Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 11:16 pm GMT

PDB ID	:	6ZXA
EMDB ID	:	EMD-11516
Title	:	LH2 complex from Marichromatium purpuratum
Authors	:	Gardiner, A.T.; Naydenova, K.; Castro-Hartmann, P.; Nguyen-Phan, T.C.; Russo, C.J.; Sader, K.; Hunter, C.N.; Cogdell, R.J.; Qian, P.
Deposited on	:	2020-07-29
Resolution	:	2.38 Å(reported)
Based on initial model	:	1LGH

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

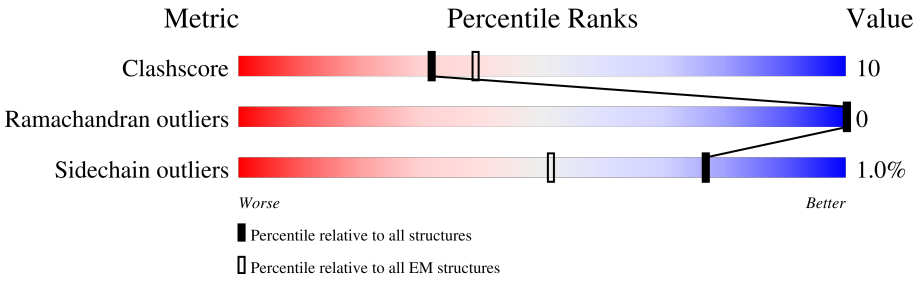
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.38 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	70	7% 73% 24% ••
1	C	70	10% 74% 23% ••
1	E	70	9% 74% 23% ••
1	G	70	9% 73% 24% ••
1	I	70	9% 73% 24% ••
1	K	70	9% 73% 24% ••
1	M	70	9% 73% 24% ••
2	B	48	83% 8% 8%

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Mol	Chain	Length	Quality of chain
2	D	48	77% 15% 8%
2	F	48	81% 10% 8%
2	H	48	85% 6% 8%
2	J	48	79% 12% 8%
2	L	48	81% 10% 8%
2	N	48	77% 15% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8442 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 LHC domain-containing protein.

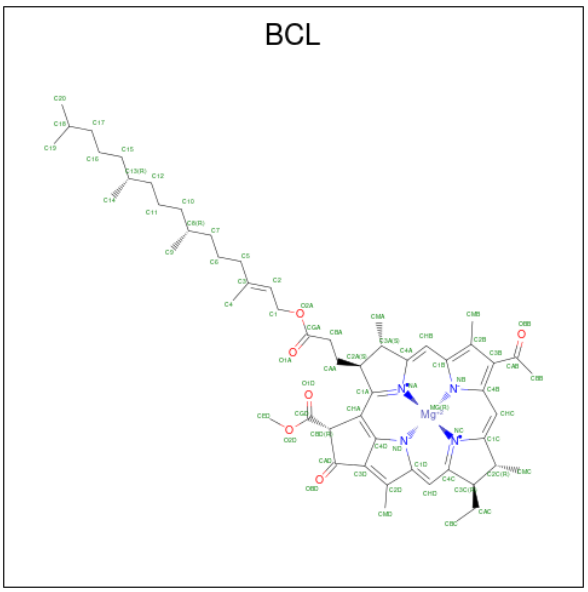
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	69	Total	C	N	O	S	0	0
			556	371	87	94	4		
1	C	69	Total	C	N	O	S	0	0
			556	371	87	94	4		
1	E	69	Total	C	N	O	S	0	0
			556	371	87	94	4		
1	G	69	Total	C	N	O	S	0	0
			556	371	87	94	4		
1	I	69	Total	C	N	O	S	0	0
			556	371	87	94	4		
1	K	69	Total	C	N	O	S	0	0
			556	371	87	94	4		
1	M	69	Total	C	N	O	S	0	0
			556	371	87	94	4		

- Molecule 2 is a protein called Light-harvesting protein B:800-850 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	44	Total	C	N	O	S	0	0
			366	244	62	59	1		
2	D	44	Total	C	N	O	S	0	0
			366	244	62	59	1		
2	F	44	Total	C	N	O	S	0	0
			366	244	62	59	1		
2	H	44	Total	C	N	O	S	0	0
			366	244	62	59	1		
2	J	44	Total	C	N	O	S	0	0
			366	244	62	59	1		
2	L	44	Total	C	N	O	S	0	0
			366	244	62	59	1		
2	N	44	Total	C	N	O	S	0	0
			366	244	62	59	1		

- Molecule 3 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$)

(labeled as "Ligand of Interest" by depositor).



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

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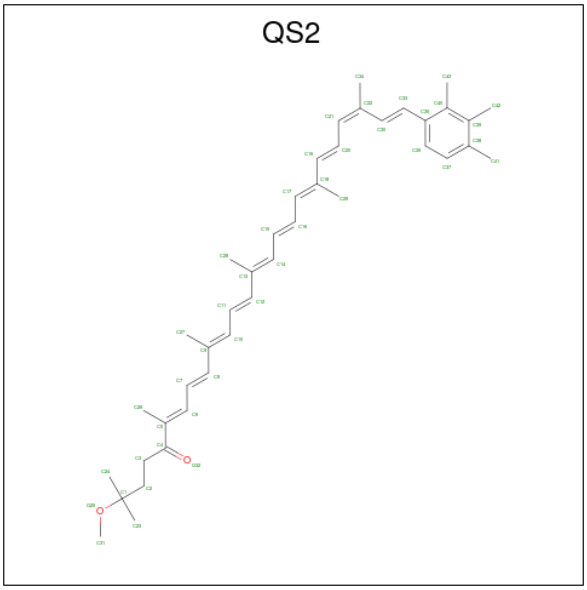
Mol	Chain	Residues	Atoms					AltConf
3	J	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
3	J	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
3	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
3	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
3	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	N	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
3	N	1	Total	C	Mg	N	O	0
			132	110	2	8	12	

- Molecule 4 is 9-cis-okenone (three-letter code: QS2) (formula: $C_{41}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			43	41	2	
4	B	1	Total	C	O	0
			43	41	2	
4	E	1	Total	C	O	0
			43	41	2	

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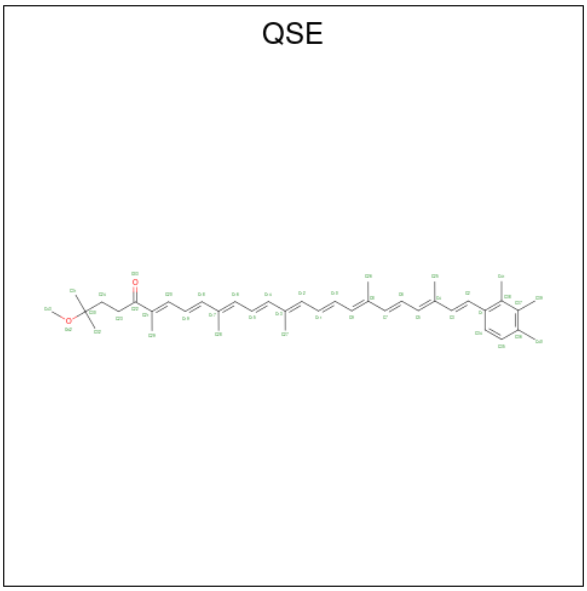
Mol	Chain	Residues	Atoms	AltConf
4	G	1	Total C O 43 41 2	0
4	I	1	Total C O 43 41 2	0
4	K	1	Total C O 43 41 2	0
4	M	1	Total C O 43 41 2	0

- Molecule 5 is all-trans okenone (three-letter code: QSE) (formula: $C_{41}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	C	1	Total C O 43 41 2	0
5	E	1	Total C O 43 41 2	0
5	F	1	Total C O 43 41 2	0
5	H	1	Total C O 43 41 2	0
5	J	1	Total C O 43 41 2	0
5	M	1	Total C O 43 41 2	0
5	N	1	Total C O 43 41 2	0

3 Residue-property plots (i)

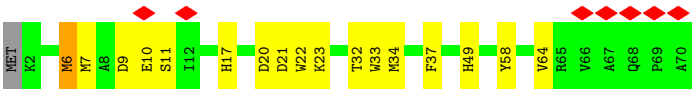
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: LHC domain-containing protein

Chain A:

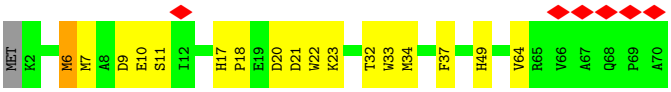
• Molecule 1: LHC domain-containing protein

Chain C:



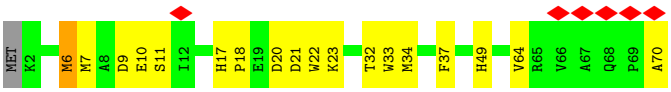
• Molecule 1: LHC domain-containing protein

Chain E:



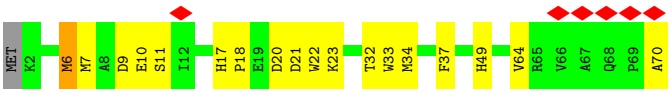
• Molecule 1: LHC domain-containing protein

Chain G:



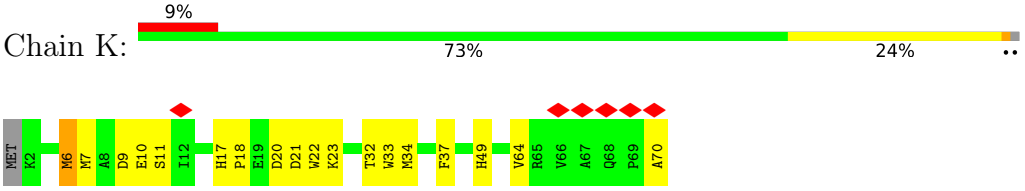
• Molecule 1: LHC domain-containing protein

Chain I:



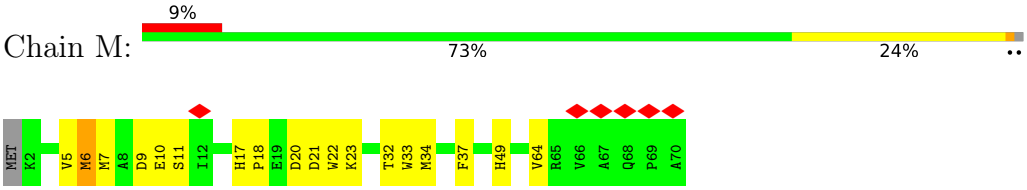
• Molecule 1: LHC domain-containing protein

Chain K:



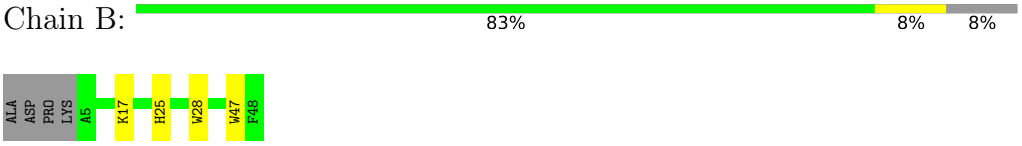
• Molecule 1: LHC domain-containing protein

Chain M:



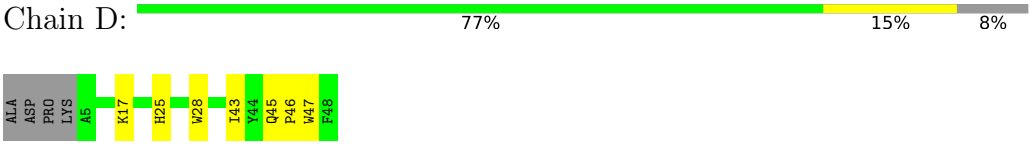
• Molecule 2: Light-harvesting protein B:800-850 subunit beta

Chain B:



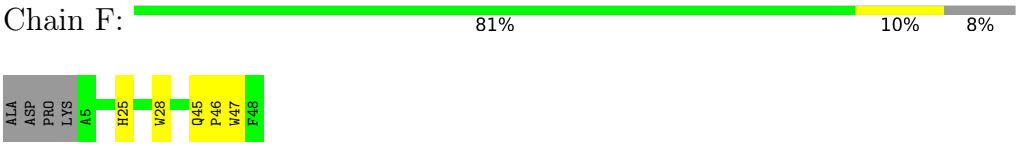
• Molecule 2: Light-harvesting protein B:800-850 subunit beta

Chain D:



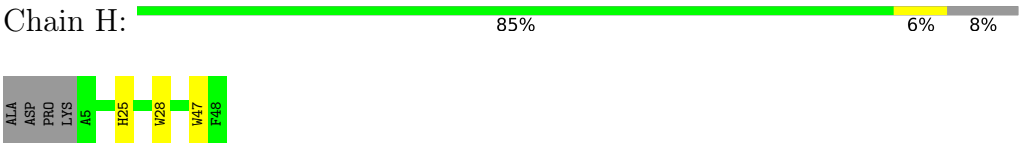
• Molecule 2: Light-harvesting protein B:800-850 subunit beta

Chain F:



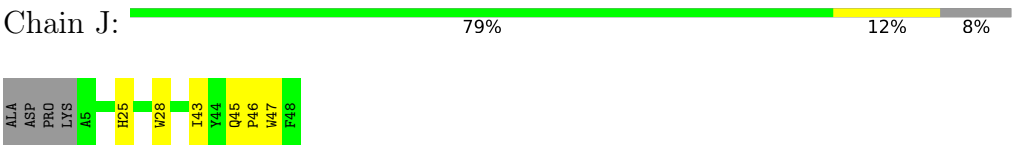
• Molecule 2: Light-harvesting protein B:800-850 subunit beta

Chain H:



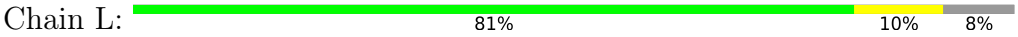
• Molecule 2: Light-harvesting protein B:800-850 subunit beta

Chain J:



• Molecule 2: Light-harvesting protein B:800-850 subunit beta

Chain L:



• Molecule 2: Light-harvesting protein B:800-850 subunit beta

Chain N:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	414511	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.7	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0167	Depositor
Map size (Å)	330.752, 330.752, 330.752	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.646, 0.646, 0.646	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QS2, BCL, QSE

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	0.39	0/577	0.57	0/791
1	C	0.39	0/577	0.57	0/791
1	E	0.39	0/577	0.57	0/791
1	G	0.39	0/577	0.57	0/791
1	I	0.39	0/577	0.57	0/791
1	K	0.39	0/577	0.57	0/791
1	M	0.39	0/577	0.57	0/791
2	B	0.37	0/383	0.44	0/526
2	D	0.37	0/383	0.44	0/526
2	F	0.37	0/383	0.44	0/526
2	H	0.37	0/383	0.44	0/526
2	J	0.37	0/383	0.44	0/526
2	L	0.37	0/383	0.44	0/526
2	N	0.37	0/383	0.44	0/526
All	All	0.38	0/6720	0.52	0/9219

