



## Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 09:33 pm GMT

PDB ID : 7ZE8  
EMDB ID : EMD-14685  
Title : PucE-LH2 complex from Rps. palustris  
Authors : Qian, P.; Cogdell, R.J.; Nguyen-Phan, T.C.  
Deposited on : 2022-03-30  
Resolution : 3.60 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

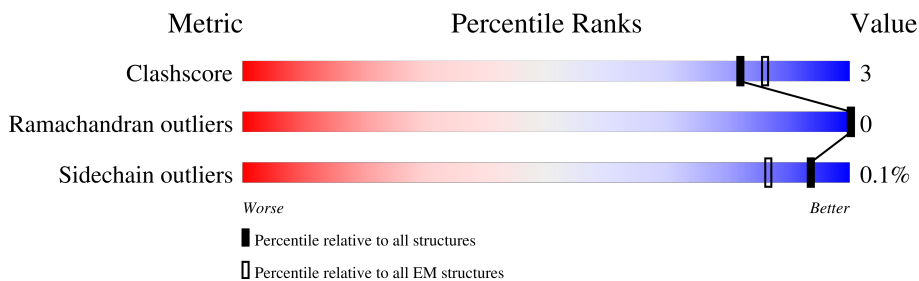
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	A	59	76% 5% 19%
1	C	59	78% 19%
1	E	59	73% 7% 19%
1	G	59	76% 19%
1	I	59	78% 19%
1	K	59	78% 19%
1	M	59	76% 19%
1	O	59	75% 5% 19%

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Mol	Chain	Length	Quality of chain
1	Q	59	 78% 19%
2	B	51	 90% 10%
2	D	51	 86% 10%
2	F	51	 84% 10%
2	H	51	 82% 8% 10%
2	J	51	 88% 10%
2	L	51	 86% 10%
2	N	51	 86% 10%
2	P	51	 82% 8% 10%
2	R	51	 90% 10%
3	S	97	 29% 92% 5% 10%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10068 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 Light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	48	382	255	63	63	1	0	0
1	C	48	382	255	63	63	1	0	0
1	E	48	382	255	63	63	1	0	0
1	G	48	382	255	63	63	1	0	0
1	I	48	382	255	63	63	1	0	0
1	K	48	382	255	63	63	1	0	0
1	M	48	382	255	63	63	1	0	0
1	O	48	382	255	63	63	1	0	0
1	Q	48	382	255	63	63	1	0	0

- Molecule 2 is a protein called Light-harvesting protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	46	371	246	62	63	0	0
2	D	46	371	246	62	63	0	0
2	F	46	371	246	62	63	0	0
2	H	46	371	246	62	63	0	0
2	J	46	371	246	62	63	0	0
2	L	46	371	246	62	63	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	N	46	Total 371	C 246	N 62	O 63	0	0
2	P	46	Total 371	C 246	N 62	O 63	0	0
2	R	46	Total 371	C 246	N 62	O 63	0	0

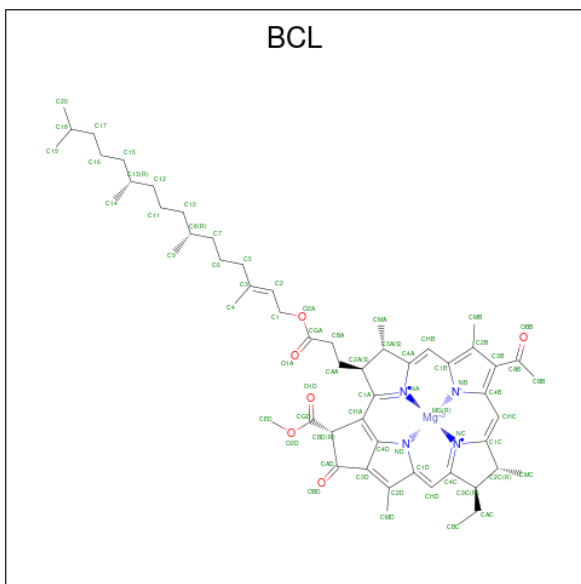
- Molecule 3 is a protein called PucA-LH2-gamma.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	S	94	Total 744	C 482	N 117	O 145	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	23	GLY	SER	conflict	UNP A0A2R4GRK2
S	82	ASP	GLU	conflict	UNP A0A2R4GRK2

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
4	A	1	Total 132	C 110	Mg 2	N 8	O 12	0

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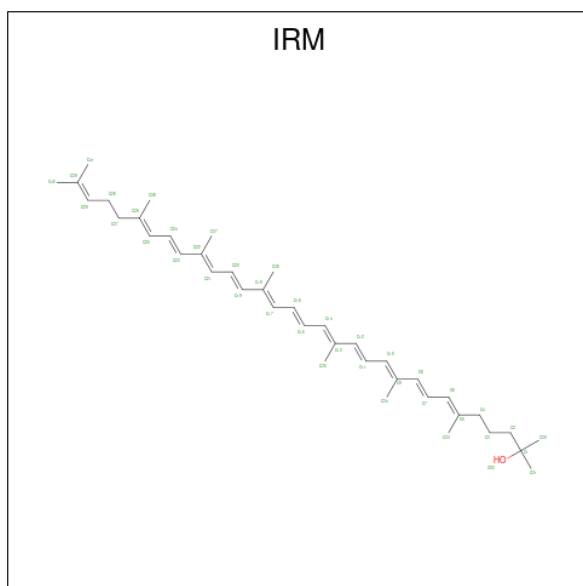
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
4	A	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	C	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	C	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	E	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	E	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	G	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	G	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	I	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	I	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	K	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	K	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	M	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	M	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	O	1	Total 132	C 110	Mg 2	N 8	O 12	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
4	O	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	Q	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	Q	1	Total 132	C 110	Mg 2	N 8	O 12	0
4	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	S	1	Total 396	C 330	Mg 6	N 24	O 36	0
4	S	1	Total 396	C 330	Mg 6	N 24	O 36	0
4	S	1	Total 396	C 330	Mg 6	N 24	O 36	0
4	S	1	Total 396	C 330	Mg 6	N 24	O 36	0
4	S	1	Total 396	C 330	Mg 6	N 24	O 36	0
4	S	1	Total 396	C 330	Mg 6	N 24	O 36	0

- Molecule 5 is 1,2-Dihydro-psi,psi-caroten-1-ol (three-letter code: IRM) (formula: C<sub>40</sub>H<sub>58</sub>O) (labeled as "Ligand of Interest" by depositor).




Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			41	40	1	
5	B	1	Total	C	O	0
			41	40	1	
5	C	1	Total	C	O	0
			41	40	1	
5	D	1	Total	C	O	0
			41	40	1	
5	G	1	Total	C	O	0
			41	40	1	
5	H	1	Total	C	O	0
			41	40	1	
5	I	1	Total	C	O	0
			41	40	1	
5	K	1	Total	C	O	0
			41	40	1	
5	P	1	Total	C	O	0
			41	40	1	

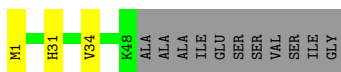


### 3 Residue-property plots


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

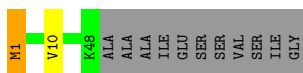
- Molecule 1: Light-harvesting protein

Chain A: 



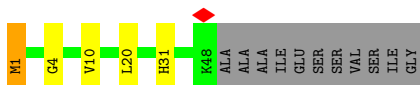
- Molecule 1: Light-harvesting protein

Chain C: 



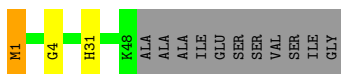
- Molecule 1: Light-harvesting protein

Chain E: 



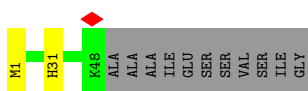
- Molecule 1: Light-harvesting protein

Chain G: 

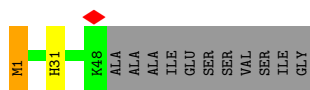
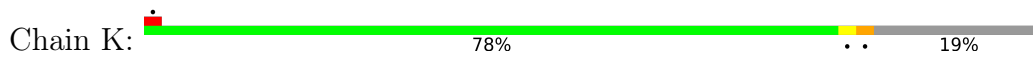


- Molecule 1: Light-harvesting protein

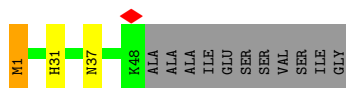
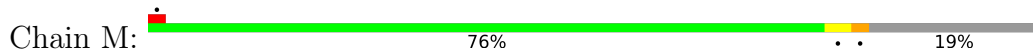
Chain I: 



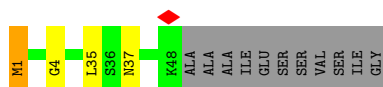
- Molecule 1: Light-harvesting protein



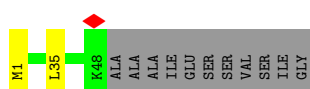
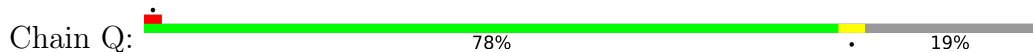
• Molecule 1: Light-harvesting protein



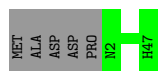
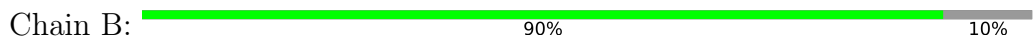
• Molecule 1: Light-harvesting protein



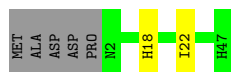
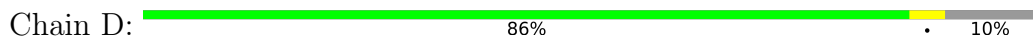
• Molecule 1: Light-harvesting protein



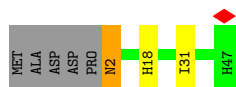
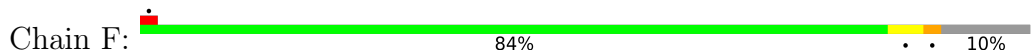
• Molecule 2: Light-harvesting protein



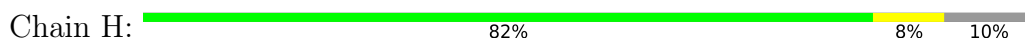
• Molecule 2: Light-harvesting protein



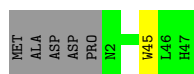
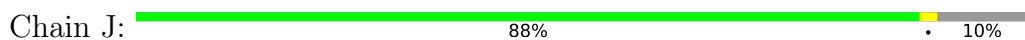
• Molecule 2: Light-harvesting protein



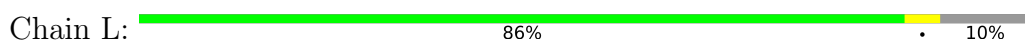
• Molecule 2: Light-harvesting protein



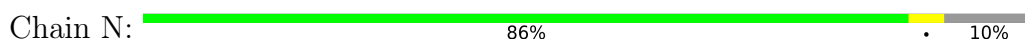
• Molecule 2: Light-harvesting protein



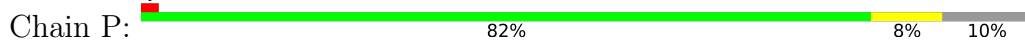
• Molecule 2: Light-harvesting protein



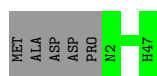
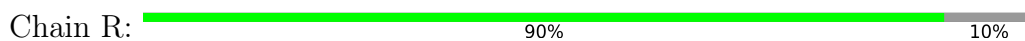
• Molecule 2: Light-harvesting protein



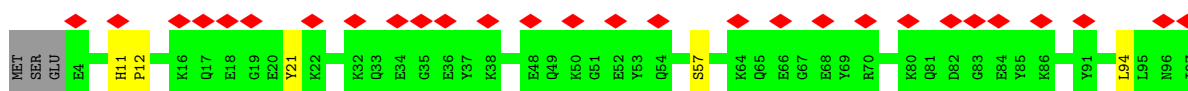
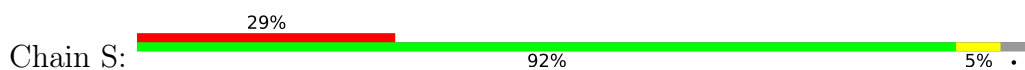
• Molecule 2: Light-harvesting protein



• Molecule 2: Light-harvesting protein



• Molecule 3: PucA-LH2-gamma



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	400518	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42.42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.351	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0347	Depositor
Map size ( $\text{\AA}$ )	195.0, 195.0, 195.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.65, 0.65, 0.65	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CXM, BCL, IRM

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	A	0.23	0/382	0.46	0/524
1	C	0.23	0/382	0.46	0/524
1	E	0.23	0/382	0.48	0/524
1	G	0.23	0/382	0.47	0/524
1	I	0.23	0/382	0.45	0/524
1	K	0.23	0/382	0.45	0/524
1	M	0.23	0/382	0.46	0/524
1	O	0.23	0/382	0.46	0/524
1	Q	0.23	0/382	0.47	0/524
2	B	0.23	0/384	0.44	0/524
2	D	0.23	0/384	0.44	0/524
2	F	0.23	0/384	0.43	0/524
2	H	0.23	0/384	0.44	0/524
2	J	0.23	0/384	0.43	0/524
2	L	0.22	0/384	0.43	0/524
2	N	0.23	0/384	0.41	0/524
2	P	0.23	0/384	0.42	0/524
2	R	0.23	0/384	0.43	0/524
3	S	0.25	0/763	0.49	0/1023
All	All	0.23	0/7657	0.45	0/10455

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	382	0	399	2	0
1	C	382	0	399	3	0
1	E	382	0	399	5	0
1	G	382	0	399	3	0
1	I	382	0	399	1	0
1	K	382	0	399	4	0
1	M	382	0	399	4	0
1	O	382	0	399	4	0
1	Q	382	0	399	1	0
2	B	371	0	364	0	0
2	D	371	0	364	2	0
2	F	371	0	364	4	0
2	H	371	0	364	4	0
2	J	371	0	364	1	0
2	L	371	0	364	3	0
2	N	371	0	364	2	0
2	P	371	0	364	4	0
2	R	371	0	364	0	0
3	S	744	0	730	4	0
4	A	132	0	148	3	0
4	B	66	0	74	2	0
4	C	132	0	148	4	0
4	D	66	0	74	1	0
4	E	132	0	148	4	0
4	F	66	0	74	1	0
4	G	132	0	148	3	0
4	H	66	0	74	1	0
4	I	132	0	148	1	0
4	J	66	0	74	2	0
4	K	132	0	148	1	0
4	L	66	0	74	2	0
4	M	132	0	148	2	0
4	N	66	0	74	2	0
4	O	132	0	148	3	0
4	P	66	0	74	1	0
4	Q	132	0	148	2	0
4	R	66	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	396	0	444	2	0
5	A	41	0	0	0	0
5	B	41	0	0	0	0
5	C	41	0	0	0	0
5	D	41	0	0	0	0
5	G	41	0	0	0	0
5	H	41	0	0	0	0
5	I	41	0	0	0	0
5	K	41	0	0	0	0
5	P	41	0	0	0	0
All	All	10068	0	10039	51	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 3.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:CXM:SD	2:H:26:ARG:NH2	2.71	0.64
4:C:102:BCL:H42	4:D:102:BCL:H203	1.79	0.63
4:Q:101:BCL:H42	4:R:101:BCL:H203	1.81	0.62
1:K:1:CXM:SD	2:L:26:ARG:NH2	2.73	0.61
1:M:1:CXM:ON2	2:N:18:HIS:NE2	2.32	0.60
4:E:102:BCL:HED1	4:G:101:BCL:H202	1.88	0.56
4:O:102:BCL:H42	4:P:102:BCL:H203	1.88	0.56
1:C:1:CXM:ON2	2:D:18:HIS:NE2	2.34	0.55
1:E:1:CXM:ON2	2:F:18:HIS:NE2	2.38	0.55
4:E:102:BCL:HHC	4:E:102:BCL:HBB2	1.89	0.54
1:K:1:CXM:HG2	2:L:22:ILE:HD13	1.90	0.54
1:E:10:VAL:HG11	4:G:101:BCL:H192	1.90	0.53
4:K:102:BCL:HBB2	4:K:102:BCL:HHC	1.90	0.53
4:N:101:BCL:HMA1	4:O:101:BCL:HMA1	1.91	0.53
4:O:102:BCL:HBB2	4:O:102:BCL:HHC	1.92	0.52
4:A:102:BCL:HHC	4:A:102:BCL:HBB2	1.91	0.52
4:C:102:BCL:HBB2	4:C:102:BCL:HHC	1.90	0.52
4:G:102:BCL:HBB2	4:G:102:BCL:HHC	1.92	0.51
1:M:1:CXM:HG3	2:N:22:ILE:HD13	1.93	0.50
4:M:101:BCL:HHC	4:M:101:BCL:HBB2	1.92	0.50
4:I:102:BCL:HHC	4:I:102:BCL:HBB2	1.92	0.50
2:P:22:ILE:HD12	3:S:94:LEU:HD12	1.93	0.49
4:Q:101:BCL:HHC	4:Q:101:BCL:HBB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:101:BCL:HED3	2:F:31:ILE:HG22	1.95	0.48
2:P:21:VAL:O	2:P:25:THR:HG23	2.13	0.48
2:H:23:ASP:OD2	3:S:21:TYR:OH	2.20	0.47
1:E:31:HIS:CE1	4:F:101:BCL:HMD1	2.51	0.46
4:C:102:BCL:HED2	1:E:20:LEU:HD13	1.98	0.45
2:F:2:ASN:HD22	2:F:2:ASN:N	2.15	0.45
1:C:10:VAL:HG11	4:E:101:BCL:H192	1.99	0.45
1:C:1:CXM:HA	2:D:22:ILE:HD11	1.98	0.44
2:J:45:TRP:CZ2	4:J:101:BCL:HHC	2.52	0.44
3:S:11:HIS:CG	3:S:12:PRO:HA	2.53	0.43
1:G:4:GLY:HA2	2:H:18:HIS:CG	2.54	0.43
3:S:57:SER:HA	4:S:103:BCL:C4C	2.49	0.43
1:I:31:HIS:CE1	4:J:101:BCL:HMD1	2.55	0.42
1:O:1:CXM:HG3	2:P:22:ILE:HD13	2.01	0.42
4:B:102:BCL:HMA1	4:C:101:BCL:HMA1	2.02	0.42
2:H:30:ALA:HB1	4:S:105:BCL:H192	2.01	0.42
1:A:34:VAL:HG11	4:A:101:BCL:HBC1	2.02	0.41
4:L:101:BCL:HMA1	4:M:102:BCL:HMA1	2.02	0.41
1:O:4:GLY:HA2	2:P:18:HIS:CG	2.55	0.41
1:E:4:GLY:HA2	2:F:18:HIS:CG	2.56	0.41
1:K:31:HIS:CE1	4:L:101:BCL:HMD1	2.56	0.41
1:M:37:ASN:ND2	1:O:35:LEU:HD21	2.35	0.41
1:A:31:HIS:CE1	4:B:102:BCL:HMD1	2.56	0.41
1:M:31:HIS:CE1	4:N:101:BCL:HMD1	2.56	0.41
1:O:37:ASN:ND2	1:Q:35:LEU:HD21	2.36	0.40
1:G:31:HIS:CE1	4:H:102:BCL:HMD1	2.55	0.40
1:K:1:CXM:HA	2:L:22:ILE:HD11	2.04	0.40
4:A:102:BCL:HHC	4:A:102:BCL:CBB	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
1	C	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
1	E	46/59 (78%)	46 (100%)	0	0	100	100
1	G	46/59 (78%)	46 (100%)	0	0	100	100
1	I	46/59 (78%)	46 (100%)	0	0	100	100
1	K	46/59 (78%)	46 (100%)	0	0	100	100
1	M	46/59 (78%)	46 (100%)	0	0	100	100
1	O	46/59 (78%)	46 (100%)	0	0	100	100
1	Q	46/59 (78%)	46 (100%)	0	0	100	100
2	B	44/51 (86%)	42 (96%)	2 (4%)	0	100	100
2	D	44/51 (86%)	43 (98%)	1 (2%)	0	100	100
2	F	44/51 (86%)	44 (100%)	0	0	100	100
2	H	44/51 (86%)	44 (100%)	0	0	100	100
2	J	44/51 (86%)	44 (100%)	0	0	100	100
2	L	44/51 (86%)	44 (100%)	0	0	100	100
2	N	44/51 (86%)	43 (98%)	1 (2%)	0	100	100
2	P	44/51 (86%)	44 (100%)	0	0	100	100
2	R	44/51 (86%)	43 (98%)	1 (2%)	0	100	100
3	S	92/97 (95%)	83 (90%)	9 (10%)	0	100	100
All	All	902/1087 (83%)	886 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	41/48 (85%)	41 (100%)	0	100	100
1	C	41/48 (85%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	41/48 (85%)	41 (100%)	0	100	100
1	G	41/48 (85%)	41 (100%)	0	100	100
1	I	41/48 (85%)	41 (100%)	0	100	100
1	K	41/48 (85%)	41 (100%)	0	100	100
1	M	41/48 (85%)	41 (100%)	0	100	100
1	O	41/48 (85%)	41 (100%)	0	100	100
1	Q	41/48 (85%)	41 (100%)	0	100	100
2	B	38/42 (90%)	38 (100%)	0	100	100
2	D	38/42 (90%)	38 (100%)	0	100	100
2	F	38/42 (90%)	37 (97%)	1 (3%)	46	74
2	H	38/42 (90%)	38 (100%)	0	100	100
2	J	38/42 (90%)	38 (100%)	0	100	100
2	L	38/42 (90%)	38 (100%)	0	100	100
2	N	38/42 (90%)	38 (100%)	0	100	100
2	P	38/42 (90%)	38 (100%)	0	100	100
2	R	38/42 (90%)	38 (100%)	0	100	100
3	S	78/81 (96%)	78 (100%)	0	100	100
All	All	789/891 (89%)	788 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	2	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	GLN
1	G	2	ASN
1	I	3	GLN
1	K	3	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CXM	A	1	1,4	8,10,11	2.13	2 (25%)	7,11,13	2.23	3 (42%)
1	CXM	I	1	1,4	8,10,11	2.11	2 (25%)	7,11,13	2.23	3 (42%)
1	CXM	G	1	1,4	8,10,11	2.12	2 (25%)	7,11,13	1.95	1 (14%)
1	CXM	K	1	1,4	8,10,11	2.13	2 (25%)	7,11,13	2.27	3 (42%)
1	CXM	M	1	1,4	8,10,11	2.13	2 (25%)	7,11,13	2.15	2 (28%)
1	CXM	O	1	1,4	8,10,11	2.12	2 (25%)	7,11,13	2.15	3 (42%)
1	CXM	Q	1	1,4	8,10,11	2.12	2 (25%)	7,11,13	2.23	3 (42%)
1	CXM	E	1	1,4	8,10,11	2.12	2 (25%)	7,11,13	2.21	3 (42%)
1	CXM	C	1	1,4	8,10,11	2.12	2 (25%)	7,11,13	2.06	3 (42%)

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
1	CXM	A	1	1,4	-	5/9/10/12	-
1	CXM	I	1	1,4	-	3/9/10/12	-
1	CXM	G	1	1,4	-	2/9/10/12	-
1	CXM	K	1	1,4	-	4/9/10/12	-
1	CXM	M	1	1,4	-	2/9/10/12	-
1	CXM	O	1	1,4	-	3/9/10/12	-
1	CXM	Q	1	1,4	-	3/9/10/12	-
1	CXM	E	1	1,4	-	1/9/10/12	-
1	CXM	C	1	1,4	-	3/9/10/12	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	1	CXM	CN-N	4.12	1.42	1.35
1	A	1	CXM	CN-N	4.07	1.42	1.35
1	K	1	CXM	CN-N	4.07	1.42	1.35
1	C	1	CXM	CN-N	4.06	1.42	1.35
1	Q	1	CXM	CN-N	4.06	1.42	1.35
1	E	1	CXM	CN-N	4.06	1.42	1.35
1	G	1	CXM	CN-N	4.05	1.42	1.35
1	I	1	CXM	CN-N	4.03	1.42	1.35
1	O	1	CXM	CN-N	4.03	1.42	1.35
1	K	1	CXM	ON1-CN	3.43	1.28	1.21
1	O	1	CXM	ON1-CN	3.41	1.28	1.21
1	G	1	CXM	ON1-CN	3.41	1.28	1.21
1	A	1	CXM	ON1-CN	3.40	1.28	1.21
1	Q	1	CXM	ON1-CN	3.40	1.28	1.21
1	M	1	CXM	ON1-CN	3.40	1.28	1.21
1	I	1	CXM	ON1-CN	3.39	1.28	1.21
1	E	1	CXM	ON1-CN	3.37	1.27	1.21
1	C	1	CXM	ON1-CN	3.36	1.27	1.21

