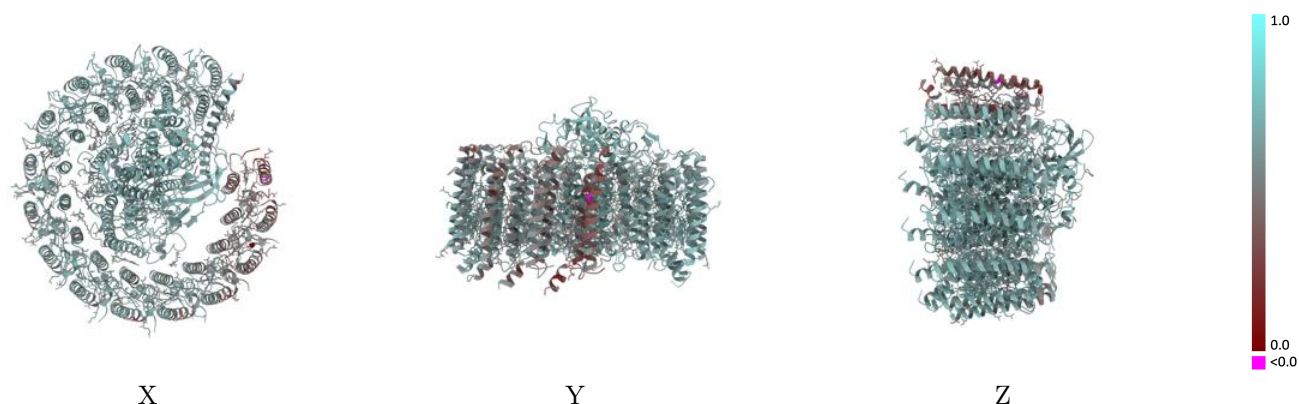
This section contains information regarding the fit between EMDB map EMD-39255 and PDB model 8YGL. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



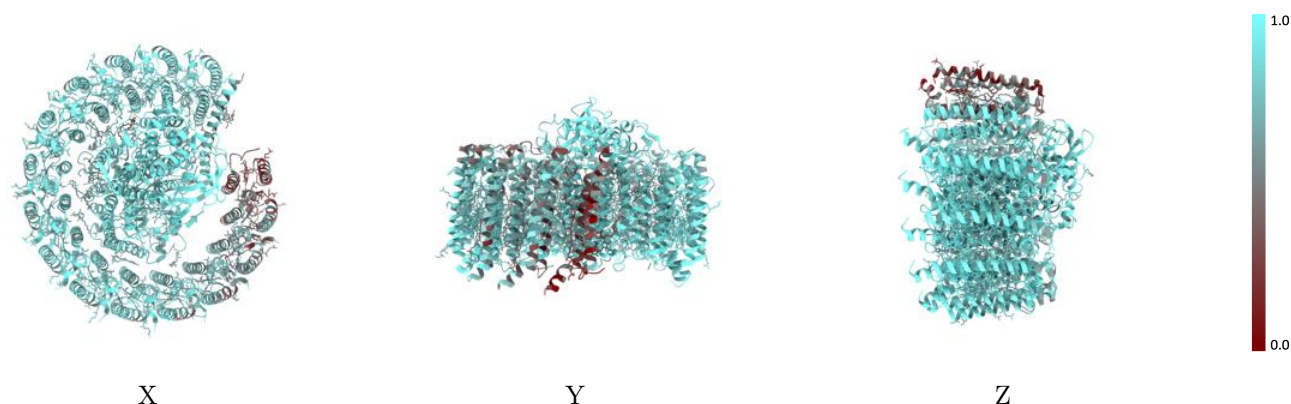
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



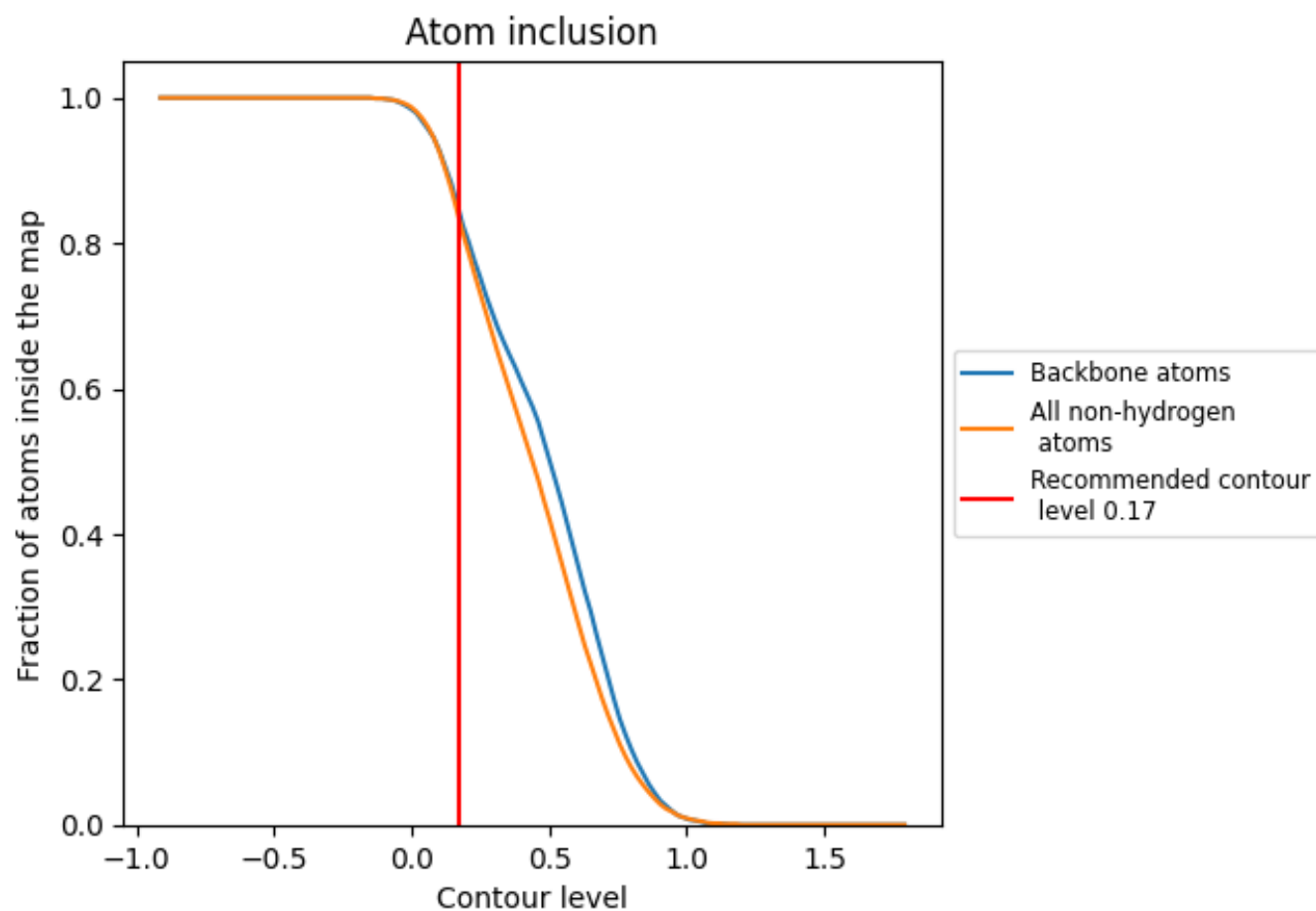
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.5900
0	 0.8640	 0.6040
1	 0.5490	 0.4500
2	 0.5300	 0.4490
3	 0.7230	 0.5090
7	 0.8760	 0.6170
8	 0.8720	 0.6090
9	 0.9310	 0.6320
A	 0.8760	 0.6090
B	 0.8820	 0.6280
C	 0.6790	 0.5110
D	 0.8980	 0.6180
E	 0.8920	 0.6180
F	 0.9330	 0.6410
G	 0.8600	 0.6060
H	 0.8980	 0.6200
I	 0.9070	 0.6260
J	 0.7980	 0.5650
K	 0.9200	 0.6200
L	 0.9210	 0.6370
M	 0.9220	 0.6380
N	 0.8350	 0.5880
O	 0.8940	 0.6120
P	 0.8390	 0.5850
Q	 0.9300	 0.6320
R	 0.8400	 0.5990
S	 0.8790	 0.5890
T	 0.8040	 0.5660
U	 0.8730	 0.6010
V	 0.8060	 0.5740
W	 0.8340	 0.5620
X	 0.8220	 0.5830
Z	 0.5810	 0.4510
a	 0.3170	 0.3490
b	 0.2530	 0.3280