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	E	0	2
1	G	0	2
1	I	0	2
1	K	0	2
1	M	0	2
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLU	Peptide
1	A	6	MET	Peptide
1	C	10	GLU	Peptide
1	C	6	MET	Peptide
1	E	10	GLU	Peptide
1	E	6	MET	Peptide
1	G	10	GLU	Peptide
1	G	6	MET	Peptide
1	I	10	GLU	Peptide
1	I	6	MET	Peptide
1	K	10	GLU	Peptide
1	K	6	MET	Peptide
1	M	10	GLU	Peptide
1	M	6	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	556	0	546	18	0
1	C	556	0	546	18	0
1	E	556	0	546	20	0
1	G	556	0	546	22	0
1	I	556	0	546	20	0
1	K	556	0	546	21	0
1	M	556	0	546	23	0
2	B	366	0	338	5	0
2	D	366	0	338	9	0
2	F	366	0	338	6	0
2	H	366	0	338	4	0
2	J	366	0	338	7	0
2	L	366	0	338	7	0
2	N	366	0	338	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	66	0	74	0	0
3	B	132	0	148	2	0
3	C	66	0	74	0	0
3	D	132	0	148	2	0
3	E	66	0	74	1	0
3	F	132	0	148	2	0
3	G	66	0	74	1	0
3	H	132	0	148	2	0
3	I	66	0	74	1	0
3	J	132	0	148	2	0
3	K	66	0	74	1	0
3	L	132	0	148	2	0
3	M	66	0	74	3	0
3	N	132	0	148	2	0
4	A	43	0	0	1	0
4	B	43	0	0	0	0
4	E	43	0	0	0	0
4	G	43	0	0	0	0
4	I	43	0	0	0	0
4	K	43	0	0	0	0
4	M	43	0	0	1	0
5	C	43	0	0	1	0
5	E	43	0	0	1	0
5	F	43	0	0	1	0
5	H	43	0	0	1	0
5	J	43	0	0	1	0
5	M	43	0	0	1	0
5	N	43	0	0	0	0
All	All	8442	0	7742	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (154) 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)
2:B:25:HIS:HA	1:C:6:MET:HG3	1.73	0.70
2:D:25:HIS:HA	1:E:6:MET:HG3	1.78	0.66
2:F:25:HIS:HA	1:G:6:MET:HG3	1.78	0.65
1:A:6:MET:HG3	2:N:25:HIS:HA	1.77	0.64
2:J:28:TRP:CE2	1:K:7:MET:HB2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:25:HIS:HA	1:M:6:MET:HG3	1.82	0.61
1:K:21:ASP:C	1:K:23:LYS:H	2.05	0.60
1:C:21:ASP:C	1:C:23:LYS:H	2.05	0.60
2:H:25:HIS:HA	1:I:6:MET:HG3	1.82	0.60
1:I:21:ASP:C	1:I:23:LYS:H	2.05	0.60
1:G:21:ASP:C	1:G:23:LYS:H	2.05	0.60
1:A:49:HIS:CE1	3:B:102:BCL:HMD1	2.37	0.60
1:E:21:ASP:C	1:E:23:LYS:H	2.05	0.60
1:M:21:ASP:C	1:M:23:LYS:H	2.05	0.60
1:A:21:ASP:C	1:A:23:LYS:H	2.05	0.59
1:K:70:ALA:HB3	2:N:43:ILE:HA	1.83	0.59
2:B:47:TRP:HA	1:M:64:VAL:HA	1.86	0.57
2:H:28:TRP:CE2	1:I:7:MET:HB2	2.40	0.56
2:J:25:HIS:HA	1:K:6:MET:HG3	1.86	0.56
2:D:28:TRP:CE2	1:E:7:MET:HB2	2.42	0.55
1:C:49:HIS:CE1	3:D:102:BCL:HMD1	2.43	0.54
1:M:23:LYS:HB3	5:M:101:QSE:C40	2.38	0.54
1:K:64:VAL:HA	2:N:47:TRP:HA	1.90	0.53
2:F:28:TRP:CE2	1:G:7:MET:HB2	2.43	0.53
1:M:17:HIS:O	1:M:20:ASP:N	2.42	0.53
1:E:17:HIS:O	1:E:20:ASP:N	2.42	0.53
1:A:7:MET:HB2	2:N:28:TRP:CE2	2.44	0.53
1:A:17:HIS:O	1:A:20:ASP:N	2.42	0.53
1:C:17:HIS:O	1:C:20:ASP:N	2.42	0.53
1:E:23:LYS:HB3	5:E:101:QSE:C40	2.39	0.53
1:I:17:HIS:O	1:I:20:ASP:N	2.42	0.53
1:G:17:HIS:O	1:G:20:ASP:N	2.42	0.52
1:K:17:HIS:O	1:K:20:ASP:N	2.42	0.52
2:L:28:TRP:CE2	1:M:7:MET:HB2	2.44	0.52
1:I:64:VAL:HA	2:L:47:TRP:HA	1.92	0.52
1:E:64:VAL:HA	2:H:47:TRP:HA	1.91	0.51
1:G:21:ASP:O	1:G:23:LYS:N	2.43	0.51
1:K:33:TRP:O	1:K:34:MET:HB3	2.10	0.51
1:C:23:LYS:HB3	5:C:101:QSE:C40	2.39	0.51
1:E:33:TRP:O	1:E:34:MET:HB3	2.10	0.51
1:I:21:ASP:O	1:I:23:LYS:N	2.44	0.51
1:C:33:TRP:O	1:C:34:MET:HB3	2.10	0.51
1:M:49:HIS:CE1	3:N:103:BCL:HMD1	2.45	0.51
1:E:49:HIS:CE1	3:F:103:BCL:HMD1	2.46	0.51
1:M:33:TRP:O	1:M:34:MET:HB3	2.11	0.51
1:M:21:ASP:O	1:M:23:LYS:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ASP:O	1:E:23:LYS:N	2.44	0.50
1:I:33:TRP:O	1:I:34:MET:HB3	2.10	0.50
1:I:70:ALA:HB3	2:L:43:ILE:HA	1.92	0.50
1:A:21:ASP:O	1:A:23:LYS:N	2.44	0.50
1:C:21:ASP:O	1:C:23:LYS:N	2.44	0.50
1:I:49:HIS:CE1	3:J:103:BCL:HMD1	2.46	0.50
1:A:33:TRP:O	1:A:34:MET:HB3	2.11	0.50
1:C:34:MET:HA	1:C:37:PHE:HB3	1.94	0.50
1:E:34:MET:HA	1:E:37:PHE:HB3	1.94	0.50
1:G:49:HIS:CE1	3:H:103:BCL:HMD1	2.46	0.50
1:K:21:ASP:O	1:K:23:LYS:N	2.44	0.50
1:G:33:TRP:O	1:G:34:MET:HB3	2.11	0.50
1:K:18:PRO:HG3	3:K:101:BCL:HMB3	1.95	0.49
1:G:64:VAL:HA	2:J:47:TRP:HA	1.94	0.49
1:A:34:MET:HA	1:A:37:PHE:HB3	1.94	0.49
1:G:34:MET:HA	1:G:37:PHE:HB3	1.94	0.49
1:G:6:MET:HE1	1:G:9:ASP:HB3	1.94	0.49
5:F:101:QSE:C40	1:G:23:LYS:HB3	2.43	0.49
1:I:18:PRO:HG3	3:I:101:BCL:HMB3	1.95	0.49
5:H:101:QSE:C40	1:I:23:LYS:HB3	2.43	0.49
1:K:34:MET:HA	1:K:37:PHE:HB3	1.94	0.48
1:M:18:PRO:HG3	3:M:102:BCL:HMB3	1.95	0.48
1:I:34:MET:HA	1:I:37:PHE:HB3	1.94	0.48
1:M:34:MET:HA	1:M:37:PHE:HB3	1.94	0.47
1:G:21:ASP:O	1:G:22:TRP:CG	2.68	0.47
1:E:21:ASP:O	1:E:22:TRP:CG	2.68	0.47
1:E:18:PRO:HG3	3:E:102:BCL:HMB3	1.96	0.46
1:A:21:ASP:O	1:A:22:TRP:CG	2.68	0.46
1:C:21:ASP:O	1:C:22:TRP:CG	2.68	0.46
1:K:21:ASP:O	1:K:22:TRP:CG	2.68	0.46
2:D:28:TRP:CD2	1:E:7:MET:HB2	2.51	0.46
1:M:21:ASP:O	1:M:22:TRP:CG	2.68	0.46
1:G:9:ASP:OD2	1:G:9:ASP:N	2.49	0.46
1:K:49:HIS:CE1	3:L:102:BCL:HMD1	2.50	0.46
1:I:21:ASP:O	1:I:22:TRP:CG	2.68	0.46
1:E:9:ASP:OD2	1:E:9:ASP:N	2.49	0.45
1:K:9:ASP:OD2	1:K:9:ASP:N	2.49	0.45
1:C:9:ASP:OD2	1:C:9:ASP:N	2.49	0.45
1:A:22:TRP:CZ2	2:B:17:LYS:HE2	2.52	0.45
1:M:9:ASP:OD2	1:M:9:ASP:N	2.49	0.45
1:A:9:ASP:OD2	1:A:9:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:ASP:OD2	1:I:9:ASP:N	2.49	0.45
2:L:28:TRP:CD1	1:M:6:MET:HA	2.51	0.45
1:A:58:TYR:OH	2:B:47:TRP:HB3	2.16	0.45
1:C:21:ASP:O	1:C:22:TRP:CD1	2.70	0.45
1:G:21:ASP:O	1:G:22:TRP:CD1	2.70	0.45
1:E:21:ASP:O	1:E:22:TRP:CD1	2.70	0.45
1:G:18:PRO:HG3	3:G:101:BCL:HMB3	1.98	0.45
1:I:21:ASP:O	1:I:22:TRP:CD1	2.70	0.45
1:A:21:ASP:O	1:A:22:TRP:CD1	2.70	0.45
5:J:101:QSE:C40	1:K:23:LYS:HB3	2.48	0.44
3:L:101:BCL:HBB3	3:L:101:BCL:HMB1	2.00	0.44
1:M:21:ASP:O	1:M:22:TRP:CD1	2.70	0.44
1:K:21:ASP:O	1:K:22:TRP:CD1	2.70	0.44
1:M:5:VAL:HG22	4:M:103:QS2:C36	2.48	0.44
3:J:102:BCL:HBB3	3:J:102:BCL:HMB1	2.00	0.44
2:J:28:TRP:CD2	1:K:7:MET:HB2	2.52	0.44
3:D:101:BCL:HMB1	3:D:101:BCL:HBB3	2.00	0.44
1:M:17:HIS:CD2	3:M:102:BCL:HMC3	2.53	0.44
1:A:64:VAL:HA	2:D:47:TRP:HA	2.00	0.43
2:F:28:TRP:CD2	1:G:7:MET:HB2	2.53	0.43
3:N:102:BCL:HMB1	3:N:102:BCL:HBB3	2.00	0.43
1:C:21:ASP:C	1:C:23:LYS:N	2.72	0.43
3:H:102:BCL:HBB3	3:H:102:BCL:HMB1	2.00	0.43
1:C:6:MET:CE	1:C:9:ASP:HB3	2.48	0.43
1:E:6:MET:CE	1:E:9:ASP:HB3	2.48	0.43
1:E:6:MET:HE1	1:E:9:ASP:HB3	1.99	0.43
1:M:6:MET:CE	1:M:9:ASP:HB3	2.48	0.43
1:A:6:MET:CE	1:A:9:ASP:HB3	2.48	0.43
1:A:70:ALA:HB3	2:D:43:ILE:HA	2.01	0.43
1:C:64:VAL:HA	2:F:47:TRP:HA	2.00	0.43
2:D:28:TRP:CD1	1:E:6:MET:HA	2.54	0.43
1:E:21:ASP:C	1:E:23:LYS:N	2.72	0.43
3:F:102:BCL:HMB1	3:F:102:BCL:HBB3	2.00	0.43
2:D:45:GLN:HA	2:D:46:PRO:HD3	1.85	0.43
1:I:6:MET:CE	1:I:9:ASP:HB3	2.49	0.43
2:L:28:TRP:CD2	1:M:7:MET:HB2	2.53	0.43
1:G:6:MET:CE	1:G:9:ASP:HB3	2.48	0.43
4:A:102:QS2:C20	2:N:32:MET:HG3	2.49	0.42
2:B:28:TRP:CE2	1:C:7:MET:HB2	2.54	0.42
3:B:101:BCL:HBB3	3:B:101:BCL:HMB1	2.00	0.42
1:G:21:ASP:C	1:G:23:LYS:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:ASP:C	1:I:23:LYS:N	2.72	0.42
1:K:6:MET:CE	1:K:9:ASP:HB3	2.48	0.42
2:H:28:TRP:CD2	1:I:7:MET:HB2	2.53	0.42
1:A:6:MET:HE1	1:A:9:ASP:HB3	2.00	0.42
1:G:70:ALA:HB3	2:J:43:ILE:HA	2.00	0.42
1:C:22:TRP:CZ2	2:D:17:LYS:HE2	2.54	0.42
1:I:32:THR:HG23	1:I:33:TRP:CD1	2.56	0.41
1:C:58:TYR:OH	2:D:47:TRP:HB3	2.21	0.41
1:G:32:THR:HG23	1:G:33:TRP:CD1	2.56	0.41
1:M:18:PRO:HG3	3:M:102:BCL:CMB	2.51	0.41
1:M:32:THR:HG23	1:M:33:TRP:CD1	2.56	0.41
2:F:28:TRP:CD1	1:G:6:MET:HA	2.56	0.41
1:C:32:THR:HG23	1:C:33:TRP:CD1	2.56	0.41
1:E:32:THR:HG23	1:E:33:TRP:CD1	2.56	0.41
2:F:45:GLN:HA	2:F:46:PRO:HD3	1.85	0.41
2:J:45:GLN:HA	2:J:46:PRO:HD3	1.85	0.41
1:K:22:TRP:CZ2	2:L:17:LYS:HE2	2.56	0.41
1:K:32:THR:HG23	1:K:33:TRP:CD1	2.56	0.41
1:I:20:ASP:C	1:I:21:ASP:O	2.60	0.40
2:J:28:TRP:CD1	1:K:6:MET:HA	2.56	0.40
1:A:32:THR:HG23	1:A:33:TRP:CD1	2.56	0.40
1:M:21:ASP:C	1:M:23:LYS:N	2.72	0.40
1:M:20:ASP:C	1:M:21:ASP:O	2.60	0.40
1:G:20:ASP:C	1:G:21:ASP:O	2.60	0.40
1:K:20:ASP:C	1:K:21:ASP:O	2.60	0.40
2:N:45:GLN:HA	2:N:46:PRO:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	67/70 (96%)	55 (82%)	12 (18%)	0	100	100
1	C	67/70 (96%)	55 (82%)	12 (18%)	0	100	100
1	E	67/70 (96%)	55 (82%)	12 (18%)	0	100	100
1	G	67/70 (96%)	55 (82%)	12 (18%)	0	100	100
1	I	67/70 (96%)	55 (82%)	12 (18%)	0	100	100
1	K	67/70 (96%)	55 (82%)	12 (18%)	0	100	100
1	M	67/70 (96%)	55 (82%)	12 (18%)	0	100	100
2	B	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
2	D	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
2	F	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
2	H	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
2	J	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
2	L	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
2	N	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
All	All	763/826 (92%)	665 (87%)	98 (13%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	60/61 (98%)	59 (98%)	1 (2%)	60	76
1	C	60/61 (98%)	59 (98%)	1 (2%)	60	76
1	E	60/61 (98%)	59 (98%)	1 (2%)	60	76
1	G	60/61 (98%)	59 (98%)	1 (2%)	60	76
1	I	60/61 (98%)	59 (98%)	1 (2%)	60	76
1	K	60/61 (98%)	59 (98%)	1 (2%)	60	76
1	M	60/61 (98%)	59 (98%)	1 (2%)	60	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	36/39 (92%)	36 (100%)	0	100 100
2	D	36/39 (92%)	36 (100%)	0	100 100
2	F	36/39 (92%)	36 (100%)	0	100 100
2	H	36/39 (92%)	36 (100%)	0	100 100
2	J	36/39 (92%)	36 (100%)	0	100 100
2	L	36/39 (92%)	36 (100%)	0	100 100
2	N	36/39 (92%)	36 (100%)	0	100 100
All	All	672/700 (96%)	665 (99%)	7 (1%)	77 87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	C	11	SER
1	E	11	SER
1	G	11	SER
1	I	11	SER
1	K	11	SER
1	M	11	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	C	16	ASN
1	E	16	ASN
1	G	16	ASN
1	I	16	ASN
1	K	16	ASN
1	M	16	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

35 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	$\#\|Z\| > 2$
5	QSE	E	101	-	43,43,43	0.40	0	51,56,56	0.65	0
3	BCL	L	101	-	58,74,74	1.20	6 (10%)	69,115,115	1.65	15 (21%)
3	BCL	N	103	-	58,74,74	1.13	3 (5%)	69,115,115	1.49	10 (14%)
5	QSE	N	101	-	43,43,43	0.40	0	51,56,56	0.65	0
4	QS2	I	102	-	43,43,43	0.35	0	51,56,56	0.65	0
3	BCL	I	101	1	58,74,74	1.17	3 (5%)	69,115,115	1.62	13 (18%)
5	QSE	J	101	-	43,43,43	0.40	0	51,56,56	0.65	0
4	QS2	E	103	-	43,43,43	0.35	0	51,56,56	0.65	0
3	BCL	J	102	-	58,74,74	1.20	6 (10%)	69,115,115	1.65	15 (21%)
4	QS2	G	102	-	43,43,43	0.35	0	51,56,56	0.65	0
4	QS2	M	103	-	43,43,43	0.35	0	51,56,56	0.65	0
5	QSE	F	101	-	43,43,43	0.40	0	51,56,56	0.65	0
3	BCL	D	101	-	58,74,74	1.20	6 (10%)	69,115,115	1.65	15 (21%)
3	BCL	G	101	1	58,74,74	1.17	3 (5%)	69,115,115	1.62	13 (18%)
3	BCL	J	103	-	58,74,74	1.13	3 (5%)	69,115,115	1.49	10 (14%)
3	BCL	B	102	-	58,74,74	1.13	3 (5%)	69,115,115	1.49	10 (14%)
3	BCL	K	101	1	58,74,74	1.17	3 (5%)	69,115,115	1.62	13 (18%)
3	BCL	M	102	1	58,74,74	1.17	3 (5%)	69,115,115	1.62	13 (18%)
5	QSE	M	101	-	43,43,43	0.40	0	51,56,56	0.65	0
3	BCL	F	103	-	58,74,74	1.13	3 (5%)	69,115,115	1.49	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	QS2	A	102	-	43,43,43	0.35	0	51,56,56	0.65	0
4	QS2	K	102	-	43,43,43	0.35	0	51,56,56	0.65	0
3	BCL	F	102	-	58,74,74	1.20	6 (10%)	69,115,115	1.65	15 (21%)
3	BCL	A	101	1	58,74,74	1.17	3 (5%)	69,115,115	1.62	13 (18%)
3	BCL	N	102	-	58,74,74	1.20	6 (10%)	69,115,115	1.65	15 (21%)
4	QS2	B	103	-	43,43,43	0.35	0	51,56,56	0.65	0
3	BCL	C	102	1	58,74,74	1.17	3 (5%)	69,115,115	1.62	13 (18%)
3	BCL	L	102	-	58,74,74	1.13	3 (5%)	69,115,115	1.49	10 (14%)
3	BCL	B	101	-	58,74,74	1.20	6 (10%)	69,115,115	1.65	15 (21%)
3	BCL	H	103	-	58,74,74	1.13	3 (5%)	69,115,115	1.49	10 (14%)
5	QSE	H	101	-	43,43,43	0.40	0	51,56,56	0.65	0
3	BCL	E	102	1	58,74,74	1.17	3 (5%)	69,115,115	1.62	13 (18%)
5	QSE	C	101	-	43,43,43	0.40	0	51,56,56	0.65	0
3	BCL	D	102	-	58,74,74	1.13	3 (5%)	69,115,115	1.49	10 (14%)
3	BCL	H	102	-	58,74,74	1.20	6 (10%)	69,115,115	1.65	15 (21%)