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	1	CXM	ON1-CN-N	-4.76	117.03	124.85
1	E	1	CXM	ON1-CN-N	-4.64	117.23	124.85
1	I	1	CXM	ON1-CN-N	-4.62	117.27	124.85
1	A	1	CXM	ON1-CN-N	-4.61	117.29	124.85
1	M	1	CXM	ON1-CN-N	-4.57	117.34	124.85
1	O	1	CXM	ON1-CN-N	-4.51	117.46	124.85
1	Q	1	CXM	ON1-CN-N	-4.50	117.47	124.85
1	C	1	CXM	ON1-CN-N	-4.48	117.50	124.85
1	G	1	CXM	ON1-CN-N	-4.42	117.59	124.85
1	Q	1	CXM	C-CA-N	2.87	114.91	109.73
1	A	1	CXM	C-CA-N	2.68	114.56	109.73
1	K	1	CXM	C-CA-N	2.66	114.53	109.73
1	E	1	CXM	C-CA-N	2.62	114.46	109.73
1	I	1	CXM	C-CA-N	2.60	114.43	109.73
1	O	1	CXM	C-CA-N	2.36	114.00	109.73
1	M	1	CXM	C-CA-N	2.33	113.94	109.73
1	I	1	CXM	O-C-CA	-2.19	119.03	124.78
1	Q	1	CXM	O-C-CA	-2.14	119.16	124.78
1	C	1	CXM	C-CA-N	2.14	113.60	109.73
1	O	1	CXM	O-C-CA	-2.14	119.18	124.78
1	A	1	CXM	O-C-CA	-2.10	119.26	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	1	CXM	O-C-CA	-2.09	119.30	124.78
1	C	1	CXM	O-C-CA	-2.08	119.33	124.78
1	E	1	CXM	O-C-CA	-2.04	119.44	124.78

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CXM	N-CA-CB-CG
1	A	1	CXM	C-CA-CB-CG
1	A	1	CXM	O-C-CA-CB
1	C	1	CXM	N-CA-CB-CG
1	C	1	CXM	C-CA-CB-CG
1	K	1	CXM	N-CA-CB-CG
1	O	1	CXM	O-C-CA-CB
1	Q	1	CXM	O-C-CA-CB
1	G	1	CXM	CB-CG-SD-CE
1	O	1	CXM	CB-CG-SD-CE
1	Q	1	CXM	CB-CG-SD-CE
1	I	1	CXM	CB-CG-SD-CE
1	M	1	CXM	CB-CG-SD-CE
1	A	1	CXM	CB-CG-SD-CE
1	K	1	CXM	CB-CG-SD-CE
1	E	1	CXM	ON1-CN-N-CA
1	O	1	CXM	ON1-CN-N-CA
1	M	1	CXM	ON1-CN-N-CA
1	K	1	CXM	ON1-CN-N-CA
1	K	1	CXM	C-CA-CB-CG
1	Q	1	CXM	ON1-CN-N-CA
1	A	1	CXM	ON1-CN-N-CA
1	G	1	CXM	ON1-CN-N-CA
1	C	1	CXM	ON1-CN-N-CA
1	I	1	CXM	ON1-CN-N-CA
1	I	1	CXM	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	1	CXM	1	0
1	K	1	CXM	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	1	CXM	2	0
1	O	1	CXM	1	0
1	E	1	CXM	1	0
1	C	1	CXM	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BCL	J	101	-	58,74,74	1.28	5 (8%)	69,115,115	1.42	11 (15%)
4	BCL	N	101	-	58,74,74	1.26	5 (8%)	69,115,115	1.41	11 (15%)
5	IRM	C	103	-	40,40,40	0.18	0	47,49,49	0.23	0
4	BCL	C	101	-	58,74,74	1.24	4 (6%)	69,115,115	1.47	11 (15%)
4	BCL	B	102	-	58,74,74	1.29	5 (8%)	69,115,115	1.42	11 (15%)
5	IRM	H	101	-	40,40,40	0.15	0	47,49,49	0.35	0
4	BCL	O	102	1	58,74,74	1.23	4 (6%)	69,115,115	1.28	9 (13%)
4	BCL	S	105	3	58,74,74	1.29	4 (6%)	69,115,115	2.06	12 (17%)
4	BCL	C	102	1	58,74,74	1.24	5 (8%)	69,115,115	1.30	9 (13%)
4	BCL	A	102	1	58,74,74	1.25	5 (8%)	69,115,115	1.31	9 (13%)
4	BCL	P	102	-	58,74,74	1.27	5 (8%)	69,115,115	1.44	11 (15%)
4	BCL	M	102	-	58,74,74	1.22	4 (6%)	69,115,115	1.44	12 (17%)
4	BCL	R	101	-	58,74,74	1.26	5 (8%)	69,115,115	1.36	10 (14%)
4	BCL	Q	102	-	58,74,74	1.24	4 (6%)	69,115,115	1.44	12 (17%)
4	BCL	A	101	-	58,74,74	1.24	5 (8%)	69,115,115	1.47	12 (17%)
4	BCL	K	102	1	58,74,74	1.25	5 (8%)	69,115,115	1.33	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BCL	D	102	-	58,74,74	1.29	5 (8%)	69,115,115	1.43	10 (14%)
4	BCL	S	103	3	58,74,74	1.29	4 (6%)	69,115,115	1.42	12 (17%)
4	BCL	K	101	-	58,74,74	1.23	4 (6%)	69,115,115	1.43	10 (14%)
4	BCL	Q	101	1	58,74,74	1.25	5 (8%)	69,115,115	1.32	10 (14%)
4	BCL	F	101	-	58,74,74	1.26	5 (8%)	69,115,115	1.41	10 (14%)
5	IRM	B	101	-	40,40,40	0.18	0	47,49,49	0.31	0
4	BCL	I	102	1	58,74,74	1.24	5 (8%)	69,115,115	1.37	10 (14%)
5	IRM	A	103	-	40,40,40	0.17	0	47,49,49	0.28	0
4	BCL	G	102	1	58,74,74	1.24	4 (6%)	69,115,115	1.31	9 (13%)
4	BCL	I	101	-	58,74,74	1.26	5 (8%)	69,115,115	1.78	14 (20%)
5	IRM	D	101	-	40,40,40	0.18	0	47,49,49	0.29	0
4	BCL	S	102	3	58,74,74	1.27	4 (6%)	69,115,115	2.07	11 (15%)
4	BCL	E	102	1	58,74,74	1.25	4 (6%)	69,115,115	1.34	9 (13%)
5	IRM	K	103	-	40,40,40	0.15	0	47,49,49	0.30	0
4	BCL	S	101	3	58,74,74	1.29	5 (8%)	69,115,115	1.40	11 (15%)
4	BCL	M	101	1	58,74,74	1.24	5 (8%)	69,115,115	1.30	9 (13%)
4	BCL	S	106	3	58,74,74	1.30	5 (8%)	69,115,115	1.65	10 (14%)
5	IRM	I	103	-	40,40,40	0.19	0	47,49,49	0.32	0
5	IRM	G	103	-	40,40,40	0.17	0	47,49,49	0.32	0
4	BCL	E	101	-	58,74,74	1.25	4 (6%)	69,115,115	1.39	10 (14%)
4	BCL	H	102	-	58,74,74	1.27	5 (8%)	69,115,115	1.37	10 (14%)
4	BCL	O	101	-	58,74,74	1.22	4 (6%)	69,115,115	1.44	12 (17%)
4	BCL	G	101	-	58,74,74	1.24	4 (6%)	69,115,115	1.50	12 (17%)
5	IRM	P	101	-	40,40,40	0.18	0	47,49,49	0.31	0
4	BCL	L	101	-	58,74,74	1.27	5 (8%)	69,115,115	1.34	10 (14%)
4	BCL	S	104	3	58,74,74	1.28	5 (8%)	69,115,115	1.40	11 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	J	101	-	-	4/37/137/137	-
4	BCL	N	101	-	-	3/37/137/137	-
5	IRM	C	103	-	-	0/44/44/44	-
4	BCL	C	101	-	-	6/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	B	102	-	-	6/37/137/137	-
5	IRM	H	101	-	-	0/44/44/44	-
4	BCL	O	102	1	-	3/37/137/137	-
4	BCL	S	105	3	-	5/37/137/137	-
4	BCL	C	102	1	-	6/37/137/137	-
4	BCL	A	102	1	-	4/37/137/137	-
4	BCL	P	102	-	-	8/37/137/137	-
4	BCL	M	102	-	-	13/37/137/137	-
4	BCL	R	101	-	-	4/37/137/137	-
4	BCL	Q	102	-	-	10/37/137/137	-
4	BCL	A	101	-	-	10/37/137/137	-
4	BCL	K	102	1	-	8/37/137/137	-
4	BCL	D	102	-	-	8/37/137/137	-
4	BCL	S	103	3	-	9/37/137/137	-
4	BCL	K	101	-	-	8/37/137/137	-
4	BCL	Q	101	1	-	2/37/137/137	-
4	BCL	F	101	-	-	6/37/137/137	-
5	IRM	B	101	-	-	0/44/44/44	-
4	BCL	I	102	1	-	2/37/137/137	-
5	IRM	A	103	-	-	0/44/44/44	-
4	BCL	G	102	1	-	4/37/137/137	-
4	BCL	I	101	-	-	12/37/137/137	-
5	IRM	D	101	-	-	0/44/44/44	-
4	BCL	S	102	3	-	5/37/137/137	-
4	BCL	E	102	1	-	6/37/137/137	-
5	IRM	K	103	-	-	0/44/44/44	-
4	BCL	S	101	3	-	4/37/137/137	-
4	BCL	M	101	1	-	2/37/137/137	-
4	BCL	S	106	3	-	6/37/137/137	-
5	IRM	I	103	-	-	0/44/44/44	-
5	IRM	G	103	-	-	0/44/44/44	-
4	BCL	E	101	-	-	5/37/137/137	-
4	BCL	H	102	-	-	10/37/137/137	-
4	BCL	O	101	-	-	10/37/137/137	-
4	BCL	G	101	-	-	7/37/137/137	-
5	IRM	P	101	-	-	0/44/44/44	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	101	-	-	8/37/137/137	-
4	BCL	S	104	3	-	3/37/137/137	-

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	105	BCL	MG-NA	5.17	2.18	2.06
4	S	106	BCL	MG-NA	5.17	2.18	2.06
4	S	104	BCL	MG-NA	5.16	2.18	2.06
4	S	101	BCL	MG-NA	5.14	2.18	2.06
4	P	102	BCL	MG-NA	5.13	2.18	2.06
4	D	102	BCL	MG-NA	5.12	2.18	2.06
4	J	101	BCL	MG-NA	5.11	2.18	2.06
4	B	102	BCL	MG-NA	5.08	2.18	2.06
4	H	102	BCL	MG-NA	5.08	2.18	2.06
4	N	101	BCL	MG-NA	5.07	2.18	2.06
4	S	102	BCL	MG-NA	5.07	2.18	2.06
4	S	103	BCL	MG-NA	5.06	2.18	2.06
4	F	101	BCL	MG-NA	5.04	2.18	2.06
4	L	101	BCL	MG-NA	5.04	2.18	2.06
4	R	101	BCL	MG-NA	4.99	2.18	2.06
4	C	102	BCL	C1B-NB	4.96	1.39	1.35
4	G	102	BCL	MG-NA	4.92	2.18	2.06
4	A	102	BCL	MG-NA	4.91	2.17	2.06
4	K	102	BCL	MG-NA	4.90	2.17	2.06
4	K	101	BCL	MG-NA	4.89	2.17	2.06
4	I	101	BCL	C1B-NB	4.89	1.39	1.35
4	I	102	BCL	MG-NA	4.88	2.17	2.06
4	S	106	BCL	C1B-NB	4.88	1.39	1.35
4	A	102	BCL	C1B-NB	4.87	1.39	1.35
4	B	102	BCL	C1B-NB	4.87	1.39	1.35
4	K	102	BCL	C1B-NB	4.87	1.39	1.35
4	E	102	BCL	MG-NA	4.87	2.17	2.06
4	Q	101	BCL	C1B-NB	4.86	1.39	1.35
4	I	101	BCL	MG-NA	4.86	2.17	2.06
4	Q	101	BCL	MG-NA	4.85	2.17	2.06
4	A	101	BCL	MG-NA	4.85	2.17	2.06
4	G	101	BCL	C1B-NB	4.85	1.39	1.35
4	Q	102	BCL	C1B-NB	4.84	1.39	1.35
4	E	102	BCL	C1B-NB	4.83	1.39	1.35
4	O	102	BCL	C1B-NB	4.83	1.39	1.35
4	S	104	BCL	C1B-NB	4.82	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	105	BCL	C1B-NB	4.82	1.39	1.35
4	S	103	BCL	C1B-NB	4.82	1.39	1.35
4	S	101	BCL	C1B-NB	4.81	1.39	1.35
4	A	101	BCL	C1B-NB	4.81	1.39	1.35
4	E	101	BCL	MG-NA	4.81	2.17	2.06
4	C	101	BCL	MG-NA	4.80	2.17	2.06
4	L	101	BCL	C1B-NB	4.80	1.39	1.35
4	M	101	BCL	C1B-NB	4.80	1.39	1.35
4	I	102	BCL	C1B-NB	4.80	1.39	1.35
4	D	102	BCL	C1B-NB	4.79	1.39	1.35
4	M	101	BCL	MG-NA	4.78	2.17	2.06
4	C	102	BCL	MG-NA	4.78	2.17	2.06
4	R	101	BCL	C1B-NB	4.78	1.39	1.35
4	J	101	BCL	C1B-NB	4.78	1.39	1.35
4	H	102	BCL	C1B-NB	4.77	1.39	1.35
4	G	102	BCL	C1B-NB	4.77	1.39	1.35
4	N	101	BCL	C1B-NB	4.76	1.39	1.35
4	K	101	BCL	C1B-NB	4.76	1.39	1.35
4	C	101	BCL	C1B-NB	4.76	1.39	1.35
4	S	102	BCL	C1B-NB	4.76	1.39	1.35
4	P	102	BCL	C1B-NB	4.74	1.39	1.35
4	O	102	BCL	MG-NA	4.73	2.17	2.06
4	O	101	BCL	C1B-NB	4.73	1.39	1.35
4	M	102	BCL	MG-NA	4.73	2.17	2.06
4	E	101	BCL	C1B-NB	4.72	1.39	1.35
4	F	101	BCL	C1B-NB	4.72	1.39	1.35
4	Q	102	BCL	MG-NA	4.71	2.17	2.06
4	G	101	BCL	MG-NA	4.70	2.17	2.06
4	M	102	BCL	C1B-NB	4.70	1.39	1.35
4	O	101	BCL	MG-NA	4.66	2.17	2.06
4	S	106	BCL	MG-NC	3.84	2.15	2.06
4	S	103	BCL	MG-NC	3.82	2.15	2.06
4	S	101	BCL	MG-NC	3.82	2.15	2.06
4	S	105	BCL	MG-NC	3.81	2.15	2.06
4	B	102	BCL	MG-NC	3.78	2.15	2.06
4	S	104	BCL	MG-NC	3.78	2.15	2.06
4	S	102	BCL	MG-NC	3.71	2.15	2.06
4	J	101	BCL	MG-NC	3.69	2.15	2.06
4	L	101	BCL	MG-NC	3.68	2.15	2.06
4	D	102	BCL	MG-NC	3.66	2.15	2.06
4	N	101	BCL	MG-NC	3.63	2.14	2.06
4	P	102	BCL	MG-NC	3.62	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	102	BCL	MG-NC	3.60	2.14	2.06
4	H	102	BCL	MG-NC	3.58	2.14	2.06
4	I	101	BCL	MG-NC	3.58	2.14	2.06
4	F	101	BCL	MG-NC	3.57	2.14	2.06
4	G	101	BCL	MG-NC	3.56	2.14	2.06
4	E	101	BCL	MG-NC	3.54	2.14	2.06
4	C	101	BCL	MG-NC	3.53	2.14	2.06
4	O	101	BCL	MG-NC	3.50	2.14	2.06
4	G	102	BCL	MG-NC	3.49	2.14	2.06
4	E	102	BCL	MG-NC	3.49	2.14	2.06
4	Q	102	BCL	MG-NC	3.48	2.14	2.06
4	A	101	BCL	MG-NC	3.48	2.14	2.06
4	R	101	BCL	MG-NC	3.48	2.14	2.06
4	M	101	BCL	MG-NC	3.47	2.14	2.06
4	Q	101	BCL	MG-NC	3.45	2.14	2.06
4	O	102	BCL	MG-NC	3.45	2.14	2.06
4	K	102	BCL	MG-NC	3.39	2.14	2.06
4	K	101	BCL	MG-NC	3.38	2.14	2.06
4	C	102	BCL	MG-NC	3.38	2.14	2.06
4	A	102	BCL	MG-NC	3.38	2.14	2.06
4	I	102	BCL	MG-NC	3.27	2.14	2.06
4	O	101	BCL	OBD-CAD	2.29	1.25	1.22
4	G	101	BCL	OBD-CAD	2.28	1.25	1.22
4	Q	102	BCL	OBD-CAD	2.27	1.25	1.22
4	M	102	BCL	OBD-CAD	2.25	1.25	1.22
4	S	101	BCL	OBD-CAD	2.24	1.25	1.22
4	A	102	BCL	OBD-CAD	2.23	1.25	1.22
4	S	106	BCL	OBD-CAD	2.22	1.25	1.22
4	S	104	BCL	OBD-CAD	2.21	1.25	1.22
4	S	103	BCL	OBD-CAD	2.20	1.25	1.22
4	C	102	BCL	C4B-NB	2.20	1.37	1.35
4	S	102	BCL	OBD-CAD	2.19	1.25	1.22
4	C	102	BCL	OBD-CAD	2.18	1.25	1.22
4	K	102	BCL	C4B-NB	2.18	1.37	1.35
4	A	102	BCL	C4B-NB	2.18	1.37	1.35
4	A	101	BCL	OBD-CAD	2.18	1.25	1.22
4	S	105	BCL	OBD-CAD	2.18	1.25	1.22
4	S	106	BCL	C4B-NB	2.17	1.37	1.35
4	I	101	BCL	OBD-CAD	2.16	1.25	1.22
4	K	102	BCL	OBD-CAD	2.15	1.25	1.22
4	P	102	BCL	C4B-NB	2.14	1.37	1.35
4	G	102	BCL	OBD-CAD	2.13	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	102	BCL	OBD-CAD	2.12	1.25	1.22
4	F	101	BCL	OBD-CAD	2.12	1.25	1.22
4	E	102	BCL	OBD-CAD	2.12	1.25	1.22
4	A	101	BCL	C4B-NB	2.11	1.37	1.35
4	H	102	BCL	C4B-NB	2.10	1.37	1.35
4	L	101	BCL	OBD-CAD	2.09	1.25	1.22
4	E	101	BCL	OBD-CAD	2.09	1.25	1.22
4	I	101	BCL	C4B-NB	2.09	1.37	1.35
4	M	101	BCL	OBD-CAD	2.09	1.25	1.22
4	B	102	BCL	OBD-CAD	2.09	1.25	1.22
4	B	102	BCL	C4B-NB	2.09	1.37	1.35
4	R	101	BCL	C4B-NB	2.09	1.37	1.35
4	S	104	BCL	C4B-NB	2.07	1.37	1.35
4	N	101	BCL	C4B-NB	2.07	1.37	1.35
4	H	102	BCL	OBD-CAD	2.07	1.25	1.22
4	F	101	BCL	C4B-NB	2.07	1.37	1.35
4	P	102	BCL	OBD-CAD	2.07	1.25	1.22
4	Q	101	BCL	OBD-CAD	2.07	1.25	1.22
4	D	102	BCL	OBD-CAD	2.07	1.25	1.22
4	R	101	BCL	OBD-CAD	2.07	1.25	1.22
4	K	101	BCL	OBD-CAD	2.07	1.25	1.22
4	C	101	BCL	OBD-CAD	2.06	1.25	1.22
4	D	102	BCL	C4B-NB	2.06	1.37	1.35
4	S	101	BCL	C4B-NB	2.06	1.37	1.35
4	J	101	BCL	OBD-CAD	2.06	1.25	1.22
4	I	102	BCL	C4B-NB	2.05	1.37	1.35
4	L	101	BCL	C4B-NB	2.05	1.37	1.35
4	J	101	BCL	C4B-NB	2.04	1.37	1.35
4	N	101	BCL	OBD-CAD	2.03	1.25	1.22
4	O	102	BCL	OBD-CAD	2.03	1.25	1.22
4	Q	101	BCL	C4B-NB	2.00	1.37	1.35
4	M	101	BCL	C4B-NB	2.00	1.37	1.35

