



## Full wwPDB EM Validation Report ⓘ

Jul 22, 2025 – 10:25 AM EDT

PDB ID : 9EK8 / pdb\_00009ek8  
EMDB ID : EMD-48112  
Title : Light Harvesting complex 2 (LH2), B800-B850, of Rhodoblastus (Rbl.) acidophilus strain 7750  
Authors : Harris, D.; Schlau-Cohen, G.S.  
Deposited on : 2024-12-01  
Resolution : 2.35 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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

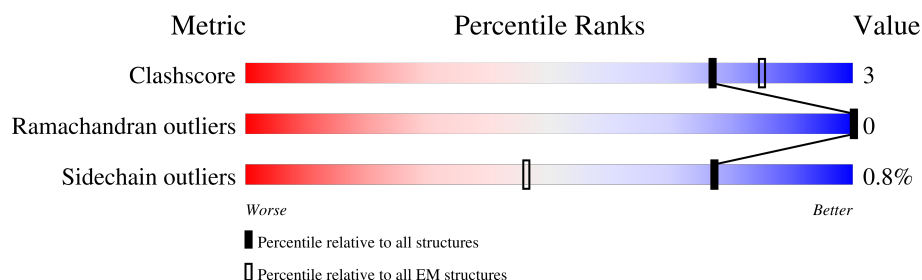
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.35 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.




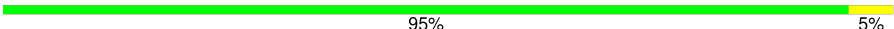
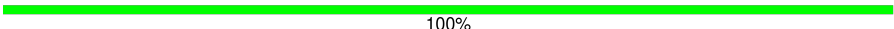
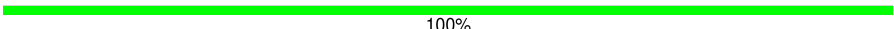
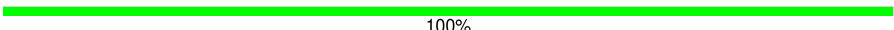
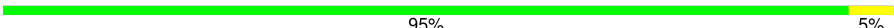
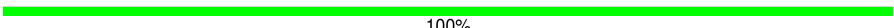
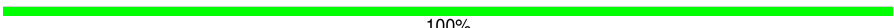
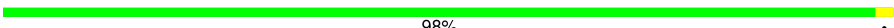

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	48	94% 6%
1	C	48	94% 6%
1	E	48	96% .
1	G	48	94% 6%
1	I	48	94% 6%
1	K	48	96% .
1	M	48	96% .
1	O	48	94% . .

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Mol	Chain	Length	Quality of chain
1	Q	48	 92%8%
2	B	41	 95%5%
2	D	41	 100%
2	F	41	 100%
2	H	41	 100%
2	J	41	 95%5%
2	L	41	 100%
2	N	41	 100%
2	P	41	 98%•
2	R	41	 95%5%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8847 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 B-800/850 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	48	Total	C	N	O	S	0	0
			369	246	60	62	1		
1	C	48	Total	C	N	O	S	0	0
			369	246	60	62	1		
1	E	48	Total	C	N	O	S	0	0
			369	246	60	62	1		
1	G	48	Total	C	N	O	S	0	0
			369	246	60	62	1		
1	I	48	Total	C	N	O	S	0	0
			369	246	60	62	1		
1	K	48	Total	C	N	O	S	0	0
			369	246	60	62	1		
1	M	48	Total	C	N	O	S	0	0
			369	246	60	62	1		
1	O	48	Total	C	N	O	S	0	0
			369	246	60	62	1		
1	Q	48	Total	C	N	O	S	0	0
			369	246	60	62	1		

- Molecule 2 is a protein called Light-harvesting protein B-800/850 beta chain.

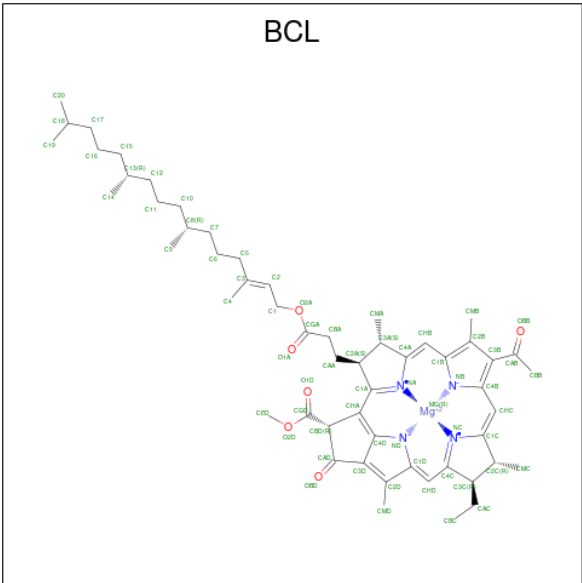
Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	41	Total	C	N	O	0	0
			324	213	53	58		
2	D	41	Total	C	N	O	0	0
			324	213	53	58		
2	F	41	Total	C	N	O	0	0
			324	213	53	58		
2	H	41	Total	C	N	O	0	0
			324	213	53	58		
2	J	41	Total	C	N	O	0	0
			324	213	53	58		
2	L	41	Total	C	N	O	0	0
			324	213	53	58		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	41	Total	C	N	O	0	0
			324	213	53	58		
2	P	41	Total	C	N	O	0	0
			324	213	53	58		
2	R	41	Total	C	N	O	0	0
			324	213	53	58		

- Molecule 3 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



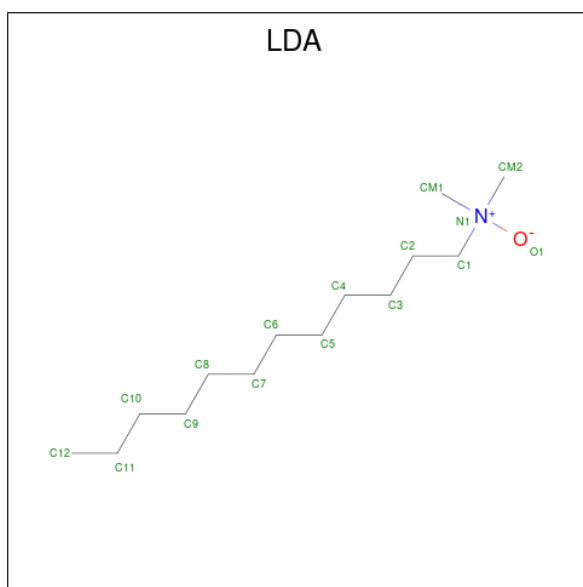
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	Mg	N	O
			66	55	1	4	6
3	A	1	Total	C	Mg	N	O
			66	55	1	4	6
3	B	1	Total	C	Mg	N	O
			66	55	1	4	6
3	C	1	Total	C	Mg	N	O
			66	55	1	4	6
3	C	1	Total	C	Mg	N	O
			66	55	1	4	6
3	D	1	Total	C	Mg	N	O
			66	55	1	4	6
3	E	1	Total	C	Mg	N	O
			66	55	1	4	6
3	E	1	Total	C	Mg	N	O
			66	55	1	4	6

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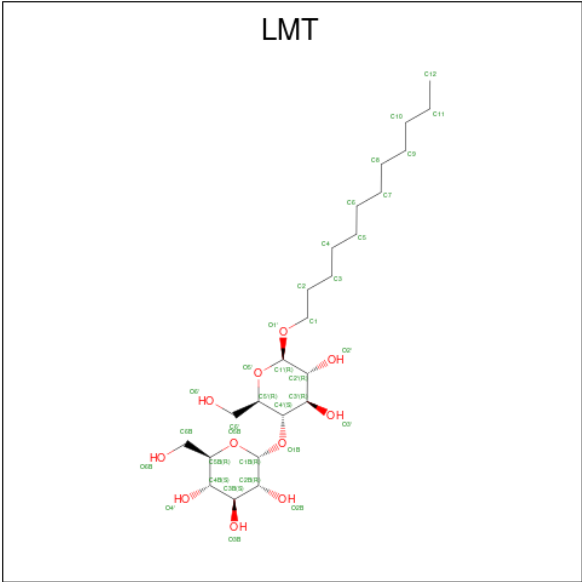
Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
3	R	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			16	14	1	1	
4	C	1	Total	C	N	O	0
			16	14	1	1	
4	E	1	Total	C	N	O	0
			16	14	1	1	
4	G	1	Total	C	N	O	0
			16	14	1	1	
4	I	1	Total	C	N	O	0
			16	14	1	1	
4	K	1	Total	C	N	O	0
			16	14	1	1	
4	M	1	Total	C	N	O	0
			16	14	1	1	
4	O	1	Total	C	N	O	0
			16	14	1	1	
4	Q	1	Total	C	N	O	0
			16	14	1	1	

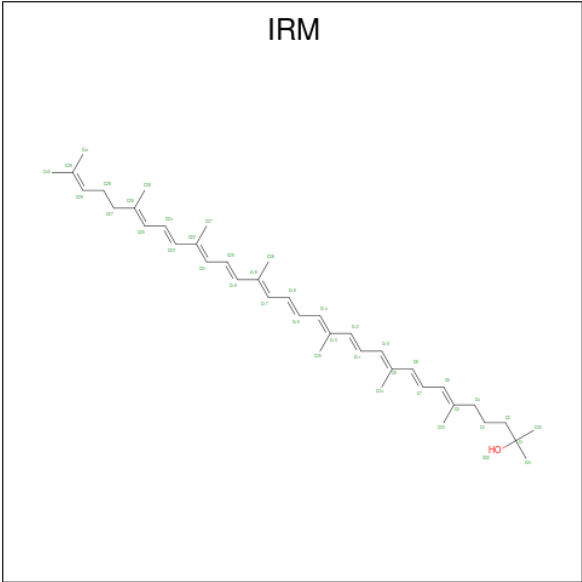
- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			35	24	11	
5	D	1	Total	C	O	0
			35	24	11	
5	F	1	Total	C	O	0
			35	24	11	
5	H	1	Total	C	O	0
			35	24	11	
5	I	1	Total	C	O	0
			35	24	11	
5	L	1	Total	C	O	0
			35	24	11	
5	N	1	Total	C	O	0
			35	24	11	
5	P	1	Total	C	O	0
			35	24	11	
5	R	1	Total	C	O	0
			35	24	11	

- Molecule 6 is 1,2-Dihydro-psi,psi-caroten-1-ol (CCD ID: IRM) (formula: C<sub>40</sub>H<sub>58</sub>O) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			41	40	1	
6	D	1	Total	C	O	0
			41	40	1	
6	E	1	Total	C	O	0
			41	40	1	
6	H	1	Total	C	O	0
			41	40	1	
6	J	1	Total	C	O	0
			41	40	1	
6	L	1	Total	C	O	0
			41	40	1	
6	N	1	Total	C	O	0
			41	40	1	
6	P	1	Total	C	O	0
			41	40	1	
6	R	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 B-800/850 alpha chain

Chain A: 



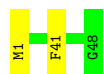
- Molecule 1: Light-harvesting protein B-800/850 alpha chain

Chain C: 



- Molecule 1: Light-harvesting protein B-800/850 alpha chain

Chain E: 



- Molecule 1: Light-harvesting protein B-800/850 alpha chain

Chain G: 

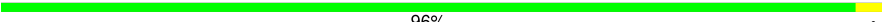


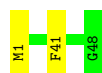
- Molecule 1: Light-harvesting protein B-800/850 alpha chain

Chain I: 



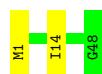
- Molecule 1: Light-harvesting protein B-800/850 alpha chain

Chain K:  96% .



- Molecule 1: Light-harvesting protein B-800/850 alpha chain

Chain M:  96% .



- Molecule 1: Light-harvesting protein B-800/850 alpha chain

Chain O:  94% . .



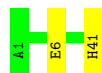
- Molecule 1: Light-harvesting protein B-800/850 alpha chain

Chain Q:  92% 8%



- Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain B:  95% 5%



- Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain F:  100%

There are no outlier residues recorded for this chain.

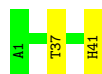
- Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain J:  95% 5%



- Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain P:  98% .



- Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain R:  95% 5%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61970	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	43.37	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	20.687	Depositor
Minimum map value	-0.159	Depositor
Average map value	-0.040	Depositor
Map value standard deviation	0.576	Depositor
Recommended contour level	0.234	Depositor
Map size (Å)	248.51999, 248.51999, 248.51999	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.654, 0.654, 0.654	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: BCL, IRM, CXM, LMT, LDA

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	0.66	0/370	1.26	1/510 (0.2%)
1	C	0.59	0/370	1.14	1/510 (0.2%)
1	E	0.60	0/370	1.13	1/510 (0.2%)
1	G	0.60	0/370	1.12	1/510 (0.2%)
1	I	0.62	0/370	1.17	1/510 (0.2%)
1	K	0.59	0/370	1.12	1/510 (0.2%)
1	M	0.62	0/370	1.18	0/510
1	O	0.57	0/370	1.08	0/510
1	Q	0.57	0/370	1.10	1/510 (0.2%)
2	B	0.86	2/333 (0.6%)	1.26	0/453
2	D	0.57	0/333	1.05	0/453
2	F	0.58	0/333	0.99	0/453
2	H	0.57	0/333	1.03	0/453
2	J	0.59	0/333	1.03	0/453
2	L	0.60	0/333	1.02	0/453
2	N	0.55	0/333	0.96	0/453
2	P	0.60	0/333	0.99	0/453
2	R	0.61	0/333	1.05	0/453
All	All	0.61	2/6327 (0.0%)	1.10	7/8667 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	GLU	CD-OE2	-7.91	1.10	1.25
2	B	6	GLU	CD-OE1	-6.11	1.13	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	41	PHE	CA-CB-CG	5.73	119.53	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	41	PHE	CA-CB-CG	5.53	119.33	113.80
1	C	41	PHE	CA-CB-CG	5.22	119.02	113.80
1	Q	41	PHE	CA-CB-CG	5.16	118.96	113.80
1	E	41	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	41	PHE	CA-CB-CG	5.09	118.89	113.80
1	I	41	PHE	CA-CB-CG	5.01	118.81	113.80

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	A	369	0	377	0	0
1	C	369	0	377	0	0
1	E	369	0	377	0	0
1	G	369	0	377	1	0
1	I	369	0	377	0	0
1	K	369	0	377	0	0
1	M	369	0	377	0	0
1	O	369	0	377	3	0
1	Q	369	0	377	2	0
2	B	324	0	321	1	0
2	D	324	0	321	0	0
2	F	324	0	321	0	0
2	H	324	0	321	0	0
2	J	324	0	321	1	0
2	L	324	0	321	0	0
2	N	324	0	321	0	0
2	P	324	0	321	1	0
2	R	324	0	321	2	0
3	A	132	0	148	4	0
3	B	66	0	74	1	0
3	C	132	0	148	3	0
3	D	66	0	74	2	0
3	E	132	0	148	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	66	0	74	2	0
3	G	132	0	148	5	0
3	H	66	0	74	2	0
3	I	132	0	148	3	0
3	J	66	0	74	2	0
3	K	132	0	148	4	0
3	L	66	0	74	1	0
3	M	132	0	148	3	0
3	N	66	0	74	1	0
3	O	132	0	148	4	0
3	P	66	0	74	1	0
3	Q	132	0	148	4	0
3	R	66	0	74	1	0
4	A	16	0	31	0	0
4	C	16	0	31	0	0
4	E	16	0	31	0	0
4	G	16	0	31	0	0
4	I	16	0	31	0	0
4	K	16	0	31	0	0
4	M	16	0	31	0	0
4	O	16	0	31	0	0
4	Q	16	0	31	0	0
5	A	35	0	46	0	0
5	D	35	0	46	0	0
5	F	35	0	46	0	0
5	H	35	0	46	0	0
5	I	35	0	46	0	0
5	L	35	0	46	0	0
5	N	35	0	46	0	0
5	P	35	0	46	0	0
5	R	35	0	46	0	0
6	B	41	0	0	0	0
6	D	41	0	0	0	0
6	E	41	0	0	0	0
6	H	41	0	0	0	0
6	J	41	0	0	0	0
6	L	41	0	0	0	0
6	N	41	0	0	0	0
6	P	41	0	0	0	0
6	R	41	0	0	0	0
All	All	8847	0	8973	50	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 (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:301:BCL:HMB1	3:O:301:BCL:HBB3	1.82	0.62
3:Q:301:BCL:HMB1	3:Q:301:BCL:HBB3	1.82	0.61
3:A:301:BCL:HMB1	3:A:301:BCL:HBB3	1.82	0.61
3:K:301:BCL:HBB3	3:K:301:BCL:HMB1	1.82	0.61
2:B:41:HIS:O	1:Q:48:GLY:OXT	2.18	0.61
1:G:48:GLY:OXT	2:J:41:HIS:O	2.19	0.61
3:M:301:BCL:HBB3	3:M:301:BCL:HMB1	1.83	0.61
3:C:302:BCL:HBB2	3:C:302:BCL:HHC	1.84	0.60
3:Q:302:BCL:HHC	3:Q:302:BCL:HBB2	1.83	0.60
3:C:302:BCL:H43	3:D:102:BCL:H43	1.82	0.60
3:E:302:BCL:HHC	3:E:302:BCL:HBB2	1.84	0.60
3:M:302:BCL:HHC	3:M:302:BCL:HBB2	1.83	0.60
3:E:301:BCL:HMB1	3:E:301:BCL:HBB3	1.81	0.60
3:G:301:BCL:HMB1	3:G:301:BCL:HBB3	1.82	0.60
3:G:302:BCL:HBB2	3:G:302:BCL:HHC	1.83	0.60
3:I:301:BCL:HBB3	3:I:301:BCL:HMB1	1.83	0.59
3:O:302:BCL:HBB2	3:O:302:BCL:HHC	1.84	0.59
3:C:301:BCL:HBB3	3:C:301:BCL:HMB1	1.83	0.59
3:A:302:BCL:HBB2	3:A:302:BCL:HHC	1.85	0.59
3:K:302:BCL:HBB2	3:K:302:BCL:HHC	1.84	0.59
3:H:102:BCL:HBB2	3:H:102:BCL:HMB3	1.85	0.58
3:I:302:BCL:HBB2	3:I:302:BCL:HHC	1.85	0.58
3:L:102:BCL:HBB2	3:L:102:BCL:HMB3	1.88	0.55
3:N:101:BCL:HBB2	3:N:101:BCL:HMB3	1.88	0.55
3:D:102:BCL:HBB2	3:D:102:BCL:HMB3	1.88	0.54
3:J:101:BCL:HBB2	3:J:101:BCL:HMB3	1.89	0.54
1:Q:5:LYS:HE2	2:R:5:ALA:HB1	1.90	0.53
3:F:101:BCL:HBB2	3:F:101:BCL:HMB3	1.90	0.53
3:P:101:BCL:HMB3	3:P:101:BCL:HBB2	1.89	0.53
3:B:101:BCL:CBB	3:B:101:BCL:HMB1	2.41	0.51
3:R:102:BCL:HMB1	3:R:102:BCL:CBB	2.41	0.51
1:O:48:GLY:OXT	2:R:41:HIS:O	2.36	0.44
3:O:301:BCL:HMB1	3:O:301:BCL:CBB	2.47	0.44
3:Q:301:BCL:HMB1	3:Q:301:BCL:CBB	2.47	0.43
3:A:301:BCL:HMB1	3:A:301:BCL:CBB	2.46	0.43
3:Q:302:BCL:HED2	3:Q:302:BCL:CAD	2.48	0.43
3:G:302:BCL:H42	3:H:102:BCL:H171	2.00	0.43
3:G:302:BCL:HED2	3:G:302:BCL:CAD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1:CXM:ON1	2:P:12:HIS:NE2	2.45	0.43
3:I:301:BCL:HMB1	3:I:301:BCL:CBB	2.48	0.42
3:A:302:BCL:HED2	3:A:302:BCL:CAD	2.50	0.42
3:G:301:BCL:HMB1	3:G:301:BCL:CBB	2.49	0.42
3:O:302:BCL:HED2	3:O:302:BCL:CAD	2.50	0.42
3:E:301:BCL:HMB1	3:E:301:BCL:CBB	2.48	0.42
3:K:301:BCL:HMB1	3:K:301:BCL:CBB	2.48	0.42
3:M:301:BCL:HMB1	3:M:301:BCL:CBB	2.48	0.41
3:K:302:BCL:CAD	3:K:302:BCL:HED2	2.50	0.41
3:J:101:BCL:HMB3	3:J:101:BCL:CBB	2.50	0.40
1:O:2:ASN:OD1	1:O:2:ASN:N	2.54	0.40
3:F:101:BCL:HMB3	3:F:101:BCL:CBB	2.52	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	A	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
1	C	46/48 (96%)	46 (100%)	0	0	100	100
1	E	46/48 (96%)	46 (100%)	0	0	100	100
1	G	46/48 (96%)	46 (100%)	0	0	100	100
1	I	46/48 (96%)	46 (100%)	0	0	100	100
1	K	46/48 (96%)	46 (100%)	0	0	100	100
1	M	46/48 (96%)	46 (100%)	0	0	100	100
1	O	46/48 (96%)	46 (100%)	0	0	100	100
1	Q	46/48 (96%)	46 (100%)	0	0	100	100
2	B	39/41 (95%)	39 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	39/41 (95%)	39 (100%)	0	0	100	100
2	F	39/41 (95%)	39 (100%)	0	0	100	100
2	H	39/41 (95%)	39 (100%)	0	0	100	100
2	J	39/41 (95%)	39 (100%)	0	0	100	100
2	L	39/41 (95%)	39 (100%)	0	0	100	100
2	N	39/41 (95%)	39 (100%)	0	0	100	100
2	P	39/41 (95%)	39 (100%)	0	0	100	100
2	R	39/41 (95%)	39 (100%)	0	0	100	100
All	All	765/801 (96%)	764 (100%)	1 (0%)	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	A	37/37 (100%)	36 (97%)	1 (3%)	40	50
1	C	37/37 (100%)	36 (97%)	1 (3%)	40	50
1	E	37/37 (100%)	37 (100%)	0	100	100
1	G	37/37 (100%)	37 (100%)	0	100	100
1	I	37/37 (100%)	36 (97%)	1 (3%)	40	50
1	K	37/37 (100%)	37 (100%)	0	100	100
1	M	37/37 (100%)	36 (97%)	1 (3%)	40	50
1	O	37/37 (100%)	37 (100%)	0	100	100
1	Q	37/37 (100%)	37 (100%)	0	100	100
2	B	33/33 (100%)	33 (100%)	0	100	100
2	D	33/33 (100%)	33 (100%)	0	100	100
2	F	33/33 (100%)	33 (100%)	0	100	100
2	H	33/33 (100%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	33/33 (100%)	32 (97%)	1 (3%)	36	46
2	L	33/33 (100%)	33 (100%)	0	100	100
2	N	33/33 (100%)	33 (100%)	0	100	100
2	P	33/33 (100%)	33 (100%)	0	100	100
2	R	33/33 (100%)	33 (100%)	0	100	100
All	All	630/630 (100%)	625 (99%)	5 (1%)	77	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	C	14	ILE
1	I	14	ILE
2	J	37	THR
1	M	14	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
2	R	7	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1,3	9,10,11	0.80	0	9,11,13	1.62	2 (22%)
1	CXM	C	1	1,3	9,10,11	2.03	3 (33%)	9,11,13	1.54	3 (33%)
1	CXM	M	1	1,3	9,10,11	0.81	0	9,11,13	1.62	3 (33%)
1	CXM	K	1	1,3	9,10,11	0.84	0	9,11,13	1.69	3 (33%)
1	CXM	O	1	1,3	9,10,11	2.01	2 (22%)	9,11,13	1.52	3 (33%)
1	CXM	E	1	1,3	9,10,11	2.04	3 (33%)	9,11,13	1.49	3 (33%)
1	CXM	G	1	1,3	9,10,11	2.03	2 (22%)	9,11,13	1.50	3 (33%)
1	CXM	Q	1	1,3	9,10,11	2.05	3 (33%)	9,11,13	1.49	3 (33%)
1	CXM	I	1	1,3	9,10,11	0.81	0	9,11,13	1.69	2 (22%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	1	CXM	CN-N	3.98	1.42	1.35
1	E	1	CXM	CN-N	3.98	1.42	1.35
1	G	1	CXM	CN-N	3.96	1.42	1.35
1	C	1	CXM	CN-N	3.92	1.42	1.35
1	O	1	CXM	CN-N	3.89	1.42	1.35
1	G	1	CXM	ON1-CN	3.50	1.28	1.21
1	C	1	CXM	ON1-CN	3.49	1.28	1.21
1	Q	1	CXM	ON1-CN	3.48	1.28	1.21
1	O	1	CXM	ON1-CN	3.45	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1	CXM	ON1-CN	3.43	1.28	1.21
1	E	1	CXM	CA-N	-2.10	1.43	1.46
1	Q	1	CXM	CA-N	-2.05	1.43	1.46
1	C	1	CXM	CA-N	-2.04	1.43	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1	CXM	ON1-CN-N	-3.27	119.50	124.86
1	A	1	CXM	ON1-CN-N	-3.21	119.60	124.86
1	K	1	CXM	C-CA-N	3.20	115.68	109.50
1	K	1	CXM	ON1-CN-N	-3.16	119.67	124.86
1	I	1	CXM	C-CA-N	3.16	115.59	109.50
1	M	1	CXM	C-CA-N	3.07	115.43	109.50
1	M	1	CXM	ON1-CN-N	-3.00	119.94	124.86
1	A	1	CXM	C-CA-N	2.83	114.96	109.50
1	C	1	CXM	C-CA-N	2.81	114.92	109.50
1	O	1	CXM	C-CA-N	2.80	114.91	109.50
1	G	1	CXM	C-CA-N	2.78	114.87	109.50
1	Q	1	CXM	C-CA-N	2.67	114.65	109.50
1	E	1	CXM	C-CA-N	2.66	114.64	109.50
1	Q	1	CXM	ON1-CN-N	-2.49	120.77	124.86
1	E	1	CXM	ON1-CN-N	-2.46	120.81	124.86
1	C	1	CXM	ON1-CN-N	-2.44	120.86	124.86
1	O	1	CXM	ON1-CN-N	-2.43	120.87	124.86
1	G	1	CXM	ON1-CN-N	-2.40	120.92	124.86
1	C	1	CXM	O-C-CA	-2.29	118.89	124.77
1	E	1	CXM	O-C-CA	-2.25	118.98	124.77
1	Q	1	CXM	O-C-CA	-2.24	119.01	124.77
1	G	1	CXM	O-C-CA	-2.23	119.04	124.77
1	O	1	CXM	O-C-CA	-2.22	119.07	124.77
1	M	1	CXM	O-C-CA	-2.08	119.43	124.77
1	K	1	CXM	O-C-CA	-2.00	119.62	124.77