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
5	QSE	E	101	-	-	10/43/43/43	0/1/1/1
3	BCL	L	101	-	-	6/37/137/137	-
3	BCL	N	103	-	-	6/37/137/137	-
5	QSE	N	101	-	-	10/43/43/43	0/1/1/1
4	QS2	I	102	-	-	9/43/43/43	0/1/1/1
3	BCL	I	101	1	-	3/37/137/137	-
5	QSE	J	101	-	-	10/43/43/43	0/1/1/1
4	QS2	E	103	-	-	9/43/43/43	0/1/1/1
3	BCL	J	102	-	-	6/37/137/137	-
4	QS2	G	102	-	-	9/43/43/43	0/1/1/1
4	QS2	M	103	-	-	9/43/43/43	0/1/1/1
5	QSE	F	101	-	-	10/43/43/43	0/1/1/1
3	BCL	D	101	-	-	6/37/137/137	-
3	BCL	G	101	1	-	3/37/137/137	-
3	BCL	J	103	-	-	6/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BCL	B	102	-	-	6/37/137/137	-
3	BCL	K	101	1	-	3/37/137/137	-
3	BCL	M	102	1	-	3/37/137/137	-
5	QSE	M	101	-	-	10/43/43/43	0/1/1/1
3	BCL	F	103	-	-	6/37/137/137	-
4	QS2	A	102	-	-	9/43/43/43	0/1/1/1
4	QS2	K	102	-	-	9/43/43/43	0/1/1/1
3	BCL	F	102	-	-	6/37/137/137	-
3	BCL	A	101	1	-	3/37/137/137	-
3	BCL	N	102	-	-	6/37/137/137	-
4	QS2	B	103	-	-	9/43/43/43	0/1/1/1
3	BCL	C	102	1	-	3/37/137/137	-
3	BCL	L	102	-	-	6/37/137/137	-
3	BCL	B	101	-	-	6/37/137/137	-
3	BCL	H	103	-	-	6/37/137/137	-
5	QSE	H	101	-	-	10/43/43/43	0/1/1/1
3	BCL	E	102	1	-	3/37/137/137	-
5	QSE	C	101	-	-	10/43/43/43	0/1/1/1
3	BCL	D	102	-	-	6/37/137/137	-
3	BCL	H	102	-	-	6/37/137/137	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	101	BCL	MG-NA	4.64	2.17	2.06
3	E	102	BCL	MG-NA	4.64	2.17	2.06
3	I	101	BCL	MG-NA	4.64	2.17	2.06
3	K	101	BCL	MG-NA	4.64	2.17	2.06
3	M	102	BCL	MG-NA	4.64	2.17	2.06
3	A	101	BCL	MG-NA	4.64	2.17	2.06
3	C	102	BCL	MG-NA	4.63	2.17	2.06
3	F	102	BCL	MG-NA	4.47	2.16	2.06
3	N	102	BCL	MG-NA	4.47	2.16	2.06
3	B	101	BCL	MG-NA	4.47	2.16	2.06
3	D	101	BCL	MG-NA	4.46	2.16	2.06
3	J	102	BCL	MG-NA	4.46	2.16	2.06
3	L	101	BCL	MG-NA	4.46	2.16	2.06
3	H	102	BCL	MG-NA	4.46	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	103	BCL	MG-NA	4.35	2.16	2.06
3	L	102	BCL	MG-NA	4.35	2.16	2.06
3	F	103	BCL	MG-NA	4.35	2.16	2.06
3	B	102	BCL	MG-NA	4.35	2.16	2.06
3	N	103	BCL	MG-NA	4.35	2.16	2.06
3	J	103	BCL	MG-NA	4.35	2.16	2.06
3	D	102	BCL	MG-NA	4.34	2.16	2.06
3	I	101	BCL	C1B-NB	4.34	1.39	1.35
3	K	101	BCL	C1B-NB	4.34	1.39	1.35
3	C	102	BCL	C1B-NB	4.34	1.39	1.35
3	G	101	BCL	C1B-NB	4.34	1.39	1.35
3	A	101	BCL	C1B-NB	4.34	1.39	1.35
3	E	102	BCL	C1B-NB	4.34	1.39	1.35
3	M	102	BCL	C1B-NB	4.34	1.39	1.35
3	F	102	BCL	C1B-NB	4.05	1.38	1.35
3	N	102	BCL	C1B-NB	4.05	1.38	1.35
3	B	101	BCL	C1B-NB	4.04	1.38	1.35
3	H	102	BCL	C1B-NB	4.04	1.38	1.35
3	J	102	BCL	C1B-NB	4.04	1.38	1.35
3	L	101	BCL	C1B-NB	4.04	1.38	1.35
3	D	101	BCL	C1B-NB	4.03	1.38	1.35
3	H	103	BCL	C1B-NB	3.87	1.38	1.35
3	F	103	BCL	C1B-NB	3.87	1.38	1.35
3	N	103	BCL	C1B-NB	3.87	1.38	1.35
3	J	103	BCL	C1B-NB	3.87	1.38	1.35
3	L	102	BCL	C1B-NB	3.87	1.38	1.35
3	D	102	BCL	C1B-NB	3.87	1.38	1.35
3	B	102	BCL	C1B-NB	3.86	1.38	1.35
3	C	102	BCL	MG-NC	3.08	2.13	2.06
3	A	101	BCL	MG-NC	3.08	2.13	2.06
3	G	101	BCL	MG-NC	3.08	2.13	2.06
3	E	102	BCL	MG-NC	3.08	2.13	2.06
3	M	102	BCL	MG-NC	3.08	2.13	2.06
3	I	101	BCL	MG-NC	3.08	2.13	2.06
3	K	101	BCL	MG-NC	3.08	2.13	2.06
3	D	102	BCL	MG-NC	2.72	2.12	2.06
3	J	103	BCL	MG-NC	2.72	2.12	2.06
3	H	103	BCL	MG-NC	2.72	2.12	2.06
3	N	103	BCL	MG-NC	2.72	2.12	2.06
3	L	102	BCL	MG-NC	2.72	2.12	2.06
3	B	102	BCL	MG-NC	2.72	2.12	2.06
3	F	103	BCL	MG-NC	2.72	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	102	BCL	MG-NC	2.65	2.12	2.06
3	B	101	BCL	MG-NC	2.65	2.12	2.06
3	L	101	BCL	MG-NC	2.65	2.12	2.06
3	F	102	BCL	MG-NC	2.65	2.12	2.06
3	D	101	BCL	MG-NC	2.65	2.12	2.06
3	H	102	BCL	MG-NC	2.65	2.12	2.06
3	N	102	BCL	MG-NC	2.65	2.12	2.06
3	F	102	BCL	O1A-CGA	-2.52	1.15	1.22
3	H	102	BCL	O1A-CGA	-2.52	1.15	1.22
3	N	102	BCL	O1A-CGA	-2.52	1.15	1.22
3	B	101	BCL	O1A-CGA	-2.52	1.15	1.22
3	J	102	BCL	O1A-CGA	-2.52	1.15	1.22
3	L	101	BCL	O1A-CGA	-2.52	1.15	1.22
3	D	101	BCL	O1A-CGA	-2.52	1.15	1.22
3	L	101	BCL	C3D-CAD	-2.20	1.40	1.46
3	D	101	BCL	C3D-CAD	-2.20	1.40	1.46
3	F	102	BCL	C3D-CAD	-2.20	1.40	1.46
3	B	101	BCL	C3D-CAD	-2.20	1.40	1.46
3	H	102	BCL	C3D-CAD	-2.20	1.40	1.46
3	J	102	BCL	C3D-CAD	-2.20	1.40	1.46
3	N	102	BCL	C3D-CAD	-2.20	1.40	1.46
3	B	101	BCL	O2A-CGA	-2.10	1.27	1.33
3	N	102	BCL	O2A-CGA	-2.10	1.27	1.33
3	L	101	BCL	O2A-CGA	-2.10	1.27	1.33
3	D	101	BCL	O2A-CGA	-2.10	1.27	1.33
3	J	102	BCL	O2A-CGA	-2.10	1.27	1.33
3	H	102	BCL	O2A-CGA	-2.10	1.27	1.33
3	F	102	BCL	O2A-CGA	-2.10	1.27	1.33

All (266) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	102	BCL	C1-C2-C3	-5.07	117.28	126.04
3	H	102	BCL	C1-C2-C3	-5.07	117.28	126.04
3	L	101	BCL	C1-C2-C3	-5.07	117.28	126.04
3	J	102	BCL	C1-C2-C3	-5.07	117.28	126.04
3	D	101	BCL	C1-C2-C3	-5.06	117.28	126.04
3	N	102	BCL	C1-C2-C3	-5.06	117.28	126.04
3	B	101	BCL	C1-C2-C3	-5.06	117.28	126.04
3	G	101	BCL	C1-C2-C3	4.46	133.75	126.04
3	K	101	BCL	C1-C2-C3	4.45	133.75	126.04
3	C	102	BCL	C1-C2-C3	4.45	133.75	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	102	BCL	C1-C2-C3	4.45	133.75	126.04
3	E	102	BCL	C1-C2-C3	4.45	133.74	126.04
3	A	101	BCL	C1-C2-C3	4.45	133.74	126.04
3	I	101	BCL	C1-C2-C3	4.45	133.74	126.04
3	G	101	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
3	M	102	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
3	C	102	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
3	K	101	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
3	I	101	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
3	E	102	BCL	CMB-C2B-C1B	-4.36	121.77	128.46
3	A	101	BCL	CMB-C2B-C1B	-4.36	121.77	128.46
3	G	101	BCL	C4A-NA-C1A	4.30	108.64	106.71
3	E	102	BCL	C4A-NA-C1A	4.30	108.64	106.71
3	I	101	BCL	C4A-NA-C1A	4.29	108.64	106.71
3	K	101	BCL	C4A-NA-C1A	4.29	108.63	106.71
3	M	102	BCL	C4A-NA-C1A	4.29	108.63	106.71
3	A	101	BCL	C4A-NA-C1A	4.28	108.63	106.71
3	C	102	BCL	C4A-NA-C1A	4.28	108.63	106.71
3	F	102	BCL	C4A-NA-C1A	4.17	108.58	106.71
3	J	102	BCL	C4A-NA-C1A	4.16	108.58	106.71
3	N	102	BCL	C4A-NA-C1A	4.16	108.58	106.71
3	L	101	BCL	C4A-NA-C1A	4.15	108.57	106.71
3	B	101	BCL	C4A-NA-C1A	4.15	108.57	106.71
3	H	102	BCL	C4A-NA-C1A	4.15	108.57	106.71
3	D	101	BCL	C4A-NA-C1A	4.14	108.57	106.71
3	J	102	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
3	F	102	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
3	H	102	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
3	D	101	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
3	L	101	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
3	B	101	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
3	N	102	BCL	CMB-C2B-C1B	-4.05	122.24	128.46
3	D	102	BCL	C16-C15-C13	3.82	128.28	115.92
3	L	102	BCL	C16-C15-C13	3.82	128.28	115.92
3	J	103	BCL	C16-C15-C13	3.82	128.28	115.92
3	H	103	BCL	C16-C15-C13	3.82	128.27	115.92
3	F	103	BCL	C16-C15-C13	3.82	128.27	115.92
3	B	102	BCL	C16-C15-C13	3.82	128.27	115.92
3	N	103	BCL	C16-C15-C13	3.82	128.27	115.92
3	B	101	BCL	CAD-C3D-C4D	-3.72	106.39	108.47
3	H	102	BCL	CAD-C3D-C4D	-3.72	106.39	108.47
3	H	103	BCL	CMB-C2B-C1B	-3.72	122.75	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	103	BCL	CMB-C2B-C1B	-3.72	122.75	128.46
3	N	103	BCL	CMB-C2B-C1B	-3.72	122.75	128.46
3	D	102	BCL	CMB-C2B-C1B	-3.72	122.75	128.46
3	F	103	BCL	CMB-C2B-C1B	-3.72	122.75	128.46
3	F	102	BCL	CAD-C3D-C4D	-3.72	106.40	108.47
3	B	102	BCL	CMB-C2B-C1B	-3.72	122.75	128.46
3	J	102	BCL	CAD-C3D-C4D	-3.72	106.40	108.47
3	L	102	BCL	CMB-C2B-C1B	-3.72	122.75	128.46
3	N	102	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
3	D	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
3	L	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
3	D	102	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
3	B	102	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
3	J	103	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
3	L	102	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
3	N	103	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
3	F	103	BCL	CAD-C3D-C4D	-3.34	106.61	108.47
3	D	101	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
3	H	103	BCL	CAD-C3D-C4D	-3.33	106.61	108.47
3	H	102	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
3	L	101	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
3	N	102	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
3	J	102	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
3	F	102	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
3	B	101	BCL	OBD-CAD-CBD	-3.33	121.14	125.89
3	D	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
3	J	103	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
3	N	103	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
3	L	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
3	F	103	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
3	H	103	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
3	B	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
3	B	102	BCL	C4A-NA-C1A	3.21	108.15	106.71
3	F	103	BCL	C4A-NA-C1A	3.21	108.15	106.71
3	L	102	BCL	C4A-NA-C1A	3.21	108.15	106.71
3	H	103	BCL	C4A-NA-C1A	3.20	108.15	106.71
3	J	103	BCL	C4A-NA-C1A	3.20	108.14	106.71
3	N	103	BCL	C4A-NA-C1A	3.20	108.14	106.71
3	D	102	BCL	C4A-NA-C1A	3.19	108.14	106.71
3	M	102	BCL	CMB-C2B-C3B	3.18	130.63	124.68
3	C	102	BCL	CMB-C2B-C3B	3.18	130.63	124.68
3	K	101	BCL	CMB-C2B-C3B	3.18	130.63	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	101	BCL	CMB-C2B-C3B	3.18	130.63	124.68
3	E	102	BCL	CMB-C2B-C3B	3.18	130.63	124.68
3	A	101	BCL	CMB-C2B-C3B	3.18	130.62	124.68
3	I	101	BCL	CMB-C2B-C3B	3.18	130.62	124.68
3	N	102	BCL	O2D-CGD-CBD	3.18	116.91	111.27
3	B	101	BCL	O2D-CGD-CBD	3.17	116.91	111.27
3	D	101	BCL	O2D-CGD-CBD	3.17	116.91	111.27
3	H	102	BCL	O2D-CGD-CBD	3.17	116.91	111.27
3	D	101	BCL	CHA-C1A-NA	-3.17	119.13	126.40
3	L	101	BCL	CHA-C1A-NA	-3.17	119.13	126.40
3	N	102	BCL	CHA-C1A-NA	-3.17	119.13	126.40
3	J	102	BCL	O2D-CGD-CBD	3.17	116.91	111.27
3	B	101	BCL	CHA-C1A-NA	-3.17	119.13	126.40
3	H	102	BCL	CHA-C1A-NA	-3.17	119.13	126.40
3	L	101	BCL	O2D-CGD-CBD	3.17	116.91	111.27
3	J	102	BCL	CHA-C1A-NA	-3.17	119.13	126.40
3	F	102	BCL	O2D-CGD-CBD	3.17	116.90	111.27
3	F	102	BCL	CHA-C1A-NA	-3.17	119.14	126.40
3	M	102	BCL	OBD-CAD-CBD	-3.12	121.44	125.89
3	E	102	BCL	OBD-CAD-CBD	-3.12	121.44	125.89
3	K	101	BCL	OBD-CAD-CBD	-3.12	121.44	125.89
3	I	101	BCL	OBD-CAD-CBD	-3.12	121.44	125.89
3	C	102	BCL	OBD-CAD-CBD	-3.12	121.44	125.89
3	A	101	BCL	OBD-CAD-CBD	-3.12	121.44	125.89
3	G	101	BCL	OBD-CAD-CBD	-3.12	121.44	125.89
3	I	101	BCL	CHA-C1A-NA	-3.02	119.48	126.40
3	A	101	BCL	CHA-C1A-NA	-3.02	119.48	126.40
3	E	102	BCL	CHA-C1A-NA	-3.02	119.48	126.40
3	M	102	BCL	CHA-C1A-NA	-3.02	119.48	126.40
3	C	102	BCL	CHA-C1A-NA	-3.02	119.48	126.40
3	K	101	BCL	CHA-C1A-NA	-3.02	119.48	126.40
3	G	101	BCL	CHA-C1A-NA	-3.02	119.49	126.40
3	N	102	BCL	C2A-C1A-CHA	2.98	129.07	123.86
3	D	101	BCL	C2A-C1A-CHA	2.98	129.07	123.86
3	L	101	BCL	C2A-C1A-CHA	2.98	129.07	123.86
3	J	102	BCL	C2A-C1A-CHA	2.98	129.06	123.86
3	H	102	BCL	C2A-C1A-CHA	2.98	129.06	123.86
3	B	101	BCL	C2A-C1A-CHA	2.98	129.06	123.86
3	F	102	BCL	C2A-C1A-CHA	2.98	129.06	123.86
3	N	103	BCL	CHA-C1A-NA	-2.97	119.59	126.40
3	L	102	BCL	CHA-C1A-NA	-2.97	119.59	126.40
3	D	102	BCL	CHA-C1A-NA	-2.97	119.59	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	103	BCL	CHA-C1A-NA	-2.97	119.59	126.40
3	B	102	BCL	CHA-C1A-NA	-2.97	119.59	126.40
3	F	103	BCL	CHA-C1A-NA	-2.97	119.59	126.40
3	J	103	BCL	CHA-C1A-NA	-2.97	119.59	126.40
3	F	102	BCL	CED-O2D-CGD	-2.96	109.24	115.94
3	L	101	BCL	CED-O2D-CGD	-2.96	109.24	115.94
3	J	102	BCL	CED-O2D-CGD	-2.96	109.24	115.94
3	D	101	BCL	CED-O2D-CGD	-2.96	109.24	115.94
3	H	102	BCL	CED-O2D-CGD	-2.96	109.24	115.94
3	B	101	BCL	CED-O2D-CGD	-2.96	109.24	115.94
3	N	102	BCL	CED-O2D-CGD	-2.96	109.25	115.94
3	A	101	BCL	CAD-C3D-C4D	-2.94	106.83	108.47
3	M	102	BCL	CAD-C3D-C4D	-2.93	106.83	108.47
3	F	102	BCL	CMB-C2B-C3B	2.93	130.16	124.68
3	D	101	BCL	CMB-C2B-C3B	2.93	130.16	124.68
3	L	101	BCL	CMB-C2B-C3B	2.93	130.16	124.68
3	H	102	BCL	CMB-C2B-C3B	2.93	130.16	124.68
3	J	102	BCL	CMB-C2B-C3B	2.93	130.16	124.68
3	N	102	BCL	CMB-C2B-C3B	2.93	130.16	124.68
3	E	102	BCL	CAD-C3D-C4D	-2.93	106.84	108.47
3	G	101	BCL	CAD-C3D-C4D	-2.93	106.84	108.47
3	K	101	BCL	CAD-C3D-C4D	-2.93	106.84	108.47
3	B	101	BCL	CMB-C2B-C3B	2.93	130.16	124.68
3	C	102	BCL	CAD-C3D-C4D	-2.92	106.84	108.47
3	I	101	BCL	CAD-C3D-C4D	-2.92	106.84	108.47
3	L	102	BCL	C2A-C1A-CHA	2.84	128.82	123.86
3	B	102	BCL	C2A-C1A-CHA	2.84	128.82	123.86
3	N	103	BCL	C2A-C1A-CHA	2.84	128.82	123.86
3	D	102	BCL	C2A-C1A-CHA	2.84	128.82	123.86
3	F	103	BCL	C2A-C1A-CHA	2.84	128.82	123.86
3	H	103	BCL	C2A-C1A-CHA	2.83	128.82	123.86
3	J	103	BCL	C2A-C1A-CHA	2.83	128.82	123.86
3	I	101	BCL	C2A-C1A-CHA	2.76	128.69	123.86
3	M	102	BCL	C2A-C1A-CHA	2.76	128.69	123.86
3	E	102	BCL	C2A-C1A-CHA	2.76	128.69	123.86
3	A	101	BCL	C2A-C1A-CHA	2.76	128.69	123.86
3	C	102	BCL	C2A-C1A-CHA	2.76	128.69	123.86
3	K	101	BCL	C2A-C1A-CHA	2.76	128.69	123.86
3	G	101	BCL	C2A-C1A-CHA	2.76	128.68	123.86
3	C	102	BCL	C11-C10-C8	2.74	124.77	115.92
3	G	101	BCL	C11-C10-C8	2.74	124.77	115.92
3	I	101	BCL	C11-C10-C8	2.74	124.77	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	101	BCL	C11-C10-C8	2.74	124.76	115.92
3	A	101	BCL	C11-C10-C8	2.74	124.76	115.92
3	M	102	BCL	C11-C10-C8	2.74	124.76	115.92
3	E	102	BCL	C11-C10-C8	2.73	124.76	115.92
3	F	103	BCL	C17-C16-C15	2.72	125.72	113.24
3	B	102	BCL	C17-C16-C15	2.72	125.72	113.24
3	D	102	BCL	C17-C16-C15	2.72	125.72	113.24
3	N	103	BCL	C17-C16-C15	2.72	125.72	113.24
3	J	103	BCL	C17-C16-C15	2.72	125.72	113.24
3	H	103	BCL	C17-C16-C15	2.72	125.71	113.24
3	L	102	BCL	C17-C16-C15	2.71	125.71	113.24
3	F	103	BCL	CMB-C2B-C3B	2.69	129.71	124.68
3	J	103	BCL	CMB-C2B-C3B	2.69	129.71	124.68
3	D	102	BCL	CMB-C2B-C3B	2.69	129.71	124.68
3	H	103	BCL	CMB-C2B-C3B	2.69	129.71	124.68
3	N	103	BCL	CMB-C2B-C3B	2.69	129.71	124.68
3	B	102	BCL	CMB-C2B-C3B	2.69	129.70	124.68
3	L	102	BCL	CMB-C2B-C3B	2.69	129.70	124.68
3	N	102	BCL	O2D-CGD-O1D	-2.63	118.70	123.84
3	B	101	BCL	O2D-CGD-O1D	-2.63	118.70	123.84
3	H	102	BCL	O2D-CGD-O1D	-2.63	118.70	123.84
3	D	101	BCL	O2D-CGD-O1D	-2.62	118.71	123.84
3	L	101	BCL	O2D-CGD-O1D	-2.62	118.71	123.84
3	F	102	BCL	O2D-CGD-O1D	-2.62	118.71	123.84
3	J	102	BCL	O2D-CGD-O1D	-2.62	118.71	123.84
3	M	102	BCL	C17-C16-C15	2.60	125.18	113.24
3	A	101	BCL	C17-C16-C15	2.60	125.18	113.24
3	G	101	BCL	C17-C16-C15	2.60	125.18	113.24
3	C	102	BCL	C17-C16-C15	2.60	125.18	113.24
3	E	102	BCL	C17-C16-C15	2.60	125.18	113.24
3	I	101	BCL	C17-C16-C15	2.60	125.18	113.24
3	K	101	BCL	C17-C16-C15	2.60	125.18	113.24
3	N	102	BCL	CMD-C2D-C3D	2.42	129.21	124.68
3	B	101	BCL	CMD-C2D-C3D	2.42	129.21	124.68
3	H	102	BCL	CMD-C2D-C3D	2.42	129.21	124.68
3	D	101	BCL	CMD-C2D-C3D	2.42	129.21	124.68
3	F	102	BCL	CMD-C2D-C3D	2.42	129.21	124.68
3	L	101	BCL	CMD-C2D-C3D	2.42	129.21	124.68
3	J	102	BCL	CMD-C2D-C3D	2.42	129.20	124.68
3	G	101	BCL	OBB-CAB-CBB	-2.40	114.77	120.17
3	E	102	BCL	OBB-CAB-CBB	-2.40	114.77	120.17
3	M	102	BCL	OBB-CAB-CBB	-2.40	114.77	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	102	BCL	OBB-CAB-CBB	-2.40	114.77	120.17
3	K	101	BCL	OBB-CAB-CBB	-2.40	114.77	120.17
3	I	101	BCL	OBB-CAB-CBB	-2.40	114.77	120.17
3	A	101	BCL	OBB-CAB-CBB	-2.40	114.77	120.17
3	B	102	BCL	CMD-C2D-C3D	2.39	129.15	124.68
3	L	102	BCL	CMD-C2D-C3D	2.39	129.15	124.68
3	D	102	BCL	CMD-C2D-C3D	2.39	129.14	124.68
3	N	103	BCL	CMD-C2D-C3D	2.39	129.14	124.68
3	F	103	BCL	CMD-C2D-C3D	2.38	129.14	124.68
3	H	103	BCL	CMD-C2D-C3D	2.38	129.14	124.68
3	J	103	BCL	CMD-C2D-C3D	2.38	129.14	124.68
3	M	102	BCL	CMD-C2D-C3D	2.26	128.91	124.68
3	I	101	BCL	CMD-C2D-C3D	2.26	128.91	124.68
3	C	102	BCL	CMD-C2D-C3D	2.26	128.91	124.68
3	G	101	BCL	CMD-C2D-C3D	2.26	128.91	124.68
3	A	101	BCL	CMD-C2D-C3D	2.26	128.91	124.68
3	K	101	BCL	CMD-C2D-C3D	2.26	128.91	124.68
3	E	102	BCL	CMD-C2D-C3D	2.26	128.90	124.68
3	A	101	BCL	C4B-C3B-CAB	-2.20	122.88	127.13
3	E	102	BCL	C4B-C3B-CAB	-2.20	122.89	127.13
3	M	102	BCL	C4B-C3B-CAB	-2.20	122.89	127.13
3	I	101	BCL	C4B-C3B-CAB	-2.20	122.89	127.13
3	C	102	BCL	C4B-C3B-CAB	-2.19	122.89	127.13
3	G	101	BCL	C4B-C3B-CAB	-2.19	122.89	127.13
3	K	101	BCL	C4B-C3B-CAB	-2.19	122.89	127.13
3	B	101	BCL	C4B-C3B-CAB	-2.16	122.96	127.13
3	H	102	BCL	C4B-C3B-CAB	-2.16	122.96	127.13
3	D	101	BCL	C4B-C3B-CAB	-2.16	122.96	127.13
3	N	102	BCL	C4B-C3B-CAB	-2.16	122.97	127.13
3	F	102	BCL	C4B-C3B-CAB	-2.15	122.97	127.13
3	J	102	BCL	C4B-C3B-CAB	-2.15	122.97	127.13
3	L	101	BCL	C4B-C3B-CAB	-2.15	122.97	127.13
3	H	102	BCL	OBB-CAB-CBB	-2.11	115.41	120.17
3	D	101	BCL	OBB-CAB-CBB	-2.11	115.41	120.17
3	B	101	BCL	OBB-CAB-CBB	-2.11	115.41	120.17
3	L	101	BCL	OBB-CAB-CBB	-2.11	115.41	120.17
3	J	102	BCL	OBB-CAB-CBB	-2.11	115.41	120.17
3	N	102	BCL	OBB-CAB-CBB	-2.11	115.42	120.17
3	F	102	BCL	OBB-CAB-CBB	-2.11	115.42	120.17
3	D	101	BCL	OBD-CAD-C3D	2.02	131.33	127.98
3	N	102	BCL	OBD-CAD-C3D	2.02	131.33	127.98
3	L	101	BCL	OBD-CAD-C3D	2.01	131.33	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	102	BCL	OBD-CAD-C3D	2.01	131.32	127.98
3	F	102	BCL	OBD-CAD-C3D	2.01	131.32	127.98
3	J	102	BCL	OBD-CAD-C3D	2.01	131.32	127.98
3	B	101	BCL	OBD-CAD-C3D	2.01	131.32	127.98