All (350) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	102	BCL	C1-C2-C3	12.19	147.13	126.04
4	S	105	BCL	C1-O2A-CGA	9.94	142.53	116.44
4	I	101	BCL	C1-C2-C3	8.23	140.27	126.04
4	S	106	BCL	C1-O2A-CGA	8.04	137.53	116.44
4	S	105	BCL	C1-C2-C3	7.62	139.22	126.04
4	G	101	BCL	CAD-C3D-C4D	-4.60	105.91	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	101	BCL	CAD-C3D-C4D	-4.45	105.99	108.47
4	A	101	BCL	CAD-C3D-C4D	-4.31	106.06	108.47
4	M	102	BCL	CAD-C3D-C4D	-4.30	106.07	108.47
4	N	101	BCL	CMB-C2B-C1B	-4.27	121.89	128.46
4	P	102	BCL	CMB-C2B-C1B	-4.27	121.90	128.46
4	G	101	BCL	CMB-C2B-C1B	-4.27	121.91	128.46
4	F	101	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
4	I	101	BCL	CMB-C2B-C1B	-4.23	121.97	128.46
4	Q	102	BCL	CMB-C2B-C1B	-4.23	121.97	128.46
4	D	102	BCL	CAD-C3D-C4D	-4.22	106.11	108.47
4	I	101	BCL	CAD-C3D-C4D	-4.22	106.12	108.47
4	H	102	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
4	O	101	BCL	CMB-C2B-C1B	-4.21	122.00	128.46
4	J	101	BCL	CMB-C2B-C1B	-4.20	122.00	128.46
4	R	101	BCL	CMB-C2B-C1B	-4.20	122.01	128.46
4	L	101	BCL	CMB-C2B-C1B	-4.18	122.03	128.46
4	S	102	BCL	CMB-C2B-C1B	-4.18	122.04	128.46
4	S	101	BCL	CMB-C2B-C1B	-4.18	122.04	128.46
4	B	102	BCL	CMB-C2B-C1B	-4.17	122.05	128.46
4	A	101	BCL	CMB-C2B-C1B	-4.17	122.06	128.46
4	C	101	BCL	CMB-C2B-C1B	-4.17	122.06	128.46
4	S	105	BCL	CMB-C2B-C1B	-4.16	122.07	128.46
4	D	102	BCL	CMB-C2B-C1B	-4.16	122.08	128.46
4	M	102	BCL	CMB-C2B-C1B	-4.16	122.08	128.46
4	S	103	BCL	CMB-C2B-C1B	-4.13	122.12	128.46
4	E	101	BCL	CMB-C2B-C1B	-4.11	122.15	128.46
4	K	101	BCL	CMB-C2B-C1B	-4.10	122.16	128.46
4	S	104	BCL	CMB-C2B-C1B	-4.09	122.19	128.46
4	S	105	BCL	CAD-C3D-C4D	-4.05	106.21	108.47
4	Q	102	BCL	CAD-C3D-C4D	-4.00	106.24	108.47
4	O	101	BCL	CAD-C3D-C4D	-3.96	106.26	108.47
4	C	101	BCL	CAD-C3D-C4D	-3.89	106.30	108.47
4	Q	101	BCL	CAD-C3D-C4D	-3.83	106.33	108.47
4	G	102	BCL	CMB-C2B-C1B	-3.83	122.58	128.46
4	I	102	BCL	CMB-C2B-C1B	-3.82	122.60	128.46
4	M	101	BCL	CMB-C2B-C1B	-3.81	122.61	128.46
4	I	101	BCL	C2A-C1A-CHA	3.81	130.51	123.86
4	S	106	BCL	CAD-C3D-C4D	-3.80	106.35	108.47
4	S	102	BCL	C4A-NA-C1A	3.77	108.40	106.71
4	A	101	BCL	C2A-C1A-CHA	3.77	130.45	123.86
4	E	102	BCL	CMB-C2B-C1B	-3.76	122.69	128.46
4	K	102	BCL	CMB-C2B-C1B	-3.71	122.77	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	101	BCL	CMB-C2B-C1B	-3.69	122.79	128.46
4	S	106	BCL	CMB-C2B-C1B	-3.69	122.79	128.46
4	E	102	BCL	CAD-C3D-C4D	-3.67	106.42	108.47
4	B	102	BCL	CAD-C3D-C4D	-3.66	106.43	108.47
4	A	102	BCL	CMB-C2B-C1B	-3.66	122.84	128.46
4	I	102	BCL	C4A-NA-C1A	3.65	108.35	106.71
4	A	102	BCL	C4A-NA-C1A	3.64	108.34	106.71
4	C	101	BCL	C4A-NA-C1A	3.64	108.34	106.71
4	E	101	BCL	C4A-NA-C1A	3.63	108.34	106.71
4	F	101	BCL	CAD-C3D-C4D	-3.63	106.44	108.47
4	K	102	BCL	C4A-NA-C1A	3.60	108.32	106.71
4	O	102	BCL	CMB-C2B-C1B	-3.59	122.94	128.46
4	P	102	BCL	C4A-NA-C1A	3.57	108.31	106.71
4	N	101	BCL	CAD-C3D-C4D	-3.56	106.48	108.47
4	J	101	BCL	CAD-C3D-C4D	-3.56	106.48	108.47
4	C	102	BCL	CMB-C2B-C1B	-3.56	122.99	128.46
4	C	102	BCL	C4A-NA-C1A	3.52	108.29	106.71
4	G	101	BCL	C2A-C1A-CHA	3.47	129.93	123.86
4	S	101	BCL	CAD-C3D-C4D	-3.47	106.53	108.47
4	D	102	BCL	C4A-NA-C1A	3.47	108.27	106.71
4	M	101	BCL	C4A-NA-C1A	3.45	108.26	106.71
4	S	104	BCL	C4A-NA-C1A	3.44	108.25	106.71
4	E	101	BCL	CAD-C3D-C4D	-3.44	106.55	108.47
4	A	101	BCL	CHA-C1A-NA	-3.43	118.53	126.40
4	S	106	BCL	C4A-NA-C1A	3.43	108.25	106.71
4	Q	102	BCL	C2A-C1A-CHA	3.42	129.84	123.86
4	H	102	BCL	CAD-C3D-C4D	-3.41	106.57	108.47
4	C	101	BCL	C1-C2-C3	3.41	131.94	126.04
4	P	102	BCL	CAD-C3D-C4D	-3.39	106.58	108.47
4	N	101	BCL	OBD-CAD-CBD	-3.39	121.05	125.89
4	F	101	BCL	OBD-CAD-CBD	-3.39	121.05	125.89
4	O	102	BCL	OBD-CAD-CBD	-3.39	121.06	125.89
4	R	101	BCL	CAD-C3D-C4D	-3.39	106.58	108.47
4	P	102	BCL	OBD-CAD-CBD	-3.39	121.06	125.89
4	E	102	BCL	C4A-NA-C1A	3.39	108.23	106.71
4	L	101	BCL	OBD-CAD-CBD	-3.38	121.07	125.89
4	H	102	BCL	OBD-CAD-CBD	-3.37	121.08	125.89
4	B	102	BCL	OBD-CAD-CBD	-3.37	121.08	125.89
4	R	101	BCL	OBD-CAD-CBD	-3.37	121.08	125.89
4	S	101	BCL	C4A-NA-C1A	3.36	108.22	106.71
4	I	101	BCL	CHA-C1A-NA	-3.36	118.71	126.40
4	J	101	BCL	OBD-CAD-CBD	-3.35	121.11	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	104	BCL	OBD-CAD-CBD	-3.35	121.11	125.89
4	F	101	BCL	C4A-NA-C1A	3.34	108.21	106.71
4	G	102	BCL	C4A-NA-C1A	3.34	108.21	106.71
4	S	102	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
4	A	102	BCL	OBD-CAD-CBD	-3.34	121.13	125.89
4	D	102	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
4	C	102	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
4	M	101	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
4	K	101	BCL	C4A-NA-C1A	3.32	108.20	106.71
4	E	101	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
4	K	101	BCL	CHA-C1A-NA	-3.31	118.81	126.40
4	S	103	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
4	K	102	BCL	OBD-CAD-CBD	-3.31	121.17	125.89
4	N	101	BCL	C4A-NA-C1A	3.31	108.19	106.71
4	H	102	BCL	C4A-NA-C1A	3.30	108.19	106.71
4	G	102	BCL	OBD-CAD-CBD	-3.30	121.18	125.89
4	J	101	BCL	C4A-NA-C1A	3.30	108.19	106.71
4	K	101	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
4	S	105	BCL	CHA-C1A-NA	-3.28	118.89	126.40
4	I	102	BCL	OBD-CAD-CBD	-3.28	121.21	125.89
4	S	101	BCL	OBD-CAD-CBD	-3.26	121.24	125.89
4	K	101	BCL	C2A-C1A-CHA	3.25	129.54	123.86
4	S	105	BCL	OBD-CAD-CBD	-3.25	121.25	125.89
4	Q	101	BCL	C4A-NA-C1A	3.25	108.17	106.71
4	S	103	BCL	CAD-C3D-C4D	-3.23	106.67	108.47
4	I	102	BCL	CAD-C3D-C4D	-3.22	106.67	108.47
4	S	106	BCL	OBD-CAD-CBD	-3.21	121.30	125.89
4	C	101	BCL	OBD-CAD-CBD	-3.21	121.31	125.89
4	K	102	BCL	CAD-C3D-C4D	-3.20	106.69	108.47
4	O	101	BCL	C2A-C1A-CHA	3.19	129.44	123.86
4	Q	101	BCL	OBD-CAD-CBD	-3.19	121.33	125.89
4	G	102	BCL	CAD-C3D-C4D	-3.19	106.69	108.47
4	R	101	BCL	C4A-NA-C1A	3.17	108.13	106.71
4	M	102	BCL	C2A-C1A-CHA	3.16	129.38	123.86
4	A	101	BCL	OBD-CAD-CBD	-3.15	121.39	125.89
4	I	101	BCL	OBD-CAD-CBD	-3.14	121.41	125.89
4	Q	102	BCL	CHA-C1A-NA	-3.13	119.22	126.40
4	E	102	BCL	OBD-CAD-CBD	-3.13	121.42	125.89
4	N	101	BCL	CMB-C2B-C3B	3.13	130.53	124.68
4	G	101	BCL	CHA-C1A-NA	-3.12	119.25	126.40
4	F	101	BCL	CMB-C2B-C3B	3.12	130.52	124.68
4	M	102	BCL	OBD-CAD-CBD	-3.12	121.44	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	102	BCL	CMB-C2B-C3B	3.12	130.51	124.68
4	S	103	BCL	C4A-NA-C1A	3.12	108.11	106.71
4	G	101	BCL	CMB-C2B-C3B	3.11	130.50	124.68
4	O	102	BCL	C4A-NA-C1A	3.11	108.10	106.71
4	S	105	BCL	CMB-C2B-C3B	3.10	130.49	124.68
4	L	101	BCL	CAD-C3D-C4D	-3.10	106.74	108.47
4	P	102	BCL	CMB-C2B-C3B	3.10	130.47	124.68
4	Q	102	BCL	OBD-CAD-CBD	-3.09	121.48	125.89
4	S	101	BCL	CMB-C2B-C3B	3.09	130.45	124.68
4	Q	102	BCL	CMB-C2B-C3B	3.07	130.42	124.68
4	O	101	BCL	CMB-C2B-C3B	3.07	130.42	124.68
4	S	103	BCL	CMB-C2B-C3B	3.07	130.42	124.68
4	I	101	BCL	CMB-C2B-C3B	3.07	130.42	124.68
4	J	101	BCL	CHA-C1A-NA	-3.06	119.39	126.40
4	H	102	BCL	CMB-C2B-C3B	3.06	130.40	124.68
4	R	101	BCL	CMB-C2B-C3B	3.06	130.40	124.68
4	B	102	BCL	CMB-C2B-C3B	3.06	130.40	124.68
4	J	101	BCL	CMB-C2B-C3B	3.05	130.38	124.68
4	S	104	BCL	CMB-C2B-C3B	3.05	130.38	124.68
4	H	102	BCL	CHA-C1A-NA	-3.05	119.42	126.40
4	L	101	BCL	CMB-C2B-C3B	3.04	130.37	124.68
4	P	102	BCL	C1-C2-C3	-3.04	120.79	126.04
4	P	102	BCL	CHA-C1A-NA	-3.03	119.45	126.40
4	D	102	BCL	CMB-C2B-C3B	3.03	130.35	124.68
4	M	101	BCL	CAD-C3D-C4D	-3.03	106.78	108.47
4	M	102	BCL	CHA-C1A-NA	-3.03	119.46	126.40
4	C	102	BCL	CAD-C3D-C4D	-3.03	106.78	108.47
4	C	101	BCL	CMB-C2B-C3B	3.02	130.34	124.68
4	S	102	BCL	CAD-C3D-C4D	-3.02	106.78	108.47
4	A	101	BCL	CMB-C2B-C3B	3.02	130.33	124.68
4	O	101	BCL	OBD-CAD-CBD	-3.02	121.58	125.89
4	O	101	BCL	CHA-C1A-NA	-3.01	119.51	126.40
4	M	102	BCL	CMB-C2B-C3B	3.00	130.30	124.68
4	F	101	BCL	CHA-C1A-NA	-3.00	119.54	126.40
4	A	102	BCL	CAD-C3D-C4D	-2.99	106.80	108.47
4	G	101	BCL	OBD-CAD-CBD	-2.99	121.63	125.89
4	E	101	BCL	CMB-C2B-C3B	2.98	130.25	124.68
4	B	102	BCL	CHA-C1A-NA	-2.97	119.60	126.40
4	E	102	BCL	CHA-C1A-NA	-2.95	119.63	126.40
4	K	101	BCL	CMB-C2B-C3B	2.95	130.19	124.68
4	R	101	BCL	CHA-C1A-NA	-2.94	119.66	126.40
4	N	101	BCL	CHA-C1A-NA	-2.94	119.66	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	101	BCL	CHA-C1A-NA	-2.94	119.67	126.40
4	S	106	BCL	CHA-C1A-NA	-2.93	119.69	126.40
4	A	102	BCL	CHA-C1A-NA	-2.93	119.70	126.40
4	D	102	BCL	CHA-C1A-NA	-2.91	119.73	126.40
4	G	101	BCL	O2D-CGD-O1D	-2.91	118.16	123.84
4	S	104	BCL	CHA-C1A-NA	-2.89	119.78	126.40
4	G	102	BCL	CHA-C1A-NA	-2.89	119.78	126.40
4	S	104	BCL	CAD-C3D-C4D	-2.89	106.86	108.47
4	O	101	BCL	O2D-CGD-O1D	-2.89	118.19	123.84
4	S	103	BCL	CHA-C1A-NA	-2.88	119.79	126.40
4	M	102	BCL	C4A-NA-C1A	2.88	108.00	106.71
4	S	102	BCL	CHA-C1A-NA	-2.88	119.80	126.40
4	E	101	BCL	CHA-C1A-NA	-2.88	119.80	126.40
4	K	102	BCL	CHA-C1A-NA	-2.87	119.84	126.40
4	I	102	BCL	CHA-C1A-NA	-2.86	119.84	126.40
4	S	101	BCL	CHA-C1A-NA	-2.86	119.85	126.40
4	Q	101	BCL	CHA-C1A-NA	-2.85	119.88	126.40
4	C	102	BCL	CHA-C1A-NA	-2.84	119.88	126.40
4	B	102	BCL	C4A-NA-C1A	2.84	107.98	106.71
4	O	102	BCL	CHA-C1A-NA	-2.84	119.89	126.40
4	H	102	BCL	C2A-C1A-CHA	2.83	128.81	123.86
4	B	102	BCL	C2A-C1A-CHA	2.82	128.78	123.86
4	C	101	BCL	CHA-C1A-NA	-2.82	119.95	126.40
4	M	101	BCL	CHA-C1A-NA	-2.81	119.97	126.40
4	S	102	BCL	C2A-C1A-CHA	2.80	128.75	123.86
4	M	102	BCL	O2D-CGD-O1D	-2.78	118.41	123.84
4	Q	102	BCL	O2D-CGD-O1D	-2.76	118.45	123.84
4	J	101	BCL	C2A-C1A-CHA	2.76	128.68	123.86
4	R	101	BCL	C2A-C1A-CHA	2.75	128.67	123.86
4	O	102	BCL	CAD-C3D-C4D	-2.75	106.94	108.47
4	P	102	BCL	C2A-C1A-CHA	2.74	128.65	123.86
4	N	101	BCL	C2A-C1A-CHA	2.72	128.61	123.86
4	E	102	BCL	C2A-C1A-CHA	2.70	128.58	123.86
4	L	101	BCL	C4A-NA-C1A	2.70	107.92	106.71
4	S	106	BCL	C2A-C1A-CHA	2.68	128.54	123.86
4	S	104	BCL	C1-O2A-CGA	2.67	123.46	116.44
4	F	101	BCL	C2A-C1A-CHA	2.66	128.50	123.86
4	E	101	BCL	C2A-C1A-CHA	2.65	128.49	123.86
4	A	101	BCL	C4A-NA-C1A	2.64	107.89	106.71
4	S	104	BCL	C2A-C1A-CHA	2.64	128.48	123.86
4	C	102	BCL	C2A-C1A-CHA	2.61	128.43	123.86
4	I	102	BCL	C1-C2-C3	2.61	130.56	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	102	BCL	C2A-C1A-CHA	2.61	128.42	123.86
4	L	101	BCL	C2A-C1A-CHA	2.60	128.40	123.86
4	S	105	BCL	C11-C10-C8	-2.57	107.61	115.92
4	K	102	BCL	C2A-C1A-CHA	2.56	128.34	123.86
4	A	101	BCL	O2D-CGD-O1D	-2.55	118.85	123.84
4	S	101	BCL	C2A-C1A-CHA	2.55	128.32	123.86
4	G	102	BCL	CMB-C2B-C3B	2.54	129.43	124.68
4	I	102	BCL	CMB-C2B-C3B	2.53	129.42	124.68
4	I	102	BCL	C2A-C1A-CHA	2.53	128.28	123.86
4	C	101	BCL	C2A-C1A-CHA	2.53	128.28	123.86
4	E	102	BCL	CMD-C2D-C3D	2.53	129.40	124.68
4	M	101	BCL	CMB-C2B-C3B	2.52	129.40	124.68
4	Q	102	BCL	C4A-NA-C1A	2.52	107.84	106.71
4	M	101	BCL	C2A-C1A-CHA	2.52	128.27	123.86
4	S	106	BCL	CMB-C2B-C3B	2.52	129.38	124.68
4	I	101	BCL	O2D-CGD-O1D	-2.51	118.92	123.84
4	G	102	BCL	C2A-C1A-CHA	2.51	128.25	123.86
4	D	102	BCL	C2A-C1A-CHA	2.50	128.23	123.86
4	P	102	BCL	OBB-CAB-CBB	-2.50	114.55	120.17
4	J	101	BCL	OBB-CAB-CBB	-2.49	114.56	120.17
4	E	102	BCL	CMB-C2B-C3B	2.49	129.33	124.68
4	M	101	BCL	CMD-C2D-C3D	2.49	129.33	124.68
4	F	101	BCL	OBB-CAB-CBB	-2.48	114.58	120.17
4	S	103	BCL	C2A-C1A-CHA	2.48	128.20	123.86
4	G	102	BCL	CMD-C2D-C3D	2.47	129.31	124.68
4	O	101	BCL	C4A-NA-C1A	2.47	107.82	106.71
4	K	102	BCL	CMB-C2B-C3B	2.47	129.30	124.68
4	C	101	BCL	CMD-C2D-C3D	2.47	129.30	124.68
4	Q	101	BCL	CMB-C2B-C3B	2.47	129.29	124.68
4	N	101	BCL	OBB-CAB-CBB	-2.47	114.62	120.17
4	N	101	BCL	CMD-C2D-C3D	2.46	129.29	124.68
4	P	102	BCL	CMD-C2D-C3D	2.46	129.28	124.68
4	D	102	BCL	OBB-CAB-CBB	-2.46	114.63	120.17
4	J	101	BCL	CMD-C2D-C3D	2.46	129.28	124.68
4	L	101	BCL	CMD-C2D-C3D	2.46	129.27	124.68
4	S	103	BCL	CMD-C2D-C3D	2.46	129.27	124.68
4	A	102	BCL	C2A-C1A-CHA	2.45	128.15	123.86
4	A	102	BCL	CMB-C2B-C3B	2.45	129.26	124.68
4	S	103	BCL	C4B-C3B-CAB	-2.45	122.39	127.13
4	O	102	BCL	CMD-C2D-C3D	2.45	129.26	124.68
4	R	101	BCL	OBB-CAB-CBB	-2.45	114.67	120.17
4	A	102	BCL	CMD-C2D-C3D	2.45	129.25	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	101	BCL	CMD-C2D-C3D	2.44	129.25	124.68
4	F	101	BCL	CMD-C2D-C3D	2.44	129.25	124.68
4	I	101	BCL	CMD-C2D-C3D	2.44	129.24	124.68
4	B	102	BCL	CMD-C2D-C3D	2.43	129.23	124.68
4	J	101	BCL	C11-C10-C8	-2.43	108.05	115.92
4	S	105	BCL	CMD-C2D-C3D	2.43	129.23	124.68
4	R	101	BCL	CMD-C2D-C3D	2.43	129.23	124.68
4	B	102	BCL	OBB-CAB-CBB	-2.43	114.70	120.17
4	S	101	BCL	CMD-C2D-C3D	2.43	129.22	124.68
4	S	106	BCL	CMD-C2D-C3D	2.43	129.22	124.68
4	H	102	BCL	CMD-C2D-C3D	2.43	129.22	124.68
4	H	102	BCL	OBB-CAB-CBB	-2.43	114.71	120.17
4	S	102	BCL	CMD-C2D-C3D	2.42	129.21	124.68
4	C	102	BCL	CMD-C2D-C3D	2.42	129.21	124.68
4	L	101	BCL	OBB-CAB-CBB	-2.42	114.72	120.17
4	E	101	BCL	CMD-C2D-C3D	2.42	129.21	124.68
4	I	102	BCL	CMD-C2D-C3D	2.42	129.21	124.68
4	Q	101	BCL	C2A-C1A-CHA	2.42	128.09	123.86
4	S	102	BCL	OBB-CAB-CBB	-2.41	114.74	120.17
4	K	101	BCL	CMD-C2D-C3D	2.41	129.18	124.68
4	S	102	BCL	C4B-C3B-CAB	-2.41	122.48	127.13
4	S	104	BCL	CMD-C2D-C3D	2.40	129.16	124.68
4	K	102	BCL	CMD-C2D-C3D	2.39	129.16	124.68
4	S	103	BCL	OBB-CAB-CBB	-2.39	114.78	120.17
4	D	102	BCL	C4B-C3B-CAB	-2.39	122.51	127.13
4	A	101	BCL	CMD-C2D-C3D	2.39	129.15	124.68
4	D	102	BCL	CMD-C2D-C3D	2.39	129.15	124.68
4	S	105	BCL	OBB-CAB-CBB	-2.39	114.80	120.17
4	S	101	BCL	OBB-CAB-CBB	-2.39	114.80	120.17
4	O	102	BCL	CMB-C2B-C3B	2.38	129.13	124.68
4	S	105	BCL	C4B-C3B-CAB	-2.38	122.54	127.13
4	C	102	BCL	CMB-C2B-C3B	2.37	129.12	124.68
4	S	104	BCL	C4B-C3B-CAB	-2.37	122.55	127.13
4	M	102	BCL	CMD-C2D-C3D	2.36	129.09	124.68
4	S	104	BCL	OBB-CAB-CBB	-2.35	114.88	120.17
4	S	106	BCL	OBB-CAB-CBB	-2.35	114.89	120.17
4	B	102	BCL	C4B-C3B-CAB	-2.35	122.59	127.13
4	Q	102	BCL	CMD-C2D-C3D	2.34	129.05	124.68
4	R	101	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
4	J	101	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
4	O	101	BCL	O2D-CGD-CBD	2.33	115.41	111.27
4	S	101	BCL	C11-C10-C8	-2.33	108.38	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	101	BCL	CMD-C2D-C3D	2.33	129.04	124.68
4	L	101	BCL	C4B-C3B-CAB	-2.32	122.65	127.13
4	O	101	BCL	CMD-C2D-C3D	2.32	129.01	124.68
4	A	101	BCL	OBB-CAB-CBB	-2.31	114.97	120.17
4	G	102	BCL	OBB-CAB-CBB	-2.31	114.98	120.17
4	S	101	BCL	C4B-C3B-CAB	-2.31	122.67	127.13
4	A	101	BCL	O2D-CGD-CBD	2.30	115.36	111.27
4	H	102	BCL	C4B-C3B-CAB	-2.30	122.68	127.13
4	I	101	BCL	C4A-NA-C1A	2.30	107.74	106.71
4	K	101	BCL	OBB-CAB-CBB	-2.30	115.00	120.17
4	C	101	BCL	OBB-CAB-CBB	-2.30	115.00	120.17
4	I	101	BCL	OBB-CAB-CBB	-2.30	115.00	120.17
4	G	101	BCL	C4A-NA-C1A	2.29	107.74	106.71
4	N	101	BCL	C4B-C3B-CAB	-2.29	122.70	127.13
4	E	101	BCL	C4B-C3B-CAB	-2.29	122.71	127.13
4	F	101	BCL	C4B-C3B-CAB	-2.29	122.71	127.13
4	P	102	BCL	C4B-C3B-CAB	-2.28	122.72	127.13
4	M	102	BCL	OBB-CAB-CBB	-2.28	115.03	120.17
4	M	101	BCL	OBB-CAB-CBB	-2.28	115.05	120.17
4	E	101	BCL	OBB-CAB-CBB	-2.28	115.05	120.17
4	O	101	BCL	OBB-CAB-CBB	-2.27	115.07	120.17
4	Q	101	BCL	OBB-CAB-CBB	-2.27	115.07	120.17
4	I	102	BCL	OBB-CAB-CBB	-2.26	115.08	120.17
4	G	101	BCL	O2D-CGD-CBD	2.26	115.29	111.27
4	C	101	BCL	C4B-C3B-CAB	-2.26	122.76	127.13
4	G	101	BCL	OBB-CAB-CBB	-2.26	115.08	120.17
4	K	102	BCL	OBB-CAB-CBB	-2.26	115.09	120.17
4	Q	102	BCL	O2D-CGD-CBD	2.25	115.27	111.27
4	O	101	BCL	C4B-C3B-CAB	-2.25	122.78	127.13
4	A	102	BCL	OBB-CAB-CBB	-2.24	115.14	120.17
4	Q	102	BCL	OBB-CAB-CBB	-2.23	115.15	120.17
4	K	101	BCL	C4B-C3B-CAB	-2.22	122.84	127.13
4	M	102	BCL	C4B-C3B-CAB	-2.21	122.86	127.13
4	O	102	BCL	OBB-CAB-CBB	-2.21	115.20	120.17
4	E	102	BCL	OBB-CAB-CBB	-2.20	115.22	120.17
4	S	103	BCL	C16-C15-C13	2.20	123.02	115.92
4	M	102	BCL	O2D-CGD-CBD	2.18	115.15	111.27
4	C	102	BCL	OBB-CAB-CBB	-2.17	115.28	120.17
4	K	102	BCL	C16-C15-C13	2.17	122.94	115.92
4	S	103	BCL	CHD-C4C-NC	-2.15	122.69	125.08
4	I	101	BCL	O2D-CGD-CBD	2.15	115.09	111.27
4	A	101	BCL	C4B-C3B-CAB	-2.14	122.99	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	101	BCL	C4B-C3B-CAB	-2.14	123.00	127.13
4	Q	101	BCL	C1C-NC-C4C	2.14	107.67	106.71
4	I	101	BCL	C6-C7-C8	-2.13	109.02	115.92
4	G	101	BCL	C4B-C3B-CAB	-2.11	123.06	127.13
4	Q	102	BCL	C4B-C3B-CAB	-2.10	123.07	127.13
4	S	105	BCL	O2A-C1-C2	-2.05	103.24	108.64
4	N	101	BCL	C1-C2-C3	-2.03	122.53	126.04
4	B	102	BCL	C4-C3-C5	-2.01	111.88	115.27

There are no chirality outliers.