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1	CXM	O-C-CA-CB
1	M	1	CXM	O-C-CA-CB
1	O	1	CXM	O-C-CA-CB
1	E	1	CXM	C-CA-N-CN

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	O	1	CXM	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

54 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
6	IRM	H	103	-	40,40,40	2.41	13 (32%)	49,49,49	1.61	9 (18%)
6	IRM	J	102	-	40,40,40	2.75	14 (35%)	49,49,49	1.67	9 (18%)
5	LMT	L	101	-	36,36,36	0.67	0	47,47,47	0.59	0
5	LMT	A	304	-	36,36,36	0.65	0	47,47,47	0.58	0
3	BCL	D	102	2	64,74,74	3.06	6 (9%)	74,115,115	2.02	8 (10%)
4	LDA	A	303	-	13,15,15	0.92	0	14,17,17	0.60	0
3	BCL	E	302	1	64,74,74	3.13	7 (10%)	74,115,115	2.10	8 (10%)
3	BCL	O	302	1	64,74,74	3.11	7 (10%)	74,115,115	2.21	13 (17%)
3	BCL	K	302	1	64,74,74	2.99	7 (10%)	74,115,115	2.12	11 (14%)
3	BCL	O	301	1	64,74,74	3.02	7 (10%)	74,115,115	2.06	8 (10%)
3	BCL	Q	302	1	64,74,74	3.12	7 (10%)	74,115,115	2.22	11 (14%)
3	BCL	R	102	2	64,74,74	3.07	6 (9%)	74,115,115	2.05	8 (10%)
6	IRM	E	304	-	40,40,40	2.42	13 (32%)	49,49,49	1.64	10 (20%)
5	LMT	I	303	-	36,36,36	0.63	0	47,47,47	0.74	1 (2%)
3	BCL	C	301	1	64,74,74	3.03	7 (10%)	74,115,115	2.07	8 (10%)
3	BCL	L	102	2	64,74,74	3.08	6 (9%)	74,115,115	2.04	8 (10%)
5	LMT	F	102	-	36,36,36	0.66	0	47,47,47	0.55	0
4	LDA	E	303	-	13,15,15	0.97	2 (15%)	14,17,17	0.52	0
6	IRM	P	102	-	40,40,40	2.44	13 (32%)	49,49,49	1.67	10 (20%)
3	BCL	M	302	1	64,74,74	3.07	7 (10%)	74,115,115	1.96	8 (10%)
3	BCL	G	302	1	64,74,74	3.08	7 (10%)	74,115,115	2.16	10 (13%)
3	BCL	B	101	2	64,74,74	3.16	7 (10%)	74,115,115	2.10	10 (13%)
3	BCL	Q	301	1	64,74,74	2.99	7 (10%)	74,115,115	2.07	8 (10%)
3	BCL	A	301	1	64,74,74	3.03	8 (12%)	74,115,115	2.07	8 (10%)
4	LDA	Q	303	-	13,15,15	0.91	1 (7%)	14,17,17	0.61	0
4	LDA	K	303	-	13,15,15	0.96	1 (7%)	14,17,17	0.54	0
5	LMT	D	101	-	36,36,36	0.79	1 (2%)	47,47,47	0.70	1 (2%)
5	LMT	P	103	-	36,36,36	0.57	0	47,47,47	0.76	1 (2%)
3	BCL	E	301	1	64,74,74	3.06	7 (10%)	74,115,115	2.07	8 (10%)
3	BCL	M	301	1	64,74,74	2.99	8 (12%)	74,115,115	2.06	8 (10%)
4	LDA	O	303	-	13,15,15	0.94	1 (7%)	14,17,17	0.49	0
4	LDA	I	304	-	13,15,15	0.97	1 (7%)	14,17,17	0.54	0
6	IRM	D	103	-	40,40,40	2.41	13 (32%)	49,49,49	1.60	10 (20%)
6	IRM	R	103	-	40,40,40	2.43	13 (32%)	49,49,49	1.60	9 (18%)
3	BCL	I	302	1	64,74,74	3.12	7 (10%)	74,115,115	2.02	10 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	LDA	C	303	-	13,15,15	0.89	1 (7%)	14,17,17	0.54	0
6	IRM	B	102	-	40,40,40	2.43	13 (32%)	49,49,49	1.64	9 (18%)
6	IRM	L	103	-	40,40,40	2.43	13 (32%)	49,49,49	1.64	10 (20%)
3	BCL	J	101	2	64,74,74	3.16	6 (9%)	74,115,115	2.06	8 (10%)
3	BCL	N	101	2	64,74,74	3.11	6 (9%)	74,115,115	2.08	9 (12%)
4	LDA	G	303	-	13,15,15	1.01	2 (15%)	14,17,17	0.55	0
4	LDA	M	303	-	13,15,15	0.98	2 (15%)	14,17,17	0.54	0
3	BCL	P	101	2	64,74,74	3.03	6 (9%)	74,115,115	2.03	9 (12%)
5	LMT	H	101	-	36,36,36	0.74	0	47,47,47	0.67	0
5	LMT	R	101	-	36,36,36	0.65	0	47,47,47	0.58	0
3	BCL	G	301	1	64,74,74	3.01	7 (10%)	74,115,115	2.11	7 (9%)
3	BCL	I	301	1	64,74,74	2.98	7 (10%)	74,115,115	2.06	8 (10%)
5	LMT	N	103	-	36,36,36	0.63	0	47,47,47	0.58	0
6	IRM	N	102	-	40,40,40	2.43	13 (32%)	49,49,49	1.65	10 (20%)
3	BCL	A	302	1	64,74,74	3.01	7 (10%)	74,115,115	2.09	10 (13%)
3	BCL	K	301	1	64,74,74	3.00	7 (10%)	74,115,115	2.10	7 (9%)
3	BCL	F	101	2	64,74,74	3.06	6 (9%)	74,115,115	2.02	8 (10%)
3	BCL	C	302	1	64,74,74	3.13	7 (10%)	74,115,115	2.02	7 (9%)
3	BCL	H	102	2	64,74,74	3.08	6 (9%)	74,115,115	2.05	10 (13%)

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
6	IRM	H	103	-	-	5/44/44/44	-
6	IRM	J	102	-	-	5/44/44/44	-
5	LMT	L	101	-	-	4/21/61/61	0/2/2/2
5	LMT	A	304	-	-	3/21/61/61	0/2/2/2
3	BCL	D	102	2	-	2/37/137/137	-
4	LDA	A	303	-	-	0/13/13/13	-
3	BCL	E	302	1	-	10/37/137/137	-
3	BCL	O	302	1	-	9/37/137/137	-
3	BCL	K	302	1	-	4/37/137/137	-
3	BCL	O	301	1	-	1/37/137/137	-
3	BCL	Q	302	1	-	3/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BCL	R	102	2	-	4/37/137/137	-
6	IRM	E	304	-	-	5/44/44/44	-
5	LMT	I	303	-	-	5/21/61/61	0/2/2/2
3	BCL	C	301	1	-	0/37/137/137	-
3	BCL	L	102	2	-	2/37/137/137	-
5	LMT	F	102	-	-	4/21/61/61	0/2/2/2
4	LDA	E	303	-	-	0/13/13/13	-
6	IRM	P	102	-	-	5/44/44/44	-
3	BCL	M	302	1	-	3/37/137/137	-
3	BCL	G	302	1	-	4/37/137/137	-
3	BCL	B	101	2	-	5/37/137/137	-
3	BCL	Q	301	1	-	2/37/137/137	-
3	BCL	A	301	1	-	2/37/137/137	-
4	LDA	Q	303	-	-	0/13/13/13	-
4	LDA	K	303	-	-	1/13/13/13	-
5	LMT	D	101	-	-	4/21/61/61	0/2/2/2
5	LMT	P	103	-	-	4/21/61/61	0/2/2/2
3	BCL	E	301	1	-	0/37/137/137	-
3	BCL	M	301	1	-	1/37/137/137	-
4	LDA	O	303	-	-	0/13/13/13	-
4	LDA	I	304	-	-	1/13/13/13	-
6	IRM	D	103	-	-	5/44/44/44	-
6	IRM	R	103	-	-	5/44/44/44	-
3	BCL	I	302	1	-	5/37/137/137	-
4	LDA	C	303	-	-	0/13/13/13	-
6	IRM	B	102	-	-	5/44/44/44	-
6	IRM	L	103	-	-	5/44/44/44	-
3	BCL	J	101	2	-	7/37/137/137	-
3	BCL	N	101	2	-	4/37/137/137	-
4	LDA	G	303	-	-	0/13/13/13	-
4	LDA	M	303	-	-	0/13/13/13	-
3	BCL	P	101	2	-	2/37/137/137	-
5	LMT	H	101	-	-	3/21/61/61	0/2/2/2
5	LMT	R	101	-	-	4/21/61/61	0/2/2/2
3	BCL	G	301	1	-	2/37/137/137	-
3	BCL	I	301	1	-	0/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	N	103	-	-	5/21/61/61	0/2/2/2
6	IRM	N	102	-	-	5/44/44/44	-
3	BCL	A	302	1	-	3/37/137/137	-
3	BCL	K	301	1	-	0/37/137/137	-
3	BCL	F	101	2	-	4/37/137/137	-
3	BCL	C	302	1	-	4/37/137/137	-
3	BCL	H	102	2	-	9/37/137/137	-

All (313) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	101	BCL	CHC-C1C	15.32	1.47	1.33
3	E	301	BCL	CHB-C4A	15.24	1.47	1.33
3	F	101	BCL	CHC-C1C	15.13	1.47	1.33
3	A	301	BCL	CHB-C4A	15.10	1.47	1.33
3	O	301	BCL	CHB-C4A	15.07	1.47	1.33
3	C	301	BCL	CHB-C4A	15.00	1.47	1.33
3	G	301	BCL	CHB-C4A	15.00	1.47	1.33
3	N	101	BCL	CHC-C1C	14.95	1.47	1.33
3	D	102	BCL	CHC-C1C	14.95	1.47	1.33
3	R	102	BCL	CHC-C1C	14.89	1.47	1.33
3	I	302	BCL	CHC-C1C	14.88	1.47	1.33
3	Q	301	BCL	CHB-C4A	14.87	1.46	1.33
3	L	102	BCL	CHC-C1C	14.82	1.46	1.33
3	C	301	BCL	CHC-C1C	14.80	1.46	1.33
3	I	301	BCL	CHB-C4A	14.79	1.46	1.33
3	G	302	BCL	CHC-C1C	14.78	1.46	1.33
3	E	301	BCL	CHC-C1C	14.78	1.46	1.33
3	Q	302	BCL	CHC-C1C	14.76	1.46	1.33
3	K	301	BCL	CHC-C1C	14.76	1.46	1.33
3	K	301	BCL	CHB-C4A	14.73	1.46	1.33
3	O	301	BCL	CHC-C1C	14.72	1.46	1.33
3	E	302	BCL	CHC-C1C	14.69	1.46	1.33
3	M	301	BCL	CHB-C4A	14.67	1.46	1.33
3	O	302	BCL	CHC-C1C	14.66	1.46	1.33
3	B	101	BCL	CHC-C1C	14.65	1.46	1.33
3	A	302	BCL	CHC-C1C	14.65	1.46	1.33
3	M	301	BCL	CHC-C1C	14.59	1.46	1.33
3	M	302	BCL	CHC-C1C	14.58	1.46	1.33
3	C	302	BCL	CHC-C1C	14.55	1.46	1.33
3	B	101	BCL	CHB-C4A	14.54	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	BCL	CHC-C1C	14.53	1.46	1.33
3	P	101	BCL	CHC-C1C	14.53	1.46	1.33
3	G	301	BCL	CHC-C1C	14.50	1.46	1.33
3	I	301	BCL	CHC-C1C	14.44	1.46	1.33
3	Q	301	BCL	CHC-C1C	14.37	1.46	1.33
3	J	101	BCL	CHB-C4A	14.32	1.46	1.33
3	H	102	BCL	CHC-C1C	14.31	1.46	1.33
3	K	302	BCL	CHC-C1C	14.20	1.46	1.33
3	D	102	BCL	CHB-C4A	14.14	1.46	1.33
3	E	302	BCL	CHB-C4A	14.13	1.46	1.33
3	R	102	BCL	CHB-C4A	14.06	1.46	1.33
3	C	302	BCL	CHB-C4A	14.04	1.46	1.33
3	N	101	BCL	CHB-C4A	14.02	1.46	1.33
3	L	102	BCL	CHB-C4A	13.91	1.46	1.33
3	F	101	BCL	CHB-C4A	13.84	1.46	1.33
3	O	302	BCL	CHB-C4A	13.81	1.46	1.33
3	H	102	BCL	CHB-C4A	13.79	1.45	1.33
3	Q	302	BCL	CHB-C4A	13.77	1.45	1.33
3	G	302	BCL	CHB-C4A	13.71	1.45	1.33
3	M	302	BCL	CHB-C4A	13.67	1.45	1.33
3	P	101	BCL	CHB-C4A	13.54	1.45	1.33
3	K	302	BCL	CHB-C4A	13.45	1.45	1.33
3	I	302	BCL	CHB-C4A	13.43	1.45	1.33
3	A	302	BCL	CHB-C4A	13.27	1.45	1.33
3	C	302	BCL	MG-NC	11.26	2.33	2.06
3	B	101	BCL	MG-NC	11.25	2.33	2.06
3	H	102	BCL	MG-NC	11.16	2.32	2.06
3	N	101	BCL	MG-NC	10.93	2.32	2.06
3	Q	302	BCL	MG-NC	10.90	2.32	2.06
3	E	302	BCL	MG-NC	10.83	2.32	2.06
3	O	302	BCL	MG-NC	10.82	2.32	2.06
3	J	101	BCL	MG-NC	10.76	2.31	2.06
3	L	102	BCL	MG-NC	10.75	2.31	2.06
3	M	302	BCL	MG-NC	10.71	2.31	2.06
3	P	101	BCL	MG-NC	10.60	2.31	2.06
3	G	302	BCL	MG-NC	10.25	2.30	2.06
3	K	302	BCL	MG-NC	10.19	2.30	2.06
3	R	102	BCL	MG-NC	10.18	2.30	2.06
3	A	302	BCL	MG-NC	10.18	2.30	2.06
3	F	101	BCL	MG-NC	9.98	2.30	2.06
3	D	102	BCL	MG-NC	9.97	2.30	2.06
3	I	302	BCL	MG-NC	9.59	2.29	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	102	IRM	C33-C5	-8.00	1.31	1.50
6	P	102	IRM	C27-C26	-7.23	1.36	1.51
6	L	103	IRM	C27-C26	-7.23	1.36	1.51
6	B	102	IRM	C27-C26	-7.22	1.36	1.51
6	D	103	IRM	C27-C26	-7.21	1.36	1.51
6	N	102	IRM	C27-C26	-7.20	1.36	1.51
6	J	102	IRM	C27-C26	-7.14	1.36	1.51
3	I	302	BCL	MG-ND	7.13	2.19	2.05
6	H	103	IRM	C27-C26	-7.10	1.36	1.51
6	E	304	IRM	C27-C26	-7.09	1.36	1.51
6	R	103	IRM	C27-C26	-7.09	1.36	1.51
3	E	301	BCL	MG-NC	6.13	2.20	2.06
3	A	301	BCL	MG-NC	6.12	2.20	2.06
3	M	301	BCL	MG-NC	5.94	2.20	2.06
3	G	301	BCL	MG-NC	5.93	2.20	2.06
3	I	301	BCL	MG-NC	5.91	2.20	2.06
6	B	102	IRM	C27-C28	-5.86	1.34	1.53
6	D	103	IRM	C27-C28	-5.86	1.34	1.53
3	C	301	BCL	MG-NC	5.86	2.20	2.06
6	J	102	IRM	C27-C28	-5.85	1.34	1.53
6	L	103	IRM	C27-C28	-5.85	1.34	1.53
6	H	103	IRM	C27-C28	-5.84	1.34	1.53
3	Q	301	BCL	MG-NC	5.84	2.20	2.06
6	P	102	IRM	C27-C28	-5.83	1.34	1.53
6	R	103	IRM	C27-C28	-5.83	1.34	1.53
6	N	102	IRM	C27-C28	-5.82	1.34	1.53
6	E	304	IRM	C27-C28	-5.81	1.34	1.53
3	O	301	BCL	MG-NC	5.68	2.19	2.06
3	K	301	BCL	MG-NC	5.59	2.19	2.06
3	H	102	BCL	C3D-C4D	-5.45	1.31	1.44
3	M	302	BCL	C3D-C4D	-5.36	1.32	1.44
3	A	301	BCL	C3D-C4D	-5.36	1.32	1.44
3	J	101	BCL	C3D-C4D	-5.35	1.32	1.44
3	R	102	BCL	C3D-C4D	-5.35	1.32	1.44
3	C	301	BCL	MG-NA	5.34	2.19	2.06
3	L	102	BCL	C3D-C4D	-5.34	1.32	1.44
3	F	101	BCL	C3D-C4D	-5.33	1.32	1.44
3	P	101	BCL	C3D-C4D	-5.33	1.32	1.44
3	K	302	BCL	C3D-C4D	-5.32	1.32	1.44
3	N	101	BCL	C3D-C4D	-5.32	1.32	1.44
3	M	301	BCL	C3D-C4D	-5.32	1.32	1.44
3	I	302	BCL	C3D-C4D	-5.31	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	BCL	C3D-C4D	-5.30	1.32	1.44
3	B	101	BCL	C3D-C4D	-5.30	1.32	1.44
3	K	301	BCL	MG-NA	5.30	2.18	2.06
3	Q	302	BCL	C3D-C4D	-5.30	1.32	1.44
3	E	301	BCL	C3D-C4D	-5.30	1.32	1.44
3	E	302	BCL	C3D-C4D	-5.29	1.32	1.44
3	E	301	BCL	MG-NA	5.28	2.18	2.06
3	Q	301	BCL	C3D-C4D	-5.27	1.32	1.44
3	G	302	BCL	C3D-C4D	-5.26	1.32	1.44
3	A	302	BCL	C3D-C4D	-5.26	1.32	1.44
3	D	102	BCL	C3D-C4D	-5.21	1.32	1.44
3	I	301	BCL	MG-NA	5.20	2.18	2.06
3	G	301	BCL	MG-NA	5.19	2.18	2.06
3	K	301	BCL	C3D-C4D	-5.19	1.32	1.44
3	O	302	BCL	C3D-C4D	-5.17	1.32	1.44
3	O	301	BCL	MG-NA	5.16	2.18	2.06
3	C	301	BCL	C3D-C4D	-5.15	1.32	1.44
3	O	301	BCL	C3D-C4D	-5.15	1.32	1.44
6	L	103	IRM	C28-C29	-5.14	1.34	1.50
6	N	102	IRM	C28-C29	-5.13	1.34	1.50
6	B	102	IRM	C28-C29	-5.13	1.34	1.50
6	P	102	IRM	C28-C29	-5.13	1.34	1.50
6	D	103	IRM	C28-C29	-5.13	1.34	1.50
3	Q	301	BCL	MG-NA	5.12	2.18	2.06
6	J	102	IRM	C28-C29	-5.12	1.35	1.50
3	G	301	BCL	C3D-C4D	-5.08	1.32	1.44
3	I	301	BCL	C3D-C4D	-5.07	1.32	1.44
6	R	103	IRM	C28-C29	-5.05	1.35	1.50
6	E	304	IRM	C28-C29	-5.05	1.35	1.50
6	H	103	IRM	C28-C29	-5.05	1.35	1.50
3	A	301	BCL	MG-NA	5.03	2.18	2.06
3	M	301	BCL	MG-NA	4.95	2.18	2.06
6	J	102	IRM	C23-C22	-4.80	1.35	1.46
6	H	103	IRM	C23-C22	-4.74	1.35	1.46
6	N	102	IRM	C23-C22	-4.69	1.35	1.46
6	R	103	IRM	C23-C22	-4.67	1.36	1.46
6	P	102	IRM	C23-C22	-4.66	1.36	1.46
6	E	304	IRM	C23-C22	-4.65	1.36	1.46
6	B	102	IRM	C23-C22	-4.64	1.36	1.46
6	D	103	IRM	C23-C22	-4.61	1.36	1.46
6	R	103	IRM	C8-C9	-4.60	1.36	1.46
6	B	102	IRM	C8-C9	-4.58	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	102	IRM	C8-C9	-4.56	1.36	1.46
6	L	103	IRM	C23-C22	-4.56	1.36	1.46
6	R	103	IRM	C12-C13	-4.53	1.36	1.46
6	L	103	IRM	C12-C13	-4.53	1.36	1.46
6	N	102	IRM	C12-C13	-4.53	1.36	1.46
6	J	102	IRM	C8-C9	-4.51	1.36	1.46
6	J	102	IRM	C12-C13	-4.51	1.36	1.46
6	L	103	IRM	C8-C9	-4.51	1.36	1.46
6	P	102	IRM	C12-C13	-4.48	1.36	1.46
6	E	304	IRM	C8-C9	-4.48	1.36	1.46
6	H	103	IRM	C12-C13	-4.47	1.36	1.46
6	E	304	IRM	C12-C13	-4.47	1.36	1.46
6	N	102	IRM	C8-C9	-4.46	1.36	1.46
6	H	103	IRM	C8-C9	-4.46	1.36	1.46
6	D	103	IRM	C8-C9	-4.43	1.36	1.46
6	B	102	IRM	C12-C13	-4.42	1.36	1.46
6	D	103	IRM	C12-C13	-4.37	1.36	1.46
6	R	103	IRM	C19-C18	-4.31	1.36	1.46
6	E	304	IRM	C19-C18	-4.24	1.36	1.46
6	J	102	IRM	C19-C18	-4.23	1.36	1.46
6	P	102	IRM	C19-C18	-4.22	1.36	1.46
6	H	103	IRM	C19-C18	-4.20	1.37	1.46
6	N	102	IRM	C19-C18	-4.20	1.37	1.46
6	D	103	IRM	C19-C18	-4.14	1.37	1.46
6	B	102	IRM	C19-C18	-4.12	1.37	1.46
6	L	103	IRM	C19-C18	-4.11	1.37	1.46
3	Q	302	BCL	CHD-C1D	3.93	1.46	1.38
3	O	302	BCL	CHD-C1D	3.90	1.46	1.38
3	E	302	BCL	CHD-C1D	3.89	1.46	1.38
3	G	302	BCL	CHD-C1D	3.88	1.46	1.38
3	C	302	BCL	CHD-C1D	3.85	1.45	1.38
3	H	102	BCL	C1D-C2D	-3.80	1.37	1.45
3	J	101	BCL	C1D-C2D	-3.76	1.37	1.45
3	I	302	BCL	CHD-C1D	3.76	1.45	1.38
3	F	101	BCL	C1D-C2D	-3.74	1.37	1.45
3	B	101	BCL	C1D-C2D	-3.74	1.37	1.45
3	L	102	BCL	C1D-C2D	-3.74	1.37	1.45
3	N	101	BCL	C1D-C2D	-3.70	1.38	1.45
3	Q	301	BCL	C1D-C2D	-3.69	1.38	1.45
3	K	302	BCL	CHD-C1D	3.68	1.45	1.38
3	P	101	BCL	C1D-C2D	-3.66	1.38	1.45
3	D	102	BCL	C1D-C2D	-3.63	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	102	BCL	C1D-C2D	-3.63	1.38	1.45
3	M	302	BCL	CHD-C1D	3.56	1.45	1.38
3	C	301	BCL	C1D-C2D	-3.56	1.38	1.45
3	A	302	BCL	CHD-C1D	3.54	1.45	1.38
3	M	301	BCL	CHD-C1D	3.52	1.45	1.38
3	O	301	BCL	C1D-C2D	-3.51	1.38	1.45
3	M	301	BCL	C1D-C2D	-3.51	1.38	1.45
3	K	301	BCL	C1D-C2D	-3.49	1.38	1.45
3	A	301	BCL	C1D-C2D	-3.48	1.38	1.45
3	E	301	BCL	CHD-C1D	3.47	1.45	1.38
3	G	301	BCL	C1D-C2D	-3.46	1.38	1.45
3	G	301	BCL	CHD-C1D	3.44	1.45	1.38
3	E	301	BCL	C1D-C2D	-3.43	1.38	1.45
3	I	301	BCL	C1D-C2D	-3.43	1.38	1.45
3	J	101	BCL	CHD-C1D	3.43	1.45	1.38
3	K	301	BCL	CHD-C1D	3.42	1.45	1.38
3	O	301	BCL	CHD-C1D	3.41	1.45	1.38
3	E	302	BCL	C1D-C2D	-3.41	1.38	1.45
3	C	302	BCL	C1D-C2D	-3.37	1.38	1.45
3	M	302	BCL	C1D-C2D	-3.36	1.38	1.45
3	O	302	BCL	C1D-C2D	-3.36	1.38	1.45
3	Q	301	BCL	CHD-C1D	3.36	1.45	1.38
3	A	302	BCL	C1D-C2D	-3.35	1.38	1.45
3	I	301	BCL	CHD-C1D	3.35	1.44	1.38
3	K	302	BCL	C1D-C2D	-3.35	1.38	1.45
3	H	102	BCL	CHD-C1D	3.34	1.44	1.38
3	A	301	BCL	CHD-C1D	3.34	1.44	1.38
3	C	301	BCL	CHD-C1D	3.33	1.44	1.38
3	R	102	BCL	CHD-C1D	3.32	1.44	1.38
3	N	101	BCL	CHD-C1D	3.31	1.44	1.38
3	D	102	BCL	CHD-C1D	3.30	1.44	1.38
3	G	302	BCL	C1D-C2D	-3.30	1.38	1.45
3	Q	302	BCL	C1D-C2D	-3.30	1.38	1.45
3	B	101	BCL	CHD-C1D	3.28	1.44	1.38
3	Q	302	BCL	MG-ND	3.24	2.12	2.05
3	L	102	BCL	CHD-C1D	3.24	1.44	1.38
3	I	302	BCL	C1D-C2D	-3.21	1.39	1.45
3	F	101	BCL	CHD-C1D	3.20	1.44	1.38
3	P	101	BCL	CHD-C1D	3.16	1.44	1.38
3	G	302	BCL	MG-ND	2.95	2.11	2.05
6	R	103	IRM	C7-C6	-2.75	1.34	1.43
6	L	103	IRM	C7-C6	-2.70	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	102	IRM	C7-C6	-2.69	1.34	1.43
6	N	102	IRM	C7-C6	-2.68	1.34	1.43
6	J	102	IRM	C7-C6	-2.68	1.34	1.43
6	B	102	IRM	C7-C6	-2.67	1.34	1.43
6	H	103	IRM	C7-C6	-2.63	1.35	1.43
6	E	304	IRM	C7-C6	-2.62	1.35	1.43
3	C	302	BCL	MG-ND	2.61	2.11	2.05
3	E	302	BCL	MG-ND	2.60	2.10	2.05
6	D	103	IRM	C7-C6	-2.57	1.35	1.43
3	A	302	BCL	MG-ND	2.56	2.10	2.05
6	R	103	IRM	C11-C10	-2.53	1.35	1.43
6	R	103	IRM	C15-C14	-2.48	1.35	1.43
6	P	102	IRM	C11-C10	-2.48	1.35	1.43
6	J	102	IRM	C11-C10	-2.48	1.35	1.43
6	N	102	IRM	C11-C10	-2.48	1.35	1.43
6	N	102	IRM	C15-C14	-2.47	1.35	1.43
6	J	102	IRM	C15-C14	-2.46	1.35	1.43
6	L	103	IRM	C15-C14	-2.46	1.35	1.43
6	H	103	IRM	C11-C10	-2.45	1.35	1.43
3	M	302	BCL	MG-ND	2.44	2.10	2.05
6	L	103	IRM	C11-C10	-2.43	1.35	1.43
6	H	103	IRM	C15-C14	-2.43	1.35	1.43
6	J	102	IRM	C20-C21	-2.43	1.35	1.43
6	E	304	IRM	C20-C21	-2.43	1.35	1.43
6	P	102	IRM	C15-C14	-2.43	1.35	1.43
6	E	304	IRM	C11-C10	-2.43	1.35	1.43
6	D	103	IRM	C11-C10	-2.43	1.35	1.43
6	B	102	IRM	C11-C10	-2.42	1.35	1.43
6	E	304	IRM	C16-C17	-2.41	1.35	1.43
6	E	304	IRM	C15-C14	-2.41	1.35	1.43
6	L	103	IRM	C16-C17	-2.41	1.35	1.43
6	R	103	IRM	C20-C21	-2.40	1.35	1.43
6	B	102	IRM	C15-C14	-2.40	1.35	1.43
6	P	102	IRM	C20-C21	-2.40	1.35	1.43
6	N	102	IRM	C20-C21	-2.39	1.35	1.43
6	R	103	IRM	C16-C17	-2.37	1.35	1.43
6	P	102	IRM	C16-C17	-2.37	1.35	1.43
6	J	102	IRM	C16-C17	-2.37	1.35	1.43
6	B	102	IRM	C16-C17	-2.36	1.35	1.43
6	D	103	IRM	C15-C14	-2.36	1.35	1.43
6	N	102	IRM	C16-C17	-2.36	1.35	1.43
6	H	103	IRM	C16-C17	-2.35	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	103	IRM	C20-C21	-2.33	1.35	1.43
6	B	102	IRM	C20-C21	-2.32	1.36	1.43
6	D	103	IRM	C16-C17	-2.32	1.36	1.43
6	H	103	IRM	C20-C21	-2.32	1.36	1.43
6	L	103	IRM	C20-C21	-2.32	1.36	1.43
6	D	103	IRM	C24-C25	-2.30	1.36	1.43
3	A	301	BCL	MG-ND	2.30	2.10	2.05
6	E	304	IRM	C24-C25	-2.26	1.36	1.43
6	P	102	IRM	C24-C25	-2.26	1.36	1.43
6	L	103	IRM	C24-C25	-2.24	1.36	1.43
6	R	103	IRM	C24-C25	-2.23	1.36	1.43
6	J	102	IRM	C24-C25	-2.23	1.36	1.43
6	N	102	IRM	C24-C25	-2.22	1.36	1.43
3	M	301	BCL	MG-ND	2.21	2.10	2.05
6	B	102	IRM	C24-C25	-2.21	1.36	1.43
6	H	103	IRM	C24-C25	-2.20	1.36	1.43
3	O	302	BCL	CMB-C2B	-2.20	1.47	1.51
3	B	101	BCL	MG-ND	2.18	2.10	2.05
3	K	302	BCL	MG-ND	2.15	2.10	2.05
4	G	303	LDA	O1-N1	-2.12	1.36	1.42
4	I	304	LDA	O1-N1	-2.11	1.36	1.42
4	M	303	LDA	O1-N1	-2.07	1.37	1.42
4	M	303	LDA	C1-N1	2.07	1.53	1.51
4	E	303	LDA	O1-N1	-2.07	1.37	1.42
4	G	303	LDA	C1-N1	2.06	1.53	1.51
4	Q	303	LDA	O1-N1	-2.04	1.37	1.42
4	C	303	LDA	O1-N1	-2.03	1.37	1.42
4	O	303	LDA	O1-N1	-2.02	1.37	1.42
4	K	303	LDA	C1-N1	2.01	1.53	1.51
4	E	303	LDA	C1-N1	2.00	1.53	1.51
5	D	101	LMT	O1'-C1'	2.00	1.43	1.40