There are no chirality outliers.

All (238) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	101	BCL	O2A-C1-C2-C3
3	C	102	BCL	O2A-C1-C2-C3
3	E	102	BCL	O2A-C1-C2-C3
3	G	101	BCL	O2A-C1-C2-C3
3	I	101	BCL	O2A-C1-C2-C3
3	K	101	BCL	O2A-C1-C2-C3
3	M	102	BCL	O2A-C1-C2-C3
4	A	102	QS2	C23-C1-C2-C3
4	A	102	QS2	C24-C1-C2-C3
4	A	102	QS2	O25-C1-C2-C3
4	A	102	QS2	C3-C4-C5-C6
4	A	102	QS2	O32-C4-C5-C26
4	A	102	QS2	O32-C4-C5-C6
4	B	103	QS2	C23-C1-C2-C3
4	B	103	QS2	C24-C1-C2-C3
4	B	103	QS2	O25-C1-C2-C3
4	B	103	QS2	C3-C4-C5-C6
4	B	103	QS2	O32-C4-C5-C26
4	B	103	QS2	O32-C4-C5-C6
4	E	103	QS2	C23-C1-C2-C3
4	E	103	QS2	C24-C1-C2-C3
4	E	103	QS2	O25-C1-C2-C3
4	E	103	QS2	C3-C4-C5-C6
4	E	103	QS2	O32-C4-C5-C26
4	E	103	QS2	O32-C4-C5-C6
4	G	102	QS2	C23-C1-C2-C3
4	G	102	QS2	C24-C1-C2-C3
4	G	102	QS2	O25-C1-C2-C3
4	G	102	QS2	C3-C4-C5-C6
4	G	102	QS2	O32-C4-C5-C26
4	G	102	QS2	O32-C4-C5-C6
4	I	102	QS2	C23-C1-C2-C3
4	I	102	QS2	C24-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	I	102	QS2	O25-C1-C2-C3
4	I	102	QS2	C3-C4-C5-C6
4	I	102	QS2	O32-C4-C5-C26
4	I	102	QS2	O32-C4-C5-C6
4	K	102	QS2	C23-C1-C2-C3
4	K	102	QS2	C24-C1-C2-C3
4	K	102	QS2	O25-C1-C2-C3
4	K	102	QS2	C3-C4-C5-C6
4	K	102	QS2	O32-C4-C5-C26
4	K	102	QS2	O32-C4-C5-C6
4	M	103	QS2	C23-C1-C2-C3
4	M	103	QS2	C24-C1-C2-C3
4	M	103	QS2	O25-C1-C2-C3
4	M	103	QS2	C3-C4-C5-C6
4	M	103	QS2	O32-C4-C5-C26
4	M	103	QS2	O32-C4-C5-C6
5	C	101	QSE	C20-C21-C22-O33
5	C	101	QSE	C29-C21-C22-O33
5	E	101	QSE	C20-C21-C22-O33
5	E	101	QSE	C29-C21-C22-O33
5	F	101	QSE	C20-C21-C22-O33
5	F	101	QSE	C29-C21-C22-O33
5	H	101	QSE	C20-C21-C22-O33
5	H	101	QSE	C29-C21-C22-O33
5	J	101	QSE	C20-C21-C22-O33
5	J	101	QSE	C29-C21-C22-O33
5	M	101	QSE	C20-C21-C22-O33
5	M	101	QSE	C29-C21-C22-O33
5	N	101	QSE	C20-C21-C22-O33
5	N	101	QSE	C29-C21-C22-O33
3	B	102	BCL	C2A-CAA-CBA-CGA
3	D	102	BCL	C2A-CAA-CBA-CGA
3	F	103	BCL	C2A-CAA-CBA-CGA
3	H	103	BCL	C2A-CAA-CBA-CGA
3	J	103	BCL	C2A-CAA-CBA-CGA
3	L	102	BCL	C2A-CAA-CBA-CGA
3	N	103	BCL	C2A-CAA-CBA-CGA
3	B	101	BCL	C15-C16-C17-C18
3	D	101	BCL	C15-C16-C17-C18
3	F	102	BCL	C15-C16-C17-C18
3	H	102	BCL	C15-C16-C17-C18
3	J	102	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	L	101	BCL	C15-C16-C17-C18
3	N	102	BCL	C15-C16-C17-C18
5	C	101	QSE	C34-C1-C2-C3
5	E	101	QSE	C34-C1-C2-C3
5	F	101	QSE	C34-C1-C2-C3
5	H	101	QSE	C34-C1-C2-C3
5	J	101	QSE	C34-C1-C2-C3
5	M	101	QSE	C34-C1-C2-C3
5	N	101	QSE	C34-C1-C2-C3
5	C	101	QSE	C31-C30-O42-C43
5	E	101	QSE	C31-C30-O42-C43
5	F	101	QSE	C31-C30-O42-C43
5	H	101	QSE	C31-C30-O42-C43
5	J	101	QSE	C31-C30-O42-C43
5	M	101	QSE	C31-C30-O42-C43
5	N	101	QSE	C31-C30-O42-C43
5	C	101	QSE	C20-C21-C22-C23
5	E	101	QSE	C20-C21-C22-C23
5	F	101	QSE	C20-C21-C22-C23
5	H	101	QSE	C20-C21-C22-C23
5	J	101	QSE	C20-C21-C22-C23
5	M	101	QSE	C20-C21-C22-C23
5	N	101	QSE	C20-C21-C22-C23
3	A	101	BCL	C8-C10-C11-C12
3	C	102	BCL	C8-C10-C11-C12
3	E	102	BCL	C8-C10-C11-C12
3	G	101	BCL	C8-C10-C11-C12
3	I	101	BCL	C8-C10-C11-C12
3	K	101	BCL	C8-C10-C11-C12
3	M	102	BCL	C8-C10-C11-C12
5	C	101	QSE	C24-C30-O42-C43
5	E	101	QSE	C24-C30-O42-C43
5	F	101	QSE	C24-C30-O42-C43
5	H	101	QSE	C24-C30-O42-C43
5	J	101	QSE	C24-C30-O42-C43
5	M	101	QSE	C24-C30-O42-C43
5	N	101	QSE	C24-C30-O42-C43
5	C	101	QSE	C32-C30-O42-C43
5	E	101	QSE	C32-C30-O42-C43
5	F	101	QSE	C32-C30-O42-C43
5	H	101	QSE	C32-C30-O42-C43
5	J	101	QSE	C32-C30-O42-C43

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Mol	Chain	Res	Type	Atoms
5	M	101	QSE	C32-C30-O42-C43
5	N	101	QSE	C32-C30-O42-C43
5	C	101	QSE	C38-C1-C2-C3
5	E	101	QSE	C38-C1-C2-C3
5	F	101	QSE	C38-C1-C2-C3
5	H	101	QSE	C38-C1-C2-C3
5	J	101	QSE	C38-C1-C2-C3
5	M	101	QSE	C38-C1-C2-C3
5	N	101	QSE	C38-C1-C2-C3
4	A	102	QS2	C20-C21-C22-C34
4	B	103	QS2	C20-C21-C22-C34
4	E	103	QS2	C20-C21-C22-C34
4	G	102	QS2	C20-C21-C22-C34
4	I	102	QS2	C20-C21-C22-C34
4	K	102	QS2	C20-C21-C22-C34
4	M	103	QS2	C20-C21-C22-C34
3	B	101	BCL	C10-C11-C12-C13
3	D	101	BCL	C10-C11-C12-C13
3	F	102	BCL	C10-C11-C12-C13
3	H	102	BCL	C10-C11-C12-C13
3	J	102	BCL	C10-C11-C12-C13
3	L	101	BCL	C10-C11-C12-C13
3	N	102	BCL	C10-C11-C12-C13
4	A	102	QS2	C20-C21-C22-C30
4	B	103	QS2	C20-C21-C22-C30
4	E	103	QS2	C20-C21-C22-C30
4	G	102	QS2	C20-C21-C22-C30
4	I	102	QS2	C20-C21-C22-C30
4	K	102	QS2	C20-C21-C22-C30
4	M	103	QS2	C20-C21-C22-C30
3	B	102	BCL	C4-C3-C5-C6
3	D	102	BCL	C4-C3-C5-C6
3	F	103	BCL	C4-C3-C5-C6
3	H	103	BCL	C4-C3-C5-C6
3	J	103	BCL	C4-C3-C5-C6
3	L	102	BCL	C4-C3-C5-C6
3	N	103	BCL	C4-C3-C5-C6
3	B	101	BCL	C6-C7-C8-C9
3	D	101	BCL	C6-C7-C8-C9
3	F	102	BCL	C6-C7-C8-C9
3	H	102	BCL	C6-C7-C8-C9
3	J	102	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	L	101	BCL	C6-C7-C8-C9
3	N	102	BCL	C6-C7-C8-C9
3	B	101	BCL	C4-C3-C5-C6
3	D	101	BCL	C4-C3-C5-C6
3	F	102	BCL	C4-C3-C5-C6
3	H	102	BCL	C4-C3-C5-C6
3	J	102	BCL	C4-C3-C5-C6
3	L	101	BCL	C4-C3-C5-C6
3	N	102	BCL	C4-C3-C5-C6
3	B	101	BCL	C2-C3-C5-C6
3	D	101	BCL	C2-C3-C5-C6
3	F	102	BCL	C2-C3-C5-C6
3	H	102	BCL	C2-C3-C5-C6
3	J	102	BCL	C2-C3-C5-C6
3	L	101	BCL	C2-C3-C5-C6
3	N	102	BCL	C2-C3-C5-C6
3	B	102	BCL	CAA-CBA-CGA-O2A
3	D	102	BCL	CAA-CBA-CGA-O2A
3	F	103	BCL	CAA-CBA-CGA-O2A
3	H	103	BCL	CAA-CBA-CGA-O2A
3	J	103	BCL	CAA-CBA-CGA-O2A
3	L	102	BCL	CAA-CBA-CGA-O2A
3	N	103	BCL	CAA-CBA-CGA-O2A
5	C	101	QSE	C1-C2-C3-C4
5	E	101	QSE	C1-C2-C3-C4
5	F	101	QSE	C1-C2-C3-C4
5	H	101	QSE	C1-C2-C3-C4
5	J	101	QSE	C1-C2-C3-C4
5	M	101	QSE	C1-C2-C3-C4
5	N	101	QSE	C1-C2-C3-C4
3	B	102	BCL	C13-C15-C16-C17
3	D	102	BCL	C13-C15-C16-C17
3	F	103	BCL	C13-C15-C16-C17
3	H	103	BCL	C13-C15-C16-C17
3	J	103	BCL	C13-C15-C16-C17
3	L	102	BCL	C13-C15-C16-C17
3	N	103	BCL	C13-C15-C16-C17
3	B	101	BCL	C2A-CAA-CBA-CGA
3	D	101	BCL	C2A-CAA-CBA-CGA
3	F	102	BCL	C2A-CAA-CBA-CGA
3	H	102	BCL	C2A-CAA-CBA-CGA
3	J	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
3	L	101	BCL	C2A-CAA-CBA-CGA
3	N	102	BCL	C2A-CAA-CBA-CGA
4	A	102	QS2	C22-C30-C33-C35
4	B	103	QS2	C22-C30-C33-C35
4	E	103	QS2	C22-C30-C33-C35
4	G	102	QS2	C22-C30-C33-C35
4	I	102	QS2	C22-C30-C33-C35
4	K	102	QS2	C22-C30-C33-C35
4	M	103	QS2	C22-C30-C33-C35
5	C	101	QSE	C22-C23-C24-C30
5	E	101	QSE	C22-C23-C24-C30
5	F	101	QSE	C22-C23-C24-C30
5	H	101	QSE	C22-C23-C24-C30
5	J	101	QSE	C22-C23-C24-C30
5	M	101	QSE	C22-C23-C24-C30
5	N	101	QSE	C22-C23-C24-C30
3	B	102	BCL	CAA-CBA-CGA-O1A
3	D	102	BCL	CAA-CBA-CGA-O1A
3	F	103	BCL	CAA-CBA-CGA-O1A
3	H	103	BCL	CAA-CBA-CGA-O1A
3	J	103	BCL	CAA-CBA-CGA-O1A
3	L	102	BCL	CAA-CBA-CGA-O1A
3	N	103	BCL	CAA-CBA-CGA-O1A
3	B	102	BCL	C2-C3-C5-C6
3	D	102	BCL	C2-C3-C5-C6
3	F	103	BCL	C2-C3-C5-C6
3	H	103	BCL	C2-C3-C5-C6
3	J	103	BCL	C2-C3-C5-C6
3	L	102	BCL	C2-C3-C5-C6
3	N	103	BCL	C2-C3-C5-C6
3	A	101	BCL	C13-C15-C16-C17
3	C	102	BCL	C13-C15-C16-C17
3	E	102	BCL	C13-C15-C16-C17
3	G	101	BCL	C13-C15-C16-C17
3	I	101	BCL	C13-C15-C16-C17
3	K	101	BCL	C13-C15-C16-C17
3	M	102	BCL	C13-C15-C16-C17

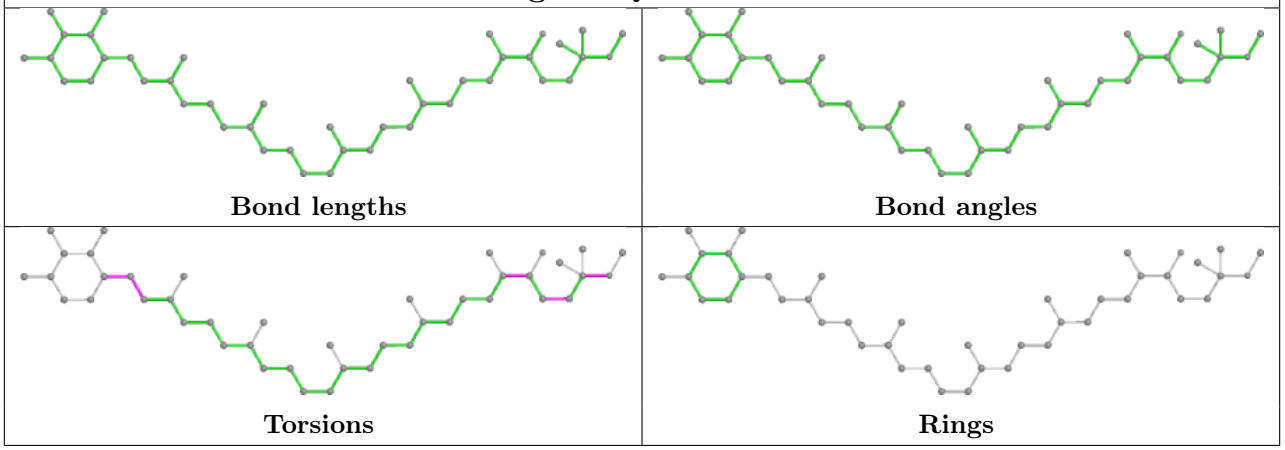
There are no ring outliers.