All (207) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	BCL	CHA-CBD-CGD-O1D
4	A	101	BCL	CAD-CBD-CGD-O1D
4	A	101	BCL	CAD-CBD-CGD-O2D
4	B	102	BCL	O2A-C1-C2-C3
4	C	102	BCL	CHA-CBD-CGD-O1D
4	G	101	BCL	CAD-CBD-CGD-O1D
4	G	101	BCL	CAD-CBD-CGD-O2D
4	I	101	BCL	CAD-CBD-CGD-O1D
4	I	101	BCL	CAD-CBD-CGD-O2D
4	K	102	BCL	C2C-C3C-CAC-CBC
4	K	102	BCL	C4C-C3C-CAC-CBC
4	K	102	BCL	CHA-CBD-CGD-O1D
4	K	102	BCL	CHA-CBD-CGD-O2D
4	M	101	BCL	CHA-CBD-CGD-O1D
4	M	101	BCL	CHA-CBD-CGD-O2D
4	M	102	BCL	CAD-CBD-CGD-O1D
4	M	102	BCL	CAD-CBD-CGD-O2D
4	O	101	BCL	CAD-CBD-CGD-O1D
4	O	101	BCL	CAD-CBD-CGD-O2D
4	O	102	BCL	CHA-CBD-CGD-O1D
4	O	102	BCL	CHA-CBD-CGD-O2D
4	P	102	BCL	CHA-CBD-CGD-O1D
4	P	102	BCL	CHA-CBD-CGD-O2D
4	Q	102	BCL	CAD-CBD-CGD-O1D
4	Q	102	BCL	CAD-CBD-CGD-O2D
4	F	101	BCL	C3-C5-C6-C7
4	K	101	BCL	C13-C15-C16-C17
4	M	102	BCL	C13-C15-C16-C17
4	O	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	O	101	BCL	C13-C15-C16-C17
4	S	103	BCL	C6-C7-C8-C9
4	I	101	BCL	C13-C15-C16-C17
4	Q	102	BCL	C13-C15-C16-C17
4	L	101	BCL	C15-C16-C17-C18
4	S	103	BCL	C6-C7-C8-C10
4	K	101	BCL	C5-C6-C7-C8
4	M	102	BCL	C5-C6-C7-C8
4	L	101	BCL	C10-C11-C12-C13
4	O	102	BCL	C13-C15-C16-C17
4	E	102	BCL	C4-C3-C5-C6
4	S	105	BCL	C4-C3-C5-C6
4	I	102	BCL	C11-C12-C13-C14
4	J	101	BCL	C3-C5-C6-C7
4	A	102	BCL	C10-C11-C12-C13
4	N	101	BCL	C15-C16-C17-C18
4	S	106	BCL	C3A-C2A-CAA-CBA
4	C	102	BCL	C16-C17-C18-C19
4	D	102	BCL	O2A-C1-C2-C3
4	G	101	BCL	C4-C3-C5-C6
4	K	101	BCL	C4-C3-C5-C6
4	S	102	BCL	C4-C3-C5-C6
4	E	101	BCL	C2-C3-C5-C6
4	K	101	BCL	C2-C3-C5-C6
4	M	102	BCL	C2-C3-C5-C6
4	Q	102	BCL	C2-C3-C5-C6
4	S	105	BCL	C2-C3-C5-C6
4	S	105	BCL	O1A-CGA-O2A-C1
4	E	101	BCL	C4-C3-C5-C6
4	M	102	BCL	C4-C3-C5-C6
4	A	101	BCL	C2-C3-C5-C6
4	E	101	BCL	C11-C10-C8-C7
4	G	101	BCL	C2-C3-C5-C6
4	I	102	BCL	C11-C12-C13-C15
4	S	102	BCL	C2-C3-C5-C6
4	S	103	BCL	C10-C11-C12-C13
4	O	101	BCL	C2A-CAA-CBA-CGA
4	Q	102	BCL	C4-C3-C5-C6
4	E	101	BCL	C11-C10-C8-C9
4	G	101	BCL	C11-C10-C8-C9
4	S	106	BCL	C1A-C2A-CAA-CBA
4	C	102	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
4	A	101	BCL	C4-C3-C5-C6
4	Q	102	BCL	C2A-CAA-CBA-CGA
4	E	102	BCL	C10-C11-C12-C13
4	D	102	BCL	C4-C3-C5-C6
4	S	104	BCL	C5-C6-C7-C8
4	S	101	BCL	C4-C3-C5-C6
4	A	101	BCL	C11-C10-C8-C7
4	C	101	BCL	C11-C10-C8-C7
4	D	102	BCL	C2-C3-C5-C6
4	G	101	BCL	C11-C10-C8-C7
4	S	101	BCL	C2-C3-C5-C6
4	A	101	BCL	C11-C10-C8-C9
4	C	101	BCL	C11-C10-C8-C9
4	D	102	BCL	C11-C10-C8-C9
4	F	101	BCL	C10-C11-C12-C13
4	S	105	BCL	CBA-CGA-O2A-C1
4	M	102	BCL	CBD-CGD-O2D-CED
4	E	102	BCL	C2-C3-C5-C6
4	G	101	BCL	C2A-CAA-CBA-CGA
4	M	102	BCL	C2A-CAA-CBA-CGA
4	L	101	BCL	C2-C1-O2A-CGA
4	H	102	BCL	C11-C10-C8-C9
4	P	102	BCL	C8-C10-C11-C12
4	D	102	BCL	C11-C10-C8-C7
4	H	102	BCL	C11-C10-C8-C7
4	Q	101	BCL	C11-C10-C8-C7
4	R	101	BCL	C11-C10-C8-C7
4	D	102	BCL	C15-C16-C17-C18
4	S	103	BCL	CAD-CBD-CGD-O2D
4	I	101	BCL	C4-C3-C5-C6
4	A	101	BCL	CHA-CBD-CGD-O2D
4	C	102	BCL	CHA-CBD-CGD-O2D
4	E	102	BCL	CHA-CBD-CGD-O1D
4	I	101	BCL	CHA-CBD-CGD-O1D
4	S	106	BCL	O1A-CGA-O2A-C1
4	O	101	BCL	C4-C3-C5-C6
4	F	101	BCL	C11-C10-C8-C9
4	Q	101	BCL	C11-C10-C8-C9
4	R	101	BCL	C11-C10-C8-C9
4	A	101	BCL	C13-C15-C16-C17
4	P	102	BCL	C3-C5-C6-C7
4	L	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
4	B	102	BCL	C11-C10-C8-C7
4	I	101	BCL	C11-C10-C8-C7
4	K	102	BCL	C12-C13-C15-C16
4	O	101	BCL	C11-C10-C8-C7
4	Q	102	BCL	C11-C10-C8-C7
4	S	104	BCL	C3-C5-C6-C7
4	M	102	BCL	O1D-CGD-O2D-CED
4	L	101	BCL	C11-C10-C8-C9
4	K	101	BCL	C3-C5-C6-C7
4	S	106	BCL	C2A-CAA-CBA-CGA
4	M	102	BCL	C8-C10-C11-C12
4	H	102	BCL	C8-C10-C11-C12
4	I	101	BCL	C2-C3-C5-C6
4	K	101	BCL	C11-C10-C8-C7
4	B	102	BCL	C11-C10-C8-C9
4	I	101	BCL	C11-C10-C8-C9
4	Q	102	BCL	C11-C10-C8-C9
4	S	106	BCL	CBA-CGA-O2A-C1
4	B	102	BCL	C4-C3-C5-C6
4	O	101	BCL	C2-C3-C5-C6
4	J	101	BCL	C11-C12-C13-C14
4	K	102	BCL	C14-C13-C15-C16
4	S	103	BCL	C4-C3-C5-C6
4	F	101	BCL	C11-C10-C8-C7
4	L	101	BCL	C2-C3-C5-C6
4	L	101	BCL	C11-C10-C8-C7
4	L	101	BCL	C3-C5-C6-C7
4	I	101	BCL	C2A-CAA-CBA-CGA
4	Q	102	BCL	C8-C10-C11-C12
4	B	102	BCL	C2-C3-C5-C6
4	K	101	BCL	C8-C10-C11-C12
4	E	102	BCL	C15-C16-C17-C18
4	O	101	BCL	C8-C10-C11-C12
4	C	102	BCL	C4-C3-C5-C6
4	S	103	BCL	C2-C3-C5-C6
4	C	101	BCL	C4-C3-C5-C6
4	H	102	BCL	C4-C3-C5-C6
4	D	102	BCL	C4C-C3C-CAC-CBC
4	N	101	BCL	C4C-C3C-CAC-CBC
4	S	105	BCL	C4C-C3C-CAC-CBC
4	H	102	BCL	C16-C17-C18-C20
4	R	101	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	C	101	BCL	C2-C3-C5-C6
4	S	102	BCL	C1-C2-C3-C4
4	H	102	BCL	C16-C17-C18-C19
4	G	102	BCL	C4-C3-C5-C6
4	R	101	BCL	C4-C3-C5-C6
4	C	102	BCL	C2-C3-C5-C6
4	F	101	BCL	C11-C12-C13-C14
4	J	101	BCL	C14-C13-C15-C16
4	K	101	BCL	C11-C10-C8-C9
4	O	101	BCL	C11-C10-C8-C9
4	C	101	BCL	CAD-CBD-CGD-O2D
4	E	101	BCL	CAD-CBD-CGD-O2D
4	M	102	BCL	C3-C5-C6-C7
4	I	101	BCL	C8-C10-C11-C12
4	K	102	BCL	CAA-CBA-CGA-O2A
4	A	101	BCL	C3-C5-C6-C7
4	N	101	BCL	O2A-C1-C2-C3
4	S	102	BCL	O2A-C1-C2-C3
4	S	103	BCL	O2A-C1-C2-C3
4	S	104	BCL	O2A-C1-C2-C3
4	D	102	BCL	C8-C10-C11-C12
4	B	102	BCL	C3-C5-C6-C7
4	A	102	BCL	CHA-CBD-CGD-O1D
4	A	102	BCL	CHA-CBD-CGD-O2D
4	E	102	BCL	CHA-CBD-CGD-O2D
4	G	102	BCL	CHA-CBD-CGD-O1D
4	G	102	BCL	CHA-CBD-CGD-O2D
4	H	102	BCL	CHA-CBD-CGD-O1D
4	H	102	BCL	CHA-CBD-CGD-O2D
4	I	101	BCL	CHA-CBD-CGD-O2D
4	Q	102	BCL	CHA-CBD-CGD-O2D
4	G	102	BCL	C2-C3-C5-C6
4	F	101	BCL	C11-C12-C13-C15
4	P	102	BCL	C16-C17-C18-C20
4	P	102	BCL	C11-C10-C8-C9
4	S	103	BCL	CAA-CBA-CGA-O2A
4	P	102	BCL	C16-C17-C18-C19
4	J	101	BCL	C8-C10-C11-C12
4	S	103	BCL	CAA-CBA-CGA-O1A
4	I	101	BCL	C3-C5-C6-C7
4	K	102	BCL	CAA-CBA-CGA-O1A
4	C	101	BCL	C8-C10-C11-C12

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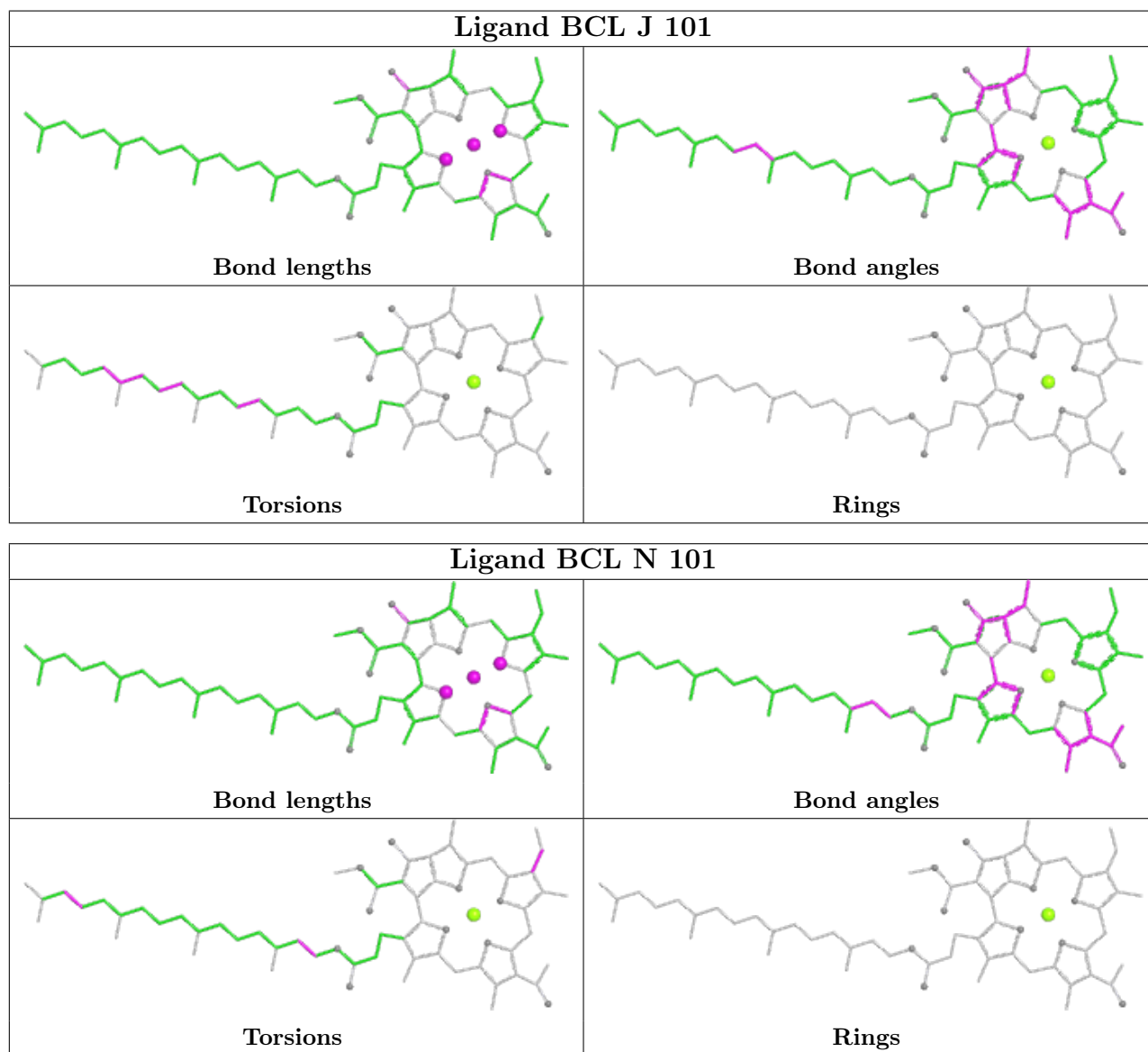
Mol	Chain	Res	Type	Atoms
4	A	102	BCL	CAD-CBD-CGD-O1D
4	H	102	BCL	C14-C13-C15-C16
4	M	102	BCL	C11-C10-C8-C9
4	H	102	BCL	C13-C15-C16-C17
4	M	102	BCL	C11-C10-C8-C7
4	P	102	BCL	C11-C10-C8-C7
4	S	101	BCL	C12-C13-C15-C16
4	S	101	BCL	CAA-CBA-CGA-O1A
4	S	102	BCL	C5-C6-C7-C8
4	S	106	BCL	C10-C11-C12-C13

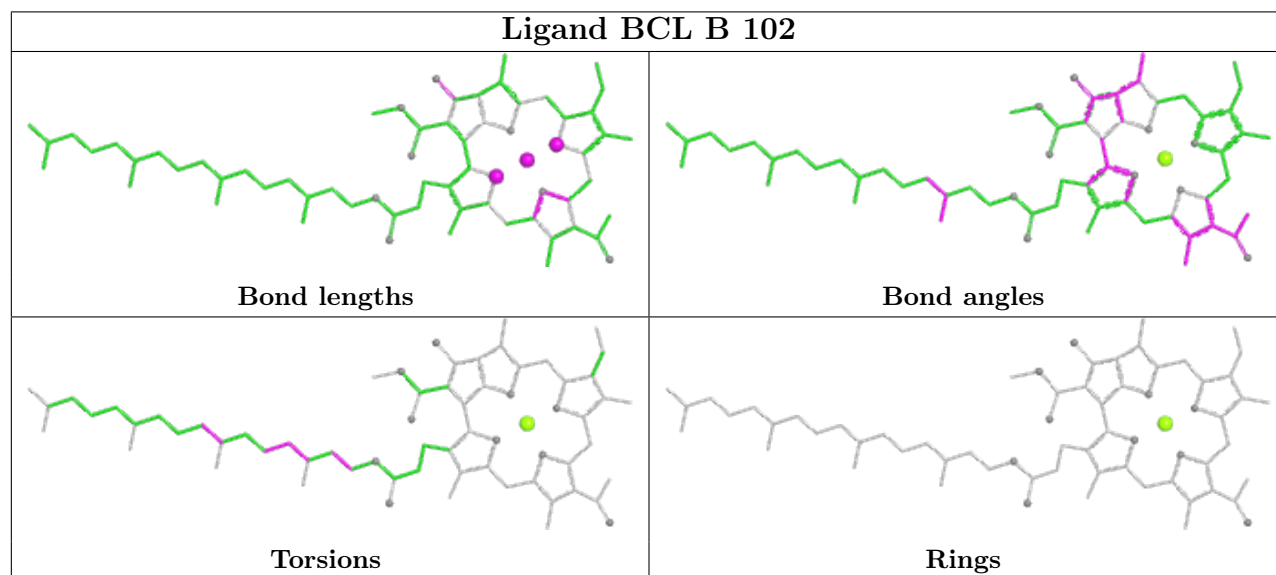
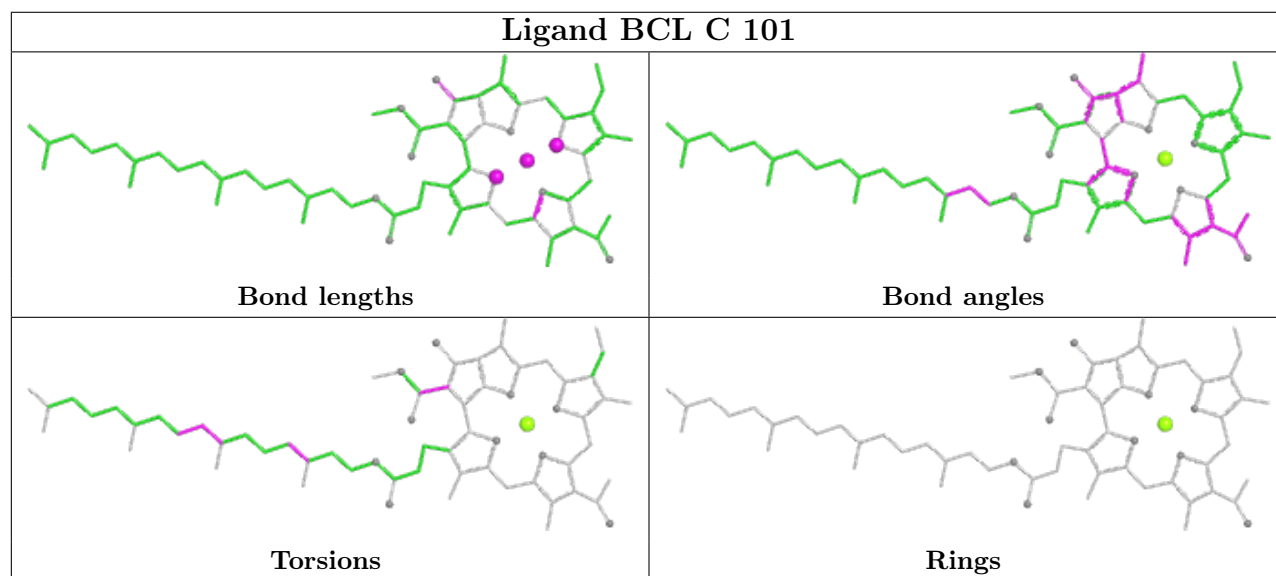
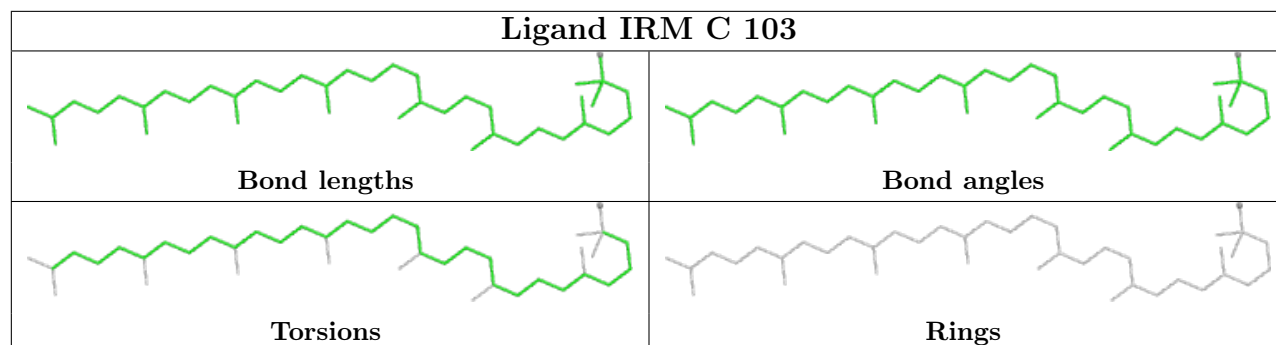
There are no ring outliers.

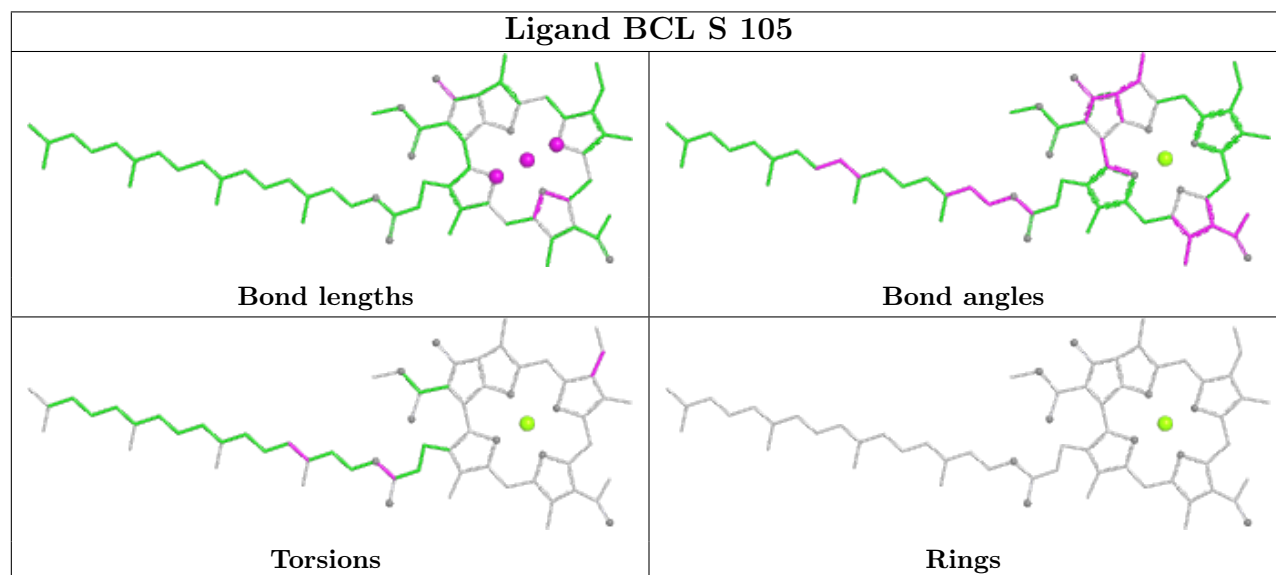
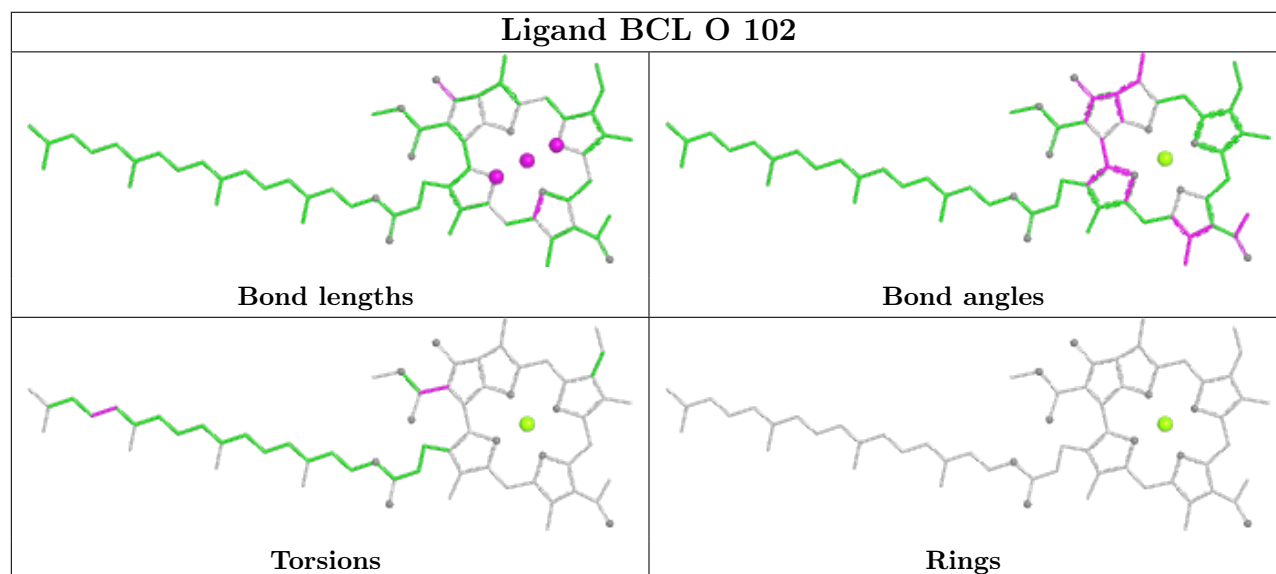
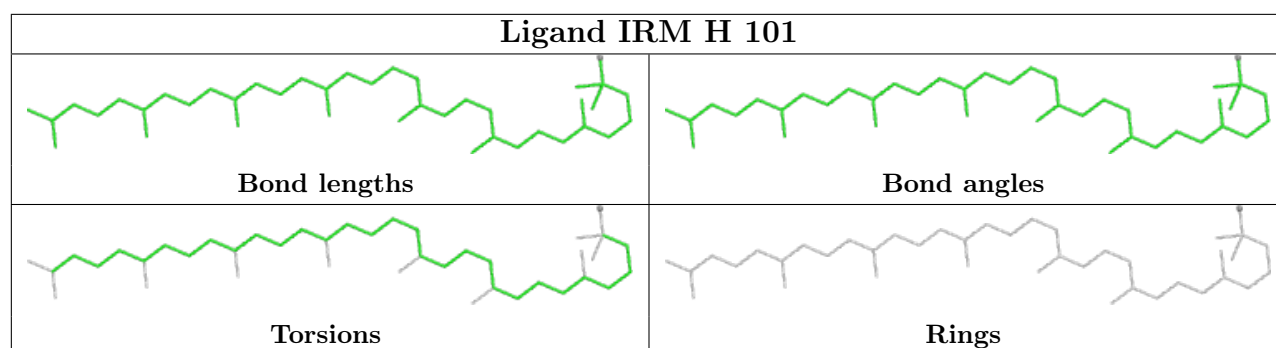
26 monomers are involved in 31 short contacts:

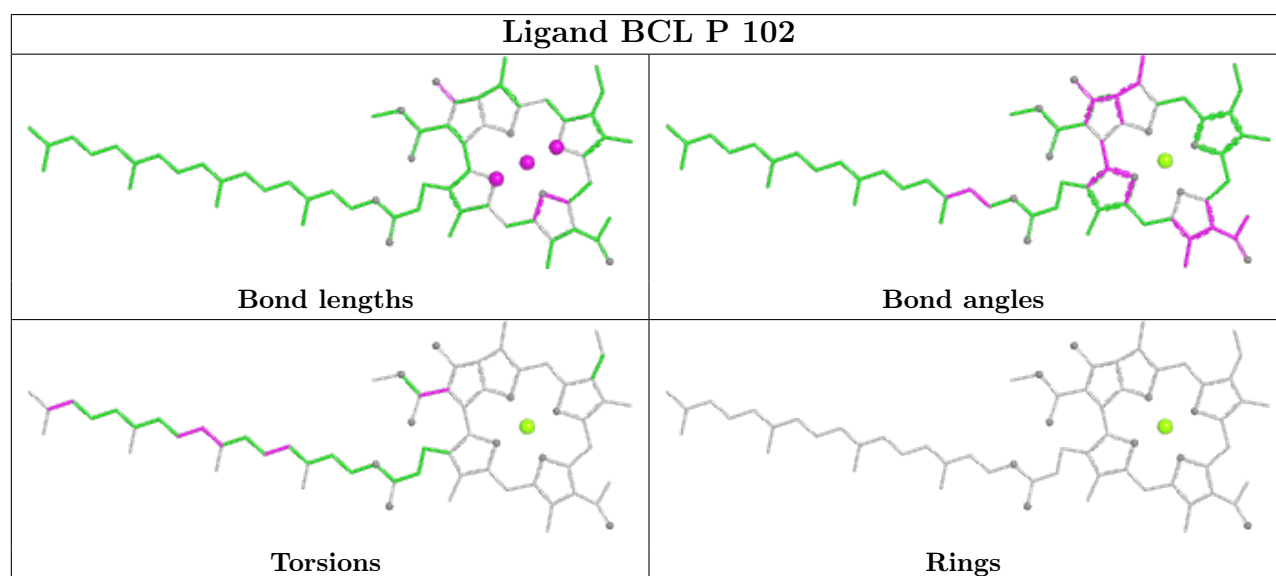
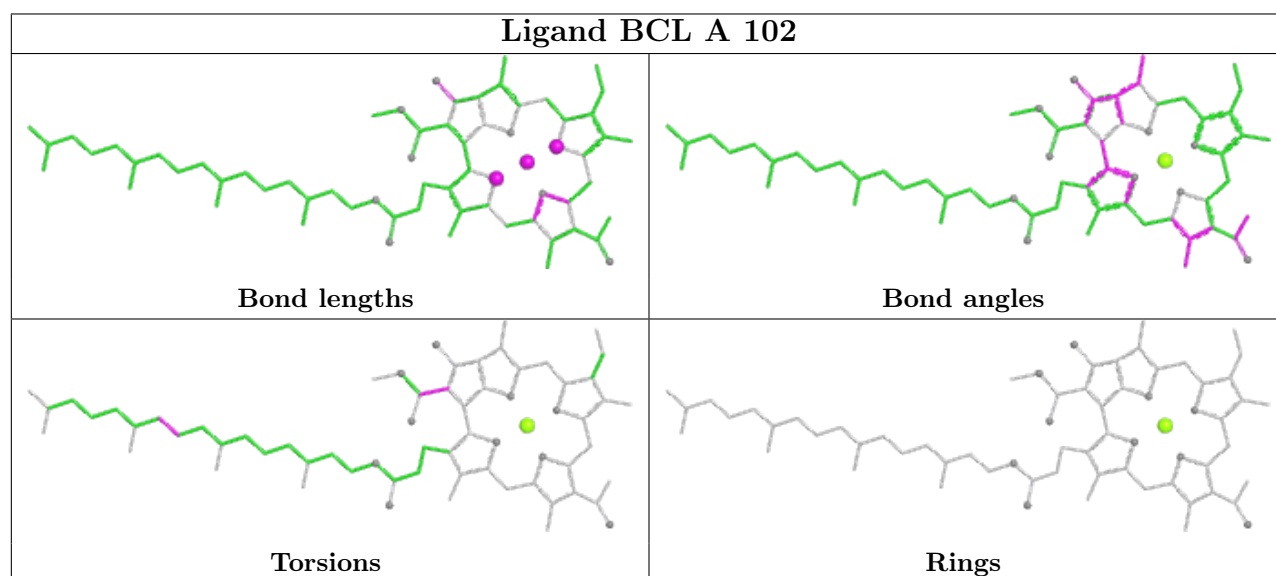
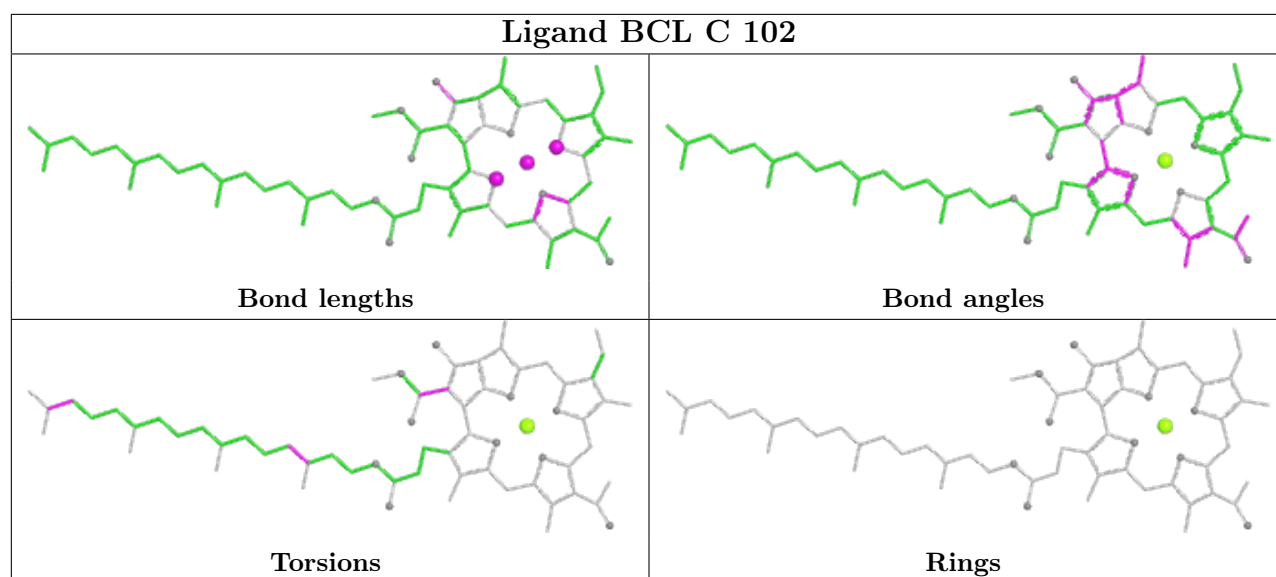
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	101	BCL	2	0
4	N	101	BCL	2	0
4	C	101	BCL	1	0
4	B	102	BCL	2	0
4	O	102	BCL	2	0
4	S	105	BCL	1	0
4	C	102	BCL	3	0
4	A	102	BCL	2	0
4	P	102	BCL	1	0
4	M	102	BCL	1	0
4	R	101	BCL	1	0
4	A	101	BCL	1	0
4	K	102	BCL	1	0
4	D	102	BCL	1	0
4	S	103	BCL	1	0
4	Q	101	BCL	2	0
4	F	101	BCL	1	0
4	I	102	BCL	1	0
4	G	102	BCL	1	0
4	E	102	BCL	2	0
4	M	101	BCL	1	0
4	E	101	BCL	2	0
4	H	102	BCL	1	0
4	O	101	BCL	1	0
4	G	101	BCL	2	0
4	L	101	BCL	2	0

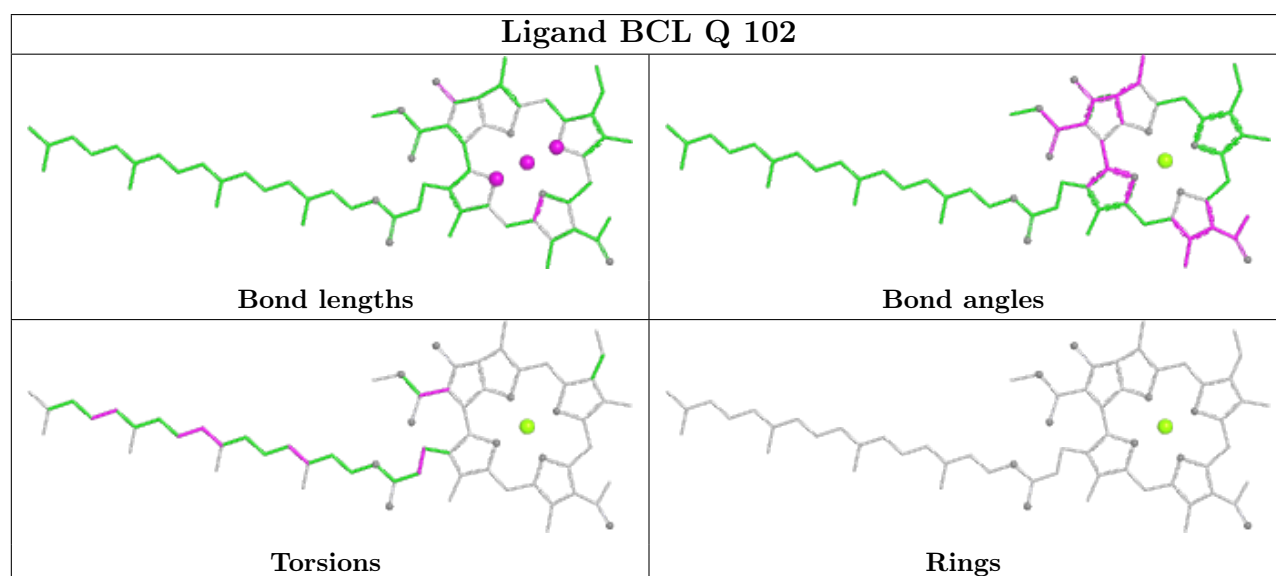
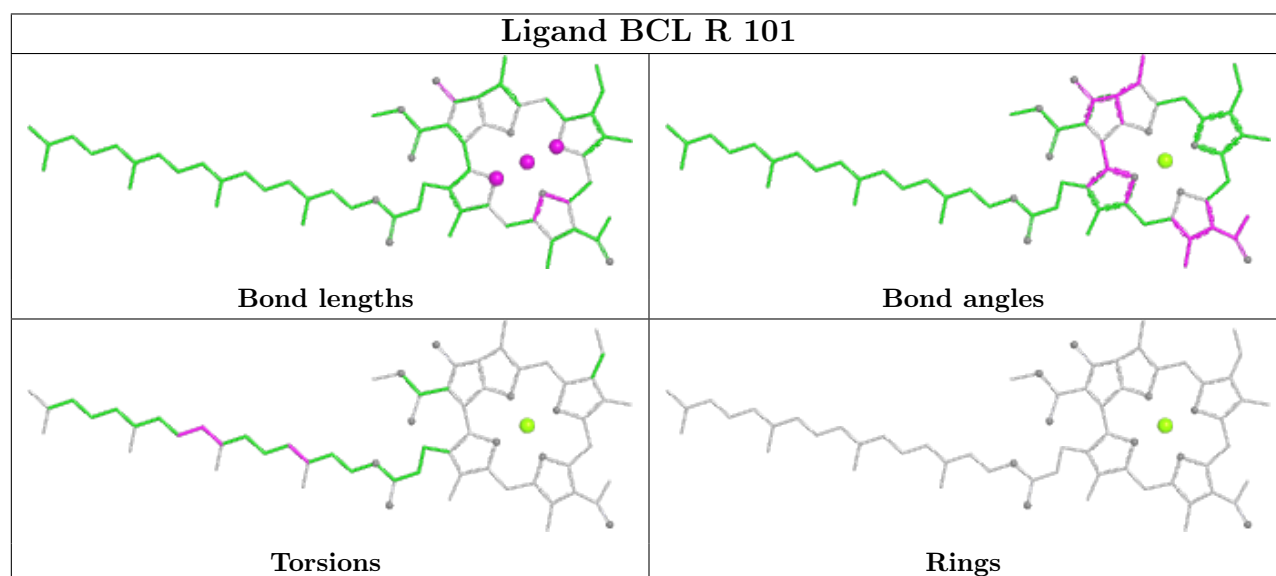
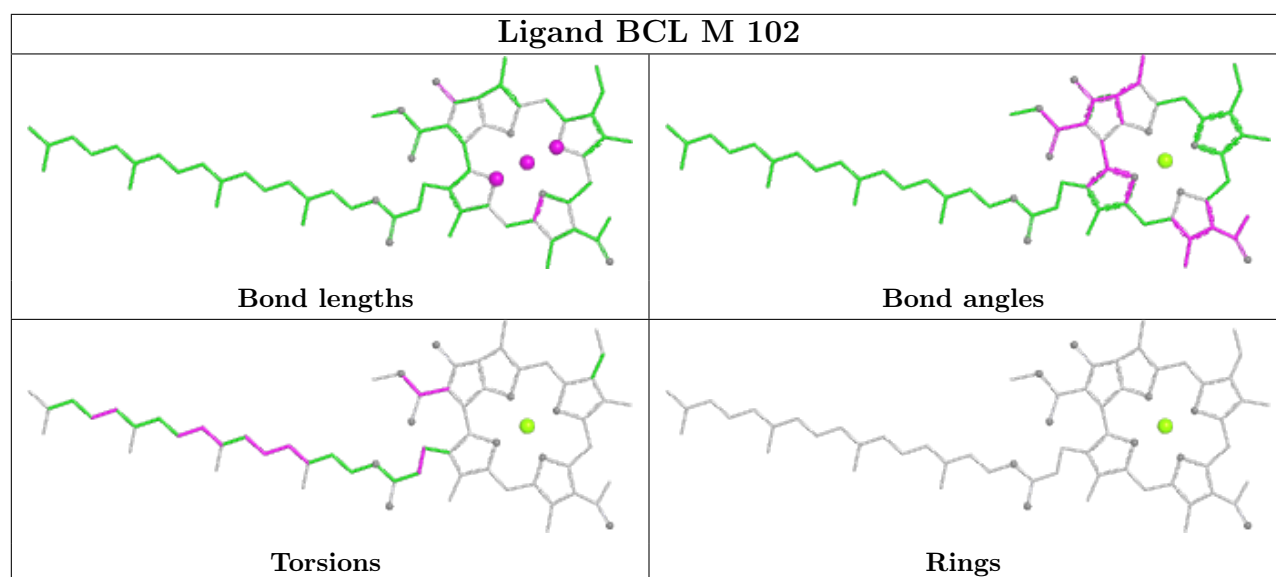
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

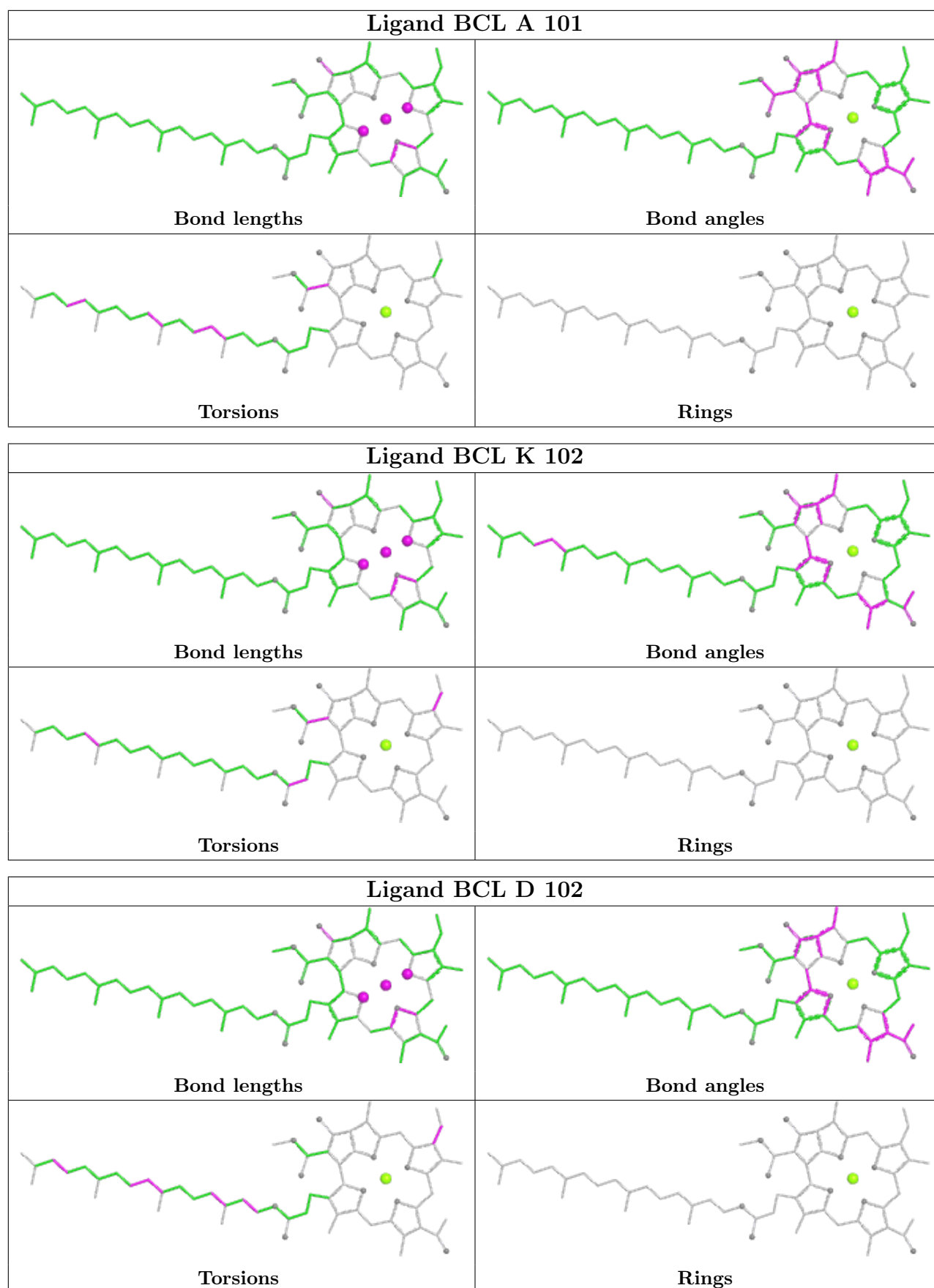




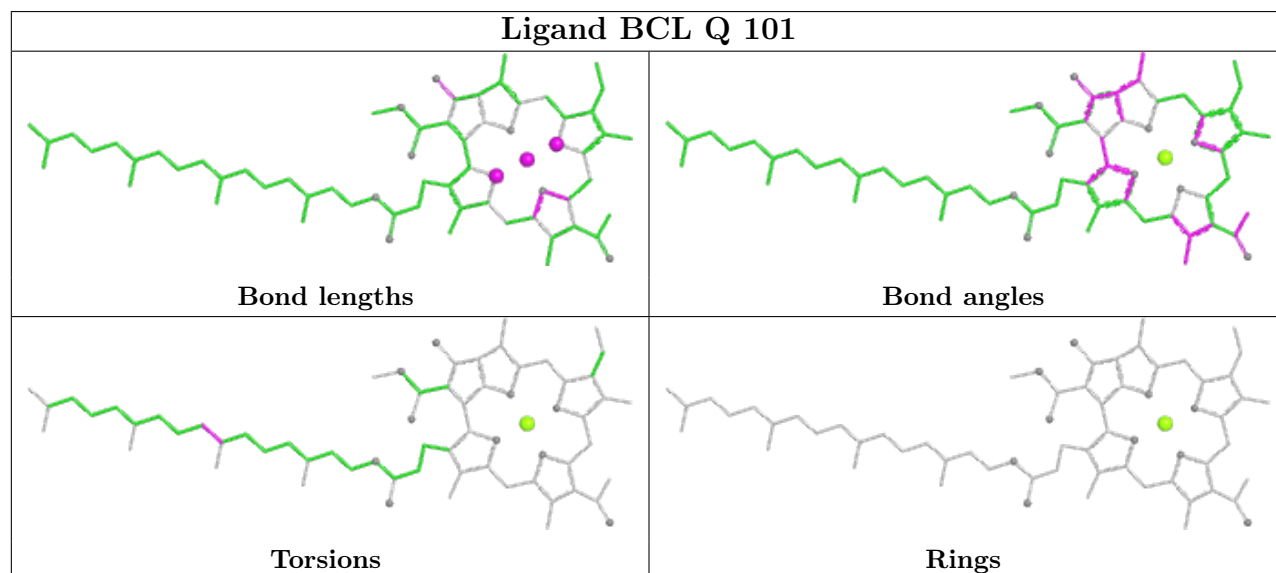
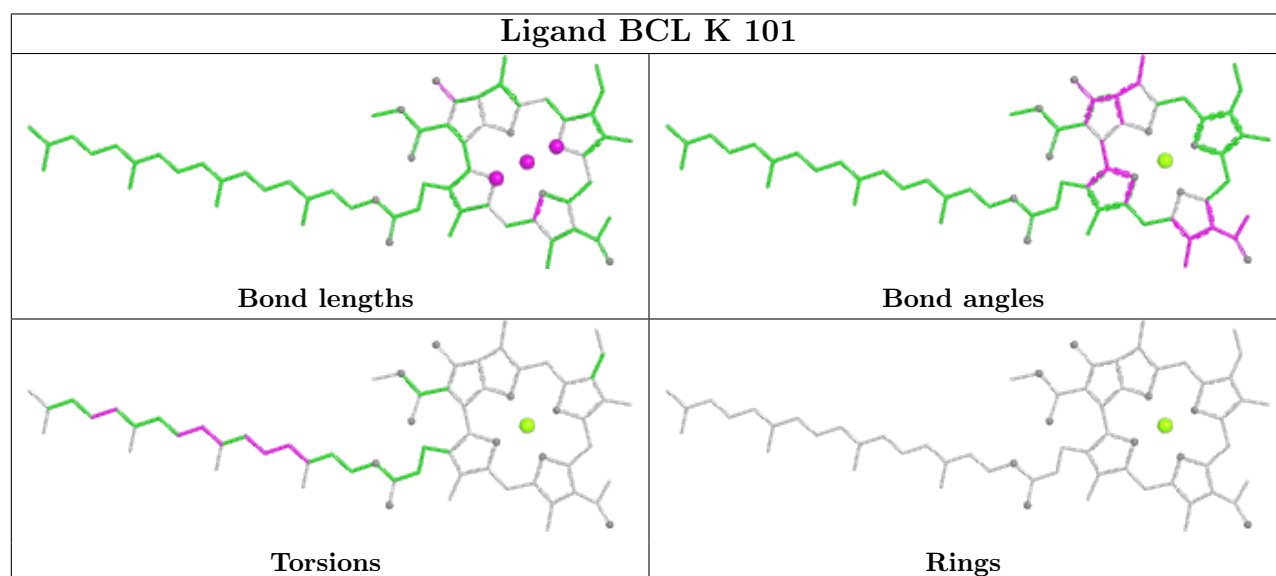
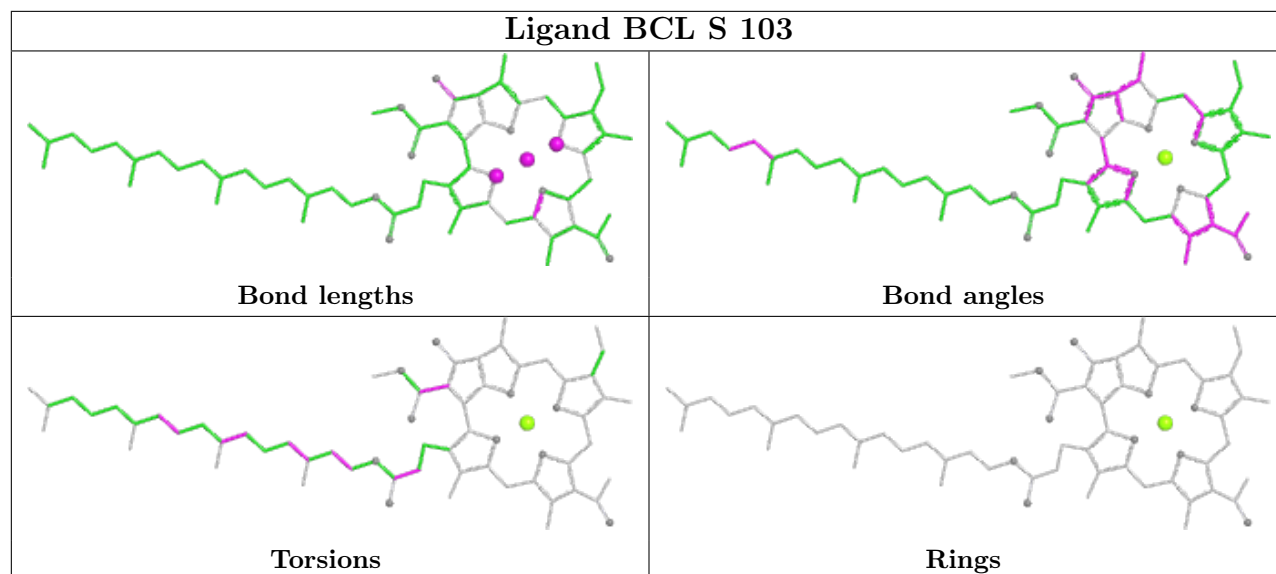