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	BCL	C4A-NA-C1A	11.13	111.76	106.68
3	A	301	BCL	C4A-NA-C1A	10.95	111.67	106.68
3	Q	301	BCL	C4A-NA-C1A	10.87	111.64	106.68
3	K	301	BCL	C4A-NA-C1A	10.81	111.61	106.68
3	O	301	BCL	C4A-NA-C1A	10.68	111.55	106.68
3	C	301	BCL	C4A-NA-C1A	10.60	111.52	106.68
3	M	301	BCL	C4A-NA-C1A	10.55	111.49	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	301	BCL	C4A-NA-C1A	10.43	111.44	106.68
3	I	301	BCL	C4A-NA-C1A	10.38	111.41	106.68
3	B	101	BCL	C4A-NA-C1A	10.09	111.28	106.68
3	N	101	BCL	C4A-NA-C1A	9.75	111.13	106.68
3	J	101	BCL	C4A-NA-C1A	9.47	111.00	106.68
3	R	102	BCL	C1C-NC-C4C	9.41	110.97	106.68
3	L	102	BCL	C4A-NA-C1A	9.37	110.95	106.68
3	C	302	BCL	C4A-NA-C1A	9.25	110.90	106.68
3	F	101	BCL	C1C-NC-C4C	9.10	110.83	106.68
3	O	302	BCL	C4A-NA-C1A	9.08	110.82	106.68
3	Q	302	BCL	C4A-NA-C1A	9.04	110.81	106.68
3	D	102	BCL	C4A-NA-C1A	9.04	110.80	106.68
3	J	101	BCL	C1C-NC-C4C	9.03	110.80	106.68
3	N	101	BCL	C1C-NC-C4C	9.03	110.80	106.68
3	L	102	BCL	C1C-NC-C4C	9.03	110.80	106.68
3	R	102	BCL	C4A-NA-C1A	8.91	110.74	106.68
3	F	101	BCL	C4A-NA-C1A	8.91	110.74	106.68
3	D	102	BCL	C1C-NC-C4C	8.90	110.74	106.68
3	E	302	BCL	C4A-NA-C1A	8.89	110.74	106.68
3	P	101	BCL	C1C-NC-C4C	8.82	110.70	106.68
3	M	302	BCL	C4A-NA-C1A	8.71	110.65	106.68
3	A	302	BCL	C4A-NA-C1A	8.66	110.63	106.68
3	B	101	BCL	C1C-NC-C4C	8.64	110.62	106.68
3	Q	302	BCL	C1C-NC-C4C	8.64	110.62	106.68
3	E	302	BCL	C1C-NC-C4C	8.61	110.61	106.68
3	G	302	BCL	C4A-NA-C1A	8.61	110.61	106.68
3	G	302	BCL	C1C-NC-C4C	8.61	110.61	106.68
3	K	302	BCL	C4A-NA-C1A	8.60	110.60	106.68
3	H	102	BCL	C4A-NA-C1A	8.59	110.60	106.68
3	P	101	BCL	C4A-NA-C1A	8.53	110.57	106.68
3	O	302	BCL	C1C-NC-C4C	8.53	110.57	106.68
3	I	302	BCL	C1C-NC-C4C	8.50	110.56	106.68
3	H	102	BCL	C1C-NC-C4C	8.35	110.49	106.68
3	E	301	BCL	C1C-NC-C4C	8.24	110.44	106.68
3	C	302	BCL	C1C-NC-C4C	8.21	110.42	106.68
3	K	301	BCL	C1C-NC-C4C	8.15	110.40	106.68
3	I	301	BCL	C1C-NC-C4C	8.10	110.38	106.68
3	G	301	BCL	C1C-NC-C4C	8.08	110.36	106.68
3	M	301	BCL	C1C-NC-C4C	7.99	110.33	106.68
3	C	301	BCL	C1C-NC-C4C	7.98	110.32	106.68
3	Q	301	BCL	C1C-NC-C4C	7.88	110.27	106.68
3	O	301	BCL	C1C-NC-C4C	7.86	110.27	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	BCL	C1C-NC-C4C	7.80	110.24	106.68
3	A	302	BCL	C1C-NC-C4C	7.79	110.23	106.68
3	K	302	BCL	C1C-NC-C4C	7.62	110.16	106.68
3	M	302	BCL	C1C-NC-C4C	7.39	110.05	106.68
3	I	302	BCL	C4A-NA-C1A	7.08	109.91	106.68
3	O	302	BCL	C1D-ND-C4D	5.97	110.50	106.31
3	Q	302	BCL	C1D-ND-C4D	5.86	110.42	106.31
3	E	302	BCL	C1D-ND-C4D	5.75	110.34	106.31
3	I	302	BCL	C1D-ND-C4D	5.74	110.34	106.31
3	C	301	BCL	C1D-ND-C4D	5.59	110.24	106.31
3	G	302	BCL	C1D-ND-C4D	5.59	110.23	106.31
3	G	301	BCL	C1D-ND-C4D	5.55	110.21	106.31
3	K	301	BCL	C1D-ND-C4D	5.54	110.20	106.31
3	E	301	BCL	C1D-ND-C4D	5.52	110.19	106.31
3	K	302	BCL	C1D-ND-C4D	5.52	110.18	106.31
3	M	301	BCL	C1D-ND-C4D	5.50	110.17	106.31
3	I	301	BCL	C1D-ND-C4D	5.50	110.17	106.31
3	M	302	BCL	C1D-ND-C4D	5.41	110.11	106.31
3	C	302	BCL	C1D-ND-C4D	5.40	110.10	106.31
3	Q	301	BCL	C1D-ND-C4D	5.36	110.07	106.31
3	E	302	BCL	C4D-CHA-C1A	5.35	127.63	121.24
3	A	302	BCL	C1D-ND-C4D	5.32	110.05	106.31
3	P	101	BCL	C1D-ND-C4D	5.28	110.02	106.31
3	E	302	BCL	C2D-C1D-ND	-5.28	104.91	110.13
3	O	301	BCL	C1D-ND-C4D	5.25	110.00	106.31
3	N	101	BCL	C1D-ND-C4D	5.23	109.98	106.31
3	Q	302	BCL	C2D-C1D-ND	-5.22	104.96	110.13
3	H	102	BCL	C1D-ND-C4D	5.22	109.97	106.31
3	I	302	BCL	C2D-C1D-ND	-5.21	104.97	110.13
3	B	101	BCL	C4D-CHA-C1A	5.21	127.45	121.24
3	A	301	BCL	C1D-ND-C4D	5.20	109.96	106.31
3	O	302	BCL	C2D-C1D-ND	-5.18	105.00	110.13
3	L	102	BCL	C1D-ND-C4D	5.18	109.94	106.31
3	O	302	BCL	C4D-CHA-C1A	5.18	127.42	121.24
3	J	101	BCL	C4D-CHA-C1A	5.15	127.39	121.24
3	R	102	BCL	C4D-CHA-C1A	5.15	127.39	121.24
3	B	101	BCL	C1D-ND-C4D	5.14	109.92	106.31
3	L	102	BCL	C4D-CHA-C1A	5.14	127.37	121.24
3	C	302	BCL	C4D-CHA-C1A	5.10	127.33	121.24
3	Q	302	BCL	C4D-CHA-C1A	5.10	127.33	121.24
3	K	302	BCL	C2D-C1D-ND	-5.10	105.08	110.13
3	C	302	BCL	C2D-C1D-ND	-5.10	105.08	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	302	BCL	C4D-CHA-C1A	5.09	127.31	121.24
3	H	102	BCL	C4D-CHA-C1A	5.08	127.31	121.24
3	G	302	BCL	C2D-C1D-ND	-5.08	105.10	110.13
3	J	101	BCL	C1D-ND-C4D	5.08	109.88	106.31
3	A	301	BCL	C4D-CHA-C1A	5.07	127.29	121.24
3	K	302	BCL	C4D-CHA-C1A	5.06	127.28	121.24
3	D	102	BCL	C1D-ND-C4D	5.04	109.85	106.31
3	M	302	BCL	C2D-C1D-ND	-5.03	105.15	110.13
3	N	101	BCL	C4D-CHA-C1A	5.00	127.20	121.24
3	A	302	BCL	C2D-C1D-ND	-4.99	105.19	110.13
3	R	102	BCL	C1D-ND-C4D	4.95	109.79	106.31
3	F	101	BCL	C1D-ND-C4D	4.95	109.78	106.31
3	I	301	BCL	C4D-CHA-C1A	4.94	127.14	121.24
3	K	301	BCL	C4D-CHA-C1A	4.92	127.12	121.24
3	A	302	BCL	C4D-CHA-C1A	4.91	127.10	121.24
3	D	102	BCL	C4D-CHA-C1A	4.90	127.09	121.24
3	F	101	BCL	C4D-CHA-C1A	4.89	127.07	121.24
3	P	101	BCL	C4D-CHA-C1A	4.86	127.04	121.24
3	H	102	BCL	C2D-C1D-ND	-4.85	105.33	110.13
3	C	301	BCL	C4D-CHA-C1A	4.82	127.00	121.24
3	E	301	BCL	C4D-CHA-C1A	4.81	126.98	121.24
3	E	301	BCL	C2D-C1D-ND	-4.81	105.36	110.13
3	Q	301	BCL	C4D-CHA-C1A	4.81	126.98	121.24
3	C	301	BCL	C2D-C1D-ND	-4.81	105.37	110.13
3	M	302	BCL	C4D-CHA-C1A	4.80	126.97	121.24
3	G	301	BCL	C2D-C1D-ND	-4.77	105.41	110.13
3	O	301	BCL	C2D-C1D-ND	-4.74	105.43	110.13
3	P	101	BCL	C2D-C1D-ND	-4.74	105.44	110.13
3	I	302	BCL	CMB-C2B-C1B	-4.72	121.55	128.46
3	Q	301	BCL	C2D-C1D-ND	-4.69	105.49	110.13
3	O	301	BCL	C4D-CHA-C1A	4.68	126.83	121.24
3	K	302	BCL	CMB-C2B-C1B	-4.68	121.60	128.46
3	Q	302	BCL	CMB-C2B-C1B	-4.66	121.62	128.46
3	I	301	BCL	C2D-C1D-ND	-4.66	105.51	110.13
3	K	301	BCL	C2D-C1D-ND	-4.66	105.52	110.13
3	B	101	BCL	C2D-C1D-ND	-4.65	105.52	110.13
3	G	301	BCL	C4D-CHA-C1A	4.65	126.80	121.24
3	M	301	BCL	C4D-CHA-C1A	4.65	126.79	121.24
3	R	102	BCL	C2D-C1D-ND	-4.64	105.53	110.13
3	M	302	BCL	CMB-C2B-C1B	-4.63	121.67	128.46
3	N	101	BCL	C2D-C1D-ND	-4.62	105.55	110.13
3	M	301	BCL	C2D-C1D-ND	-4.58	105.59	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	101	BCL	C2D-C1D-ND	-4.56	105.61	110.13
3	L	102	BCL	C2D-C1D-ND	-4.55	105.62	110.13
3	P	101	BCL	CMB-C2B-C1B	-4.55	121.79	128.46
3	F	101	BCL	C2D-C1D-ND	-4.55	105.63	110.13
3	D	102	BCL	C2D-C1D-ND	-4.54	105.64	110.13
3	I	302	BCL	C4D-CHA-C1A	4.51	126.62	121.24
3	A	301	BCL	C2D-C1D-ND	-4.50	105.67	110.13
3	Q	302	BCL	O2D-CGD-CBD	4.50	119.10	111.23
6	B	102	IRM	C23-C22-C21	4.47	126.03	119.01
3	A	302	BCL	O2D-CGD-CBD	4.44	118.99	111.23
6	L	103	IRM	C23-C22-C21	4.42	125.96	119.01
3	K	302	BCL	O2D-CGD-CBD	4.41	118.94	111.23
3	A	302	BCL	CMB-C2B-C1B	-4.39	122.02	128.46
6	D	103	IRM	C23-C22-C21	4.33	125.82	119.01
6	R	103	IRM	C23-C22-C21	4.33	125.82	119.01
3	G	302	BCL	O2D-CGD-CBD	4.33	118.79	111.23
6	P	102	IRM	C23-C22-C21	4.31	125.79	119.01
6	H	103	IRM	C23-C22-C21	4.30	125.78	119.01
6	E	304	IRM	C23-C22-C21	4.29	125.76	119.01
3	H	102	BCL	CMB-C2B-C1B	-4.29	122.17	128.46
6	P	102	IRM	C28-C27-C26	4.23	127.20	113.19
6	J	102	IRM	C23-C22-C21	4.22	125.65	119.01
3	O	302	BCL	O2D-CGD-CBD	4.18	118.54	111.23
6	J	102	IRM	C28-C27-C26	4.17	126.99	113.19
6	L	103	IRM	C28-C27-C26	4.15	126.93	113.19
3	G	302	BCL	CMB-C2B-C1B	-4.15	122.38	128.46
6	E	304	IRM	C28-C27-C26	4.13	126.88	113.19
3	E	302	BCL	CMB-C2B-C1B	-4.10	122.45	128.46
6	N	102	IRM	C23-C22-C21	4.10	125.45	119.01
6	N	102	IRM	C28-C27-C26	4.09	126.75	113.19
6	H	103	IRM	C28-C27-C26	4.08	126.71	113.19
6	B	102	IRM	C28-C27-C26	4.02	126.49	113.19
6	D	103	IRM	C28-C27-C26	3.99	126.41	113.19
6	R	103	IRM	C28-C27-C26	3.96	126.29	113.19
3	N	101	BCL	CMB-C2B-C1B	-3.95	122.67	128.46
3	H	102	BCL	C1-O2A-CGA	3.94	126.20	116.65
3	O	302	BCL	CMB-C2B-C1B	-3.93	122.70	128.46
3	F	101	BCL	CMB-C2B-C1B	-3.79	122.90	128.46
6	P	102	IRM	C24-C25-C26	3.78	133.00	127.69
3	D	102	BCL	CMB-C2B-C1B	-3.78	122.92	128.46
6	E	304	IRM	C24-C25-C26	3.75	132.97	127.69
6	J	102	IRM	C24-C25-C26	3.74	132.95	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	102	BCL	CMB-C2B-C1B	-3.74	122.98	128.46
6	D	103	IRM	C24-C25-C26	3.73	132.94	127.69
3	R	102	BCL	CMB-C2B-C1B	-3.70	123.03	128.46
3	J	101	BCL	CMB-C2B-C1B	-3.67	123.07	128.46
3	B	101	BCL	CMB-C2B-C1B	-3.64	123.12	128.46
6	H	103	IRM	C24-C25-C26	3.64	132.81	127.69
3	A	302	BCL	CED-O2D-CGD	3.63	124.16	115.92
6	B	102	IRM	C24-C25-C26	3.60	132.76	127.69
6	N	102	IRM	C24-C25-C26	3.60	132.75	127.69
3	C	302	BCL	CMB-C2B-C1B	-3.60	123.19	128.46
6	R	103	IRM	C24-C25-C26	3.57	132.71	127.69
6	R	103	IRM	C27-C28-C29	3.55	129.60	112.02
6	L	103	IRM	C24-C25-C26	3.55	132.68	127.69
6	H	103	IRM	C27-C28-C29	3.54	129.54	112.02
3	Q	302	BCL	CED-O2D-CGD	3.54	123.95	115.92
6	B	102	IRM	C27-C28-C29	3.54	129.53	112.02
6	D	103	IRM	C27-C28-C29	3.54	129.52	112.02
3	E	302	BCL	CHD-C1D-C2D	3.53	132.83	125.49
6	J	102	IRM	C27-C28-C29	3.52	129.43	112.02
3	M	301	BCL	CMB-C2B-C1B	-3.51	123.31	128.46
3	G	302	BCL	CHD-C1D-C2D	3.51	132.78	125.49
6	P	102	IRM	C27-C28-C29	3.50	129.36	112.02
6	E	304	IRM	C27-C28-C29	3.50	129.32	112.02
6	N	102	IRM	C27-C28-C29	3.49	129.28	112.02
6	L	103	IRM	C27-C28-C29	3.49	129.26	112.02
3	I	302	BCL	CHD-C1D-C2D	3.48	132.74	125.49
3	G	302	BCL	CED-O2D-CGD	3.48	123.81	115.92
3	C	302	BCL	CHD-C1D-C2D	3.45	132.67	125.49
3	K	302	BCL	CED-O2D-CGD	3.42	123.68	115.92
3	O	302	BCL	CHD-C1D-C2D	3.40	132.56	125.49
3	Q	302	BCL	CHD-C1D-C2D	3.39	132.54	125.49
3	K	301	BCL	CMB-C2B-C1B	-3.38	123.51	128.46
3	K	302	BCL	CHD-C1D-C2D	3.38	132.51	125.49
3	O	302	BCL	CED-O2D-CGD	3.37	123.57	115.92
3	Q	301	BCL	CMB-C2B-C1B	-3.36	123.54	128.46
5	I	303	LMT	C1'-O5'-C5'	3.33	120.23	113.72
3	I	301	BCL	CMB-C2B-C1B	-3.33	123.58	128.46
3	M	302	BCL	CHD-C1D-C2D	3.31	132.37	125.49
3	O	301	BCL	CMB-C2B-C1B	-3.30	123.62	128.46
3	G	301	BCL	CMB-C2B-C1B	-3.29	123.64	128.46
3	C	301	BCL	CMB-C2B-C1B	-3.29	123.64	128.46
3	A	302	BCL	CHD-C1D-C2D	3.26	132.26	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	301	BCL	CMB-C2B-C1B	-3.24	123.70	128.46
3	O	301	BCL	CHD-C1D-C2D	3.24	132.22	125.49
3	A	301	BCL	CMB-C2B-C1B	-3.22	123.74	128.46
3	E	301	BCL	CHD-C1D-C2D	3.21	132.17	125.49
3	Q	301	BCL	CHD-C1D-C2D	3.20	132.14	125.49
3	G	301	BCL	CHD-C1D-C2D	3.18	132.10	125.49
3	C	301	BCL	CHD-C1D-C2D	3.18	132.09	125.49
3	D	102	BCL	CHD-C1D-C2D	3.18	132.09	125.49
3	R	102	BCL	CHD-C1D-C2D	3.15	132.03	125.49
6	E	304	IRM	C20-C21-C22	-3.14	122.88	127.28
3	I	301	BCL	CHD-C1D-C2D	3.12	131.98	125.49
6	N	102	IRM	C20-C21-C22	-3.11	122.91	127.28
6	J	102	IRM	C20-C21-C22	-3.11	122.92	127.28
3	K	301	BCL	CHD-C1D-C2D	3.10	131.94	125.49
3	J	101	BCL	CHD-C1D-C2D	3.10	131.93	125.49
3	M	301	BCL	CHD-C1D-C2D	3.09	131.92	125.49
3	A	301	BCL	CHD-C1D-C2D	3.09	131.91	125.49
6	H	103	IRM	C37-C22-C23	-3.09	113.37	118.09
3	N	101	BCL	CHD-C1D-C2D	3.06	131.85	125.49
6	B	102	IRM	C20-C21-C22	-3.04	123.02	127.28
3	F	101	BCL	CHD-C1D-C2D	3.03	131.80	125.49
6	P	102	IRM	C20-C21-C22	-3.03	123.02	127.28
3	P	101	BCL	CHD-C1D-C2D	3.01	131.75	125.49
3	B	101	BCL	CHD-C1D-C2D	3.01	131.74	125.49
3	L	102	BCL	CHD-C1D-C2D	2.97	131.65	125.49
3	H	102	BCL	CHD-C1D-C2D	2.94	131.60	125.49
6	L	103	IRM	C20-C21-C22	-2.92	123.19	127.28
6	B	102	IRM	C37-C22-C23	-2.91	113.65	118.09
6	N	102	IRM	C36-C18-C17	-2.87	118.17	122.82
6	R	103	IRM	C20-C21-C22	-2.85	123.28	127.28
6	L	103	IRM	C37-C22-C23	-2.83	113.77	118.09
6	E	304	IRM	C37-C22-C23	-2.77	113.85	118.09
6	D	103	IRM	C37-C22-C23	-2.77	113.86	118.09
6	D	103	IRM	C20-C21-C22	-2.74	123.44	127.28
6	H	103	IRM	C20-C21-C22	-2.73	123.45	127.28
6	R	103	IRM	C37-C22-C23	-2.72	113.94	118.09
6	B	102	IRM	C36-C18-C17	-2.65	118.52	122.82
6	J	102	IRM	C36-C18-C17	-2.64	118.54	122.82
6	J	102	IRM	C37-C22-C23	-2.60	114.11	118.09
6	P	102	IRM	C37-C22-C23	-2.57	114.16	118.09
6	L	103	IRM	C36-C18-C17	-2.50	118.77	122.82
6	N	102	IRM	C37-C22-C23	-2.49	114.28	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	102	IRM	C36-C18-C17	-2.47	118.81	122.82
3	P	101	BCL	CMB-C2B-C3B	2.44	129.55	124.68
6	H	103	IRM	C36-C18-C17	-2.41	118.91	122.82
3	E	302	BCL	C1-O2A-CGA	2.41	122.48	116.65
6	L	103	IRM	C33-C5-C4	-2.38	111.09	115.23
6	R	103	IRM	C36-C18-C17	-2.38	118.96	122.82
6	N	102	IRM	C16-C17-C18	-2.38	123.94	127.28
6	D	103	IRM	C36-C18-C17	-2.35	119.01	122.82
6	J	102	IRM	C16-C17-C18	-2.33	124.01	127.28
5	P	103	LMT	C1-O1'-C1'	2.32	117.65	113.68
3	P	101	BCL	CHA-C1A-NA	-2.29	121.20	126.39
3	I	302	BCL	CHA-C1A-NA	-2.29	121.21	126.39
6	P	102	IRM	C25-C24-C23	2.26	129.76	123.20
3	H	102	BCL	CHA-C1A-NA	-2.26	121.27	126.39
6	H	103	IRM	C16-C17-C18	-2.26	124.11	127.28
6	E	304	IRM	C36-C18-C17	-2.26	119.15	122.82
3	I	302	BCL	CMB-C2B-C3B	2.26	129.20	124.68
3	O	302	BCL	C4-C3-C5	2.25	119.14	115.23
6	E	304	IRM	C16-C17-C18	-2.25	124.12	127.28
6	R	103	IRM	C25-C24-C23	2.25	129.71	123.20
6	D	103	IRM	C25-C24-C23	2.24	129.70	123.20
3	Q	302	BCL	CMB-C2B-C3B	2.23	129.13	124.68
6	E	304	IRM	C33-C5-C4	-2.22	111.37	115.23
6	P	102	IRM	C16-C17-C18	-2.21	124.17	127.28
3	Q	302	BCL	O2D-CGD-O1D	-2.21	119.55	123.85
6	B	102	IRM	C25-C24-C23	2.20	129.57	123.20
6	E	304	IRM	C25-C24-C23	2.20	129.57	123.20
3	I	302	BCL	C2A-C1A-CHA	2.20	127.68	123.87
3	B	101	BCL	C4-C3-C5	-2.19	111.43	115.23
3	K	302	BCL	O2D-CGD-O1D	-2.18	119.60	123.85
6	B	102	IRM	C16-C17-C18	-2.18	124.22	127.28
6	H	103	IRM	C25-C24-C23	2.18	129.51	123.20
6	N	102	IRM	C25-C24-C23	2.18	129.51	123.20
6	J	102	IRM	C25-C24-C23	2.17	129.49	123.20
6	P	102	IRM	C33-C5-C4	-2.17	111.47	115.23
3	E	301	BCL	CHA-C1A-NA	-2.14	121.54	126.39
3	A	301	BCL	CHA-C1A-NA	-2.14	121.54	126.39
3	L	102	BCL	CHA-C1A-NA	-2.14	121.55	126.39
3	J	101	BCL	CHA-C1A-NA	-2.14	121.55	126.39
6	D	103	IRM	C16-C17-C18	-2.13	124.29	127.28
6	L	103	IRM	C16-C17-C18	-2.12	124.30	127.28
3	R	102	BCL	CHA-C1A-NA	-2.12	121.58	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	302	BCL	CMB-C2B-C3B	2.12	128.92	124.68
3	O	302	BCL	CBA-CAA-C2A	2.11	120.07	113.79
6	L	103	IRM	C25-C24-C23	2.11	129.31	123.20
3	B	101	BCL	CHA-C1A-NA	-2.11	121.62	126.39
3	G	302	BCL	O2D-CGD-O1D	-2.11	119.75	123.85
3	N	101	BCL	CHA-C1A-NA	-2.10	121.63	126.39
3	M	302	BCL	CMB-C2B-C3B	2.10	128.88	124.68
3	H	102	BCL	CMB-C2B-C3B	2.09	128.87	124.68
3	I	301	BCL	CHA-C1A-NA	-2.09	121.65	126.39
3	B	101	BCL	C5-C3-C2	2.09	125.85	121.17
3	O	302	BCL	O2D-CGD-O1D	-2.04	119.88	123.85
3	C	301	BCL	CHA-C1A-NA	-2.04	121.77	126.39
3	D	102	BCL	CHA-C1A-NA	-2.03	121.80	126.39
3	F	101	BCL	CHA-C1A-NA	-2.03	121.80	126.39
6	N	102	IRM	C36-C18-C19	2.02	121.18	118.09
3	N	101	BCL	CMB-C2B-C3B	2.02	128.72	124.68
3	M	301	BCL	CHA-C1A-NA	-2.02	121.83	126.39
6	D	103	IRM	C33-C5-C4	-2.02	111.73	115.23
3	Q	301	BCL	CHA-C1A-NA	-2.01	121.84	126.39
3	O	301	BCL	CHA-C1A-NA	-2.00	121.85	126.39
5	D	101	LMT	O5'-C1'-C2'	-2.00	106.25	110.37
3	A	302	BCL	CMB-C2B-C3B	2.00	128.69	124.68
6	R	103	IRM	C16-C17-C18	-2.00	124.47	127.28
3	O	302	BCL	CHA-C1A-NA	-2.00	121.86	126.39