27 monomers are involved in 29 short contacts:

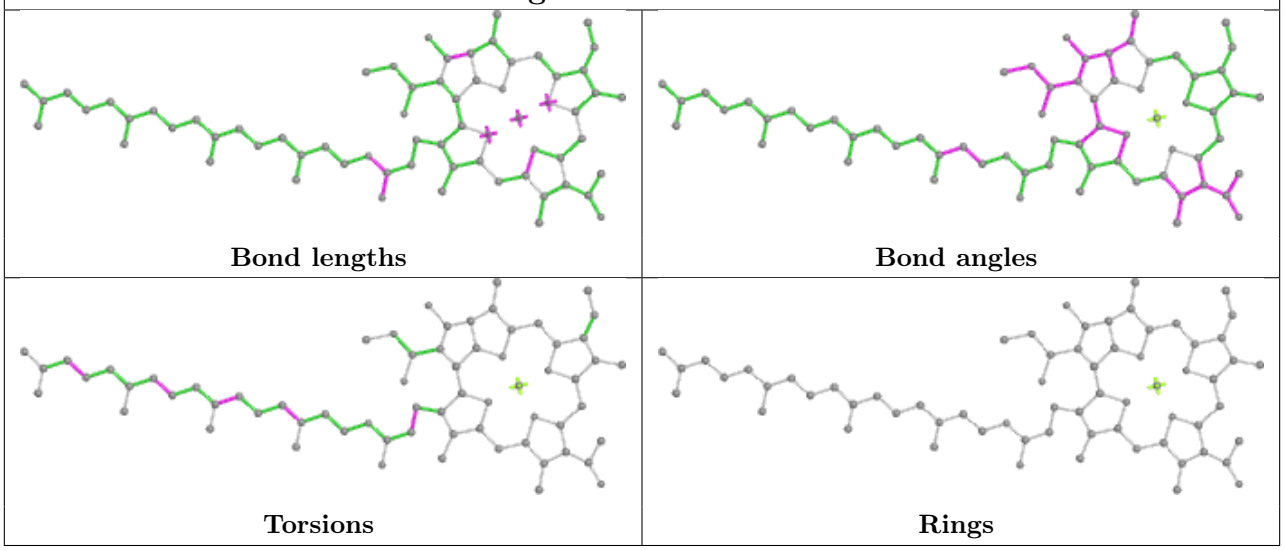
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	101	QSE	1	0
3	L	101	BCL	1	0
3	N	103	BCL	1	0
3	I	101	BCL	1	0
5	J	101	QSE	1	0
3	J	102	BCL	1	0
4	M	103	QS2	1	0
5	F	101	QSE	1	0
3	D	101	BCL	1	0
3	G	101	BCL	1	0
3	J	103	BCL	1	0
3	B	102	BCL	1	0
3	K	101	BCL	1	0
3	M	102	BCL	3	0
5	M	101	QSE	1	0
3	F	103	BCL	1	0
4	A	102	QS2	1	0
3	F	102	BCL	1	0
3	N	102	BCL	1	0
3	L	102	BCL	1	0
3	B	101	BCL	1	0
3	H	103	BCL	1	0
5	H	101	QSE	1	0
3	E	102	BCL	1	0
5	C	101	QSE	1	0
3	D	102	BCL	1	0
3	H	102	BCL	1	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 then 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.

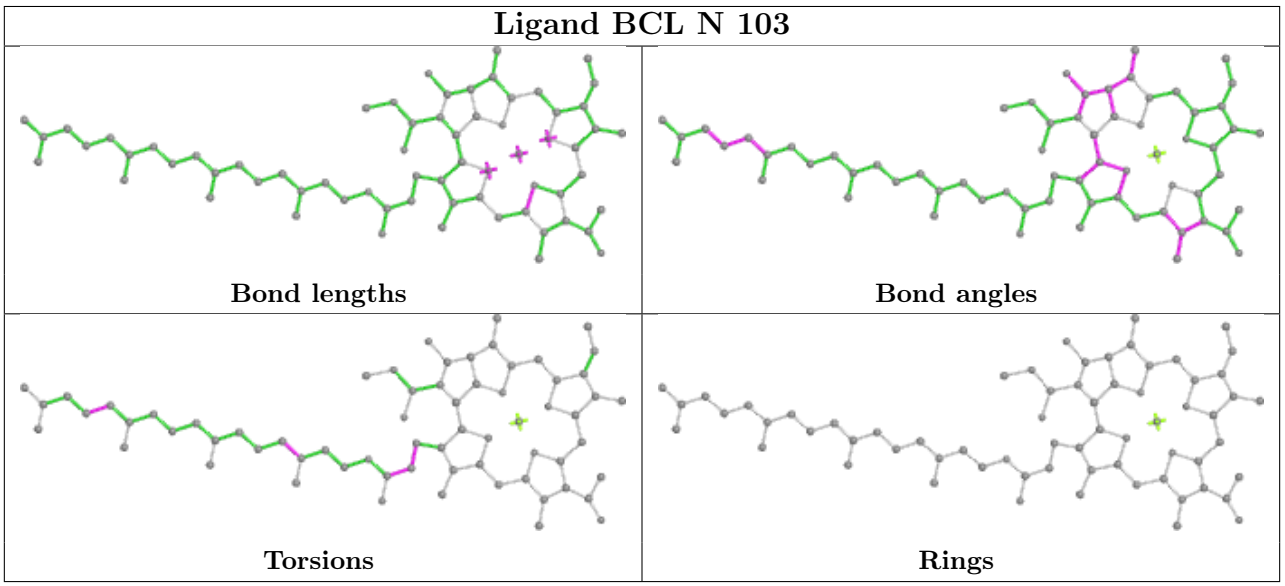
Ligand QSE E 101



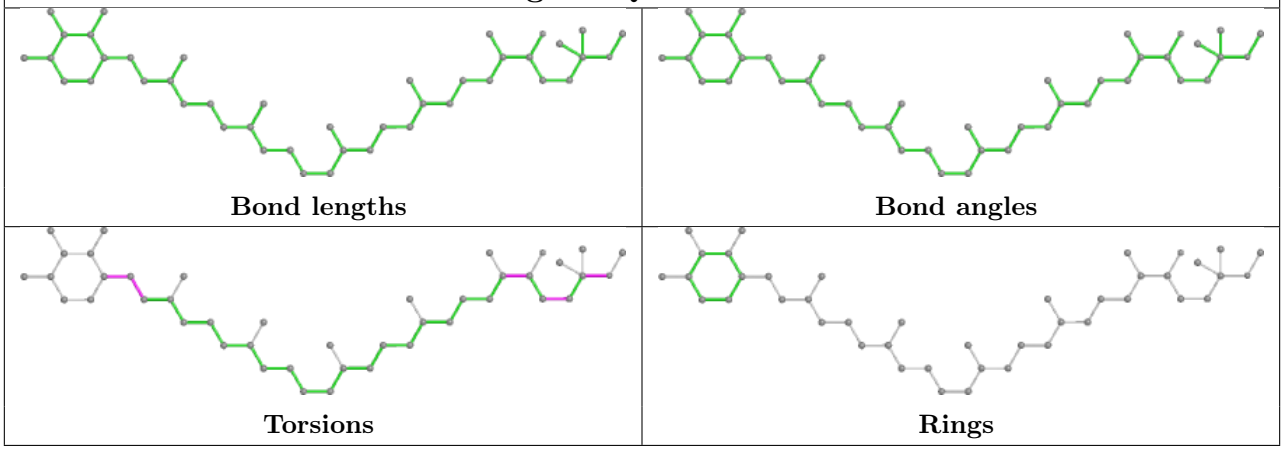
Ligand BCL L 101



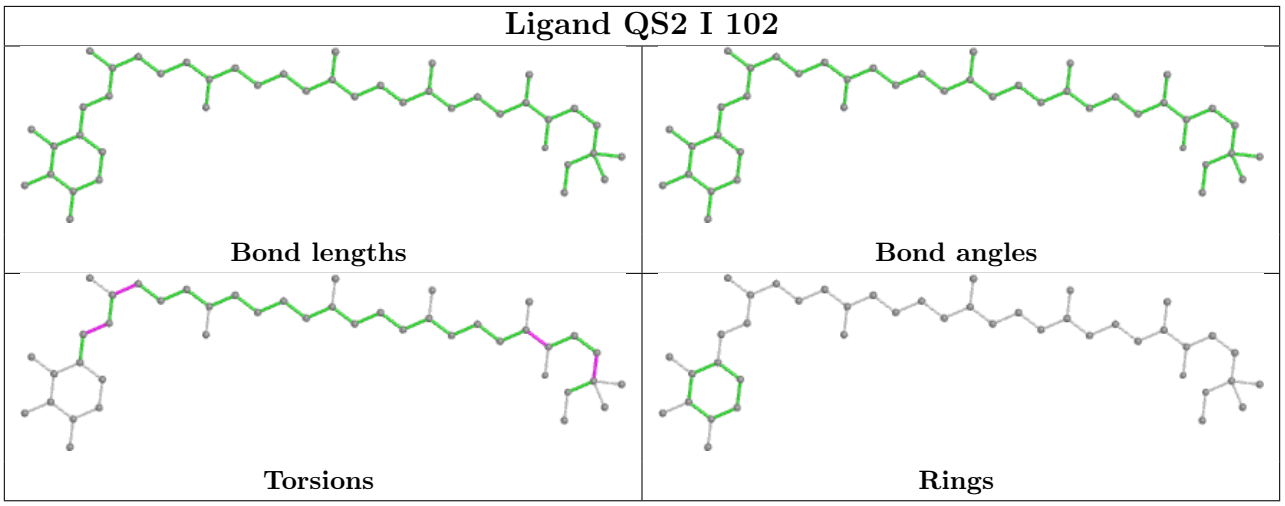
Ligand BCL N 103



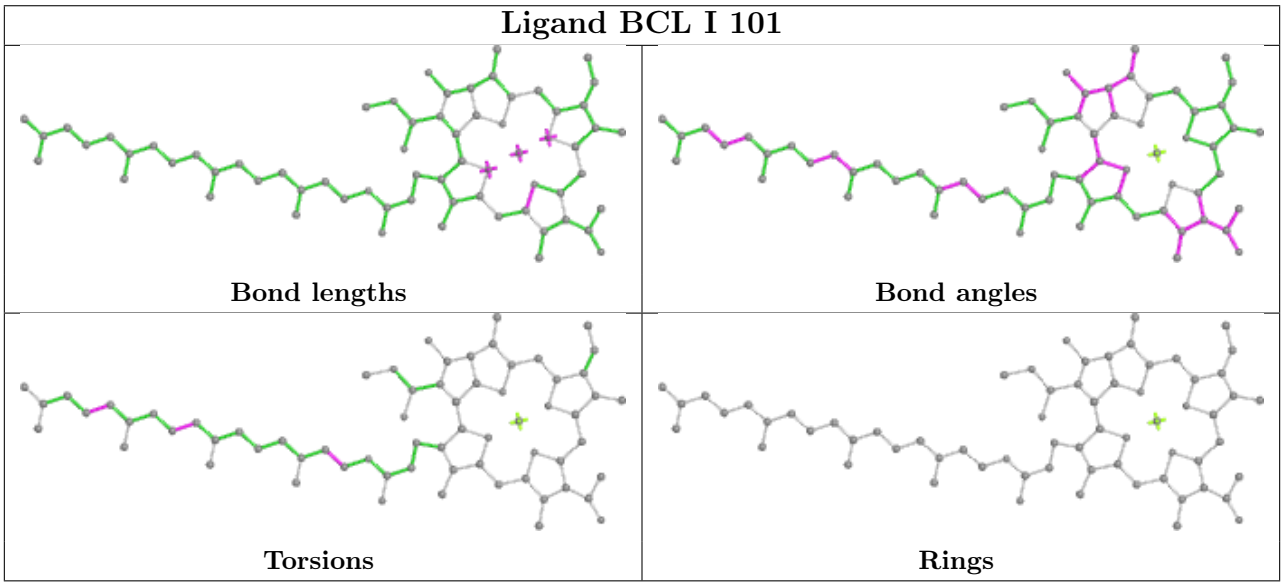
Ligand QSE N 101



Ligand QS2 I 102



Ligand BCL I 101



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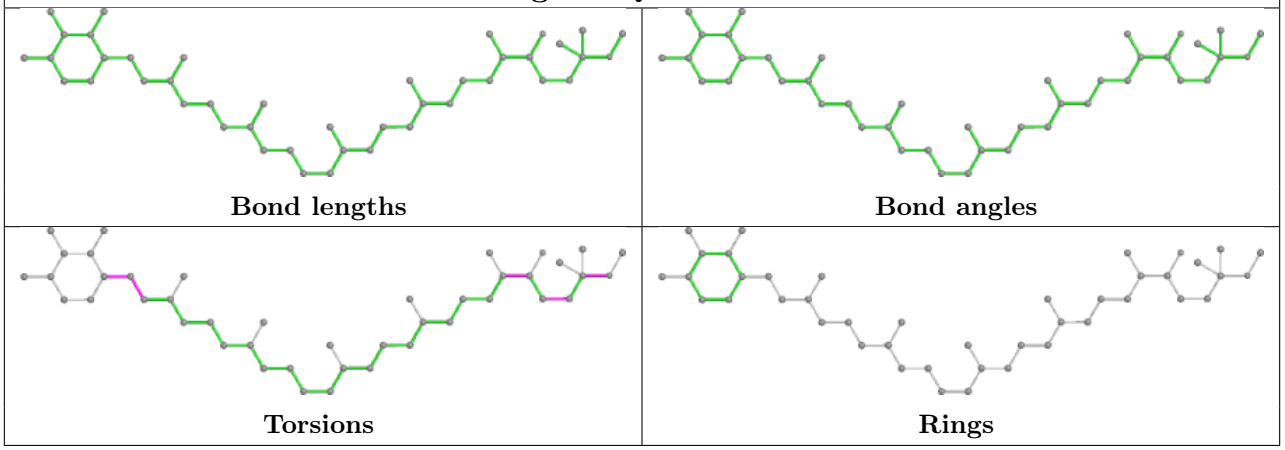
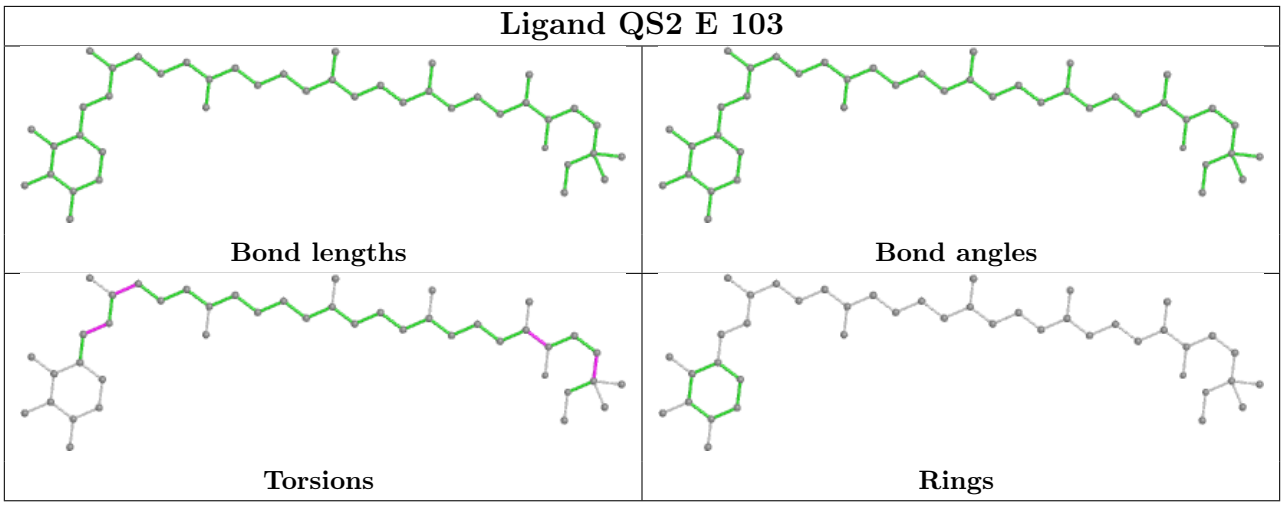
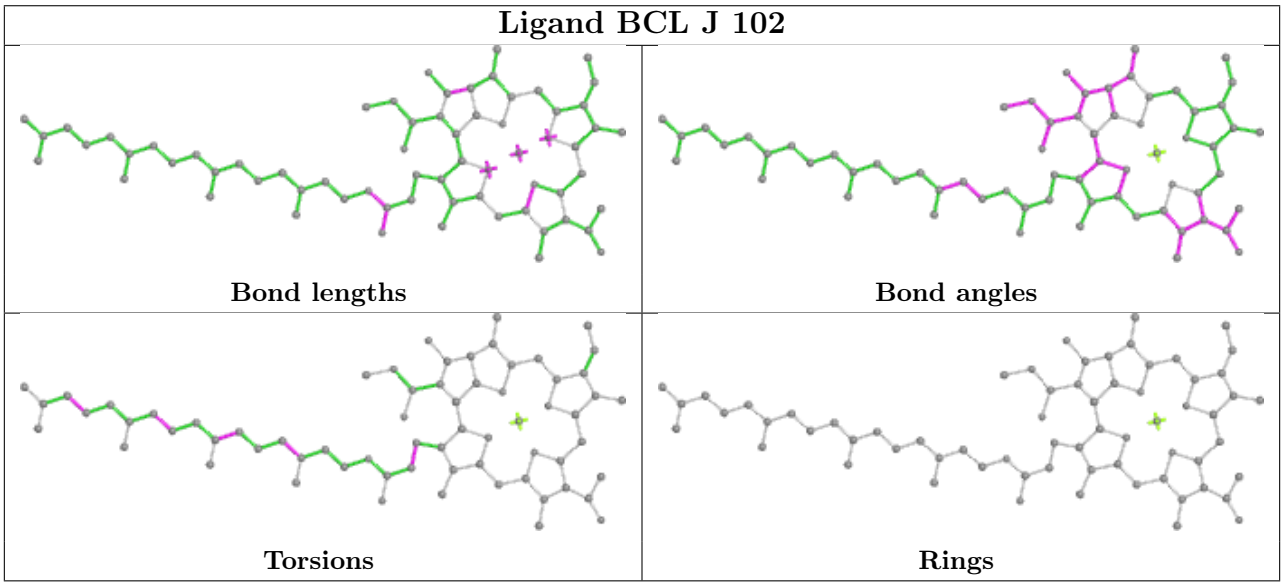