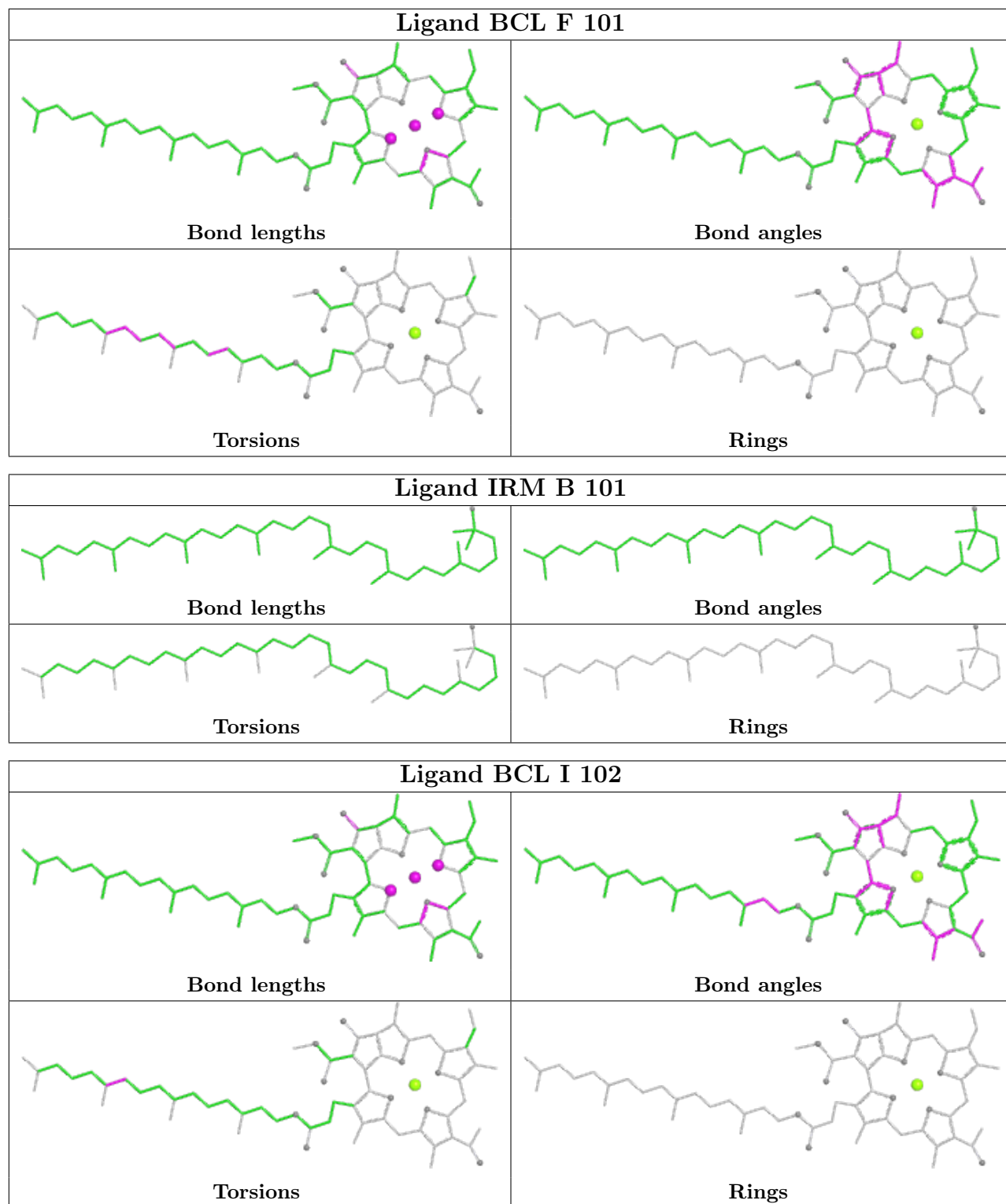


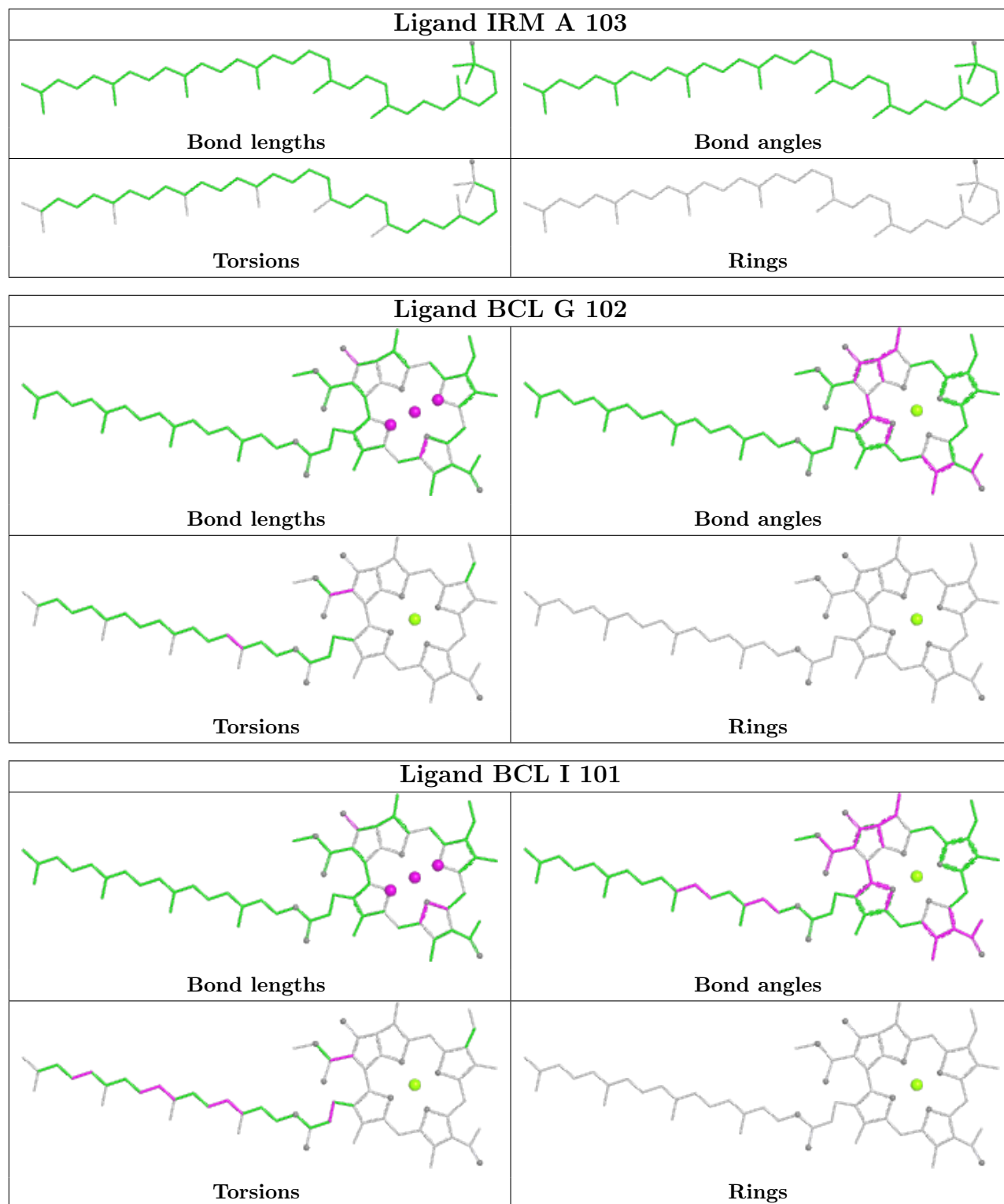


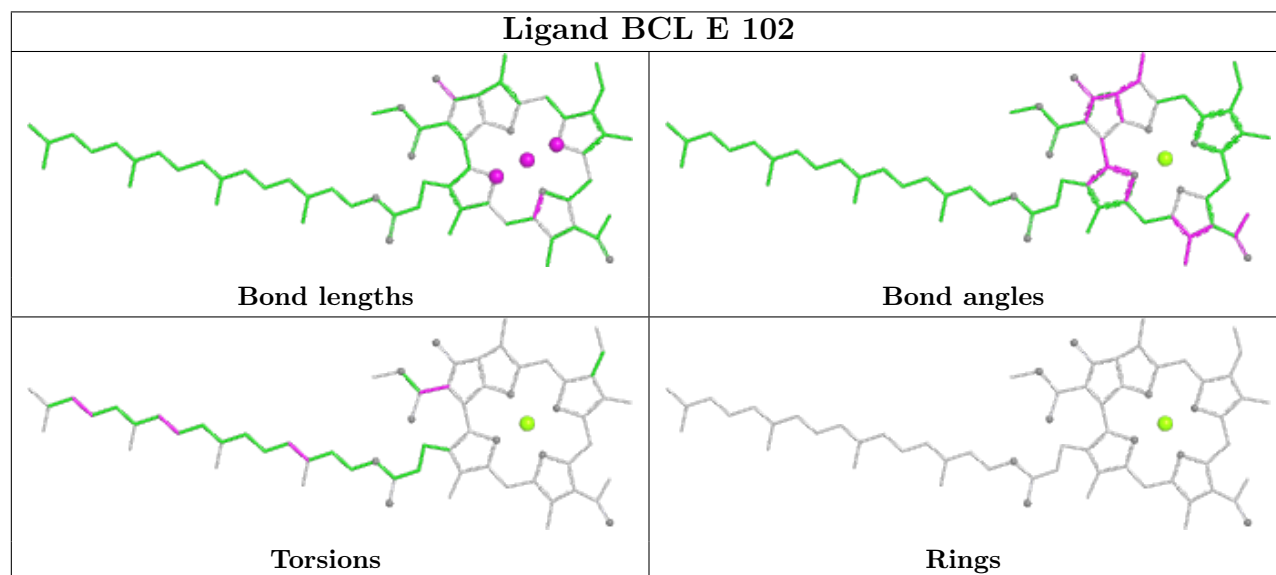
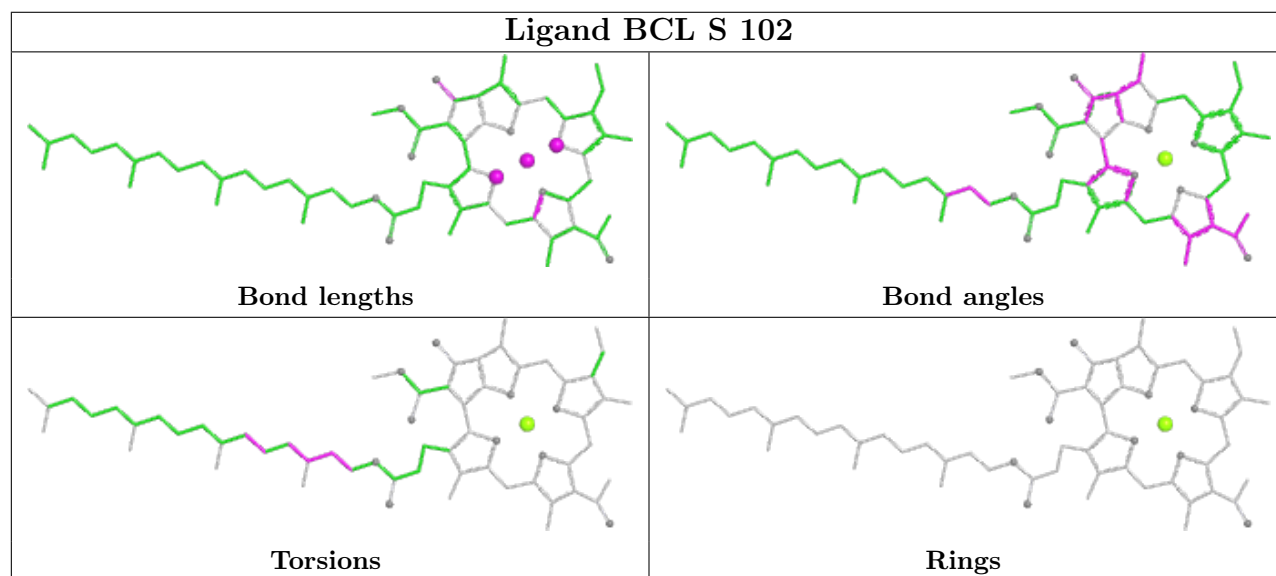
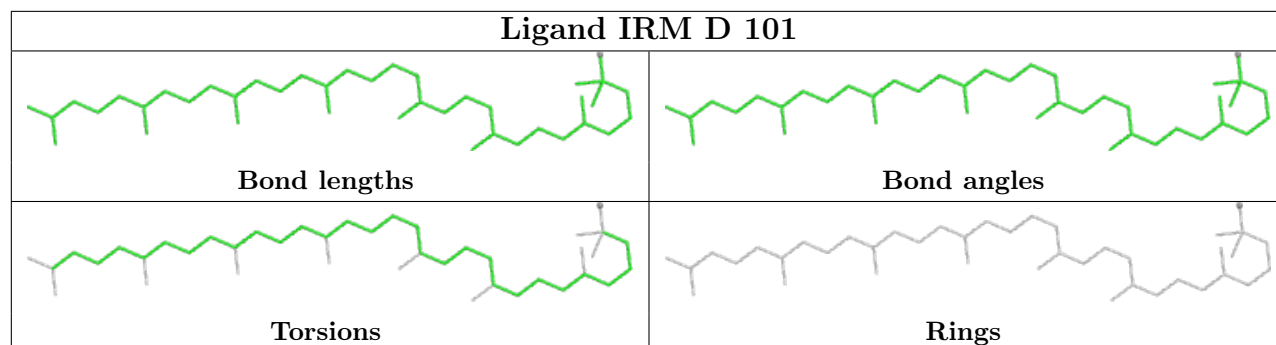


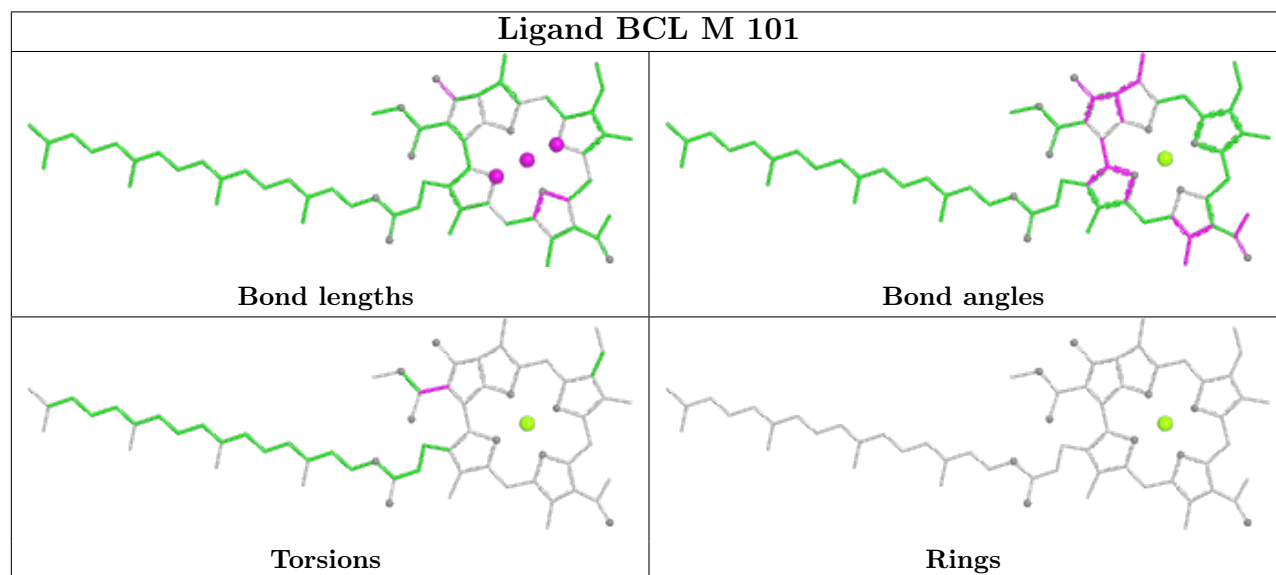
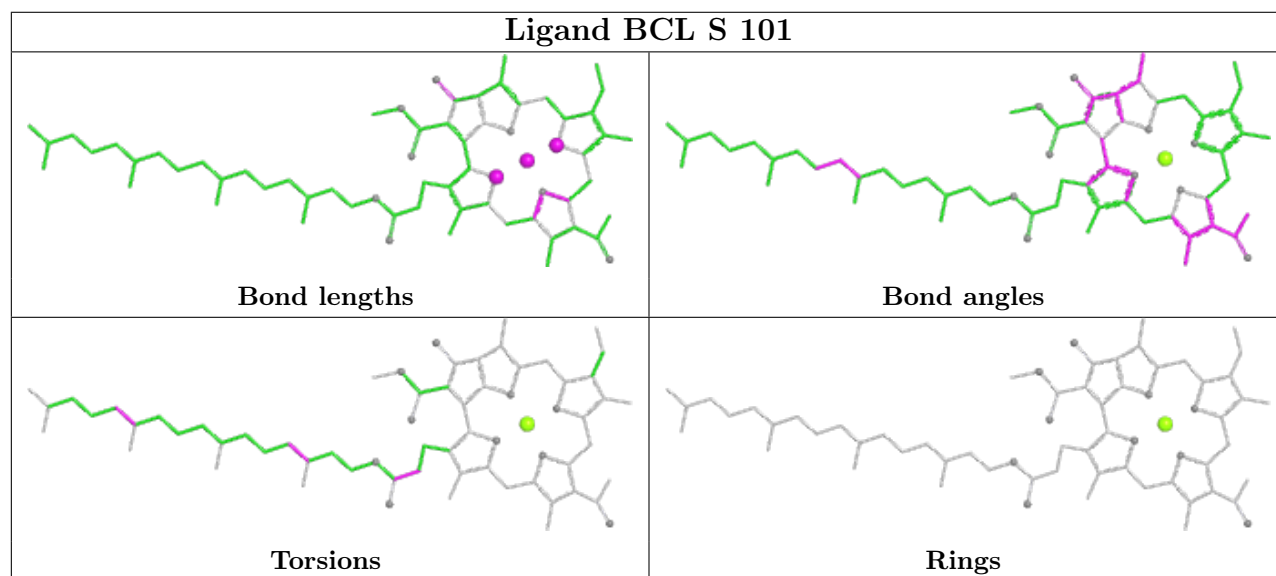
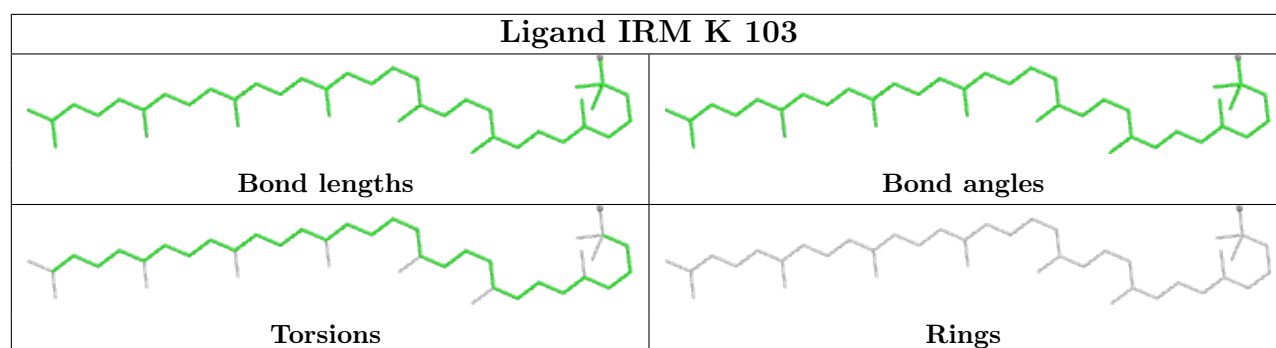