There are no chirality outliers.

All (175) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	BCL	CBD-CGD-O2D-CED
3	E	302	BCL	C1A-C2A-CAA-CBA
3	G	302	BCL	CBD-CGD-O2D-CED
3	H	102	BCL	CBA-CGA-O2A-C1
3	H	102	BCL	O1A-CGA-O2A-C1
3	K	302	BCL	CBD-CGD-O2D-CED
3	O	302	BCL	CBD-CGD-O2D-CED
3	O	302	BCL	C4-C3-C5-C6
3	Q	302	BCL	CBD-CGD-O2D-CED
4	K	303	LDA	N1-C1-C2-C3
6	B	102	IRM	C27-C28-C29-C39
6	D	103	IRM	C27-C28-C29-C39
6	E	304	IRM	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
6	H	103	IRM	C27-C28-C29-C39
6	J	102	IRM	C27-C28-C29-C39
6	L	103	IRM	C27-C28-C29-C39
6	N	102	IRM	C27-C28-C29-C39
6	P	102	IRM	C27-C28-C29-C39
6	R	103	IRM	C27-C28-C29-C39
3	A	302	BCL	O1D-CGD-O2D-CED
3	G	302	BCL	O1D-CGD-O2D-CED
3	K	302	BCL	O1D-CGD-O2D-CED
3	O	302	BCL	O1D-CGD-O2D-CED
3	Q	302	BCL	O1D-CGD-O2D-CED
3	O	302	BCL	C2-C3-C5-C6
6	B	102	IRM	C23-C24-C25-C26
6	D	103	IRM	C23-C24-C25-C26
6	E	304	IRM	C23-C24-C25-C26
6	H	103	IRM	C23-C24-C25-C26
6	J	102	IRM	C23-C24-C25-C26
6	L	103	IRM	C23-C24-C25-C26
6	N	102	IRM	C23-C24-C25-C26
6	P	102	IRM	C23-C24-C25-C26
6	R	103	IRM	C23-C24-C25-C26
3	O	302	BCL	C2A-CAA-CBA-CGA
6	B	102	IRM	C37-C22-C23-C24
6	D	103	IRM	C37-C22-C23-C24
6	E	304	IRM	C37-C22-C23-C24
6	H	103	IRM	C37-C22-C23-C24
6	J	102	IRM	C37-C22-C23-C24
6	L	103	IRM	C37-C22-C23-C24
6	N	102	IRM	C37-C22-C23-C24
6	P	102	IRM	C37-C22-C23-C24
6	R	103	IRM	C37-C22-C23-C24
6	B	102	IRM	C21-C22-C23-C24
6	D	103	IRM	C21-C22-C23-C24
6	E	304	IRM	C21-C22-C23-C24
6	H	103	IRM	C21-C22-C23-C24
6	J	102	IRM	C21-C22-C23-C24
6	L	103	IRM	C21-C22-C23-C24
6	N	102	IRM	C21-C22-C23-C24
6	P	102	IRM	C21-C22-C23-C24
6	R	103	IRM	C21-C22-C23-C24
3	E	302	BCL	C2A-CAA-CBA-CGA
3	D	102	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	D	102	BCL	C5-C6-C7-C8
3	L	102	BCL	C5-C6-C7-C8
3	R	102	BCL	C5-C6-C7-C8
5	N	103	LMT	C3-C4-C5-C6
3	P	101	BCL	C5-C6-C7-C8
3	B	101	BCL	C5-C6-C7-C8
3	H	102	BCL	C5-C6-C7-C8
3	N	101	BCL	C13-C15-C16-C17
3	E	302	BCL	C5-C6-C7-C8
5	P	103	LMT	O5'-C1'-O1'-C1
3	E	302	BCL	C2-C1-O2A-CGA
3	G	302	BCL	C8-C10-C11-C12
3	J	101	BCL	C10-C11-C12-C13
5	H	101	LMT	C4-C5-C6-C7
3	E	302	BCL	C8-C10-C11-C12
3	A	302	BCL	C8-C10-C11-C12
3	E	302	BCL	C3A-C2A-CAA-CBA
3	C	302	BCL	C5-C6-C7-C8
5	F	102	LMT	C6-C7-C8-C9
5	N	103	LMT	O1'-C1-C2-C3
3	L	102	BCL	C13-C15-C16-C17
3	R	102	BCL	C15-C16-C17-C18
5	I	303	LMT	C11-C10-C9-C8
5	R	101	LMT	C2-C3-C4-C5
5	I	303	LMT	C2-C3-C4-C5
3	P	101	BCL	C15-C16-C17-C18
3	Q	302	BCL	C8-C10-C11-C12
3	O	302	BCL	C1A-C2A-CAA-CBA
5	P	103	LMT	C2'-C1'-O1'-C1
3	H	102	BCL	C4-C3-C5-C6
3	I	302	BCL	C2-C3-C5-C6
5	I	303	LMT	O5'-C5'-C6'-O6'
3	N	101	BCL	O2A-C1-C2-C3
3	H	102	BCL	C2-C3-C5-C6
3	I	302	BCL	C4-C3-C5-C6
5	F	102	LMT	C4-C5-C6-C7
3	H	102	BCL	C11-C10-C8-C7
3	F	101	BCL	C15-C16-C17-C18
5	L	101	LMT	C2-C3-C4-C5
5	H	101	LMT	C5'-C4'-O1B-C1B
5	H	101	LMT	C3'-C4'-O1B-C1B
5	A	304	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	B	101	BCL	C11-C10-C8-C9
3	B	101	BCL	C11-C10-C8-C7
3	G	301	BCL	C15-C16-C17-C18
5	D	101	LMT	C3'-C4'-O1B-C1B
3	Q	301	BCL	C15-C16-C17-C18
3	B	101	BCL	C13-C15-C16-C17
3	H	102	BCL	C15-C16-C17-C18
5	D	101	LMT	C5'-C4'-O1B-C1B
5	N	103	LMT	C2-C3-C4-C5
3	F	101	BCL	C11-C10-C8-C7
3	E	302	BCL	CAD-CBD-CGD-O2D
3	I	302	BCL	CAD-CBD-CGD-O2D
3	O	302	BCL	CAD-CBD-CGD-O2D
3	C	302	BCL	CAD-CBD-CGD-O1D
3	E	302	BCL	CAD-CBD-CGD-O1D
3	I	302	BCL	CAD-CBD-CGD-O1D
3	H	102	BCL	C11-C10-C8-C9
3	F	101	BCL	C11-C10-C8-C9
3	N	101	BCL	C6-C7-C8-C10
3	F	101	BCL	C5-C6-C7-C8
5	P	103	LMT	C3'-C4'-O1B-C1B
3	N	101	BCL	C6-C7-C8-C9
5	I	303	LMT	C3'-C4'-O1B-C1B
5	L	101	LMT	C5'-C4'-O1B-C1B
5	L	101	LMT	C3'-C4'-O1B-C1B
6	R	103	IRM	C25-C26-C27-C28
3	R	102	BCL	C11-C10-C8-C7
5	A	304	LMT	C3'-C4'-O1B-C1B
6	B	102	IRM	C25-C26-C27-C28
3	J	101	BCL	C6-C7-C8-C9
5	P	103	LMT	C5'-C4'-O1B-C1B
3	J	101	BCL	C4-C3-C5-C6
6	D	103	IRM	C25-C26-C27-C28
5	R	101	LMT	C5'-C4'-O1B-C1B
5	A	304	LMT	C5'-C4'-O1B-C1B
3	C	302	BCL	C4-C3-C5-C6
5	D	101	LMT	C11-C10-C9-C8
5	F	102	LMT	C3'-C4'-O1B-C1B
5	F	102	LMT	C5'-C4'-O1B-C1B
3	E	302	BCL	O1A-CGA-O2A-C1
3	K	302	BCL	C4-C3-C5-C6
5	R	101	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
3	B	101	BCL	C14-C13-C15-C16
3	Q	301	BCL	C8-C10-C11-C12
3	G	301	BCL	C8-C10-C11-C12
5	I	303	LMT	C5'-C4'-O1B-C1B
6	L	103	IRM	C25-C26-C27-C28
5	N	103	LMT	C5'-C4'-O1B-C1B
3	J	101	BCL	C6-C7-C8-C10
4	I	304	LDA	C5-C6-C7-C8
6	E	304	IRM	C25-C26-C27-C28
6	H	103	IRM	C25-C26-C27-C28
6	J	102	IRM	C25-C26-C27-C28
6	N	102	IRM	C25-C26-C27-C28
6	P	102	IRM	C25-C26-C27-C28
3	J	101	BCL	C5-C6-C7-C8
3	E	302	BCL	CAA-CBA-CGA-O2A
3	M	302	BCL	CAA-CBA-CGA-O2A
5	N	103	LMT	C3'-C4'-O1B-C1B
5	L	101	LMT	C7-C8-C9-C10
3	C	302	BCL	C1A-C2A-CAA-CBA
3	O	302	BCL	CAA-CBA-CGA-O2A
3	H	102	BCL	C8-C10-C11-C12
3	I	302	BCL	C3A-C2A-CAA-CBA
3	A	301	BCL	C11-C12-C13-C14
3	M	301	BCL	C11-C12-C13-C14
3	O	301	BCL	C11-C12-C13-C14
3	R	102	BCL	C11-C10-C8-C9
3	J	101	BCL	C2-C3-C5-C6
3	O	302	BCL	CAA-CBA-CGA-O1A
5	D	101	LMT	C5-C6-C7-C8
3	G	302	BCL	CAD-CBD-CGD-O2D
3	K	302	BCL	CAD-CBD-CGD-O2D
3	M	302	BCL	CAD-CBD-CGD-O2D
5	R	101	LMT	C3-C4-C5-C6
3	J	101	BCL	C15-C16-C17-C18
3	M	302	BCL	CAA-CBA-CGA-O1A
3	A	301	BCL	C11-C12-C13-C15

There are no ring outliers.

27 monomers are involved in 44 short contacts:

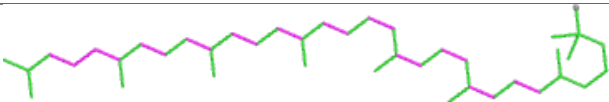
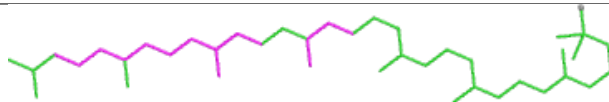
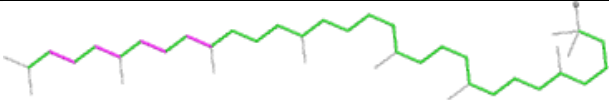
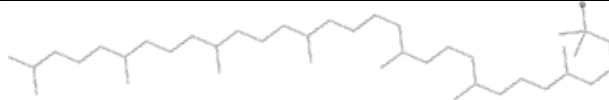
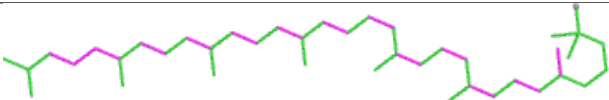
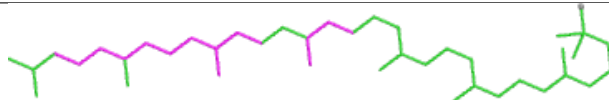
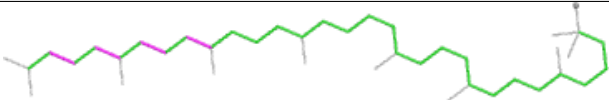
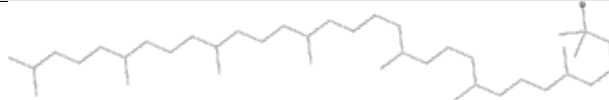
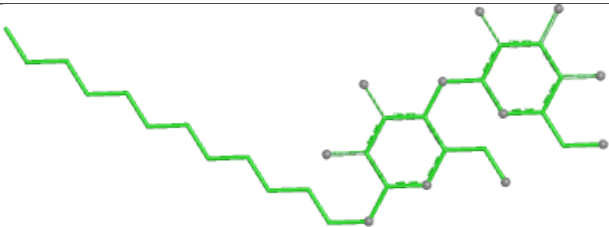
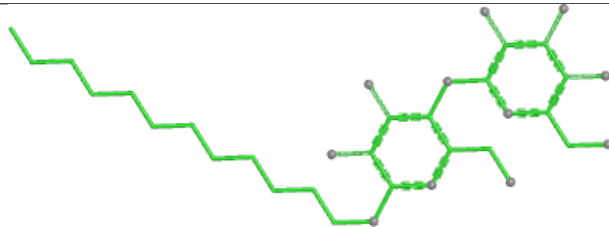
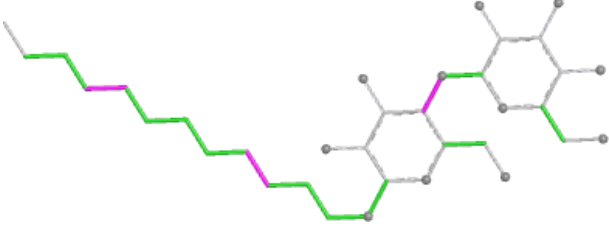
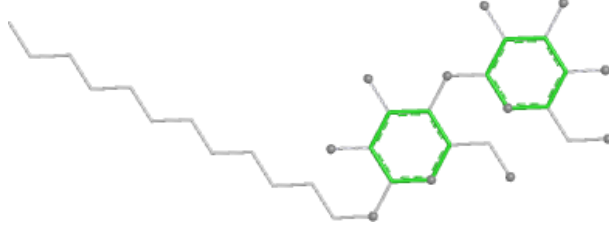
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	102	BCL	2	0

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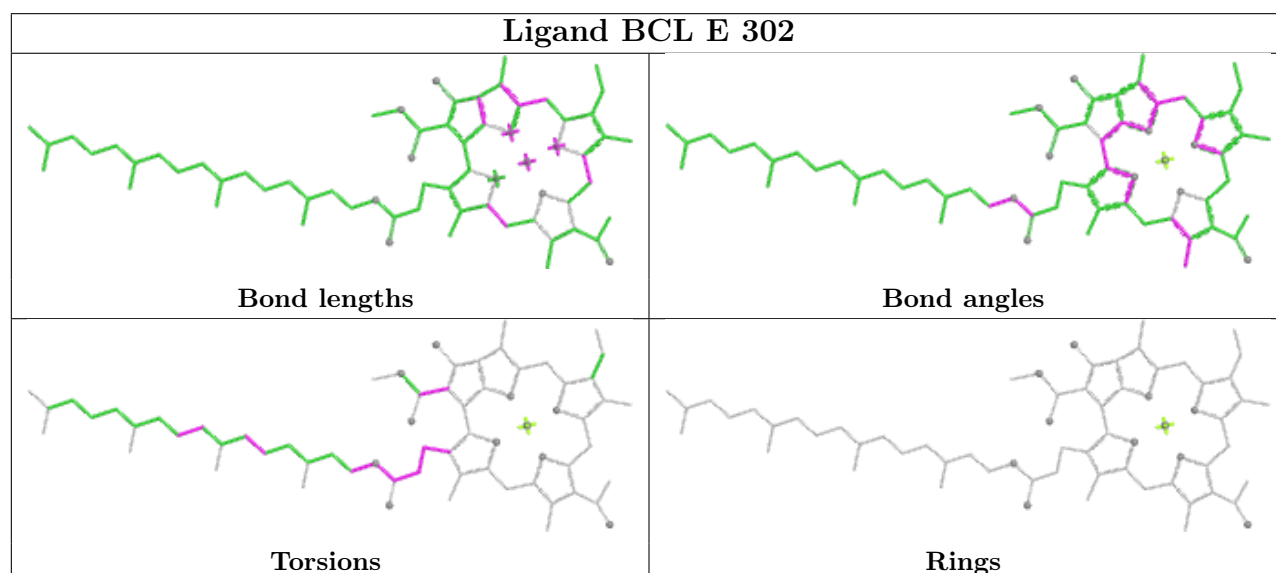
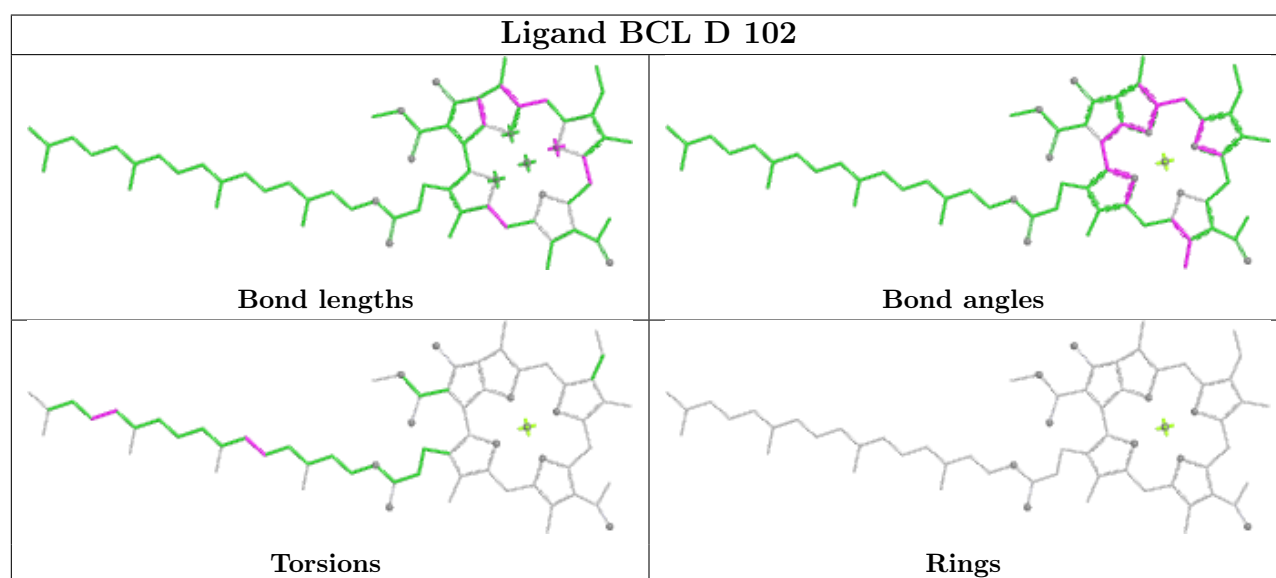
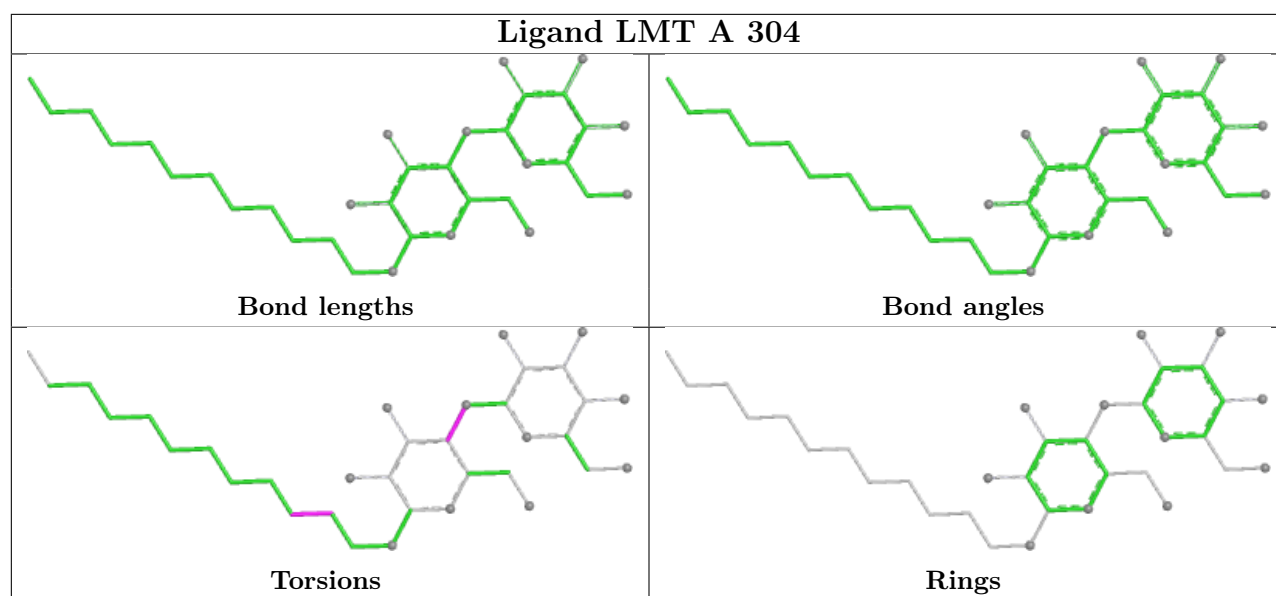
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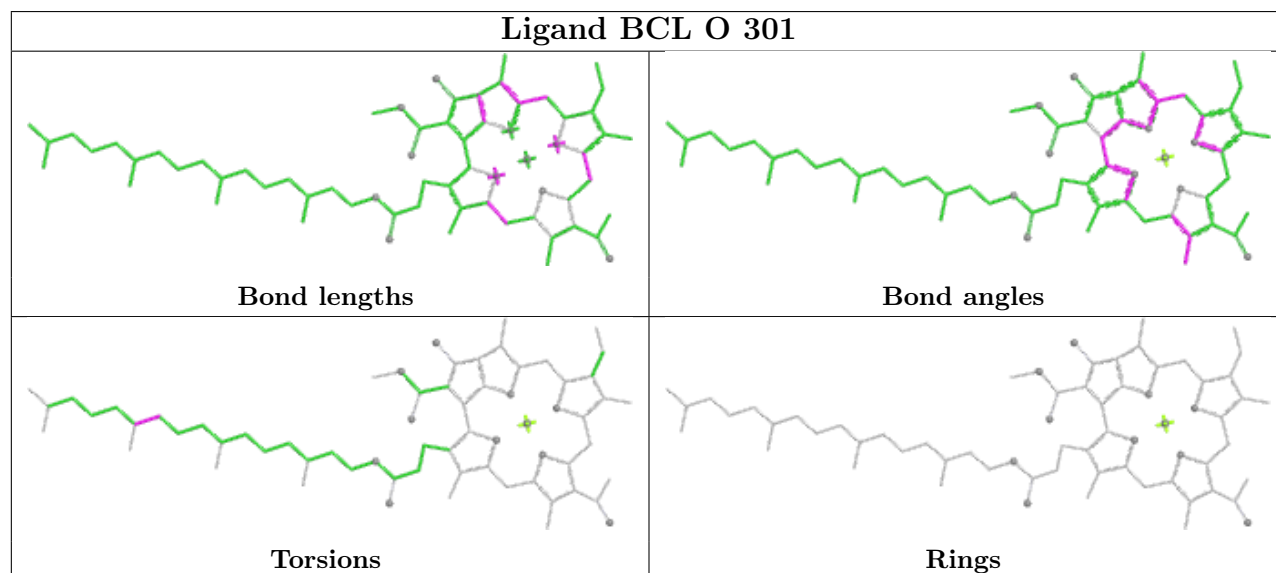
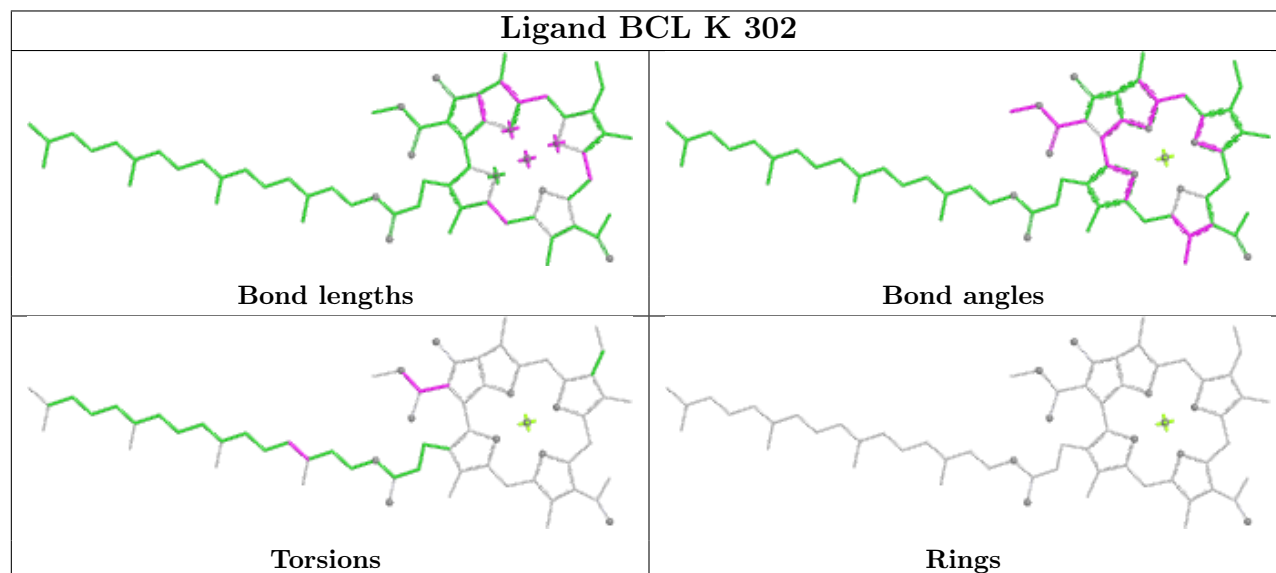
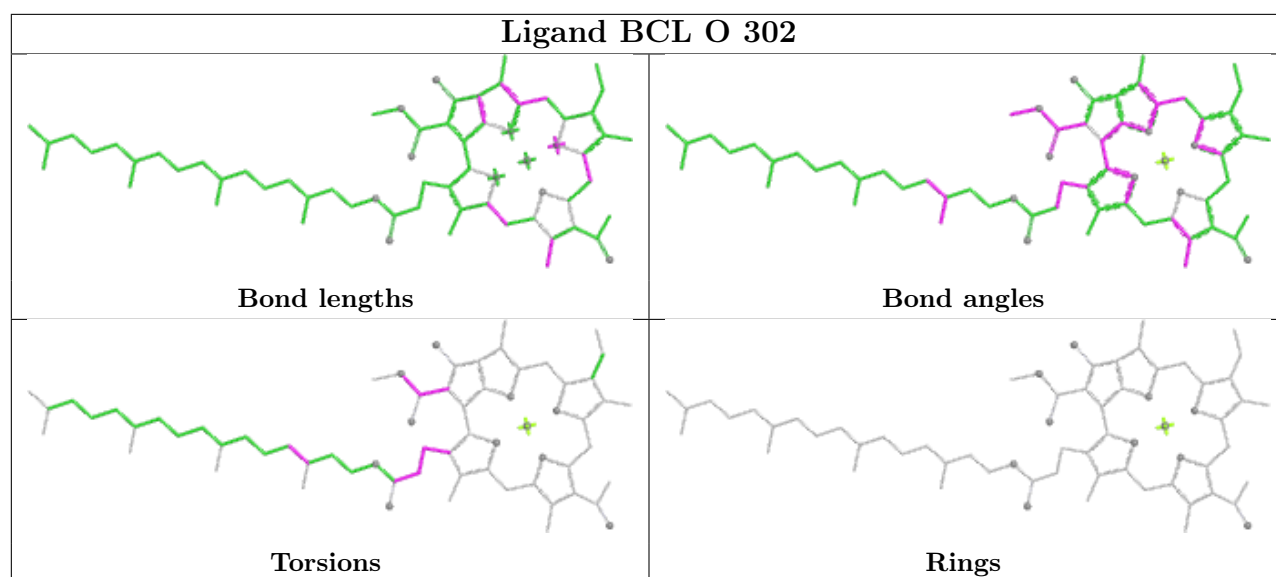
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	BCL	1	0
3	O	302	BCL	2	0
3	K	302	BCL	2	0
3	O	301	BCL	2	0
3	Q	302	BCL	2	0
3	R	102	BCL	1	0
3	C	301	BCL	1	0
3	L	102	BCL	1	0
3	M	302	BCL	1	0
3	G	302	BCL	3	0
3	B	101	BCL	1	0
3	Q	301	BCL	2	0
3	A	301	BCL	2	0
3	E	301	BCL	2	0
3	M	301	BCL	2	0
3	I	302	BCL	1	0
3	J	101	BCL	2	0
3	N	101	BCL	1	0
3	P	101	BCL	1	0
3	G	301	BCL	2	0
3	I	301	BCL	2	0
3	A	302	BCL	2	0
3	K	301	BCL	2	0
3	F	101	BCL	2	0
3	C	302	BCL	2	0
3	H	102	BCL	2	0