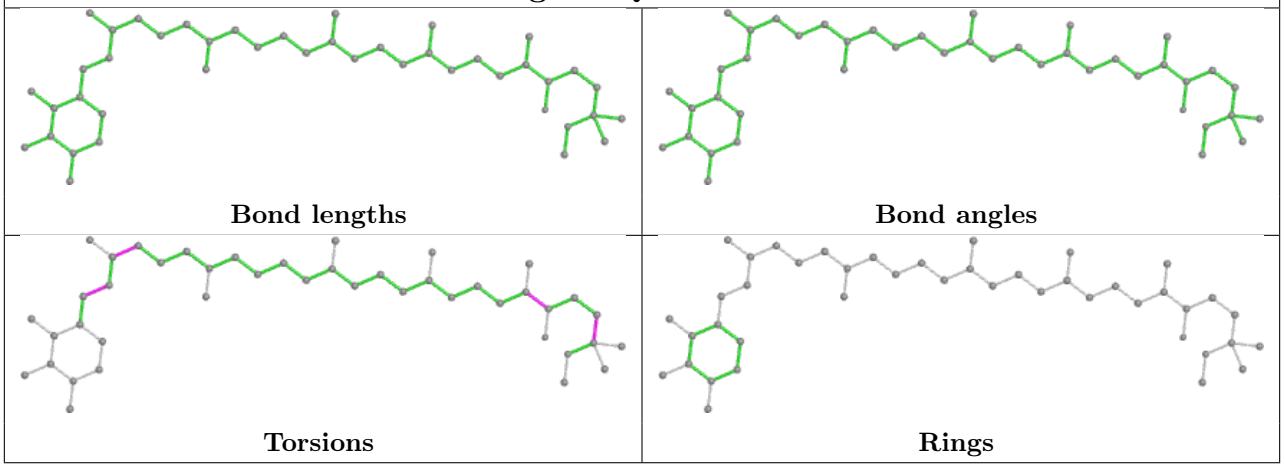
Ligand QS2 E 103



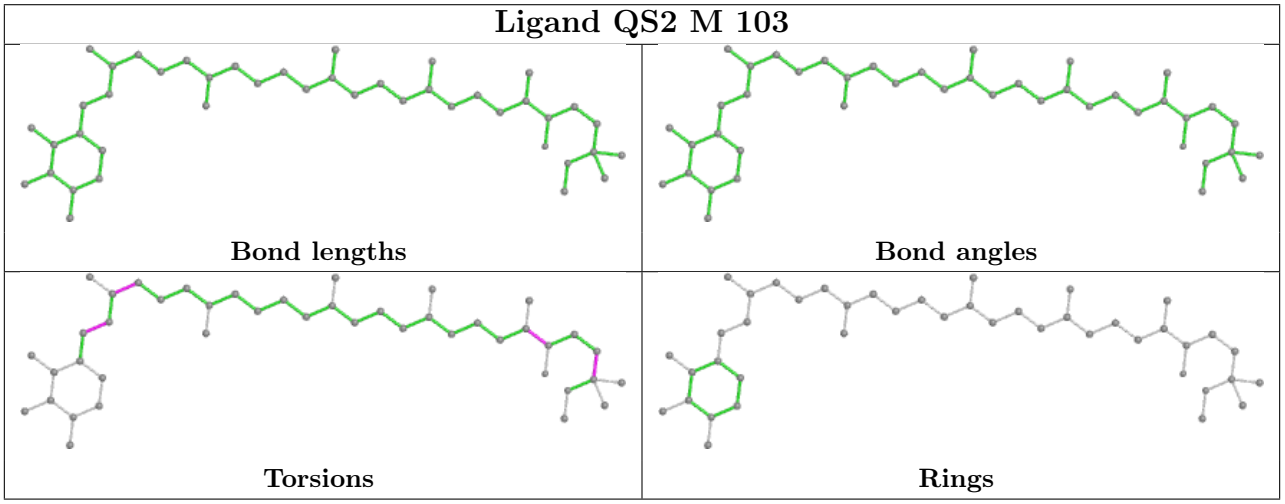
Ligand BCL J 102



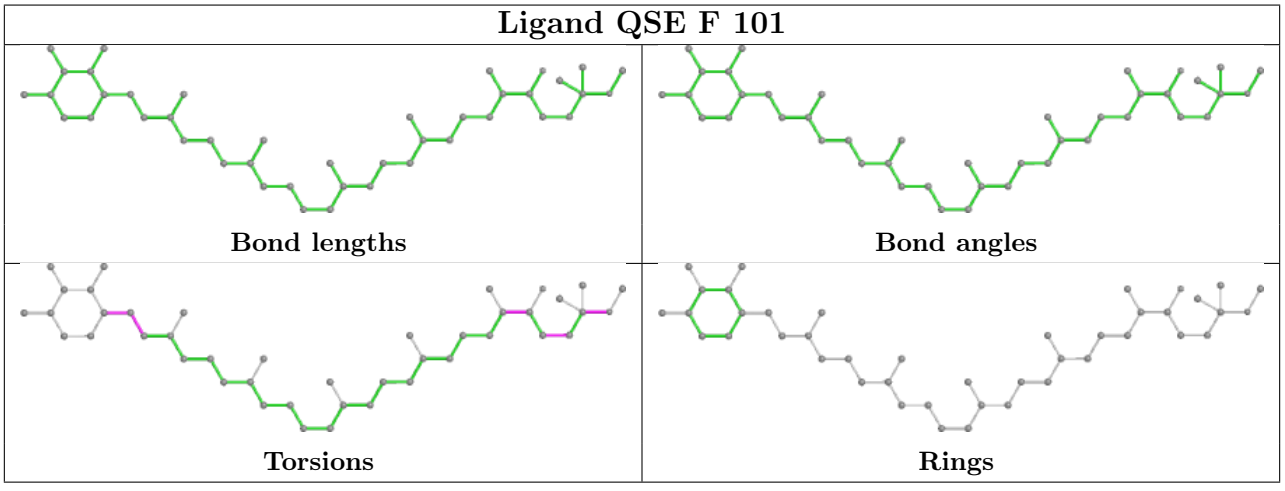
Ligand QS2 G 102



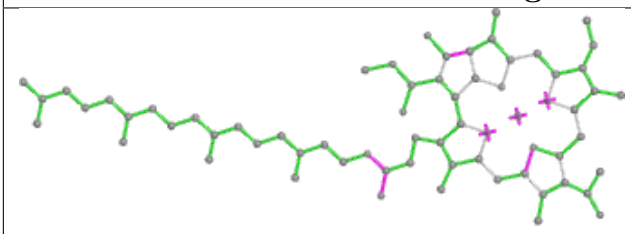
Ligand QS2 M 103



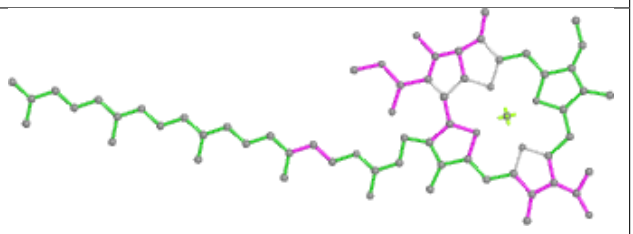
Ligand QSE F 101



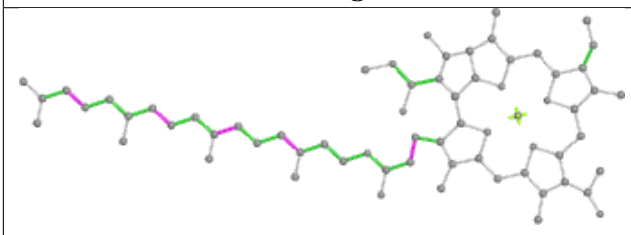
Ligand BCL D 101



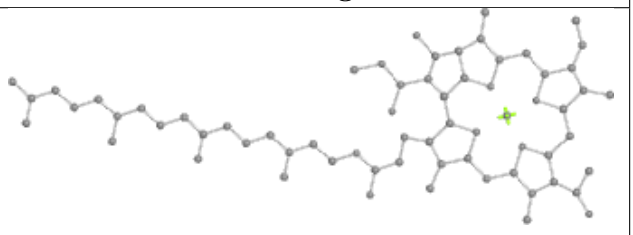
Bond lengths



Bond angles

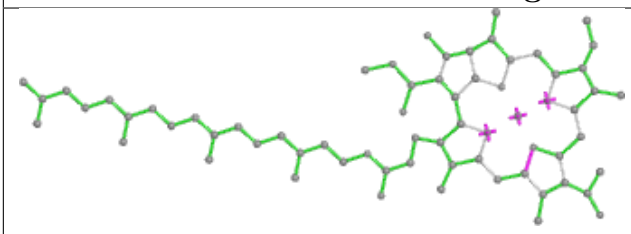


Torsions

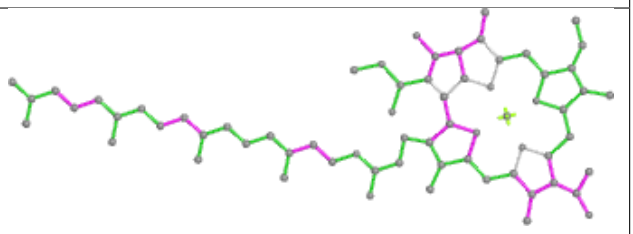


Rings

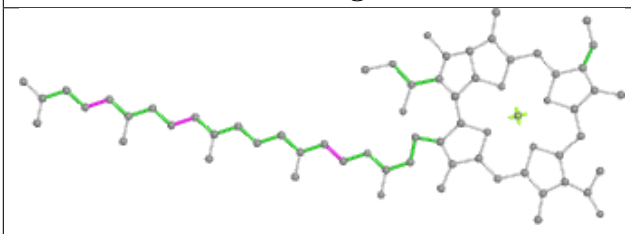
Ligand BCL G 101



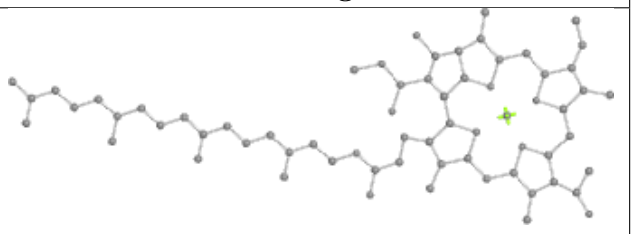
Bond lengths



Bond angles

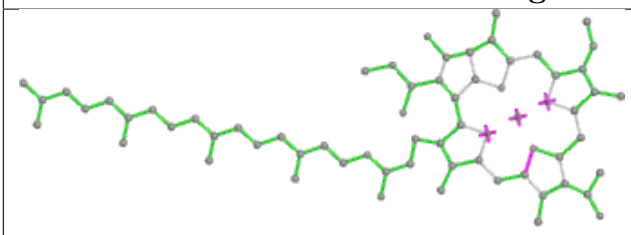


Torsions

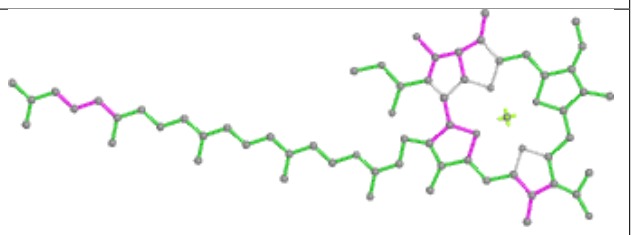


Rings

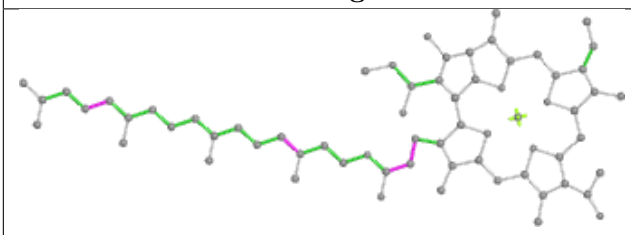