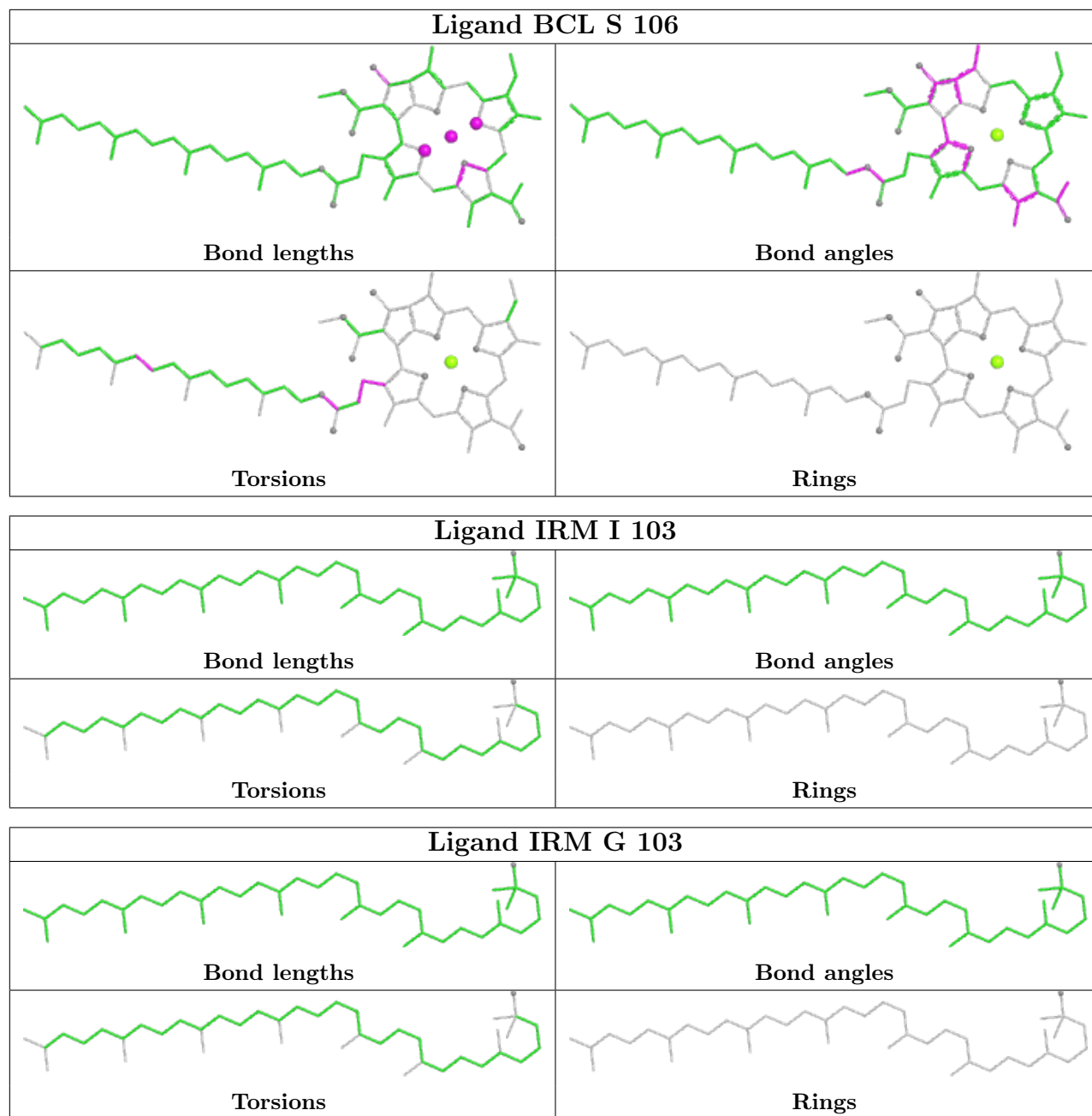


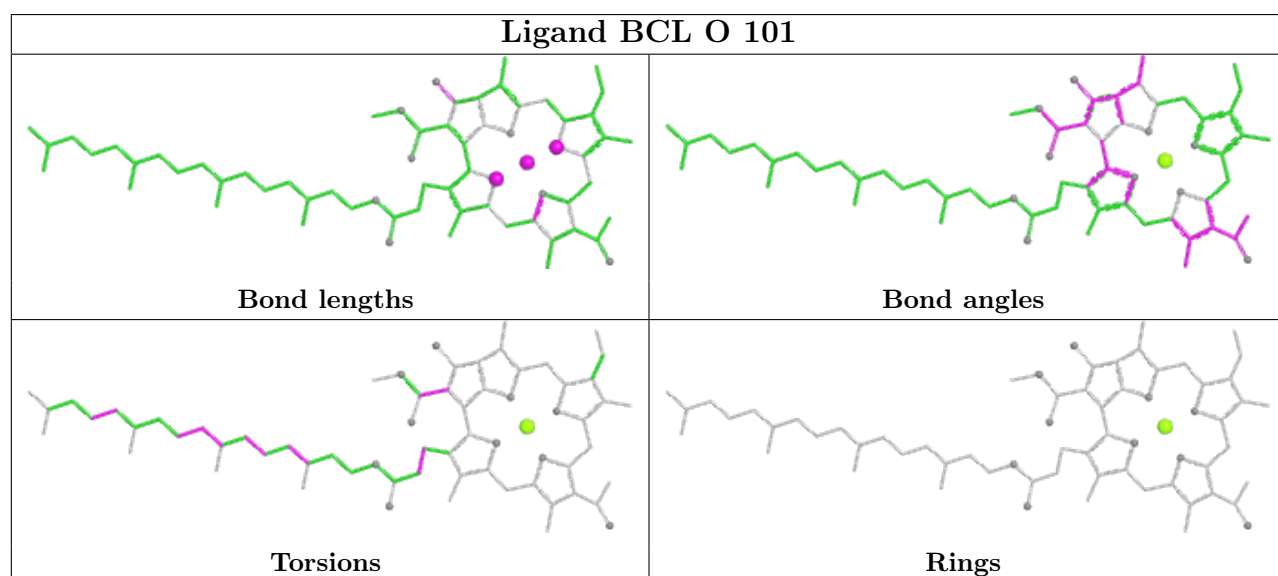
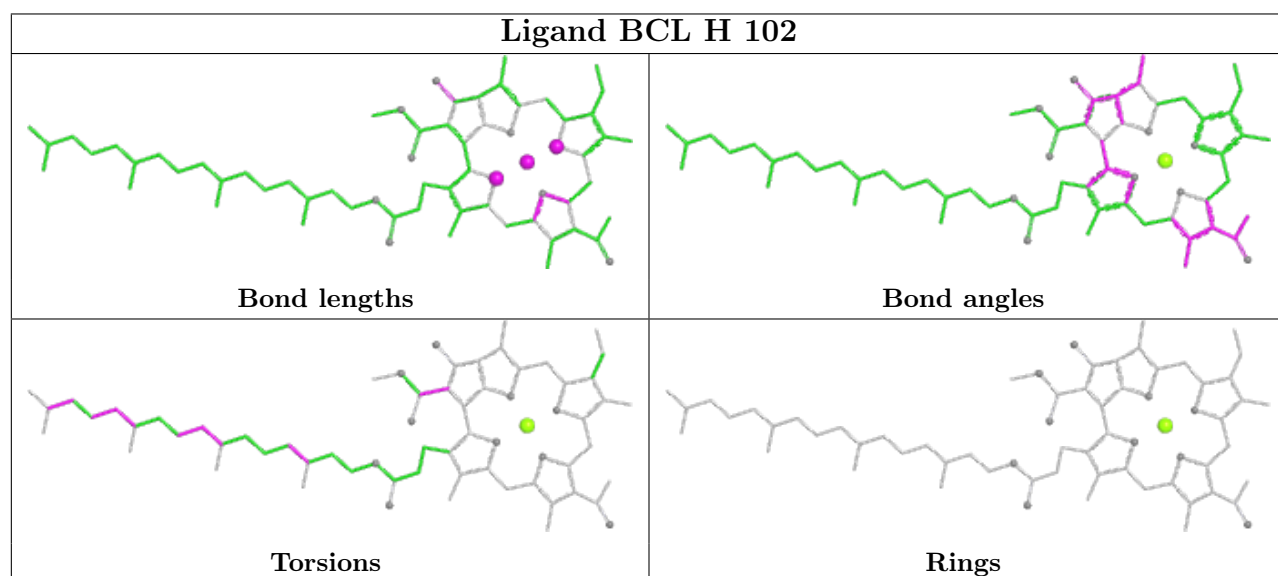
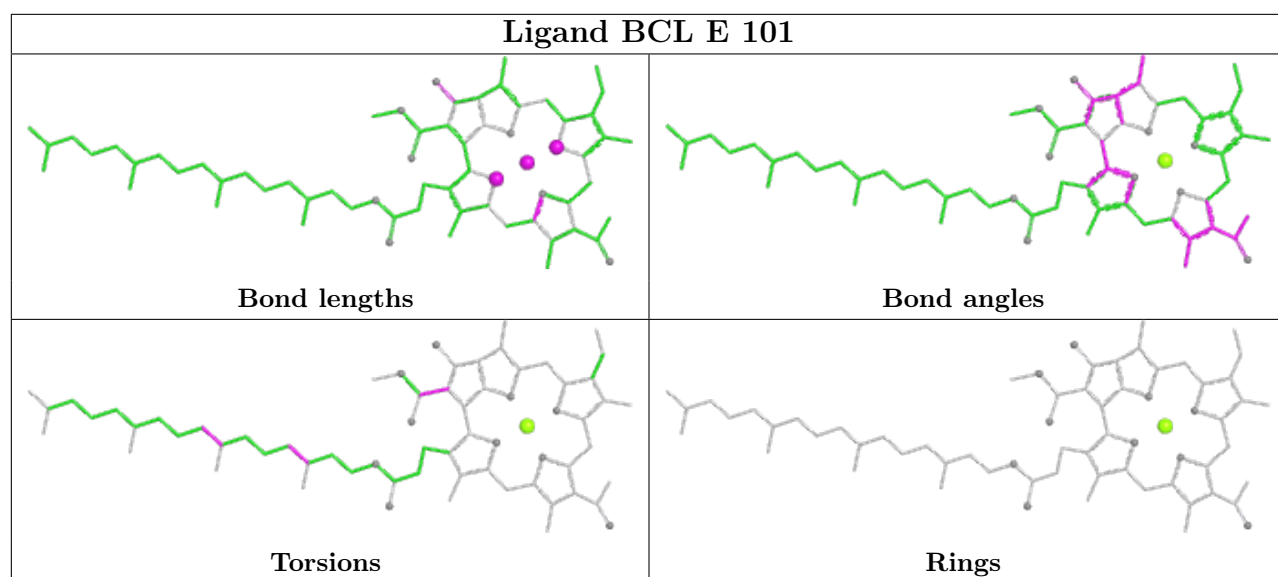


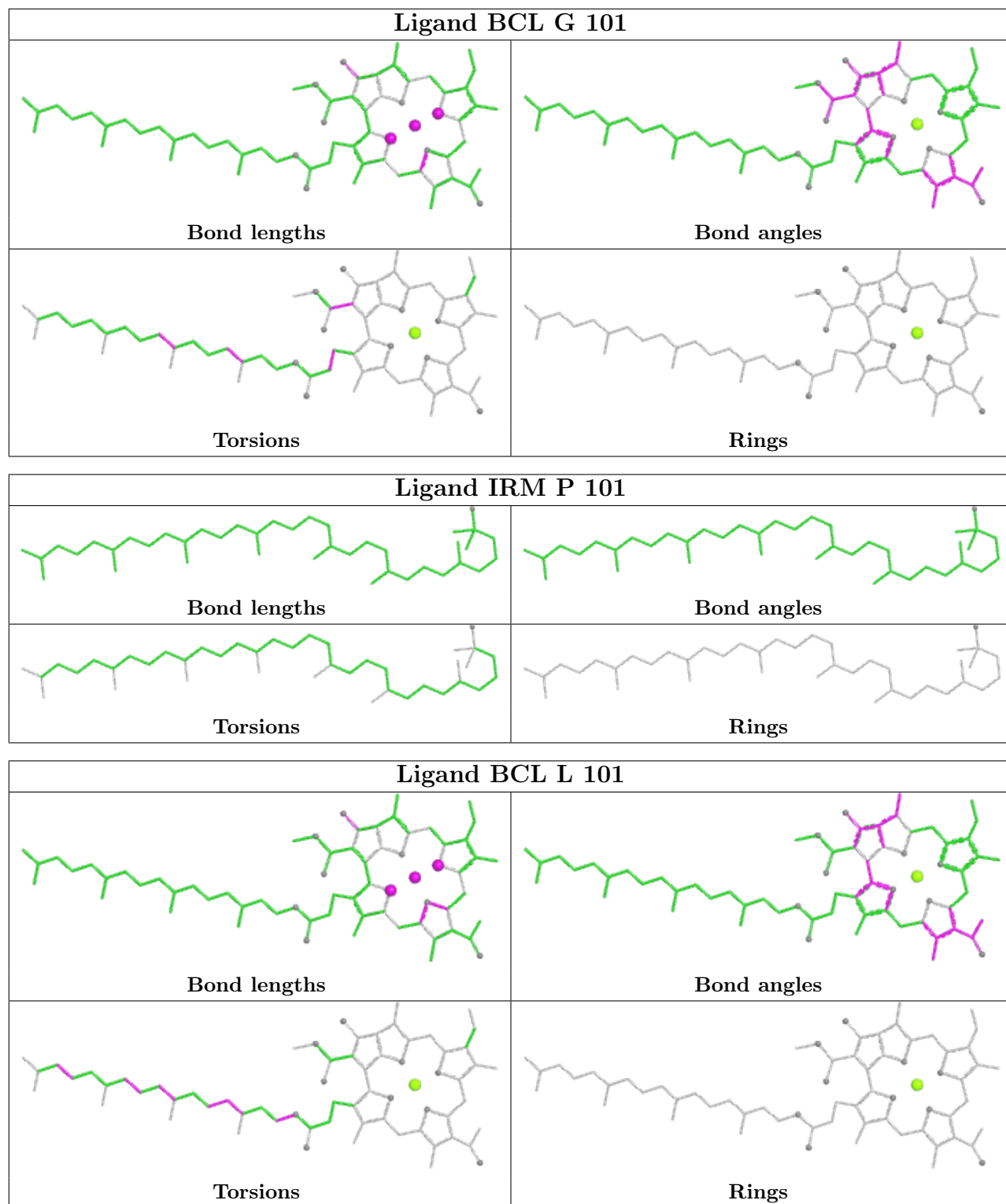




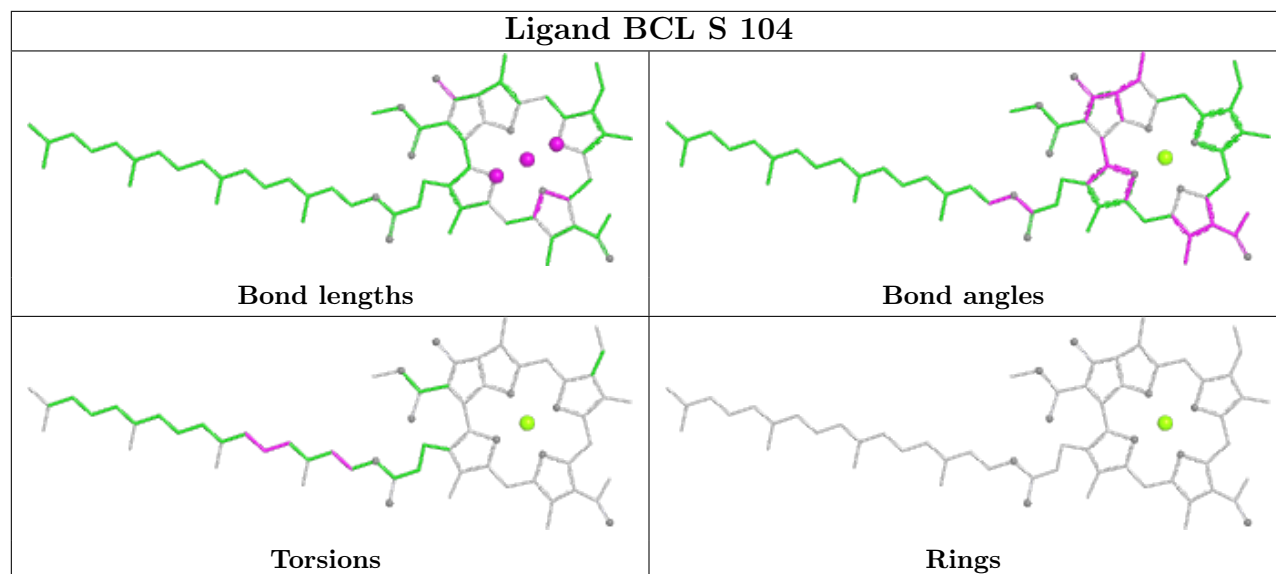












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

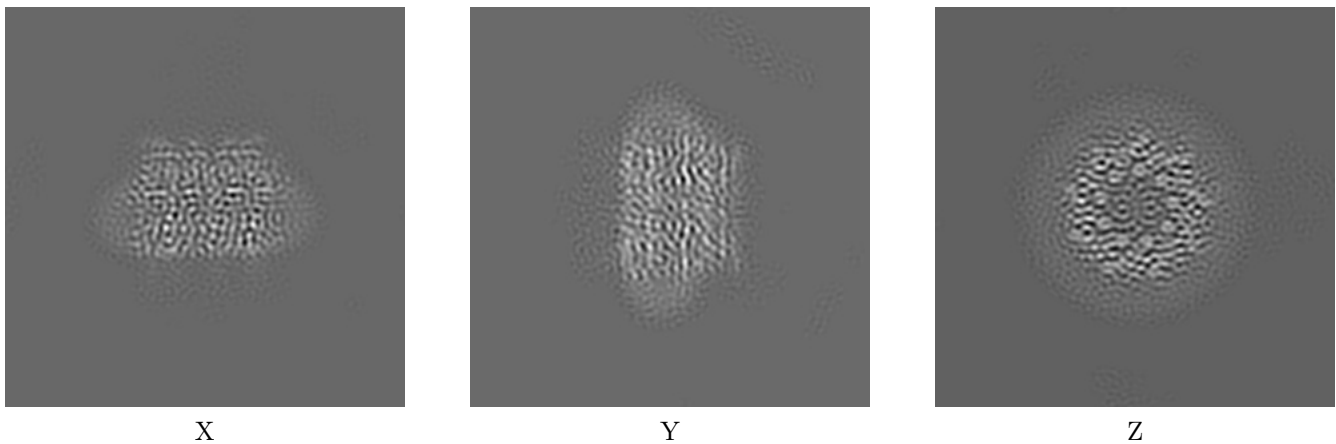
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14685. These allow visual inspection of the internal detail of the map and identification of artifacts.

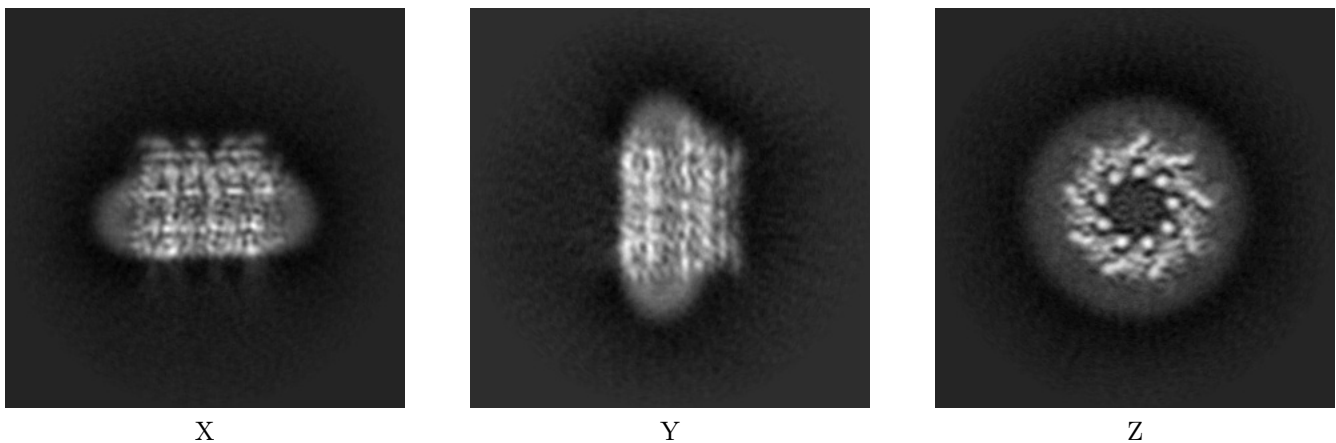
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



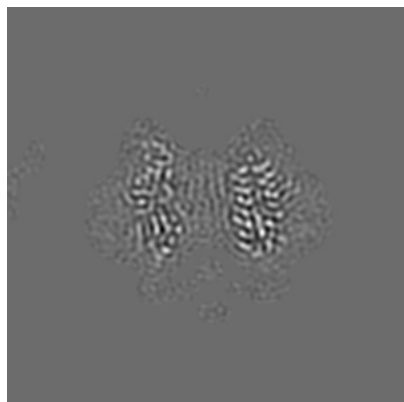
#### 6.1.2 Raw map



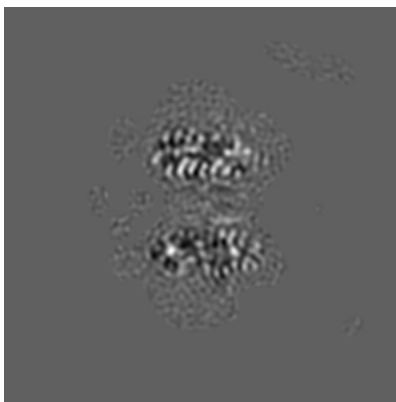
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

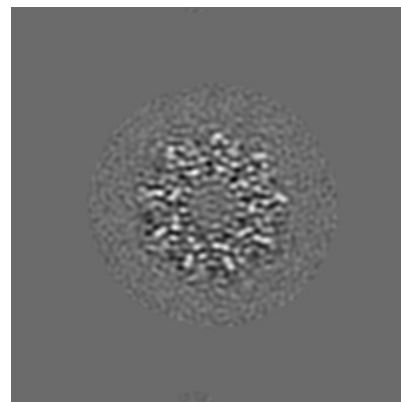
### 6.2.1 Primary map



X Index: 150

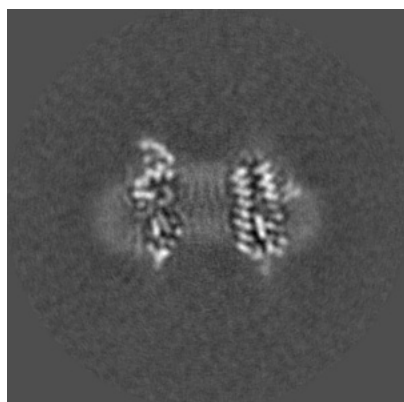


Y Index: 150

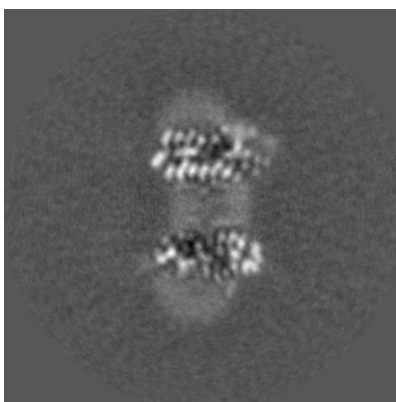


Z Index: 150

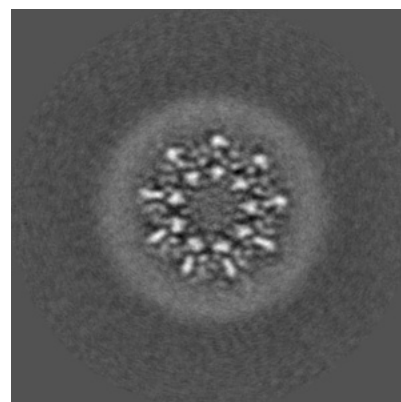
### 6.2.2 Raw map



X Index: 150



Y Index: 150

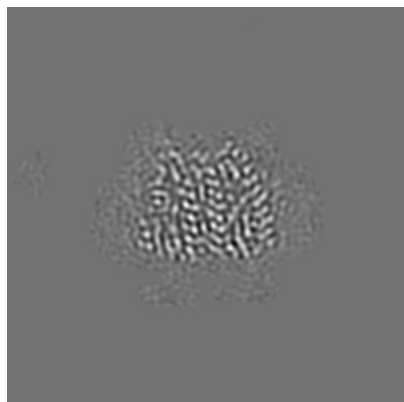


Z Index: 150

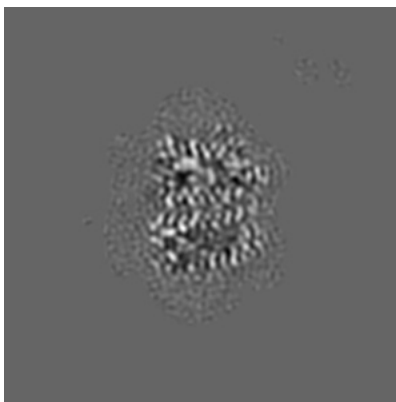
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

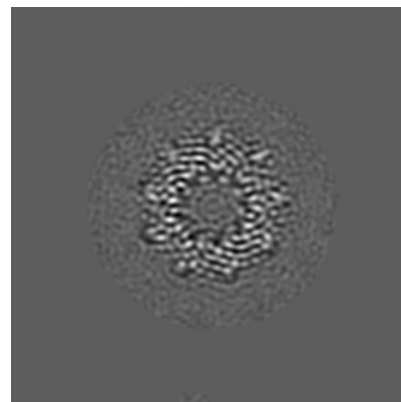
### 6.3.1 Primary map



X Index: 123

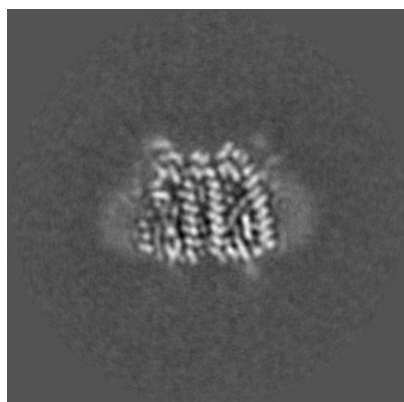


Y Index: 123

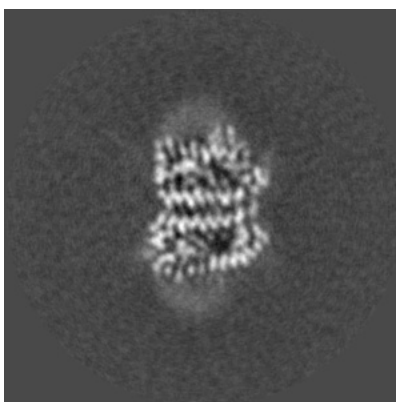


Z Index: 135

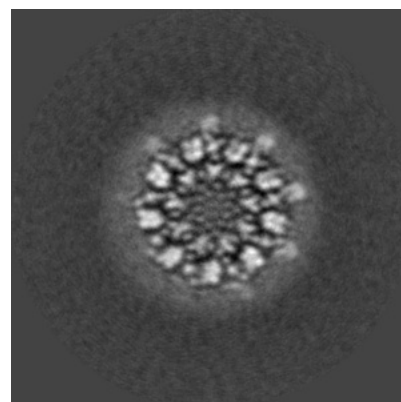
### 6.3.2 Raw map



X Index: 123



Y Index: 124

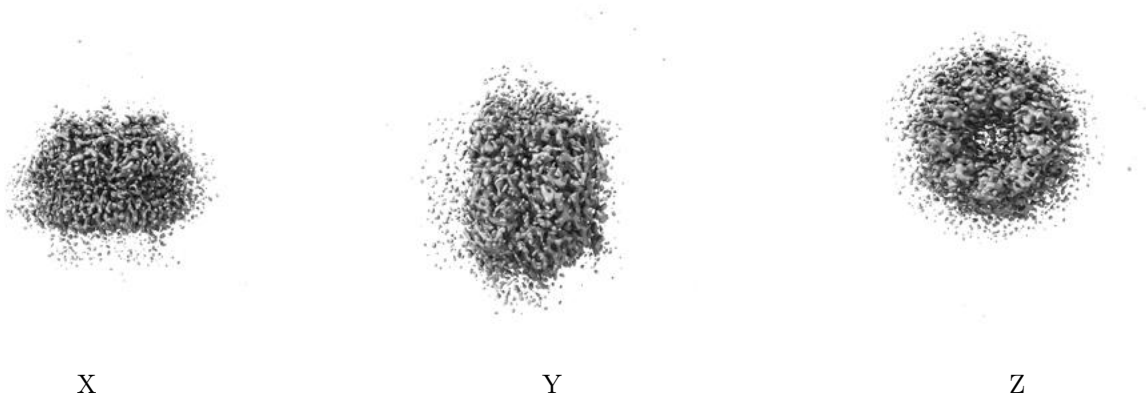


Z Index: 161

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

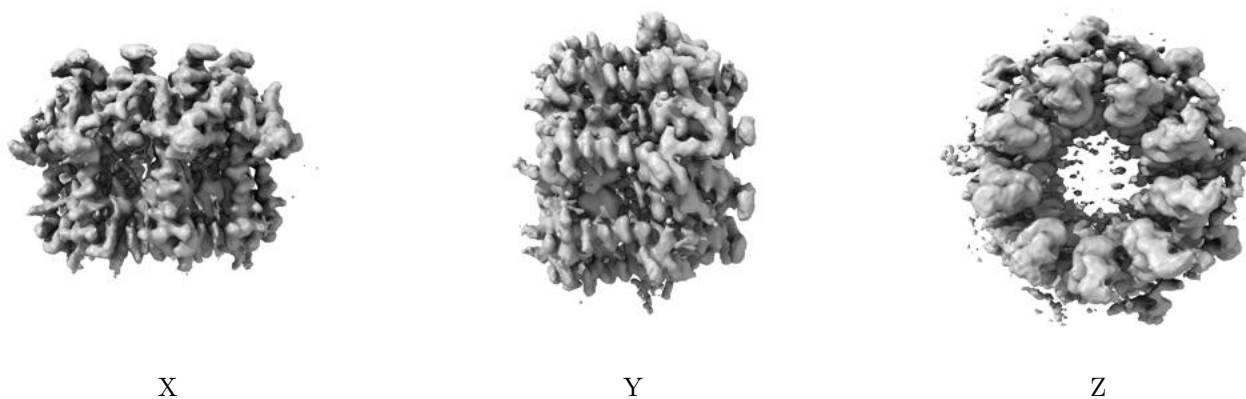
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0347. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