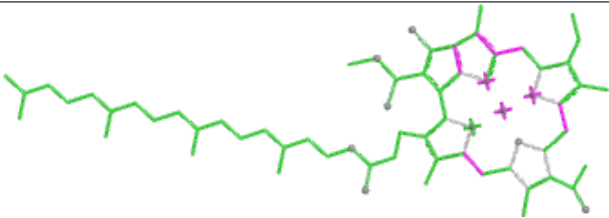
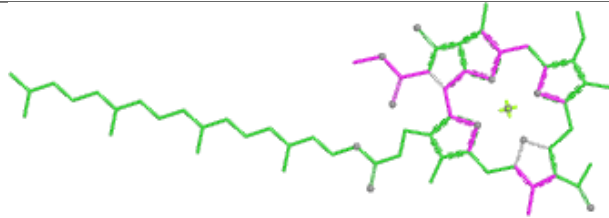
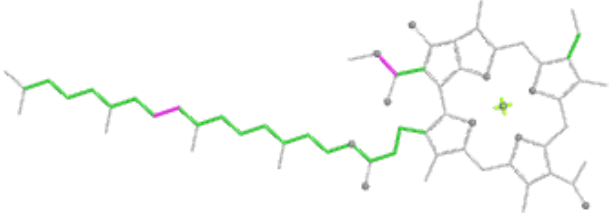
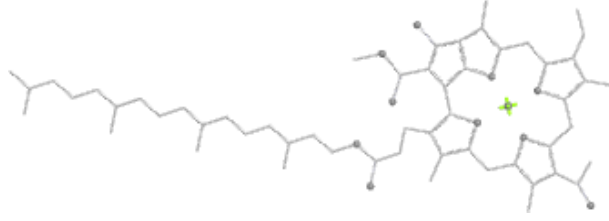
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

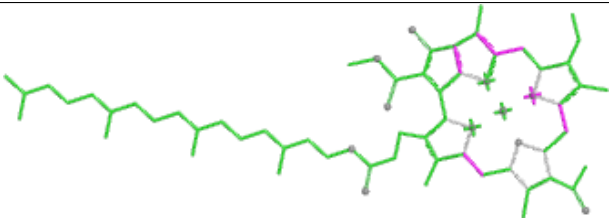
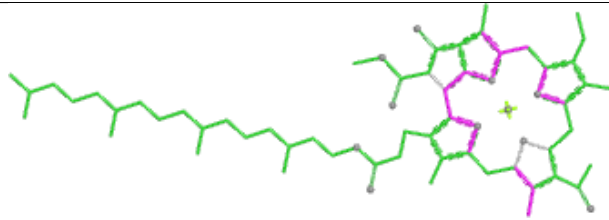
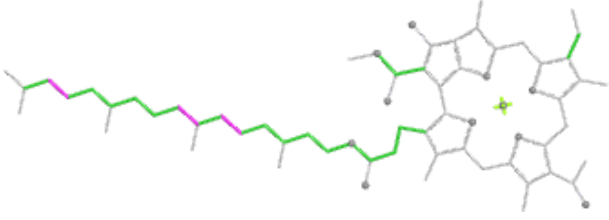
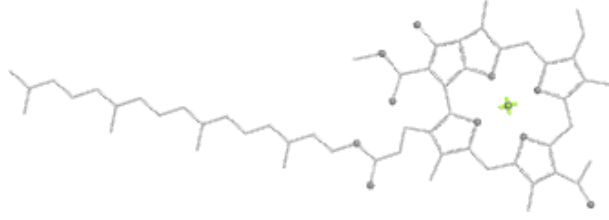
Ligand IRM H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand IRM J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT L 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

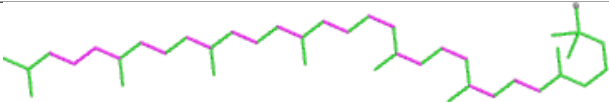
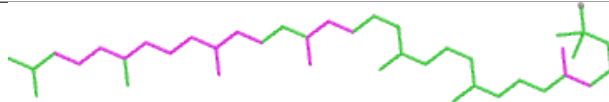
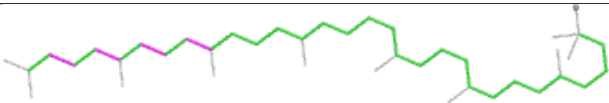
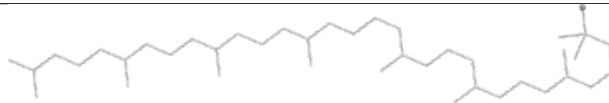


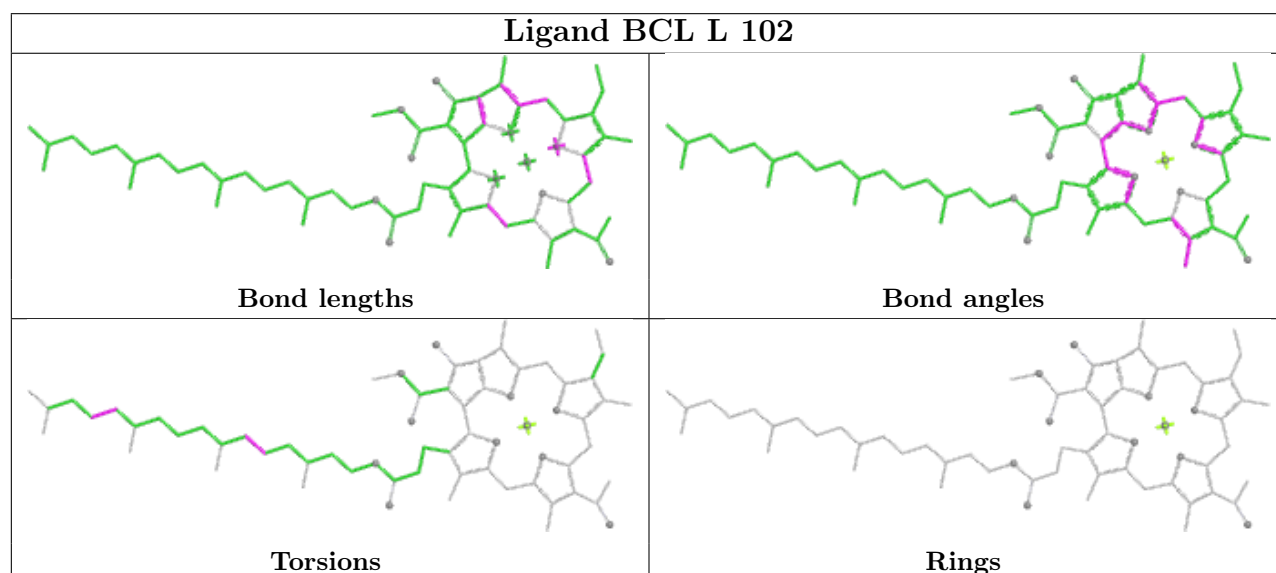
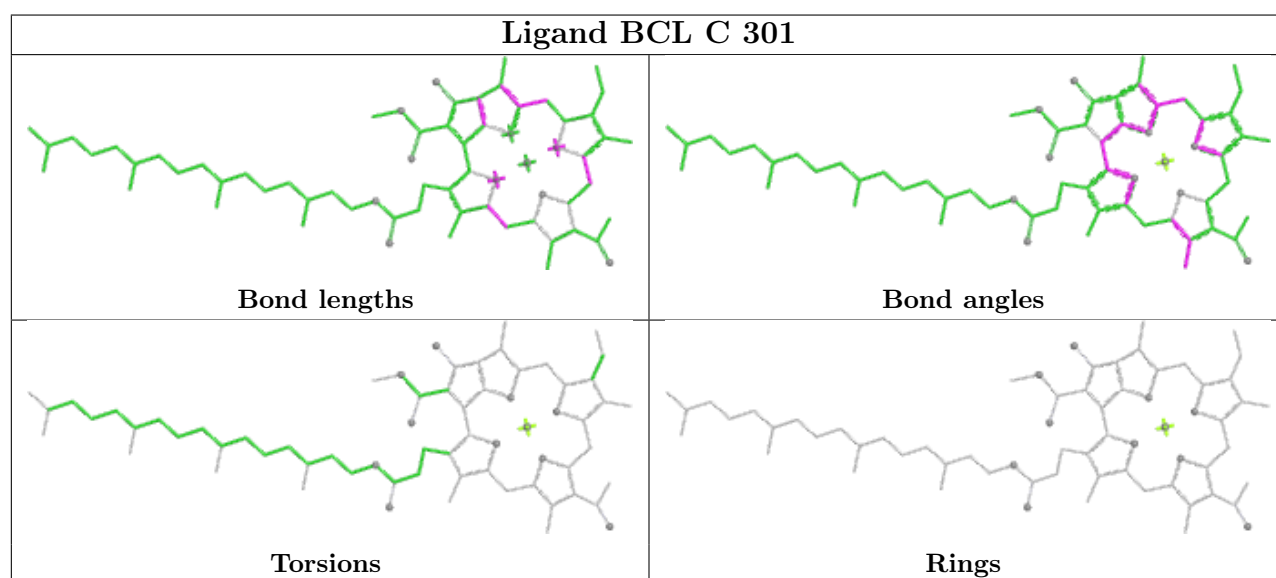
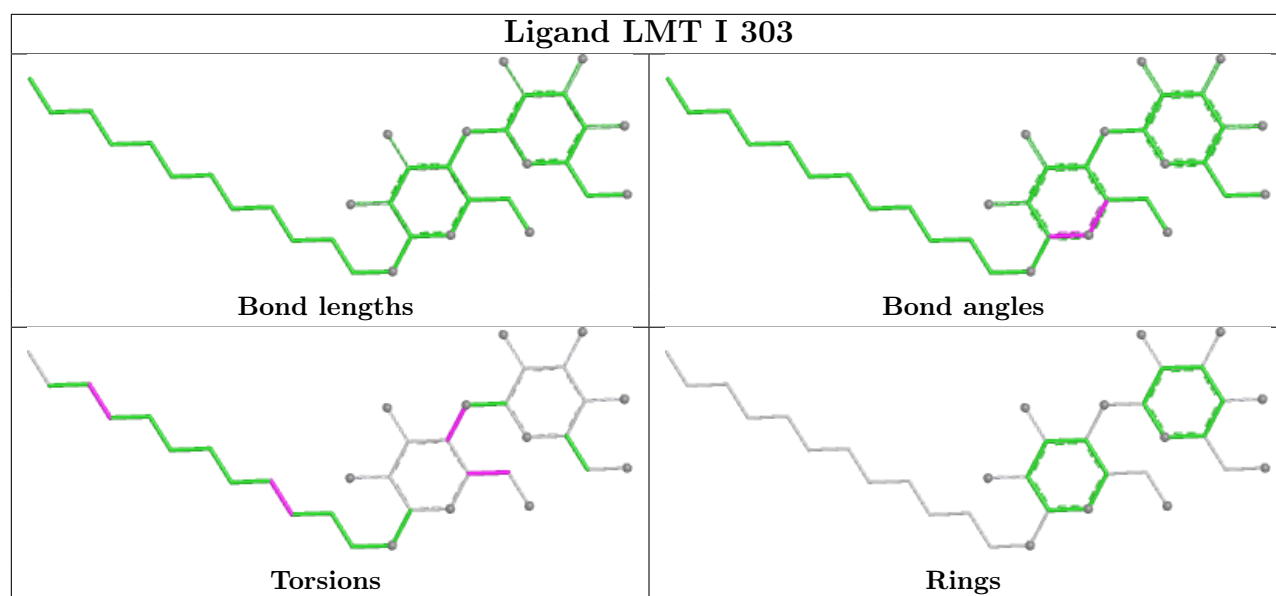


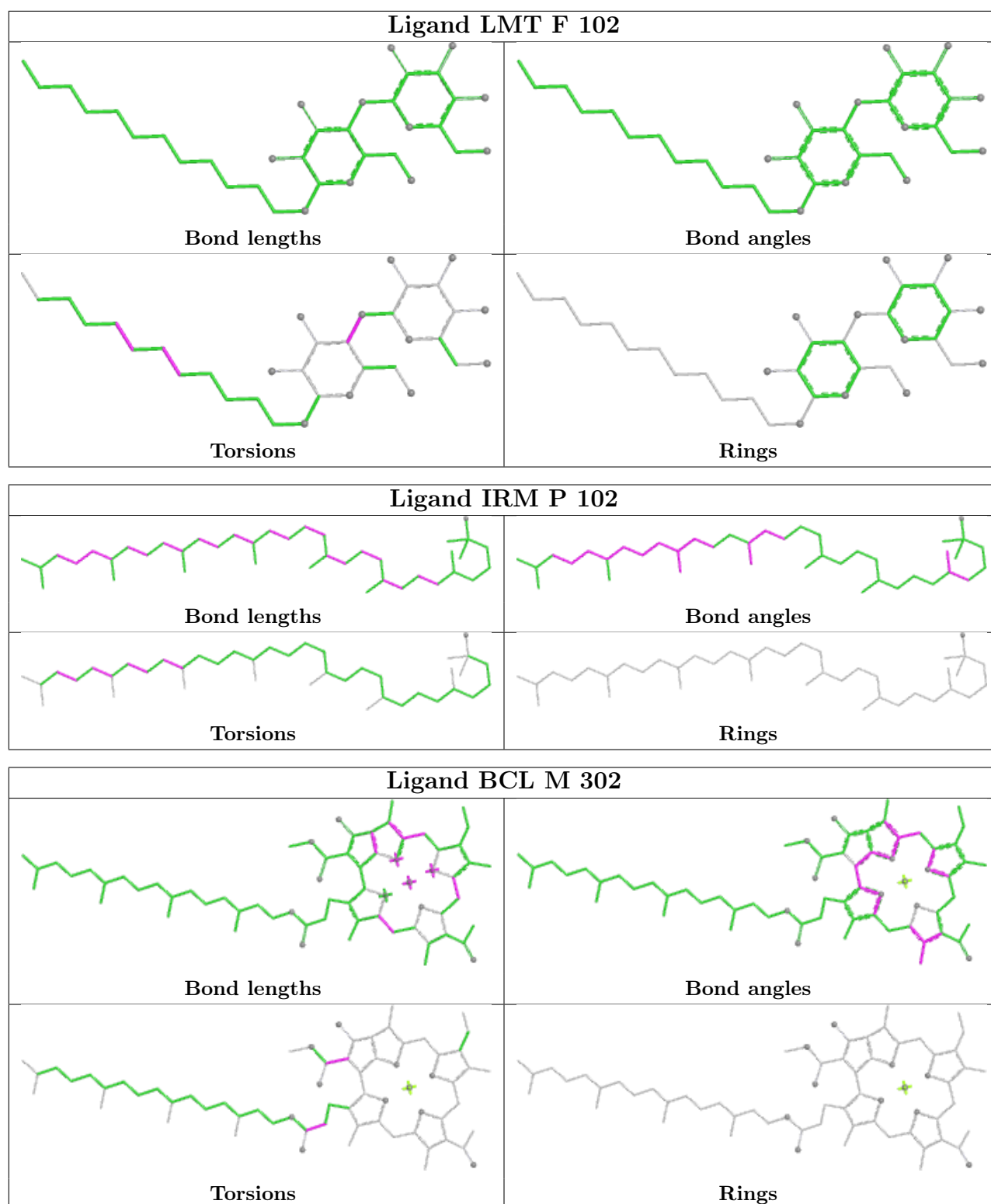


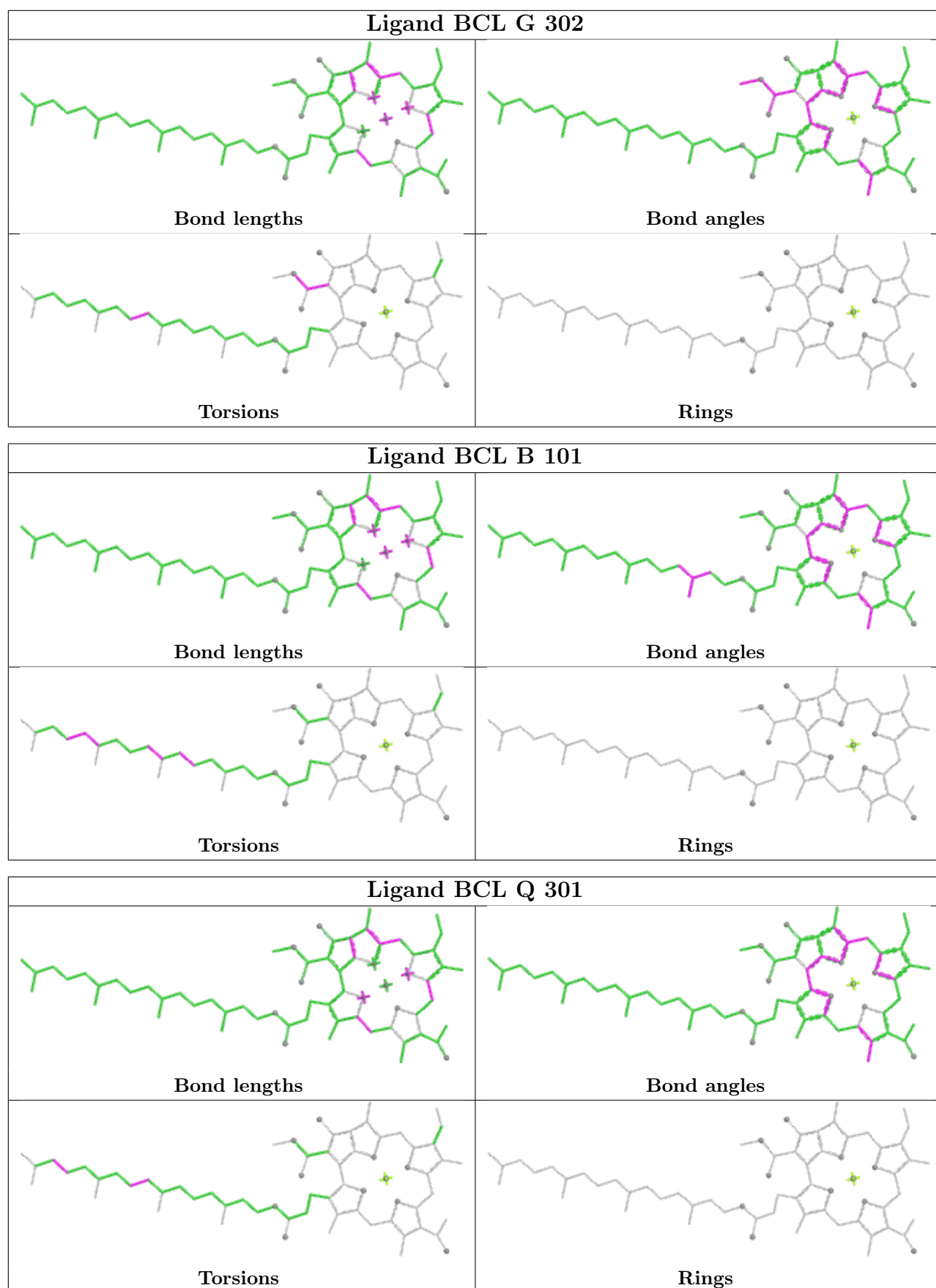
Ligand BCL Q 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