Ligand BCL J 103



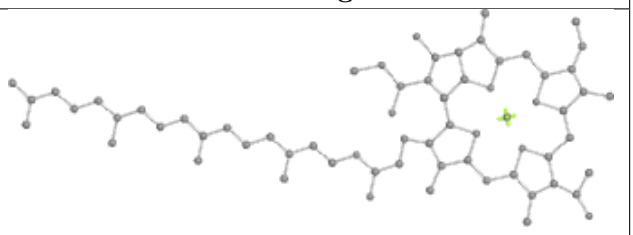
Bond lengths



Bond angles

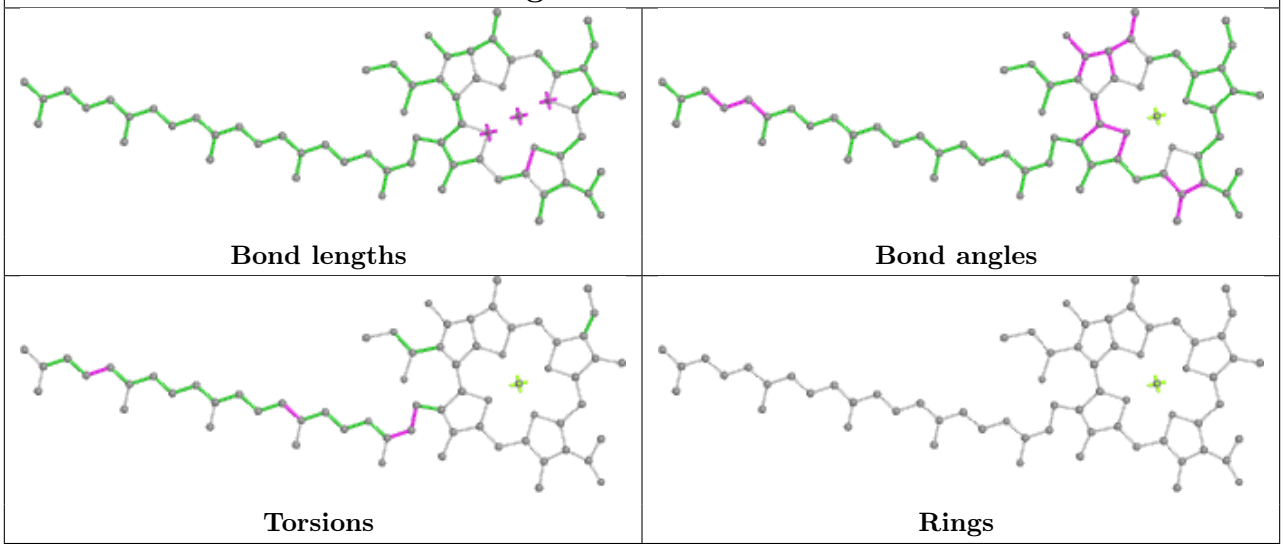


Torsions

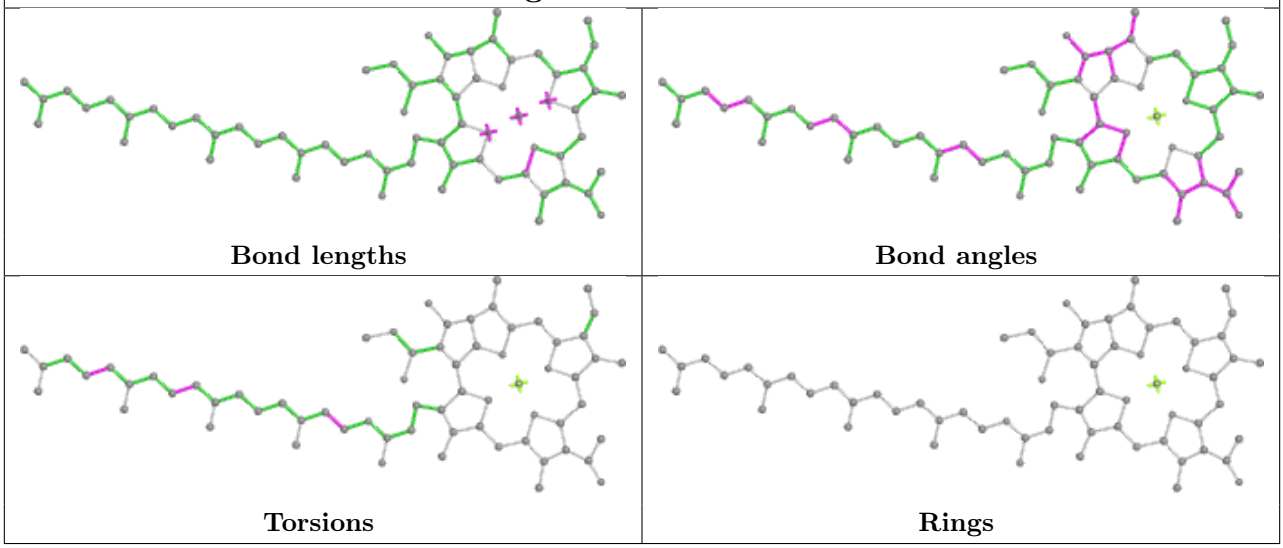


Rings

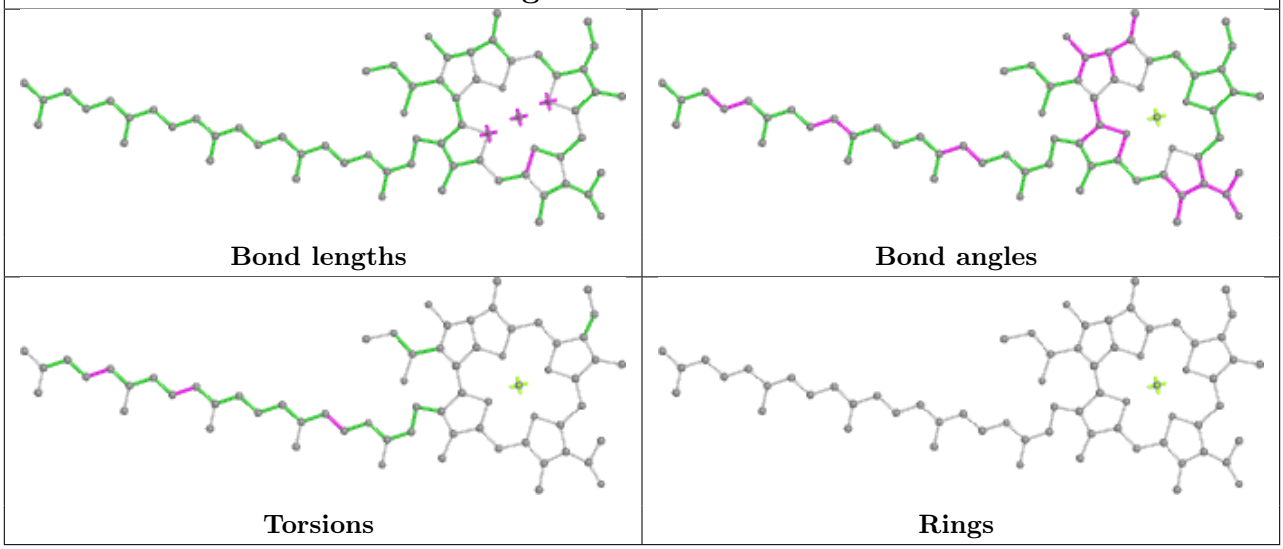
Ligand BCL B 102



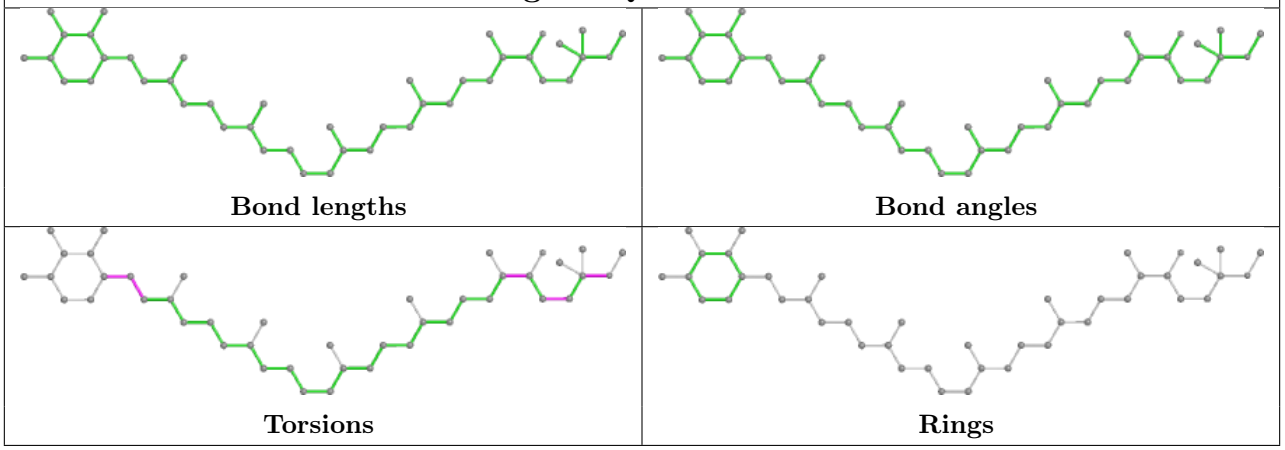
Ligand BCL K 101



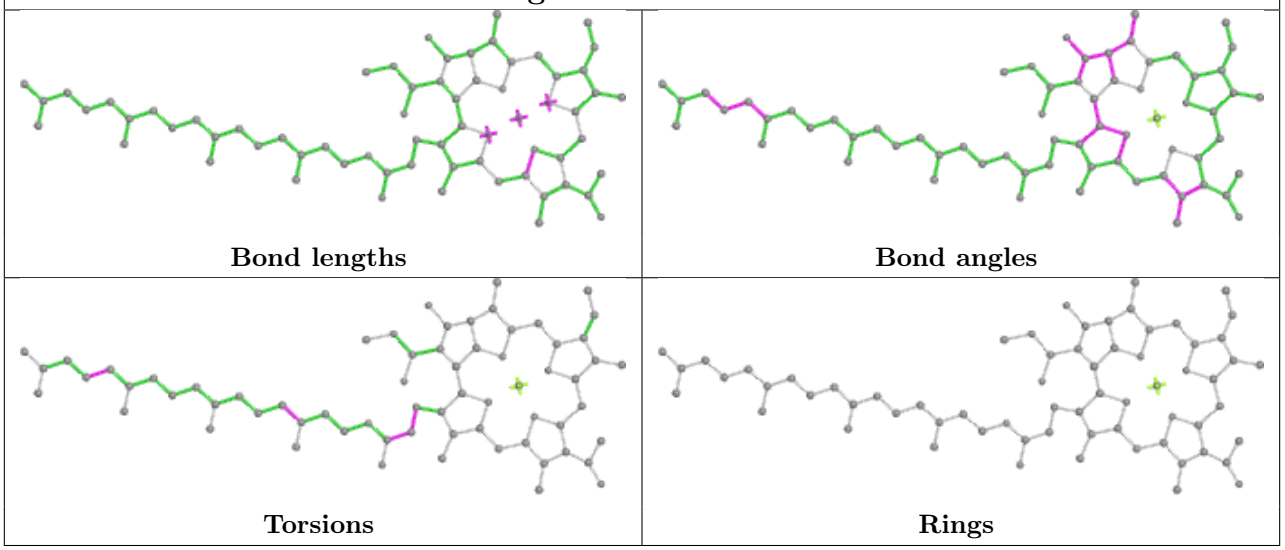
Ligand BCL M 102



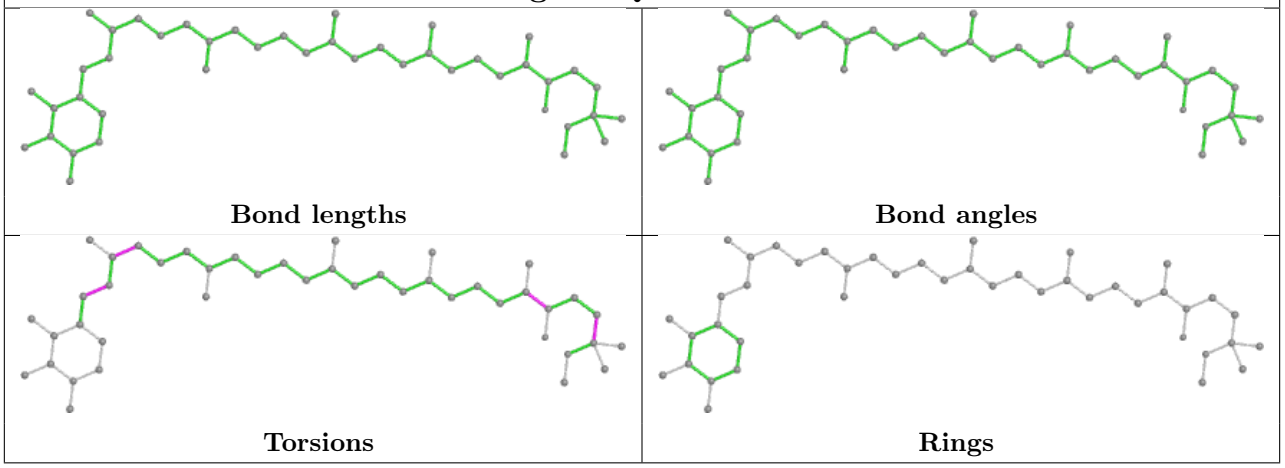
Ligand QSE M 101



Ligand BCL F 103



Ligand QS2 A 102



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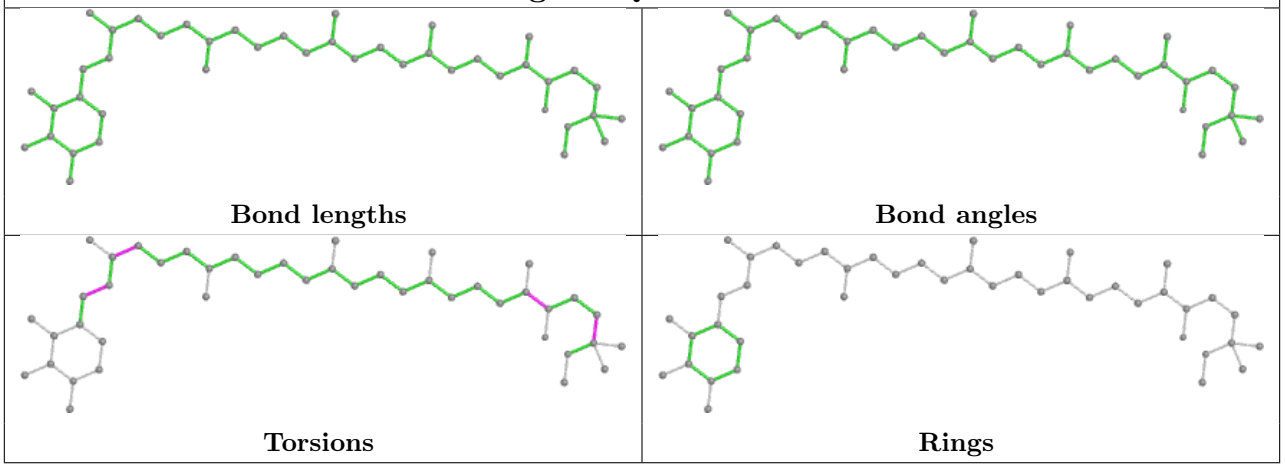
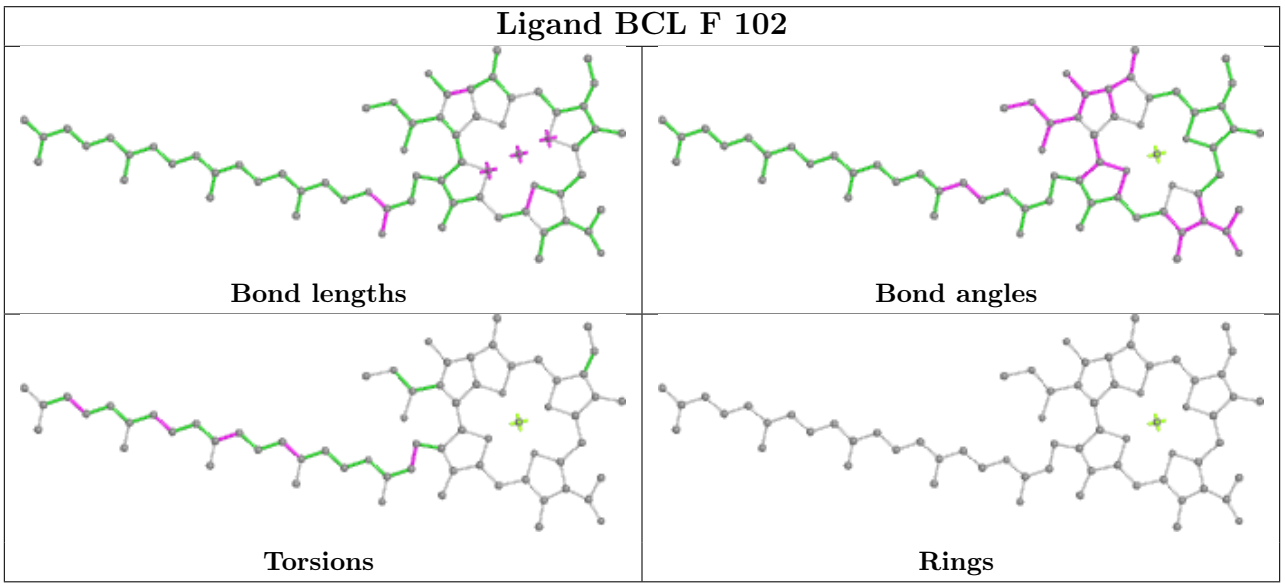


Ligand BCL F 102



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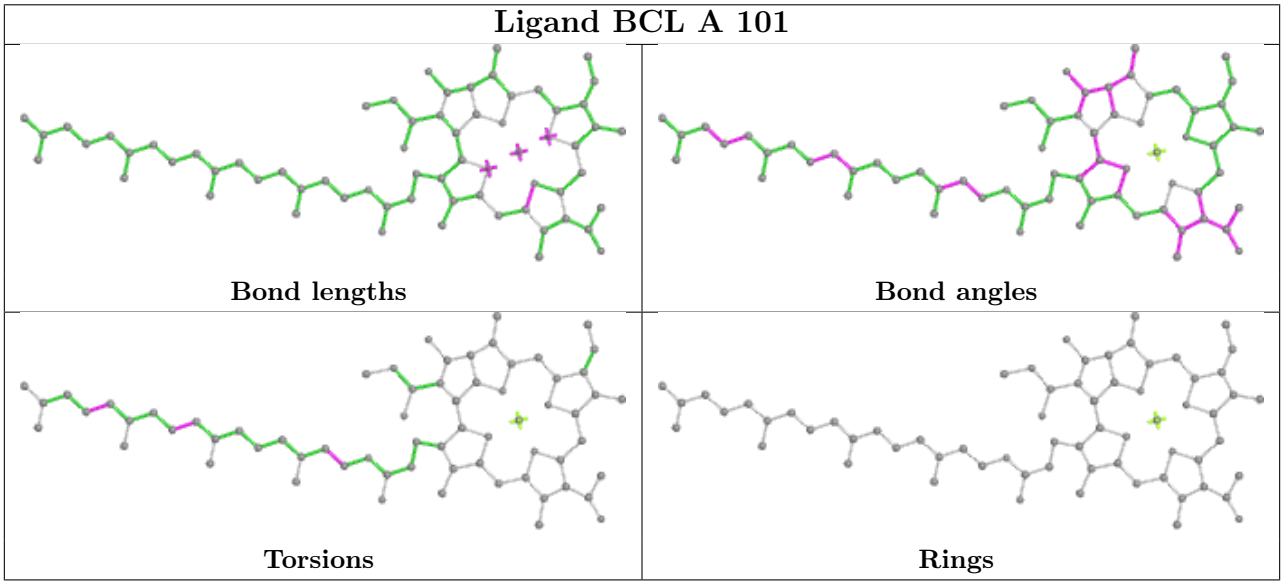
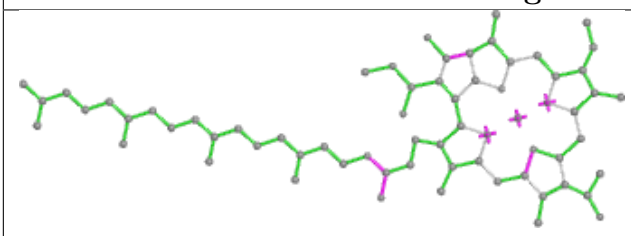
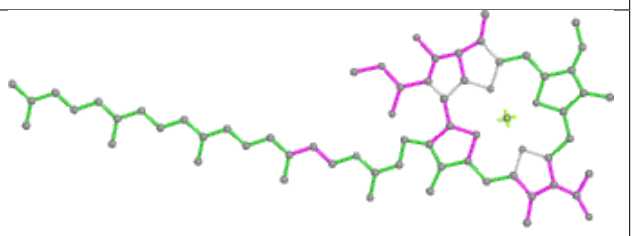