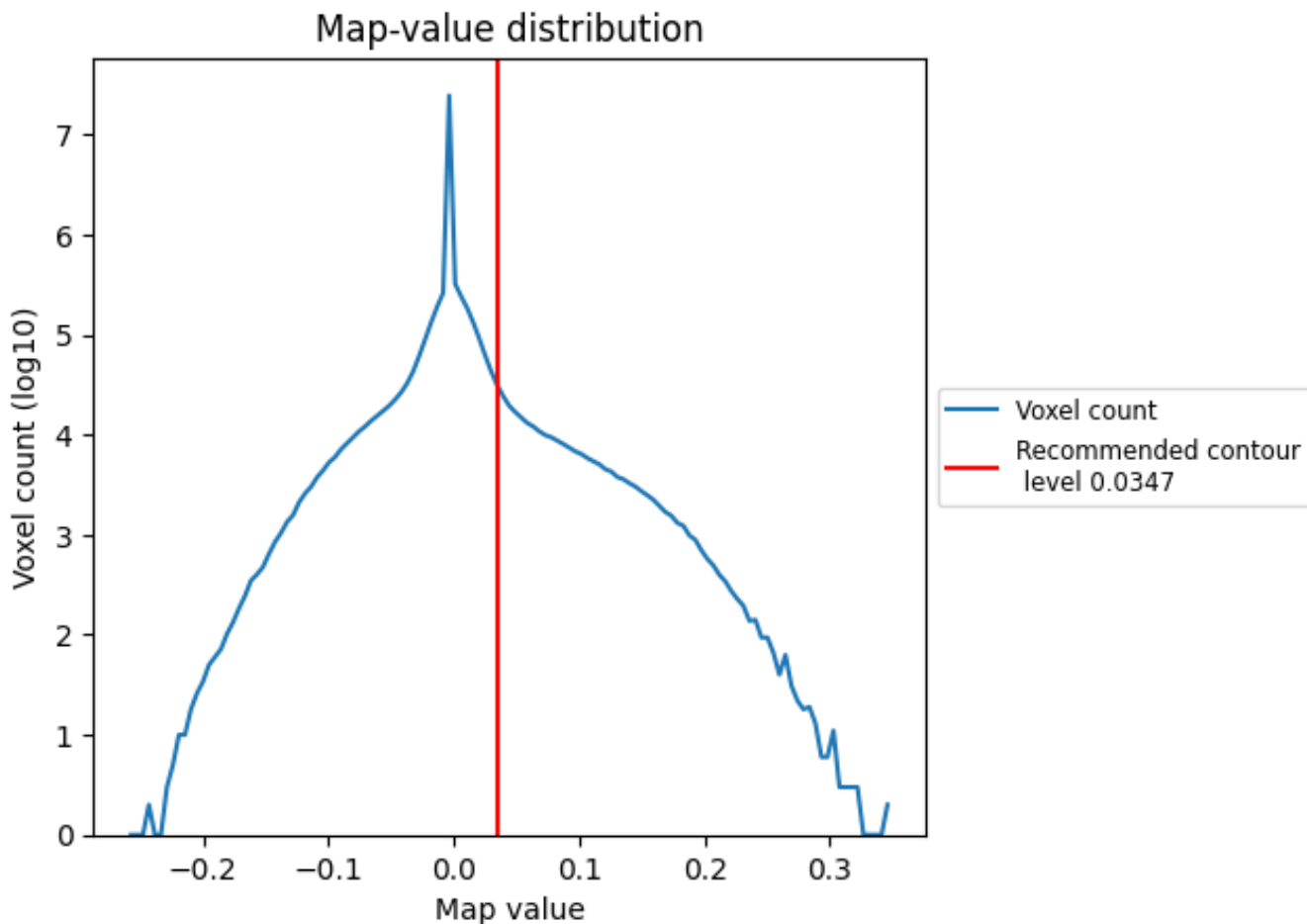
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

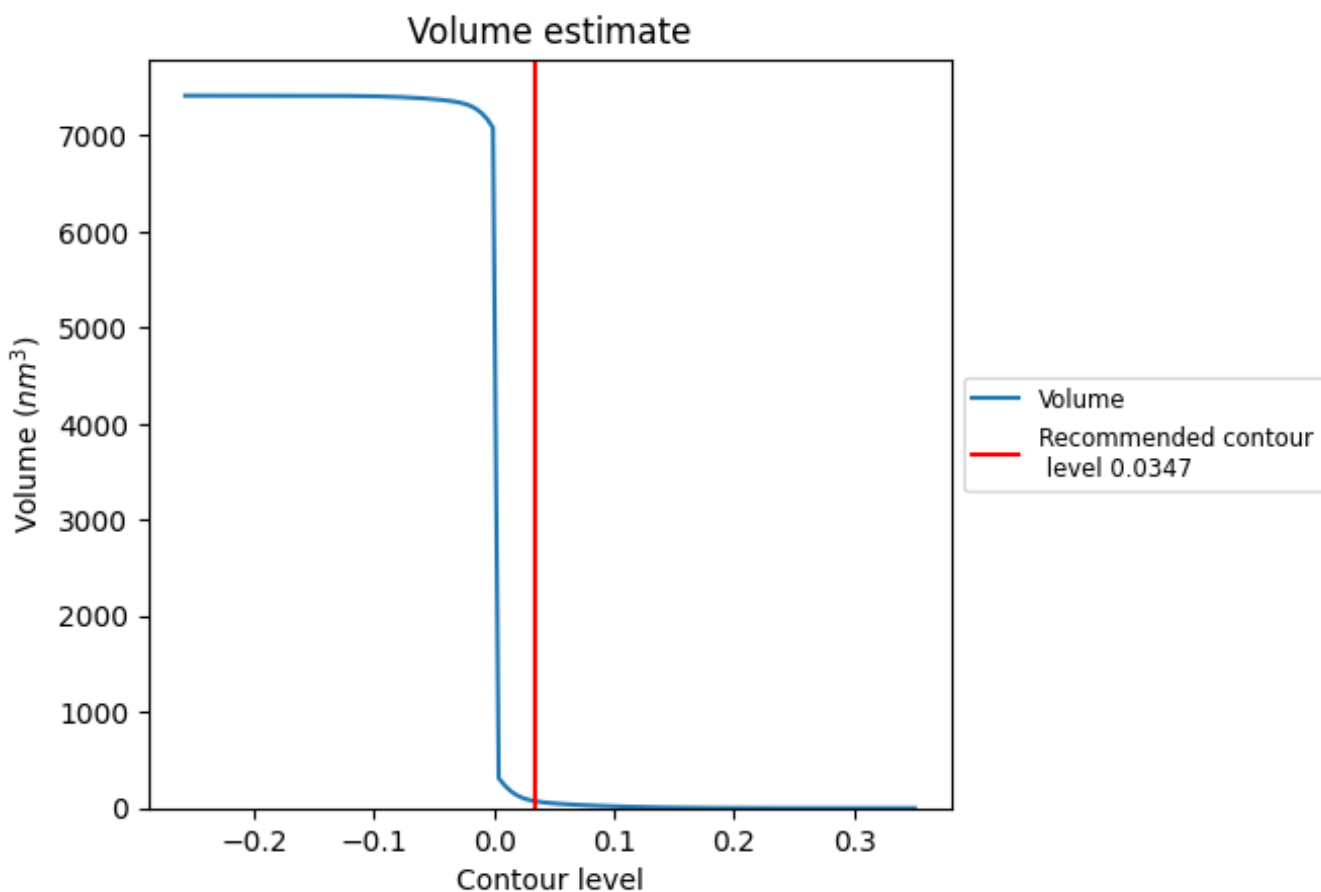
This section contains the results of statistical analysis of the map.

### 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.

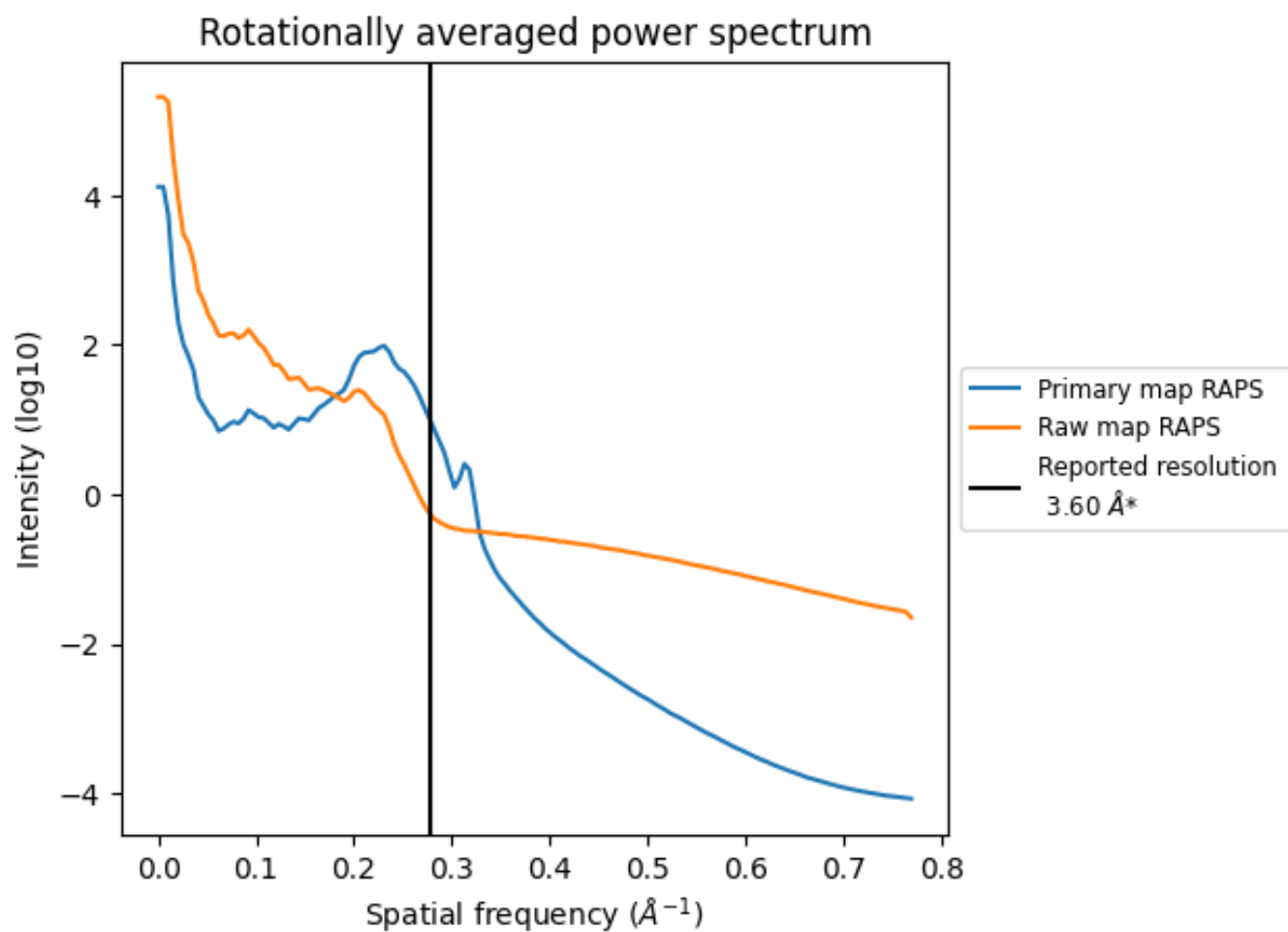
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 72  $\text{nm}^3$ ; this corresponds to an approximate mass of 65 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 i



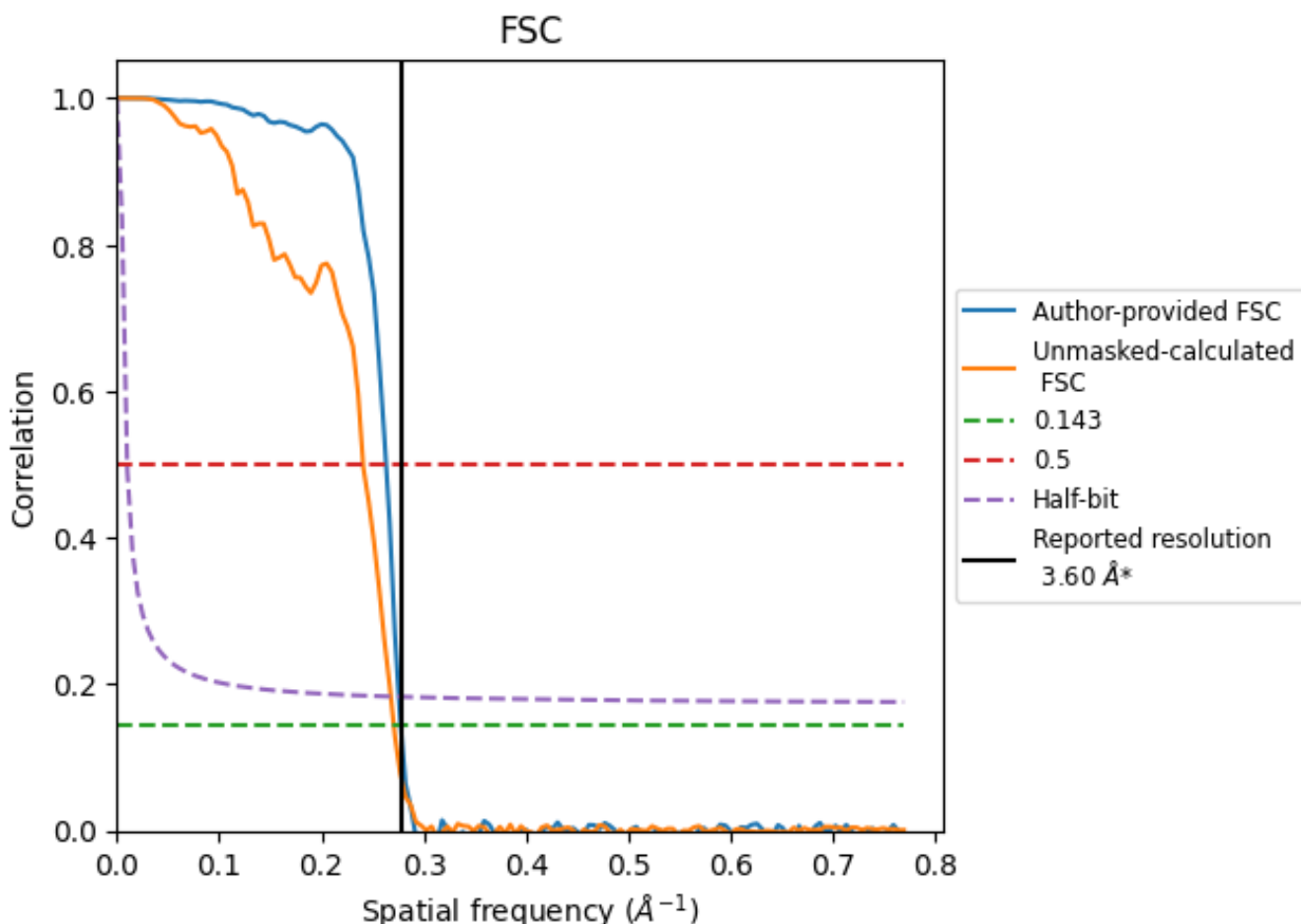
\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>



## 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 0.278  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

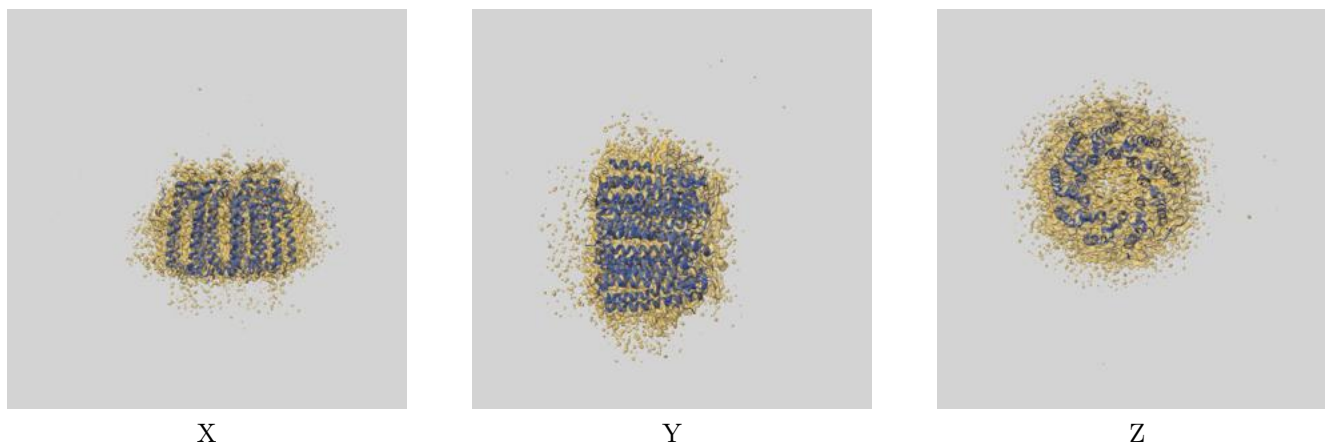
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	3.80	3.63
Unmasked-calculated*	3.69	4.15	3.73

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

## 9 Map-model fit [i](#)

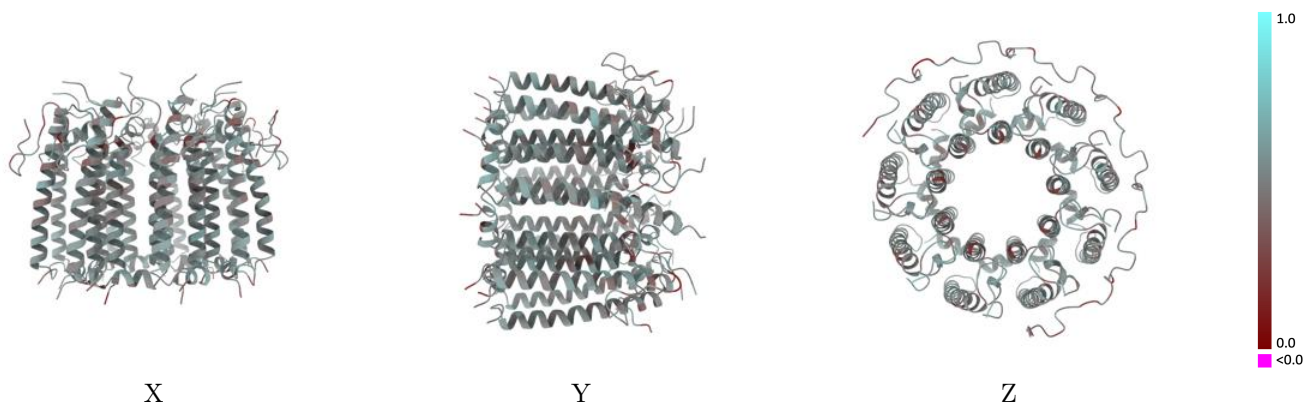
This section contains information regarding the fit between EMDB map EMD-14685 and PDB model 7ZE8. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



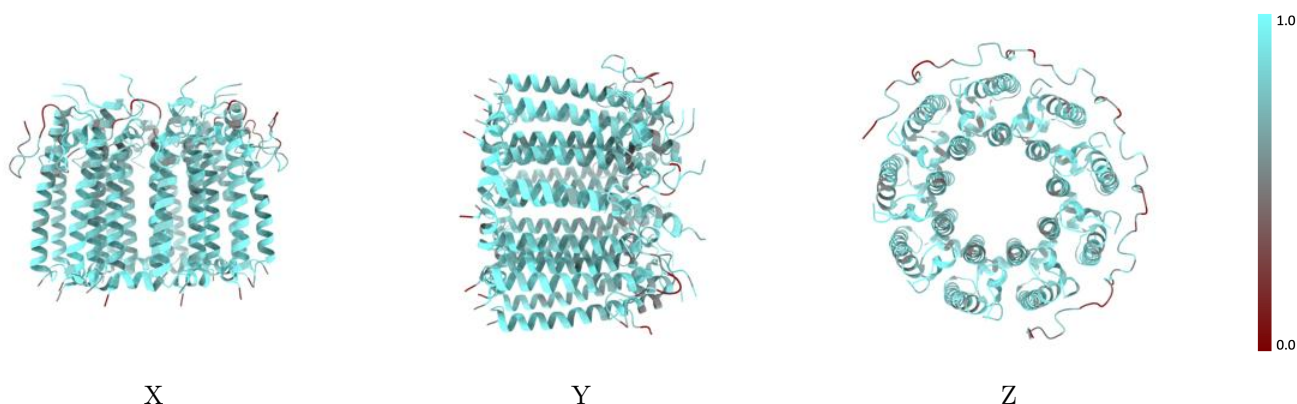
The images above show the 3D surface view of the map at the recommended contour level 0.0347 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



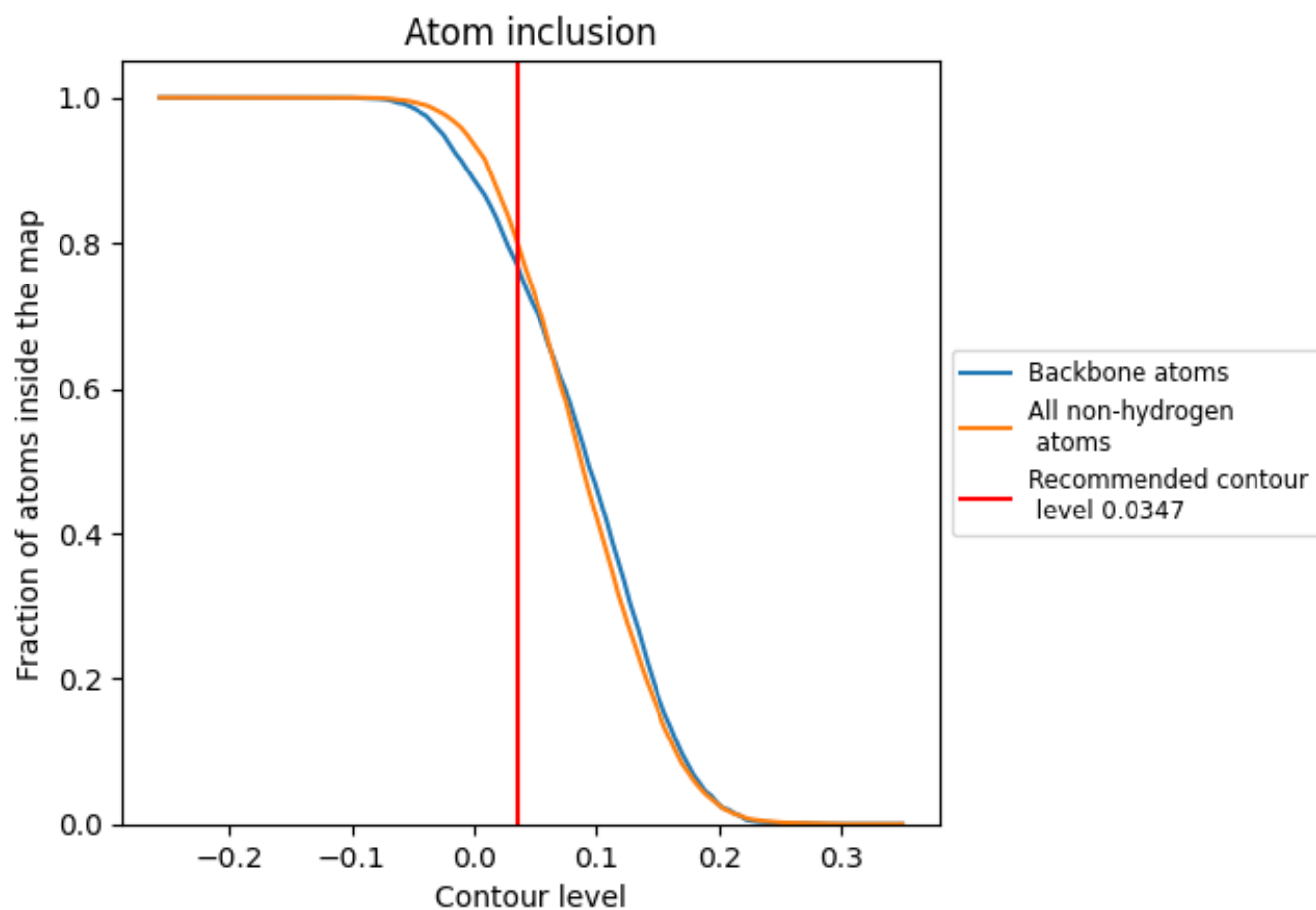
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0347).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 80% 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 (0.0347) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.5090
A	 0.8447	 0.5160
B	 0.8462	 0.5180
C	 0.8373	 0.5210
D	 0.8440	 0.5290
E	 0.8420	 0.5160
F	 0.8290	 0.5160
G	 0.8299	 0.5150
H	 0.8397	 0.5090
I	 0.8447	 0.5230
J	 0.8173	 0.5030
K	 0.8373	 0.5230
L	 0.8290	 0.5200
M	 0.8320	 0.5240
N	 0.8337	 0.5240
O	 0.8440	 0.5210
P	 0.8162	 0.5130
Q	 0.8400	 0.5160
R	 0.8009	 0.5010
S	 0.5466	 0.4490