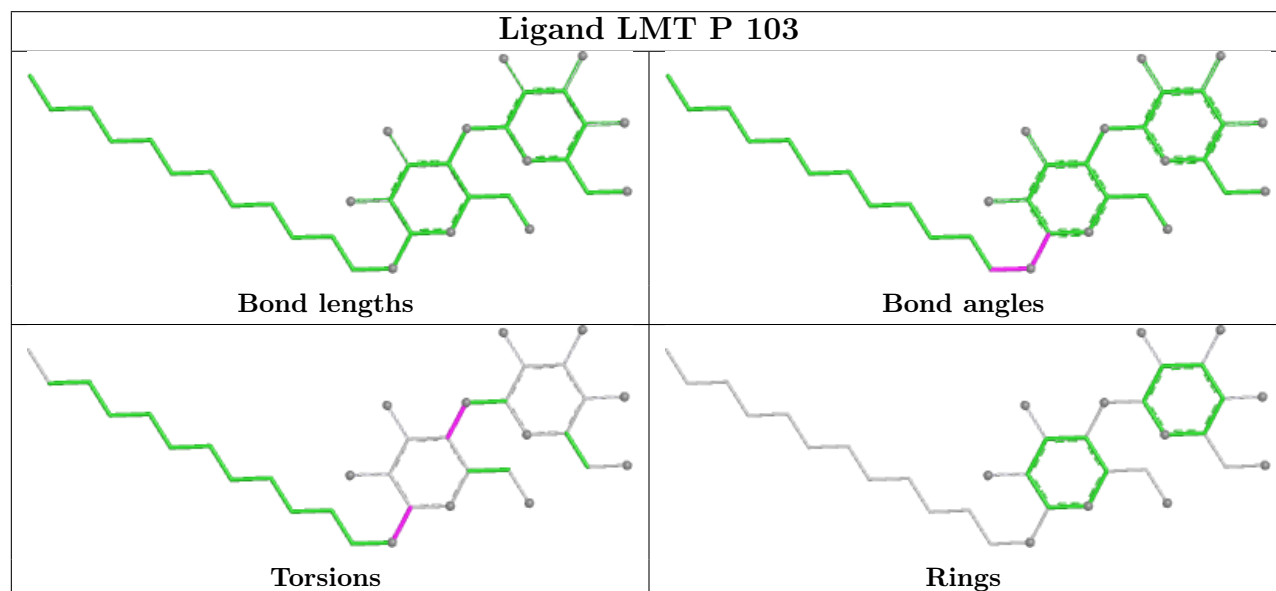
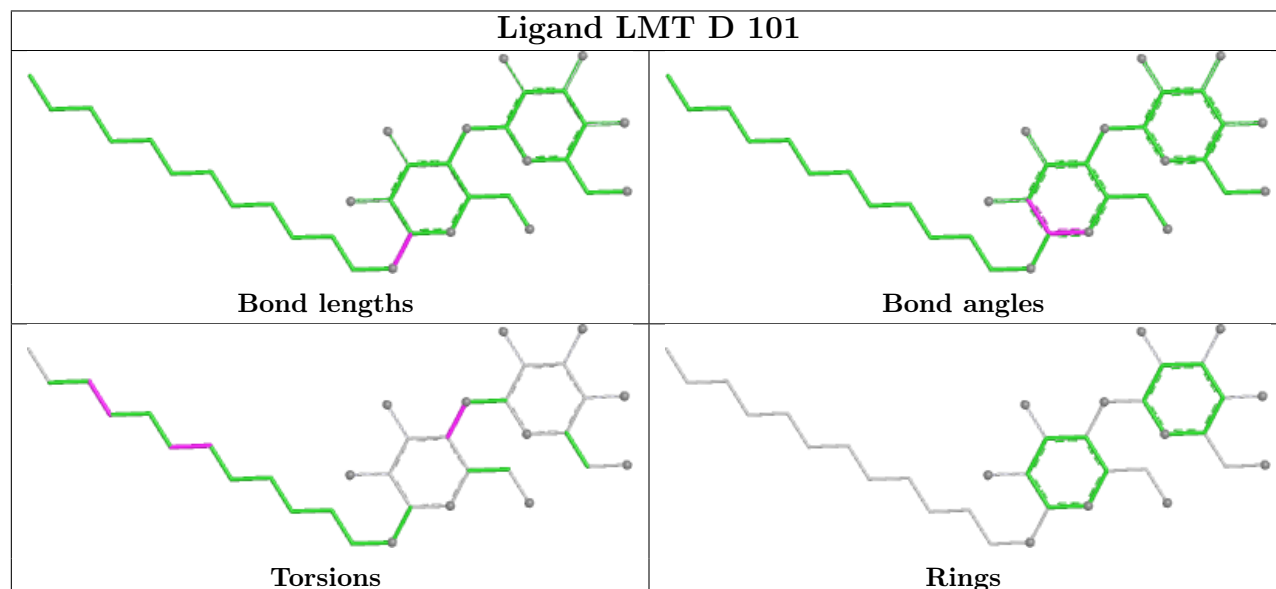
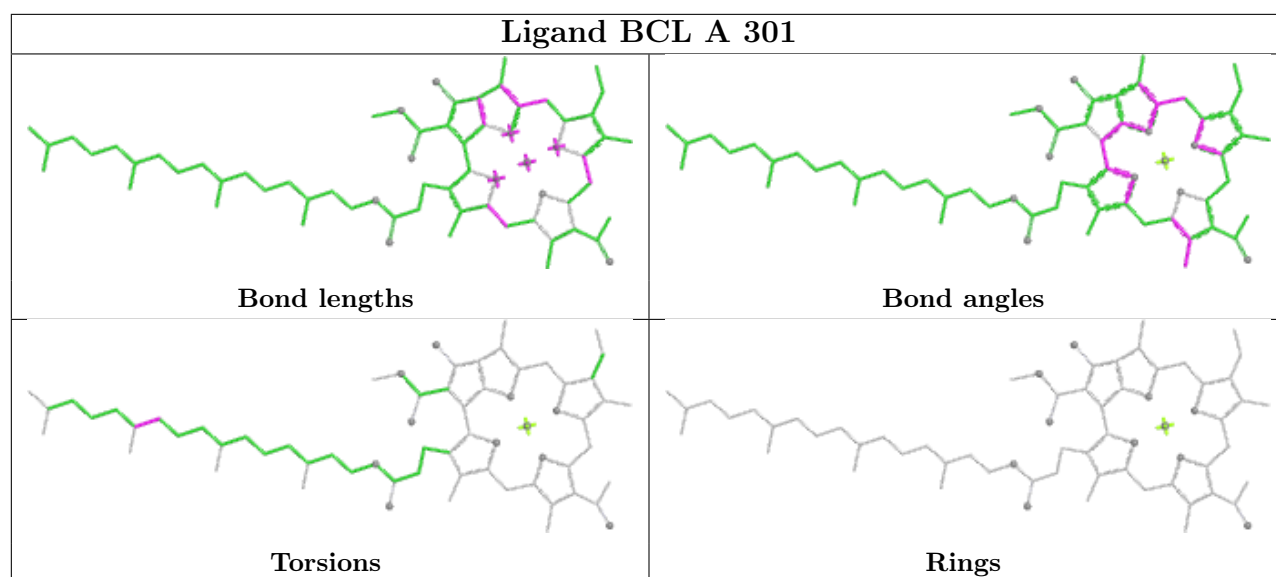
Ligand BCL R 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

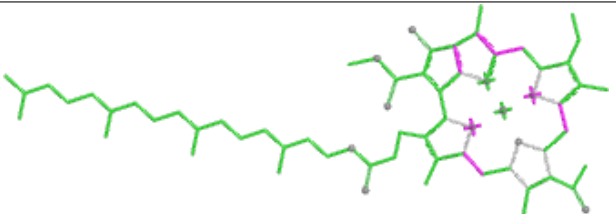
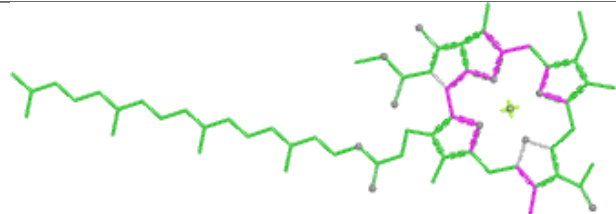
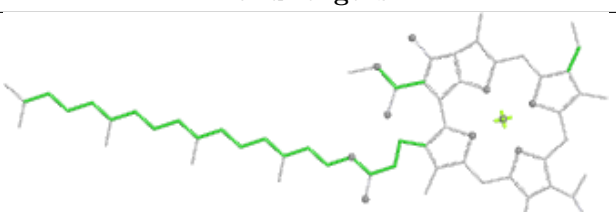
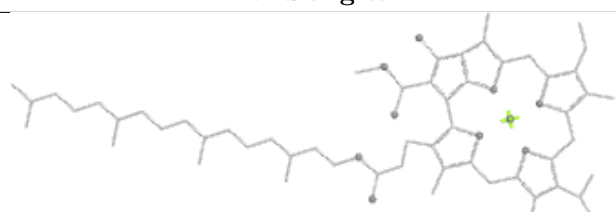
Ligand IRM E 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

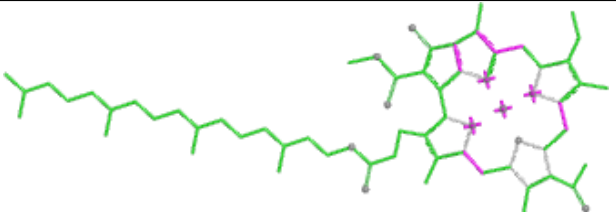
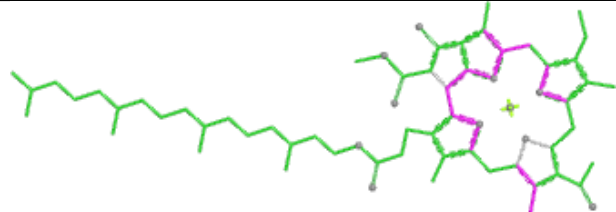
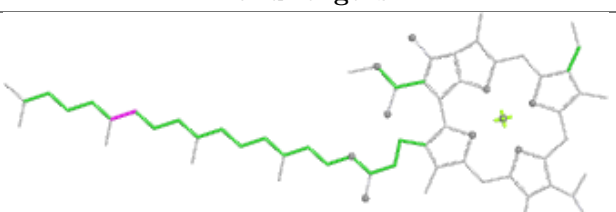
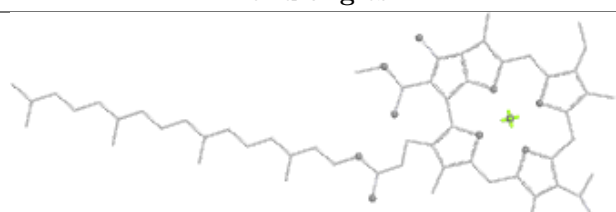


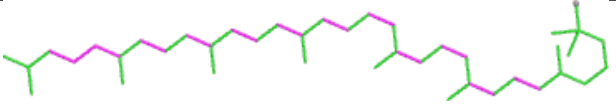
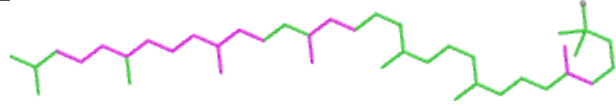
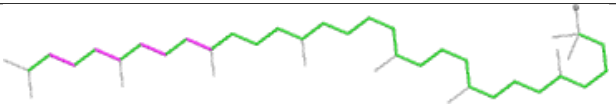
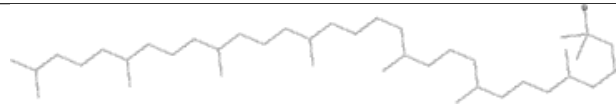




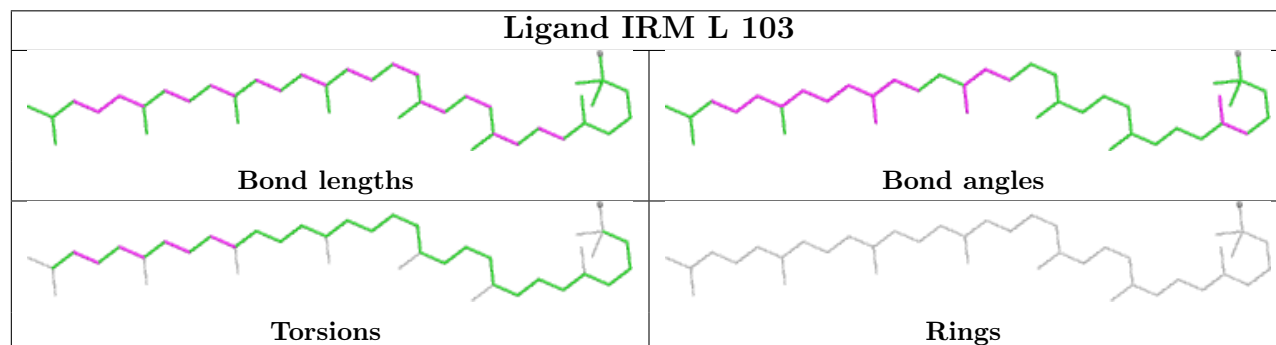
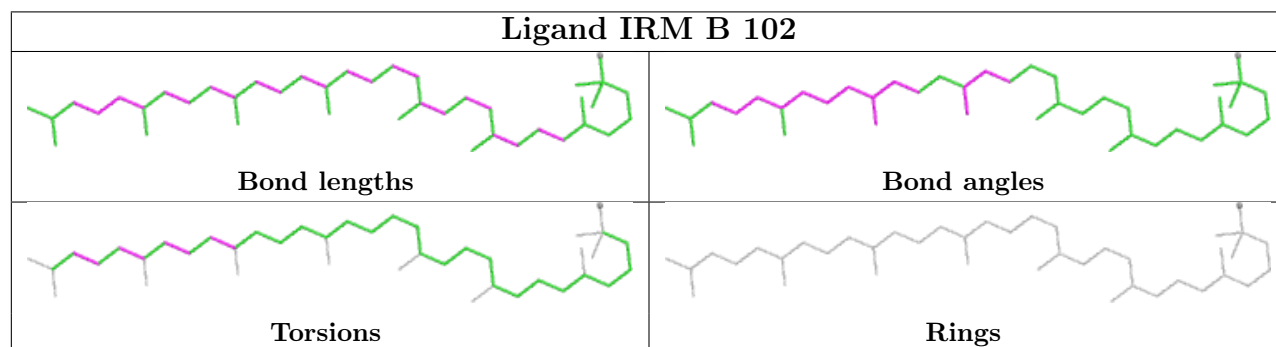
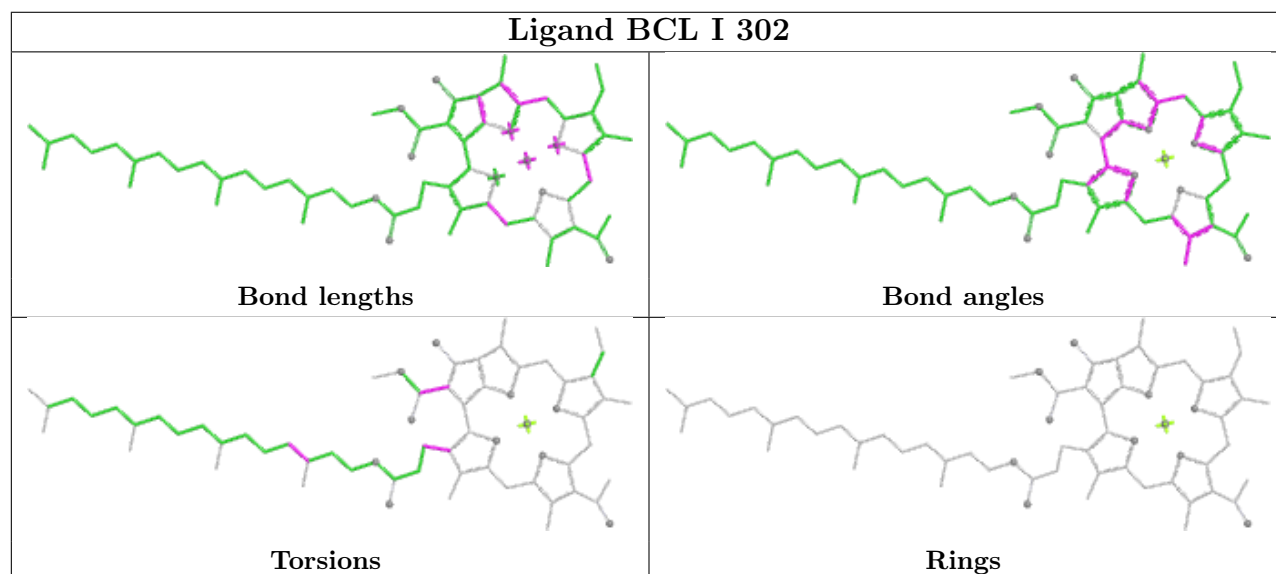
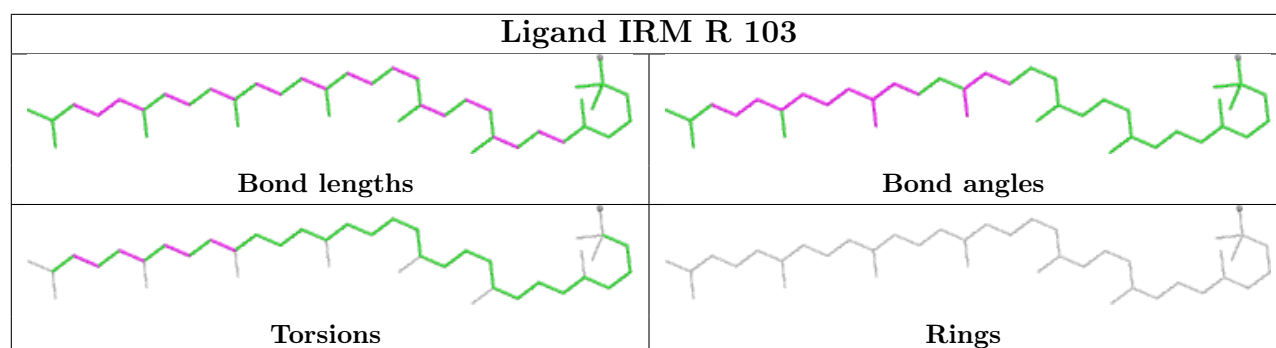


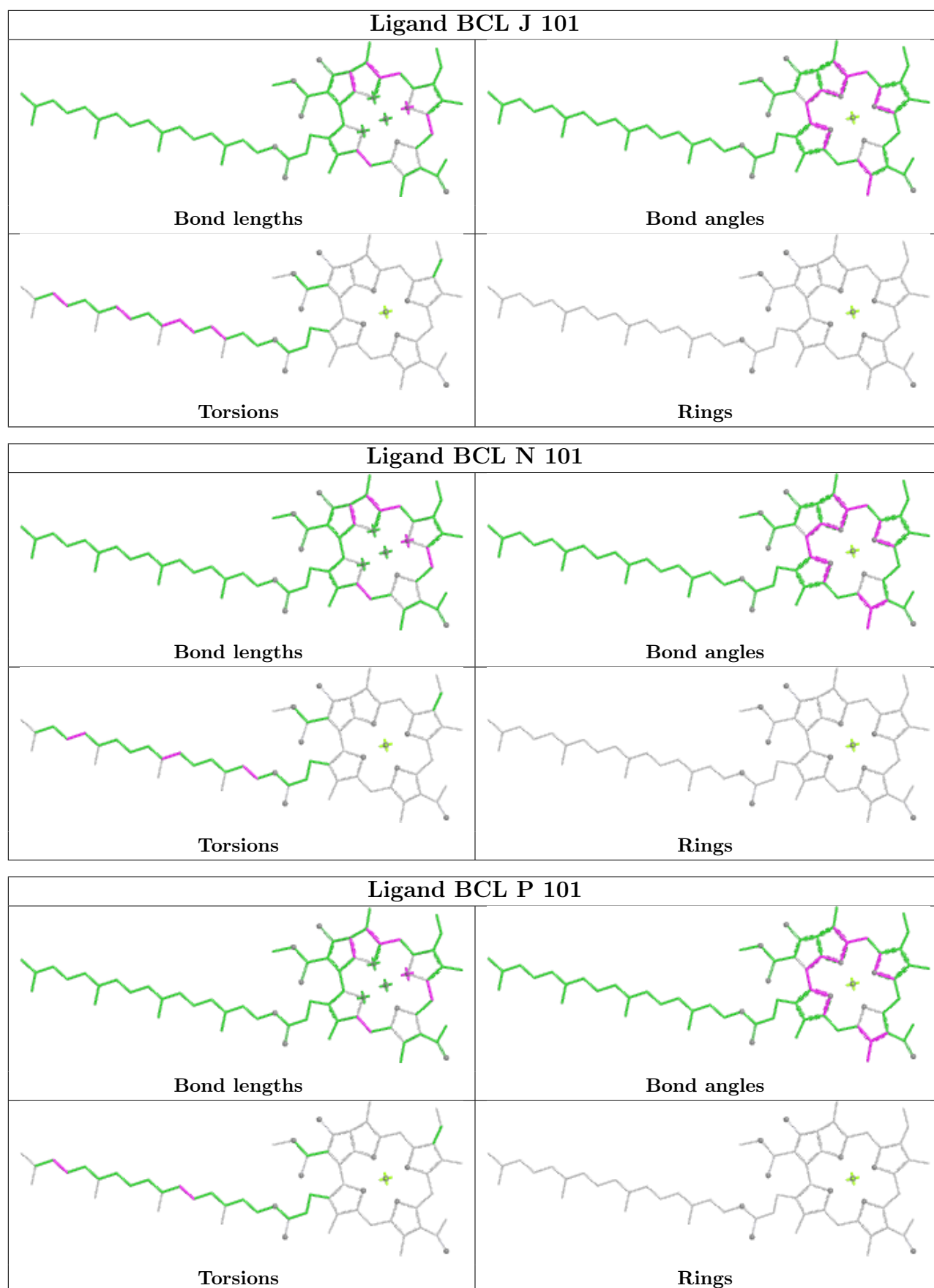
Ligand BCL E 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

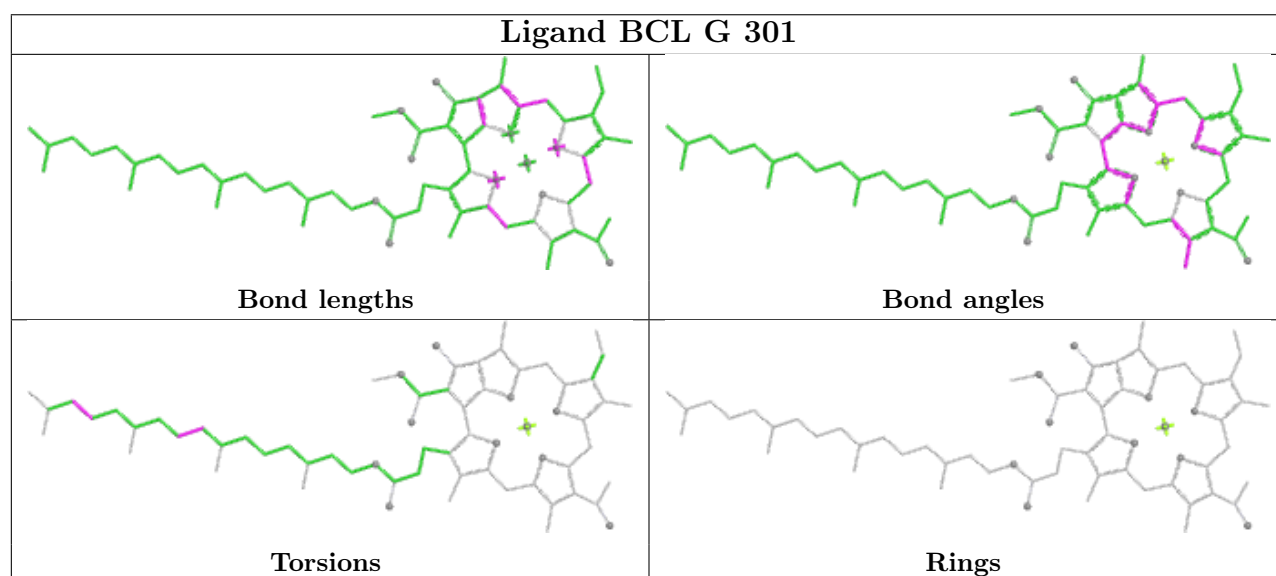
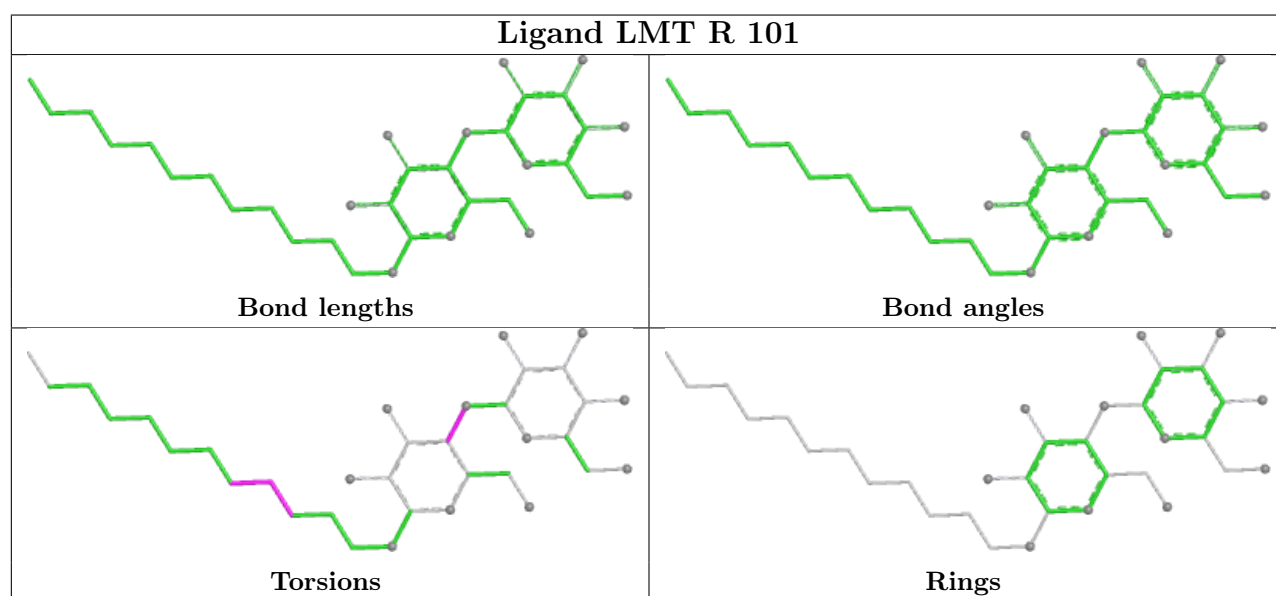
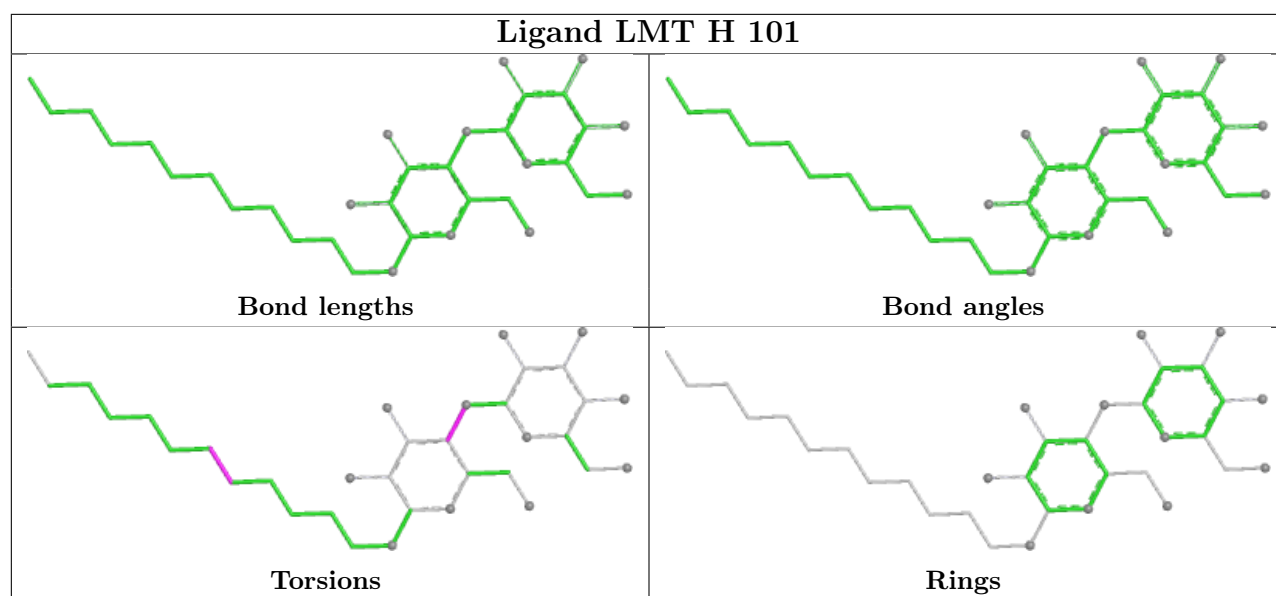
Ligand BCL M 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

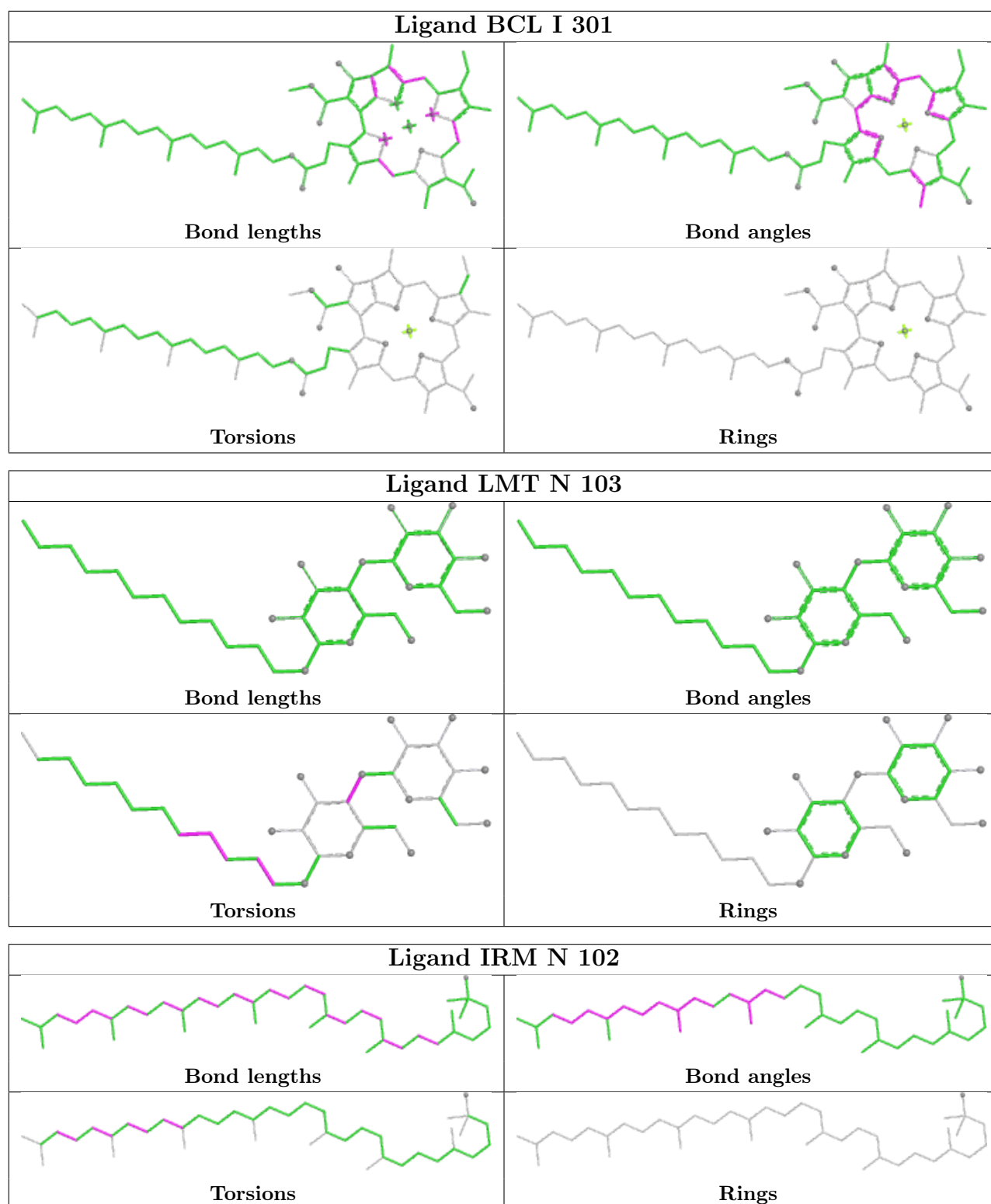
Ligand IRM D 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

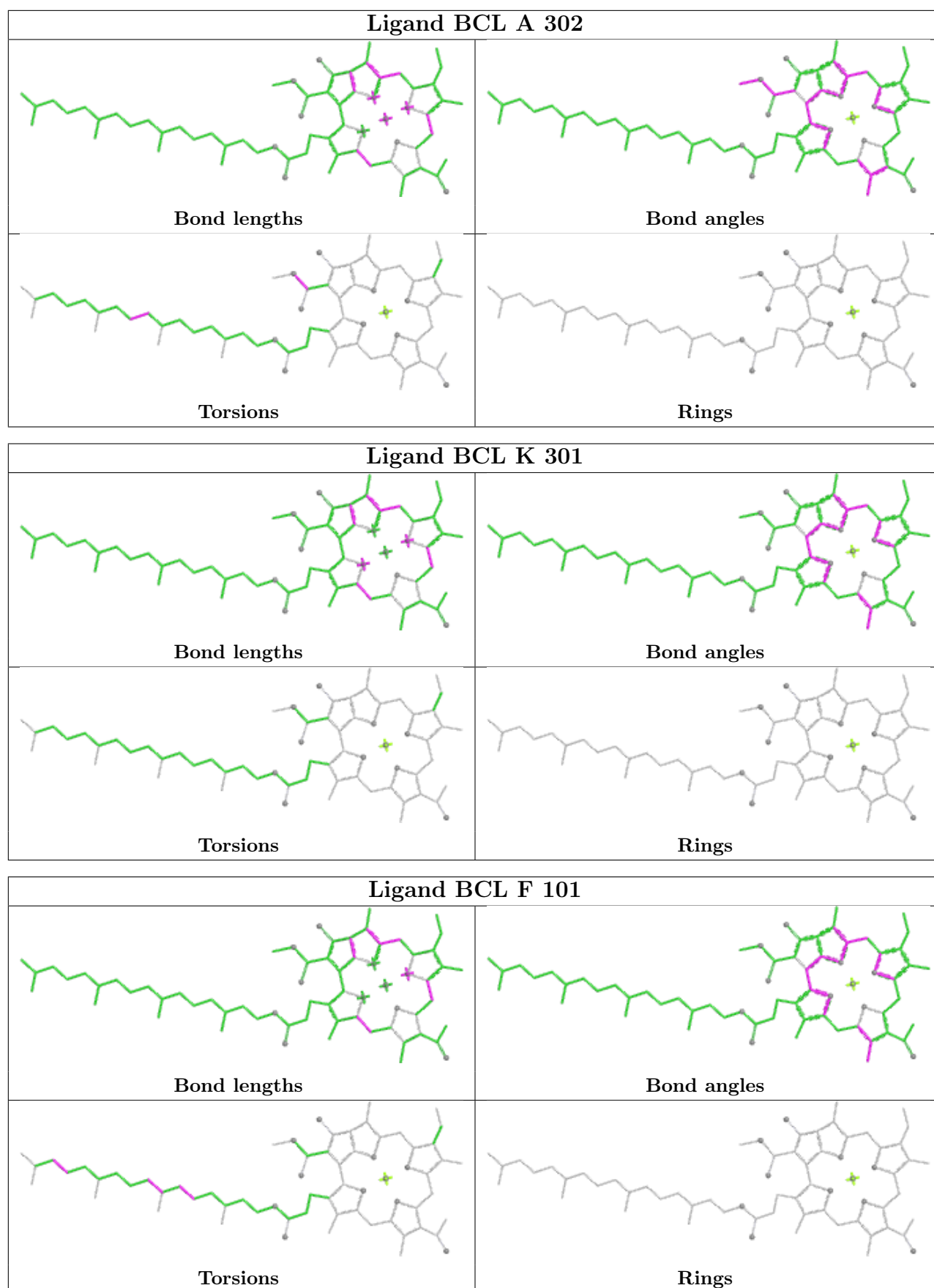


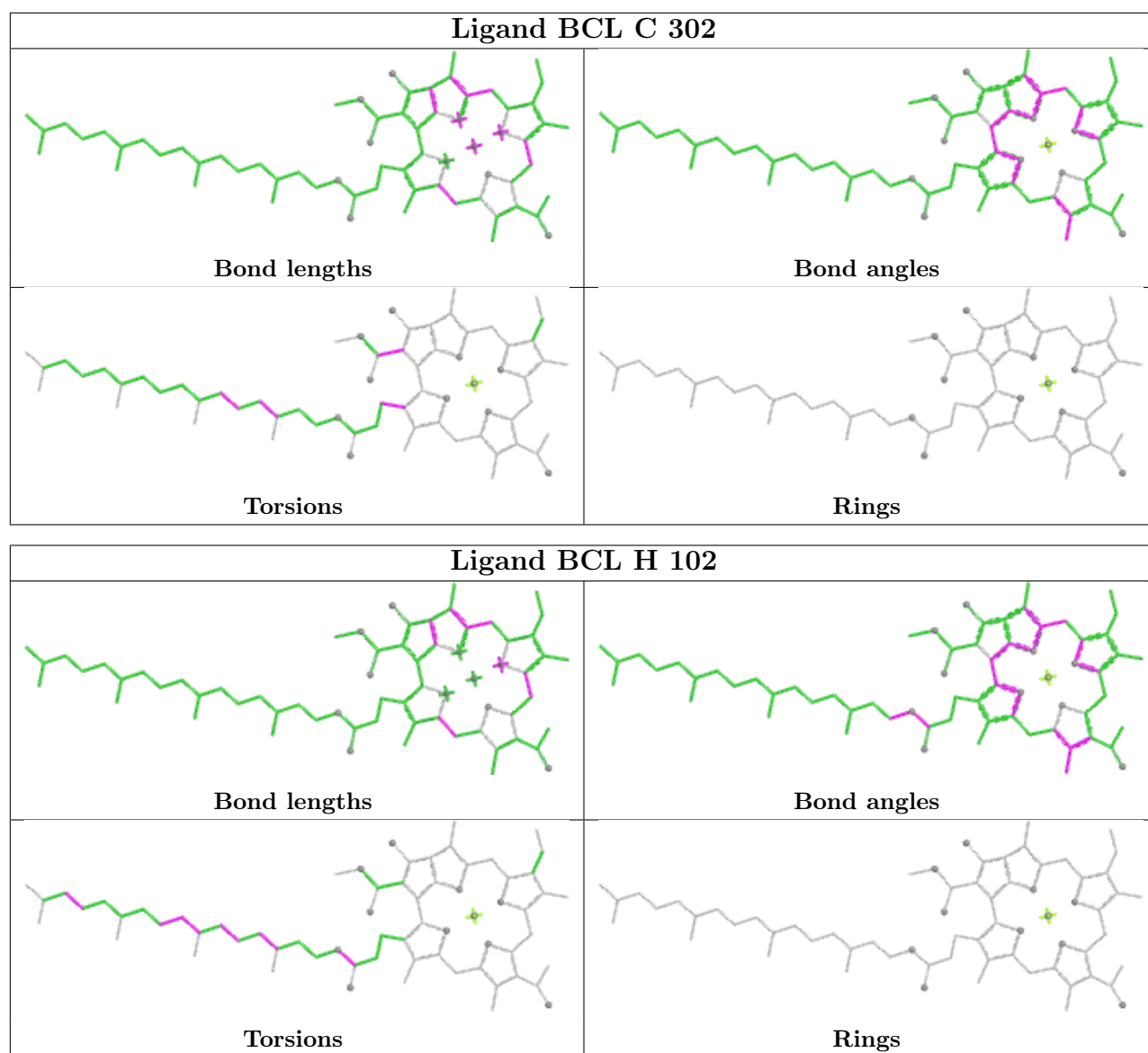












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

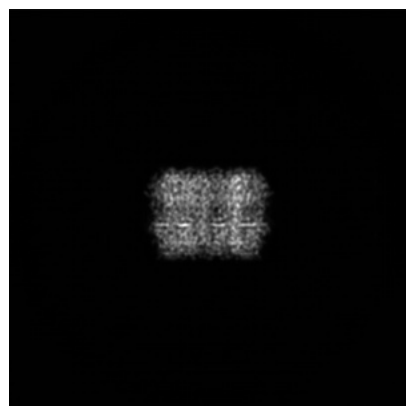
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48112. These allow visual inspection of the internal detail of the map and identification of artifacts.

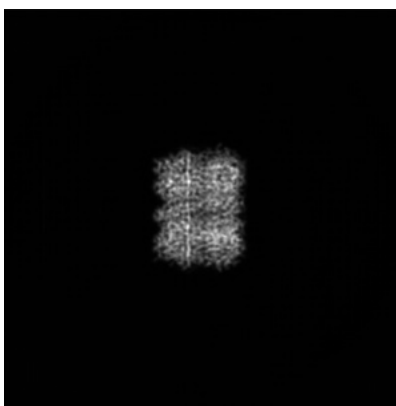
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

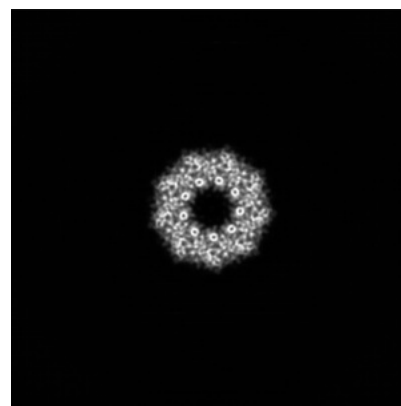
#### 6.1.1 Primary map



X

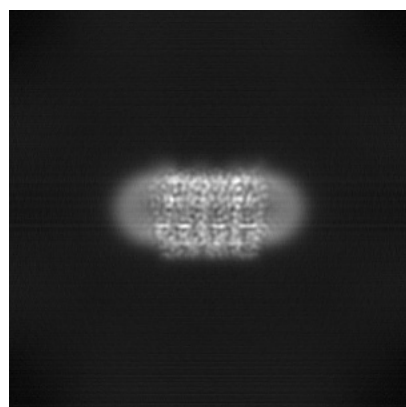


Y

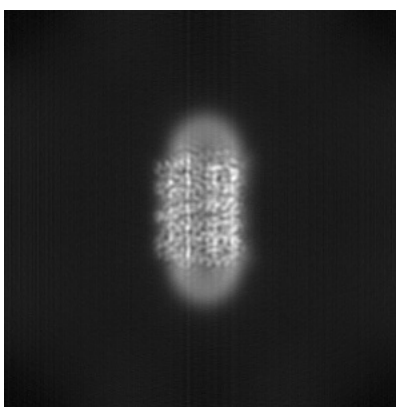


Z

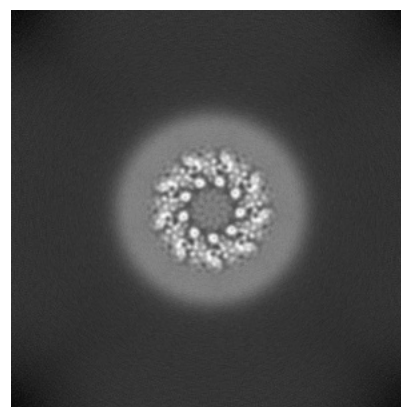
#### 6.1.2 Raw map



X



Y

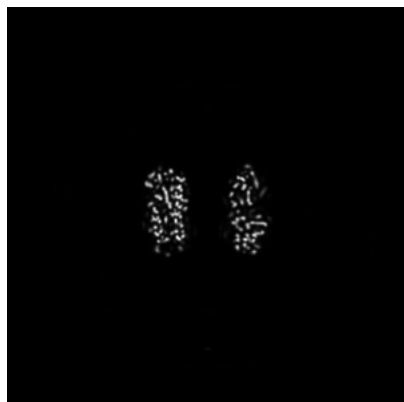


Z

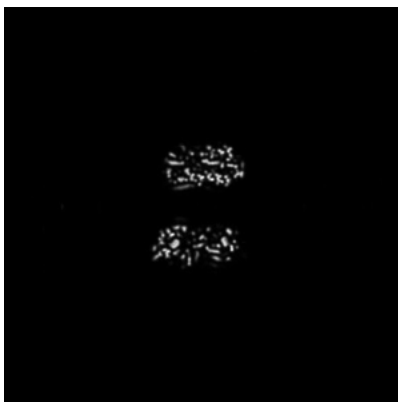
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

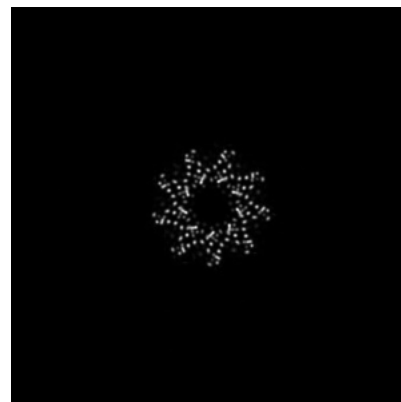
### 6.2.1 Primary map



X Index: 190



Y Index: 190

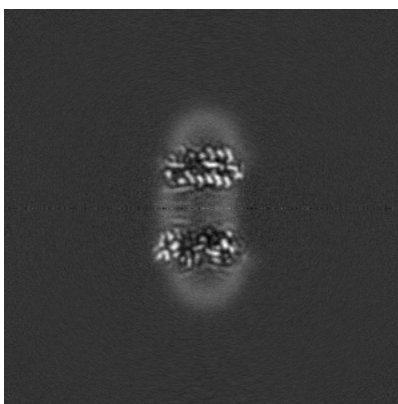


Z Index: 190

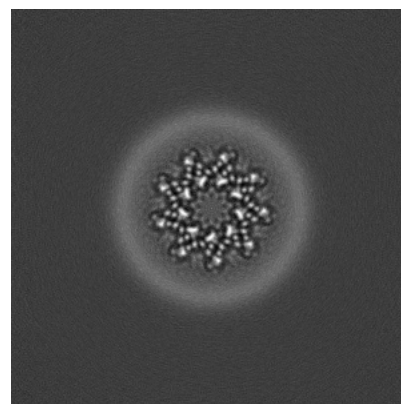
### 6.2.2 Raw map



X Index: 190



Y Index: 190



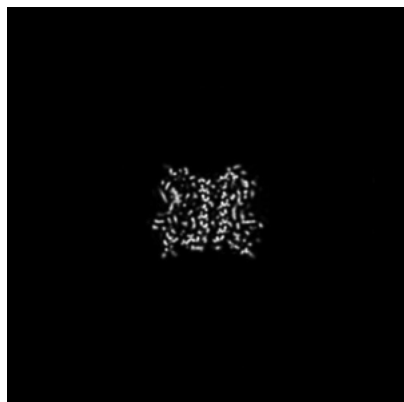
Z Index: 190

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

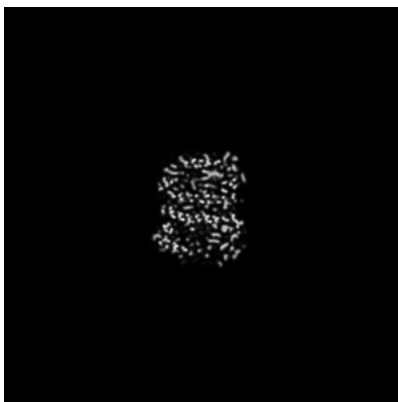


## 6.3 Largest variance slices [i](#)

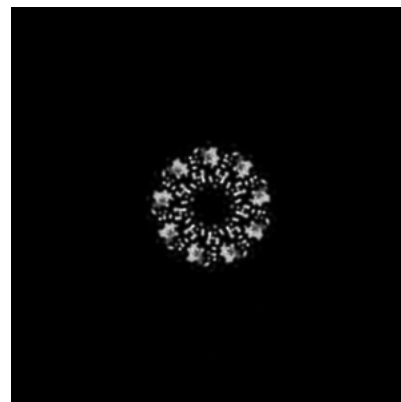
### 6.3.1 Primary map



X Index: 215

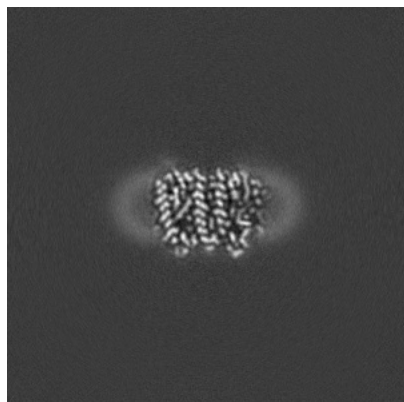


Y Index: 217

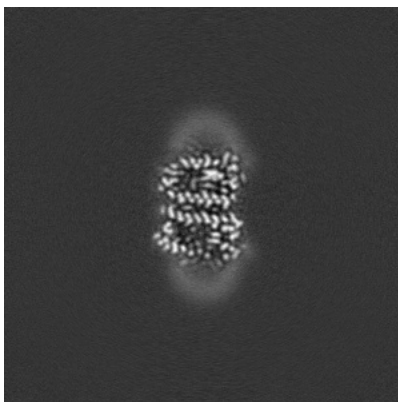


Z Index: 174

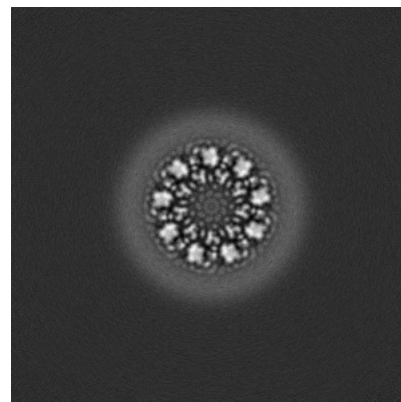
### 6.3.2 Raw map



X Index: 162



Y Index: 217

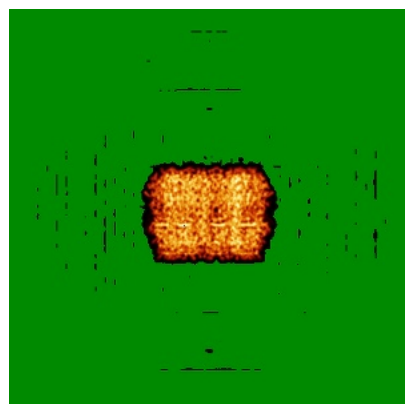


Z Index: 174

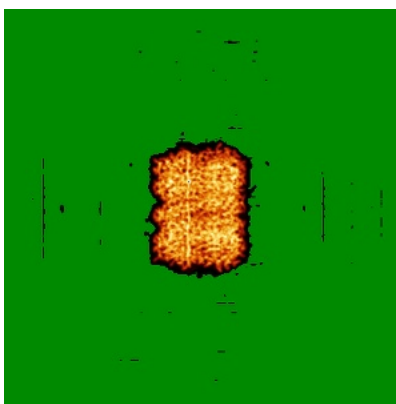
The images above show the largest variance slices of the map in three orthogonal directions.

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

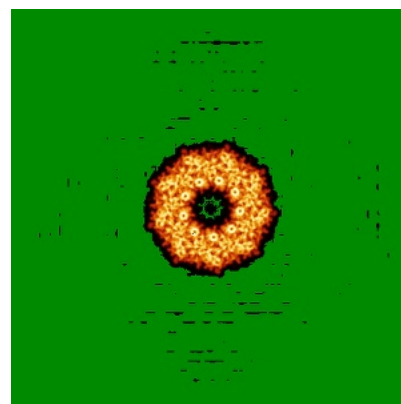
### 6.4.1 Primary map



X

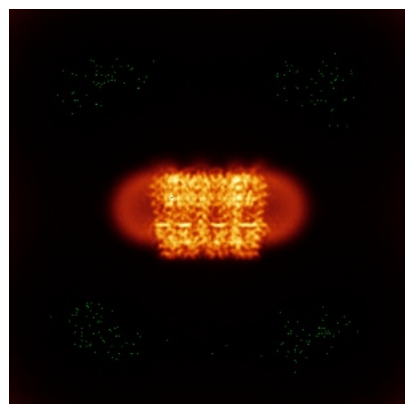


Y

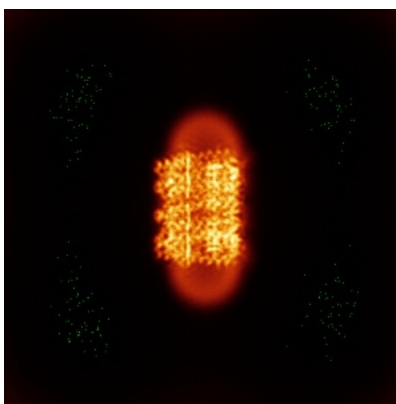


Z

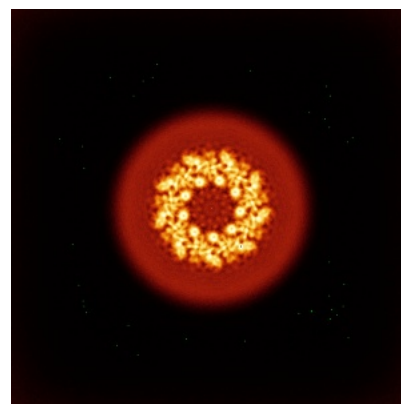
### 6.4.2 Raw map



X



Y

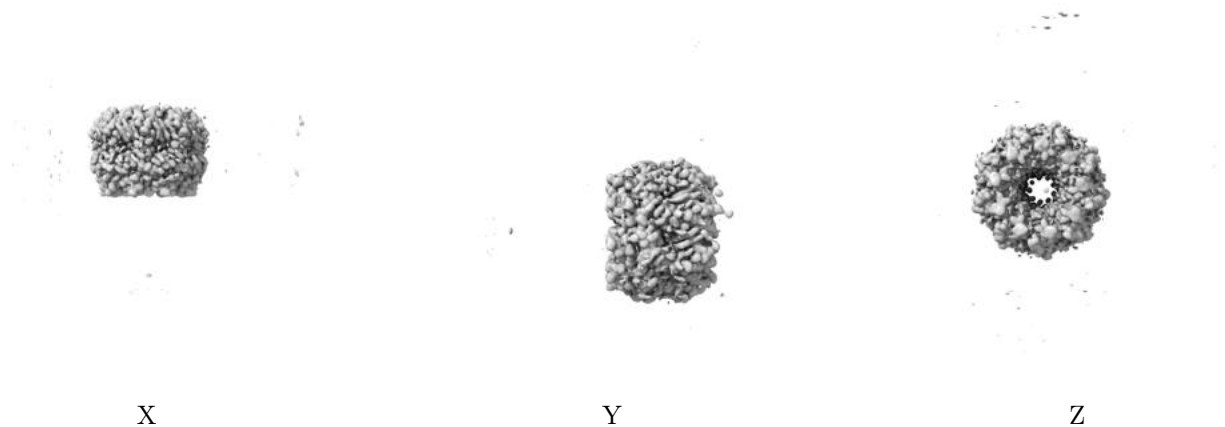


Z

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 0.234. 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.

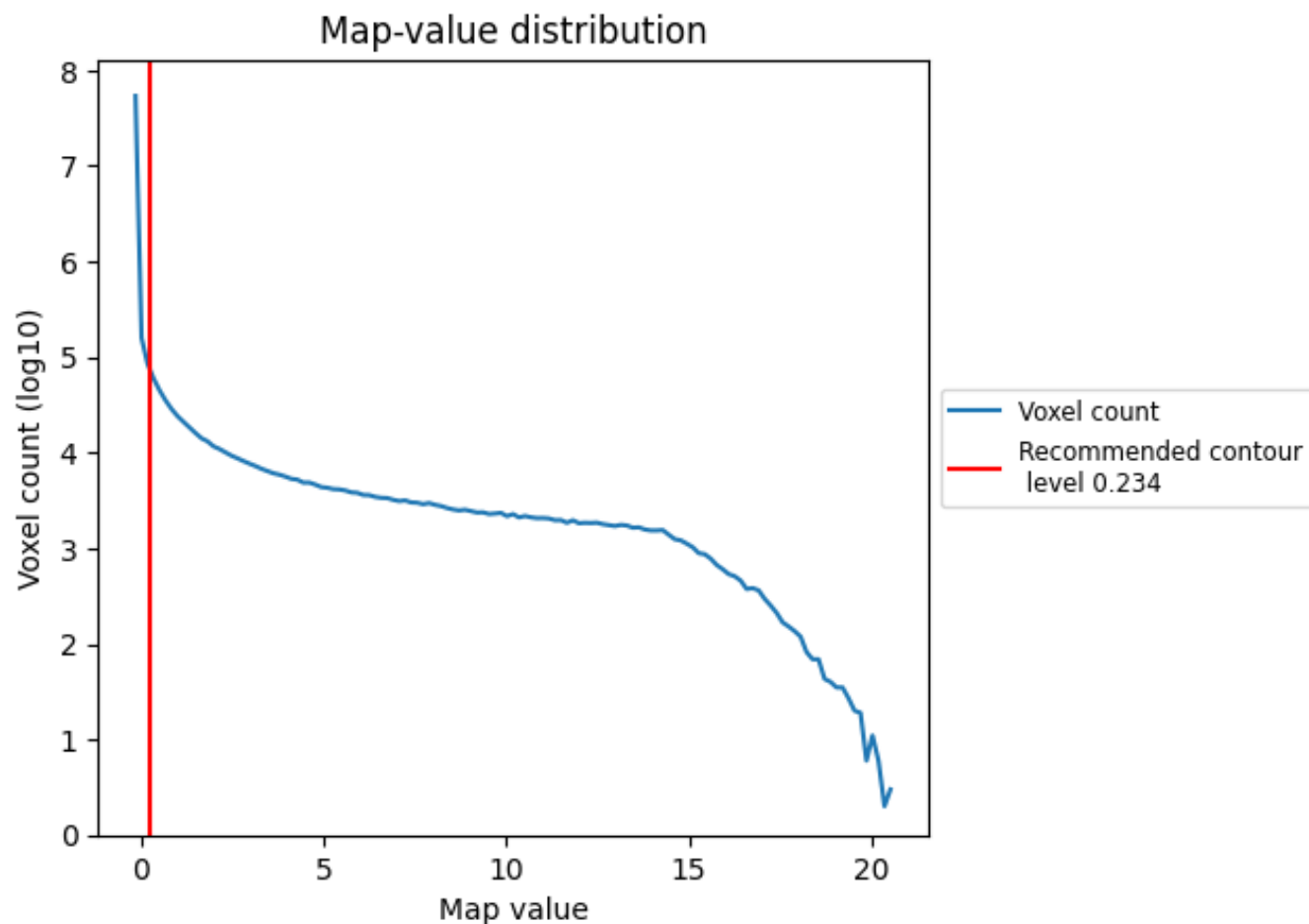
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

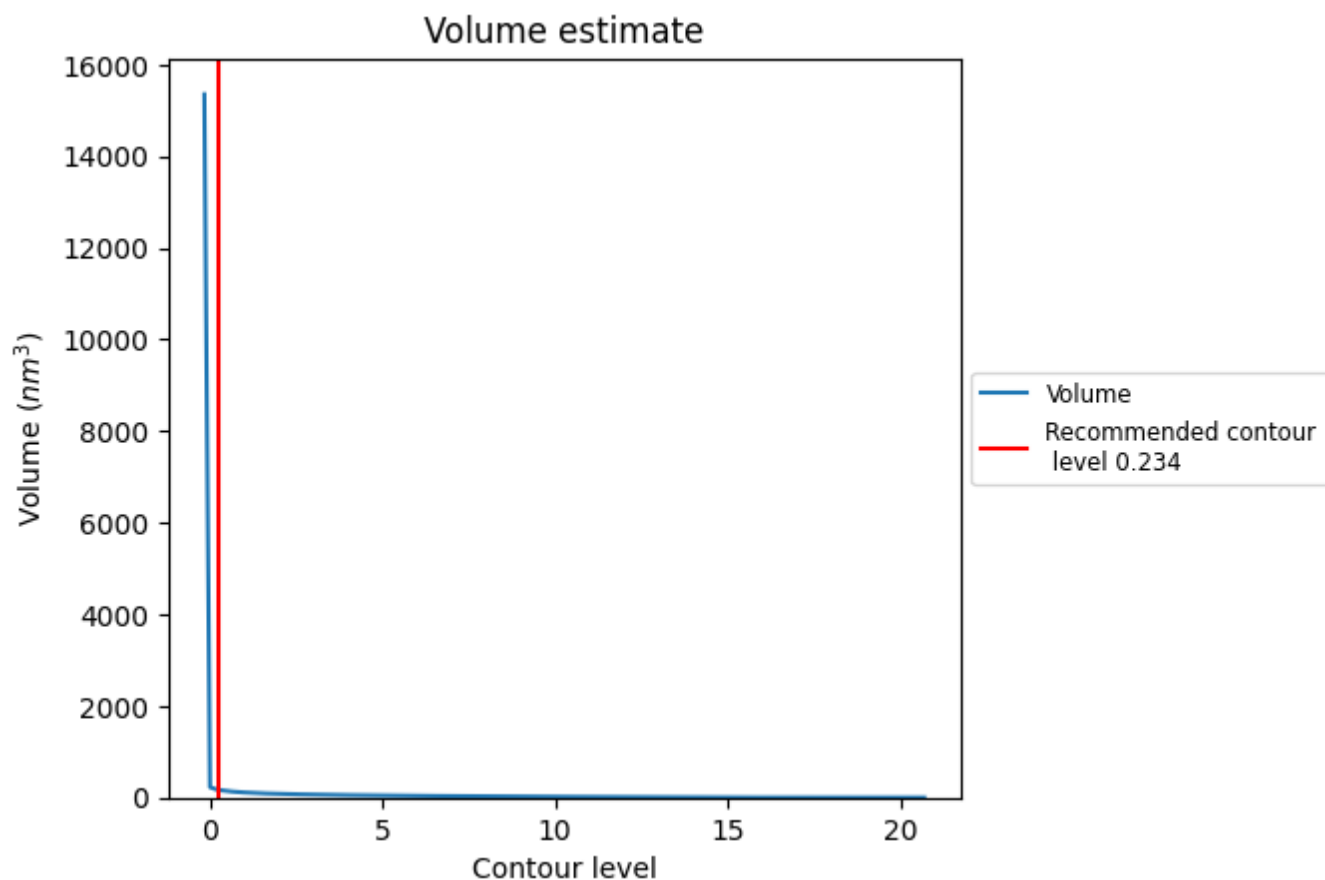
This section contains the results of statistical analysis of the map.

### 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.

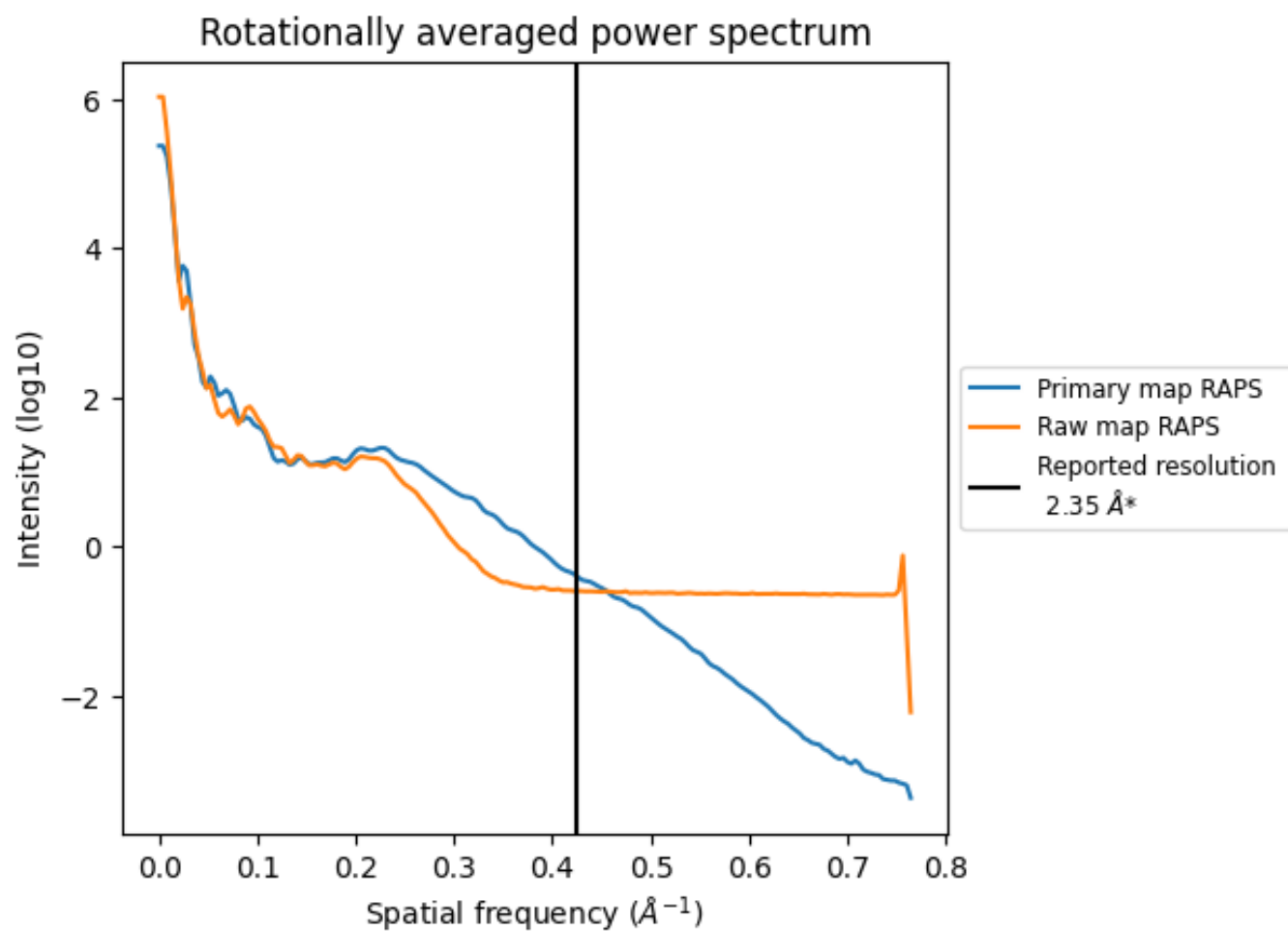
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm<sup>3</sup>; this corresponds to an approximate mass of 156 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 ⓘ

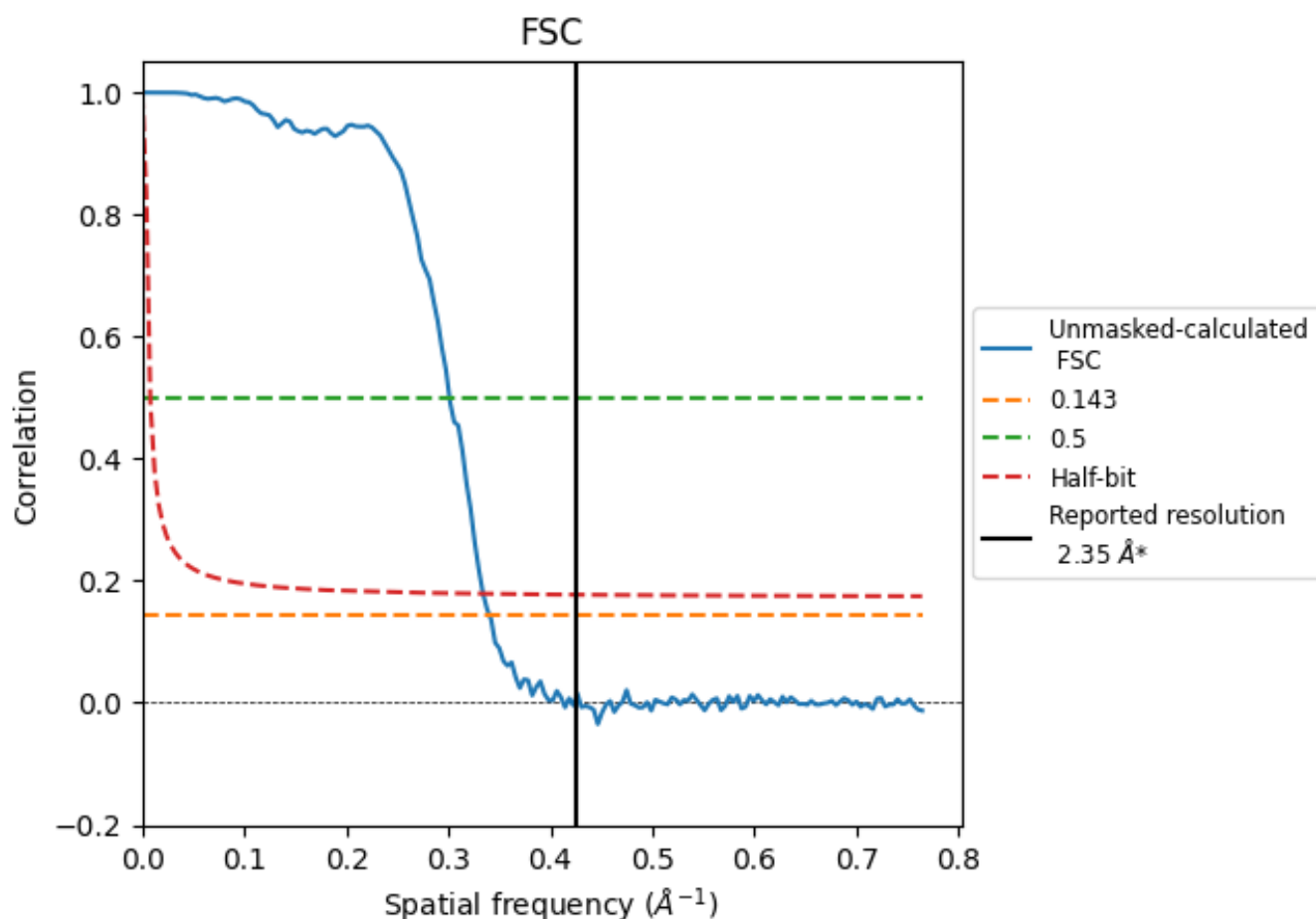


\*Reported resolution corresponds to spatial frequency of 0.426 Å<sup>-1</sup>

## 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  $0.426 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.94	3.32	2.99

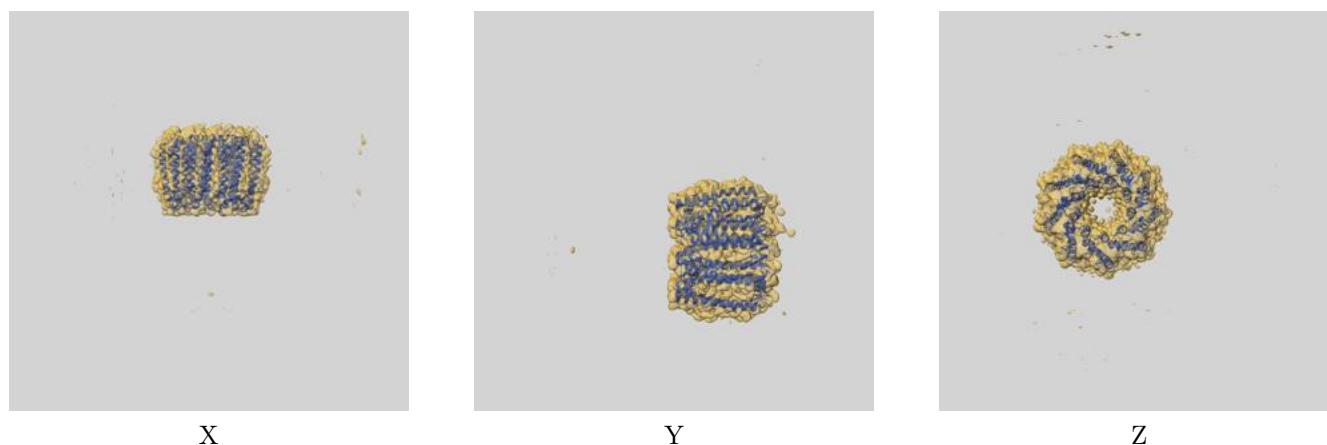
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.94 differs from the reported value 2.35 by more than 10 %



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

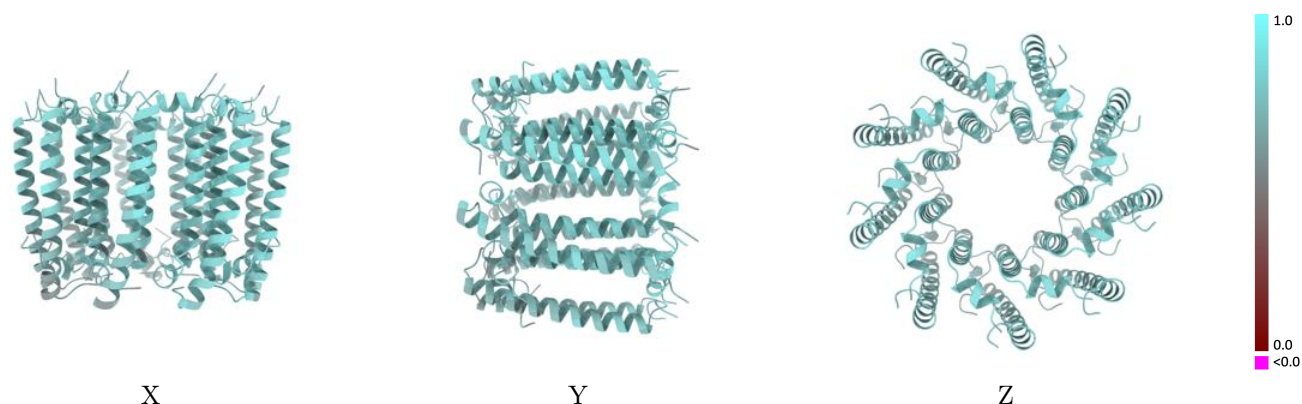
This section contains information regarding the fit between EMDB map EMD-48112 and PDB model 9EK8. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



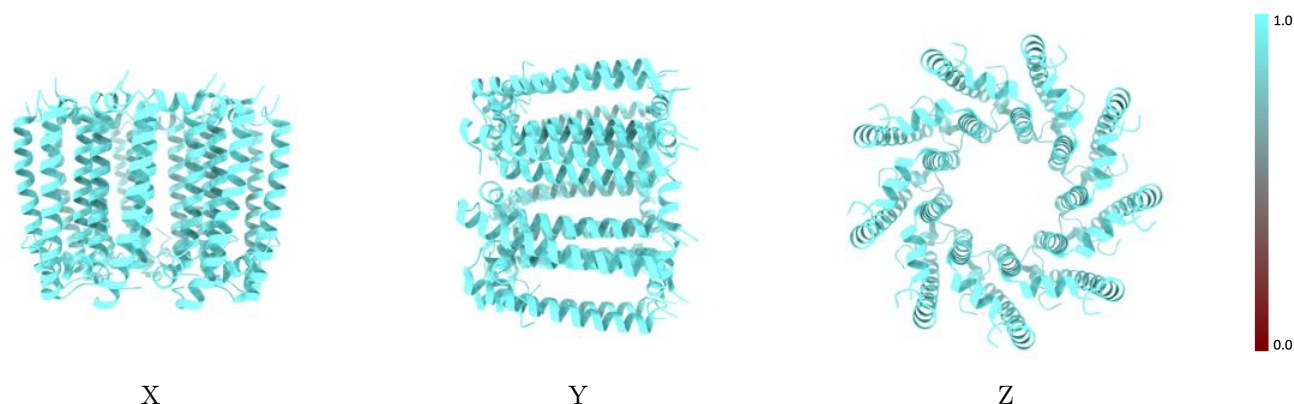
The images above show the 3D surface view of the map at the recommended contour level 0.234 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



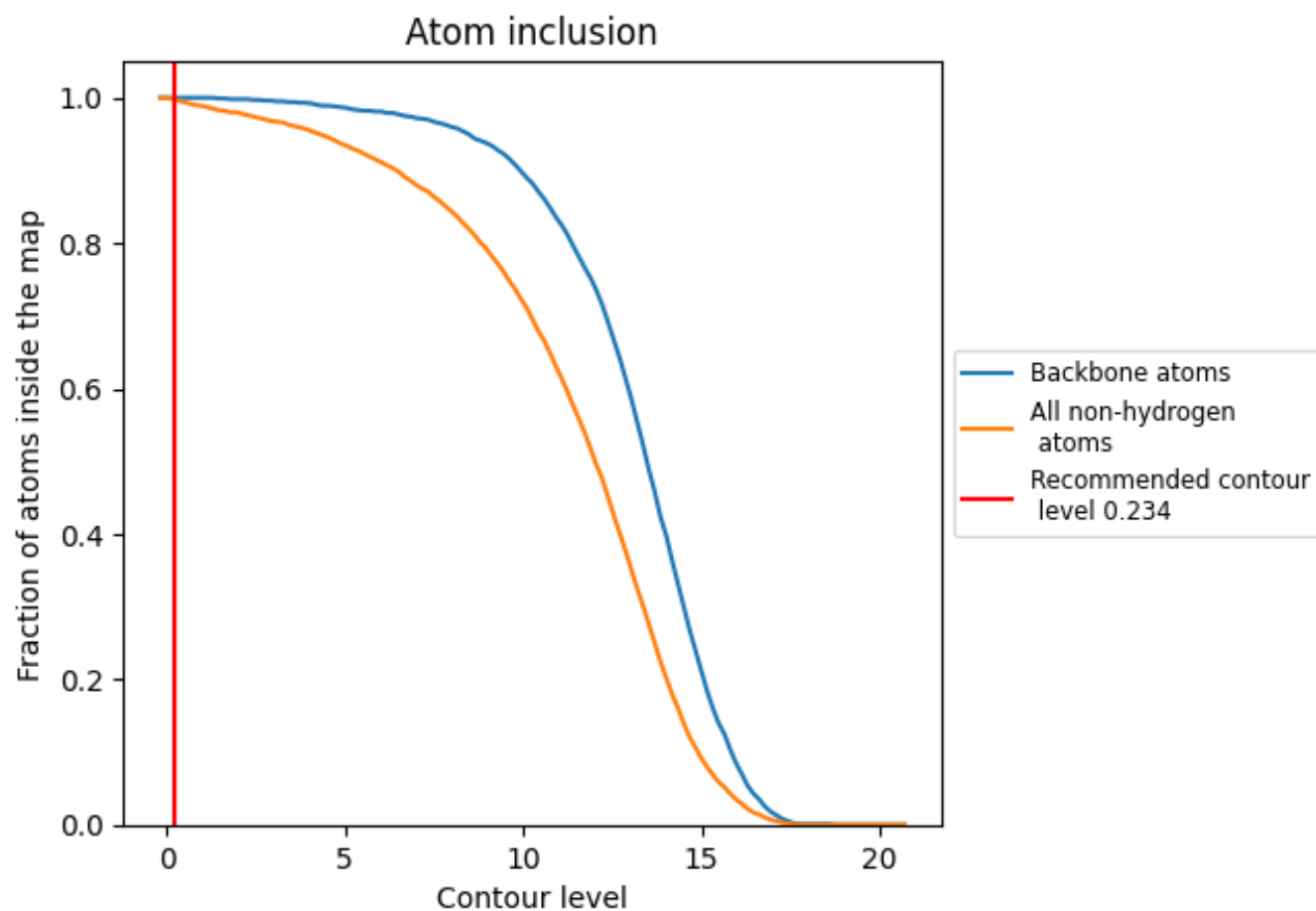
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.234).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.234) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9970	 0.6820
A	 0.9960	 0.7170
B	 1.0000	 0.7220
C	 0.9960	 0.7020
D	 0.9980	 0.6820
E	 0.9960	 0.6740
F	 1.0000	 0.6580
G	 0.9960	 0.6760
H	 0.9980	 0.6490
I	 0.9960	 0.6680
J	 1.0000	 0.6500
K	 0.9920	 0.6740
L	 1.0000	 0.6500
M	 0.9960	 0.6810
N	 1.0000	 0.6530
O	 0.9960	 0.6990
P	 1.0000	 0.6800
Q	 0.9960	 0.7190
R	 1.0000	 0.7180