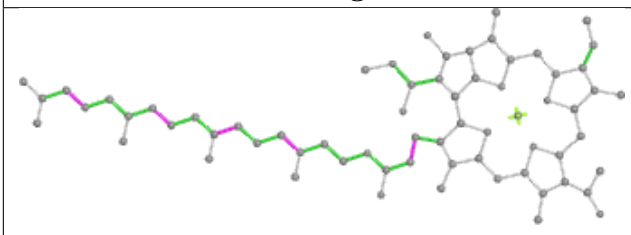
Ligand BCL N 102



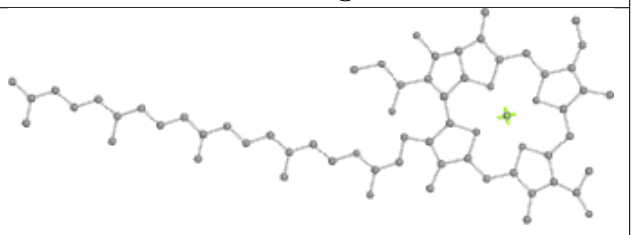
Bond lengths



Bond angles

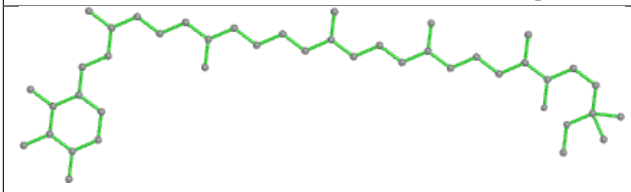


Torsions

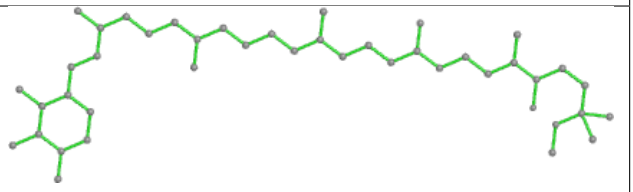


Rings

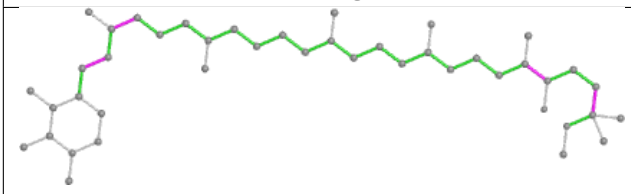
Ligand QS2 B 103



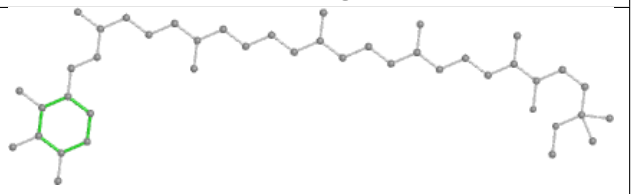
Bond lengths



Bond angles

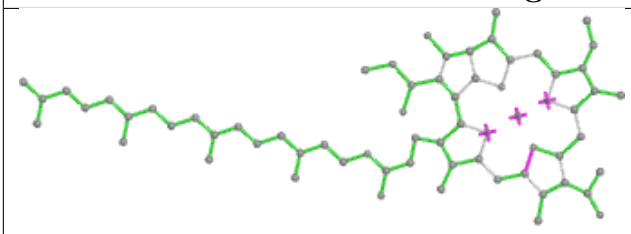


Torsions

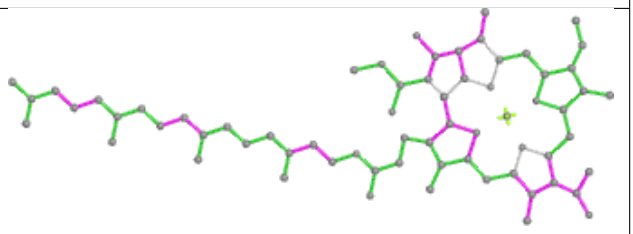


Rings

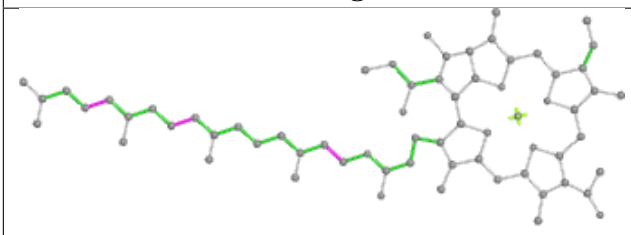
Ligand BCL C 102



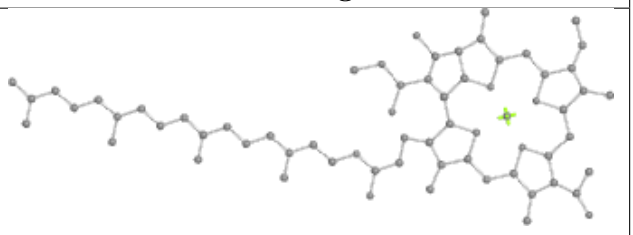
Bond lengths



Bond angles

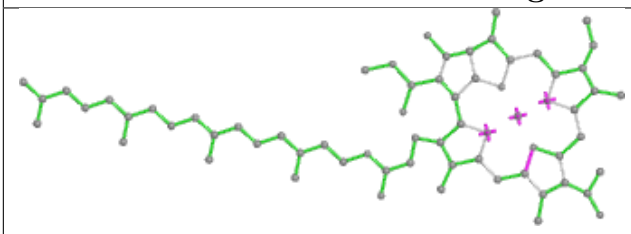


Torsions

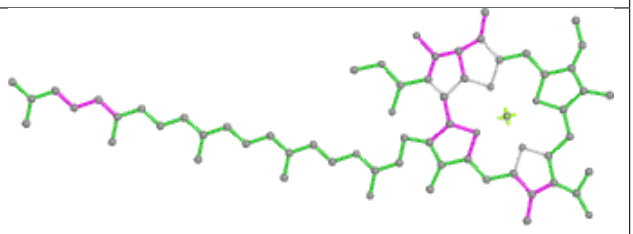


Rings

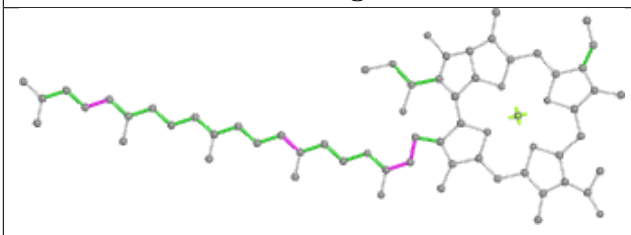
Ligand BCL L 102



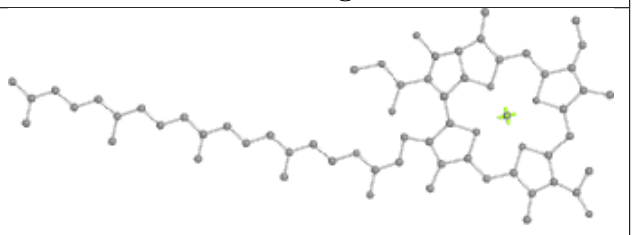
Bond lengths



Bond angles

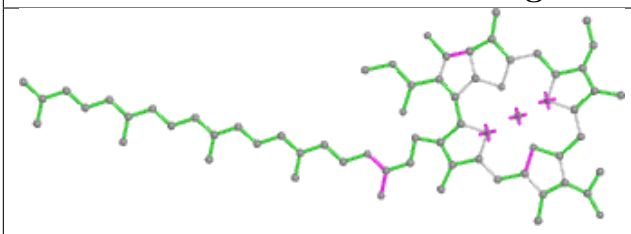


Torsions

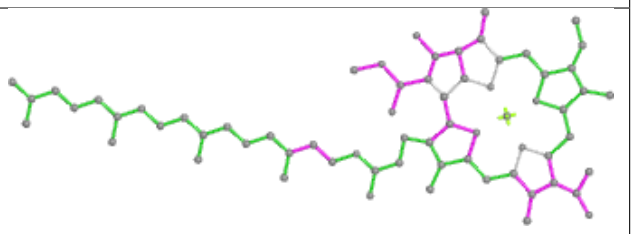


Rings

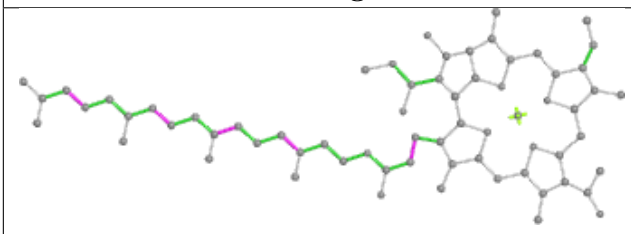
Ligand BCL B 101



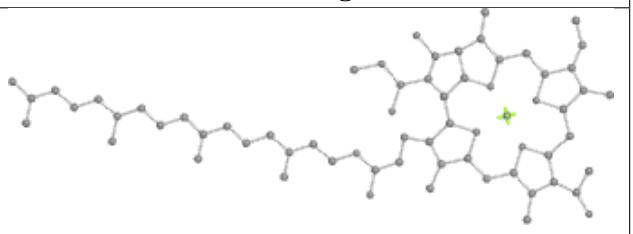
Bond lengths



Bond angles

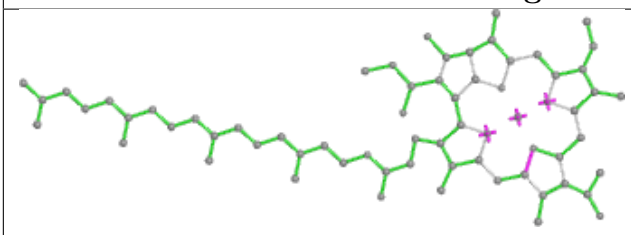


Torsions

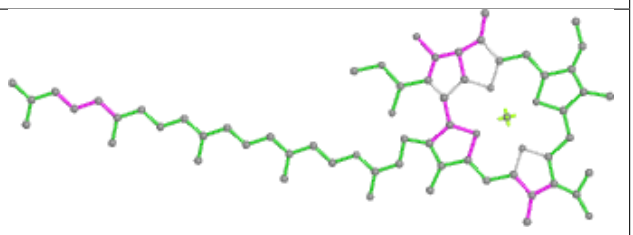


Rings

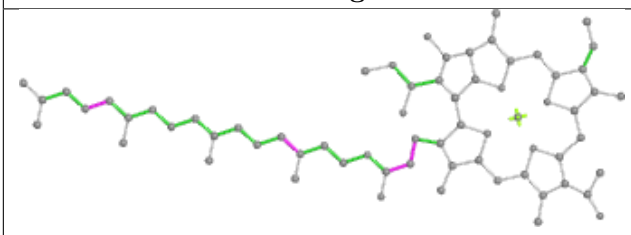
Ligand BCL H 103



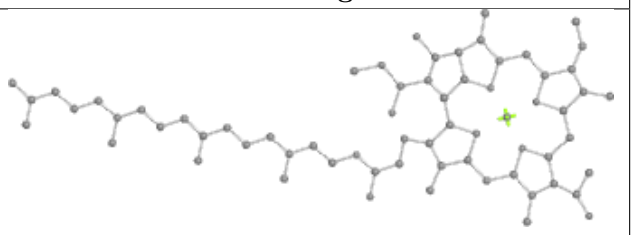
Bond lengths



Bond angles

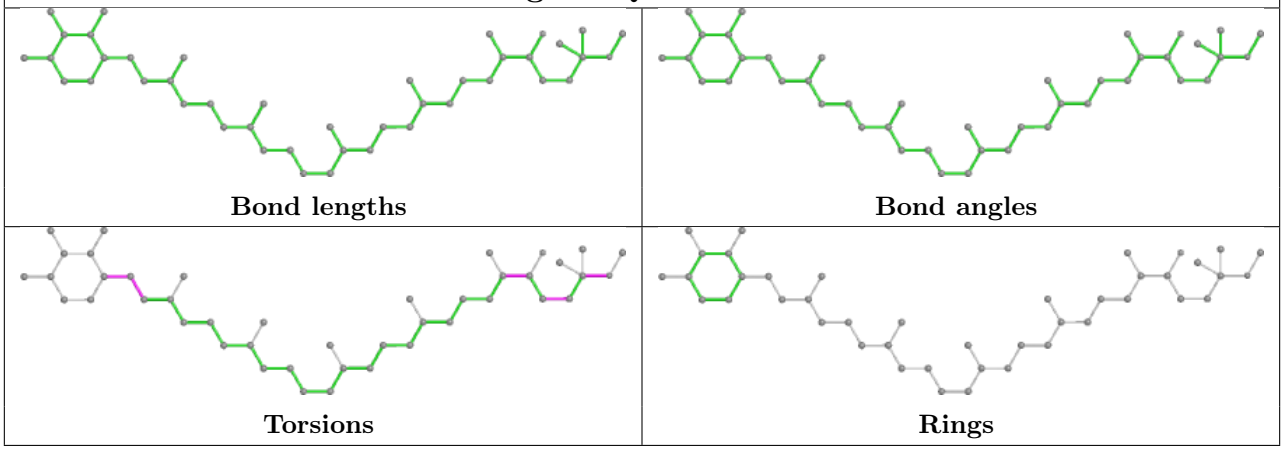


Torsions

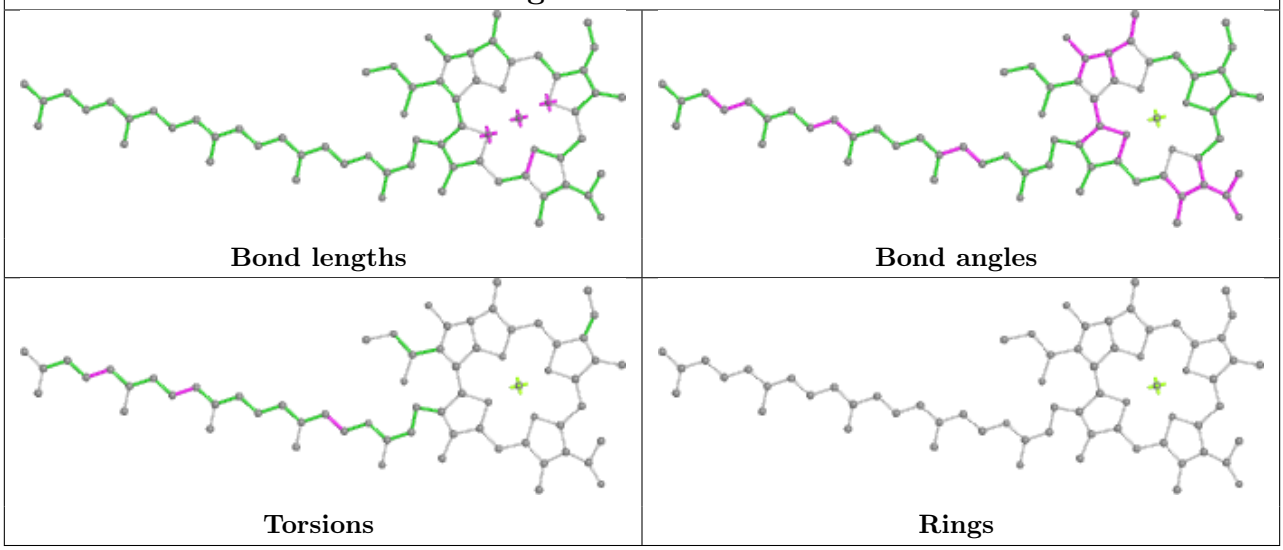


Rings

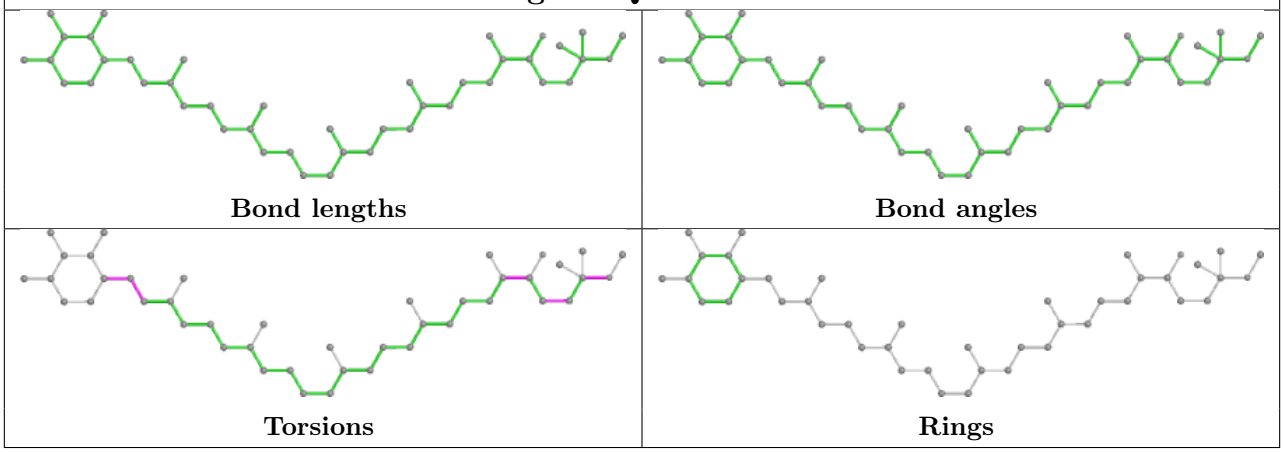
Ligand QSE H 101



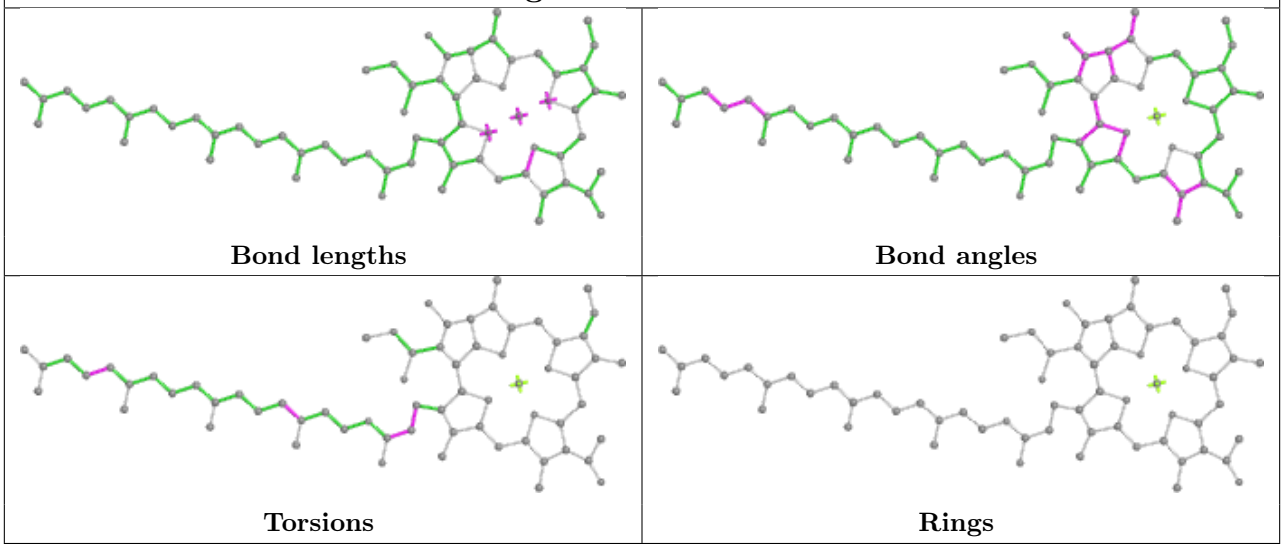
Ligand BCL E 102



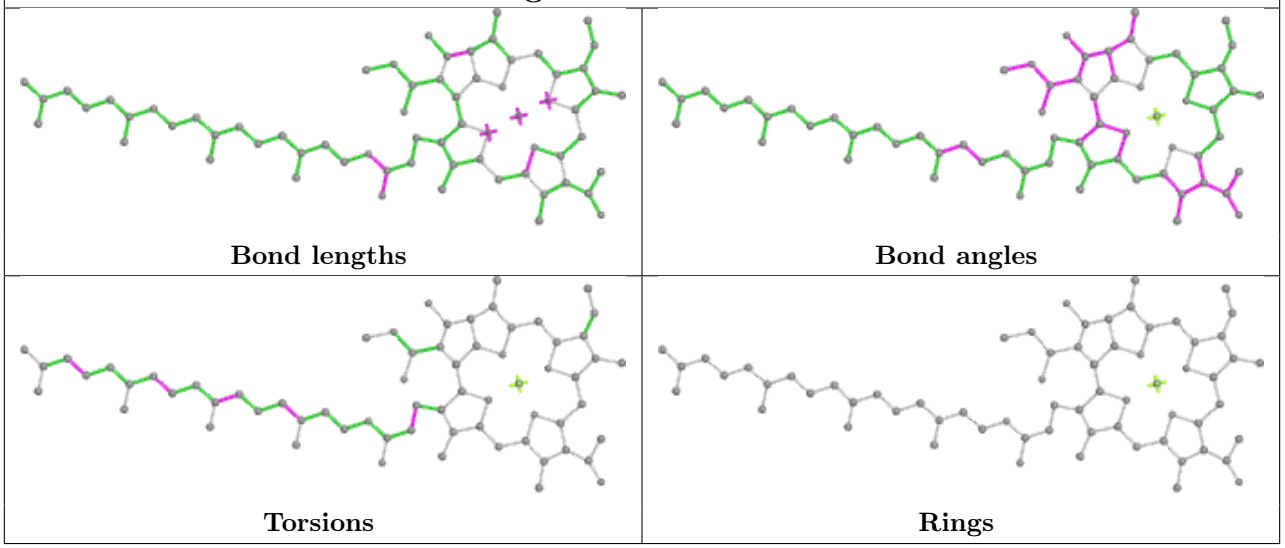
Ligand QSE C 101



Ligand BCL D 102



Ligand BCL H 102



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.

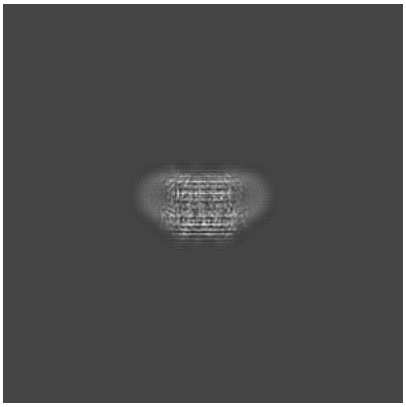
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11516. These allow visual inspection of the internal detail of the map and identification of artifacts.

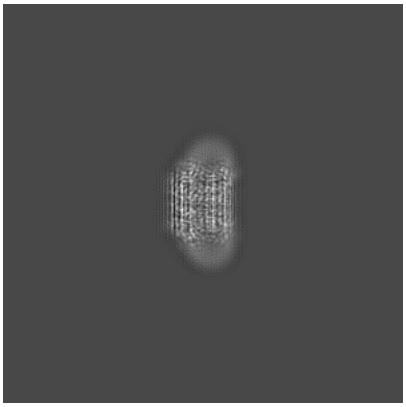
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

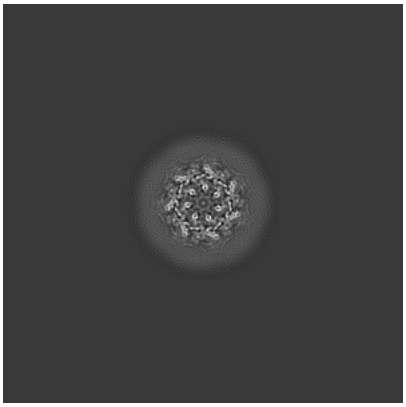
6.1.1 Primary map



X



Y

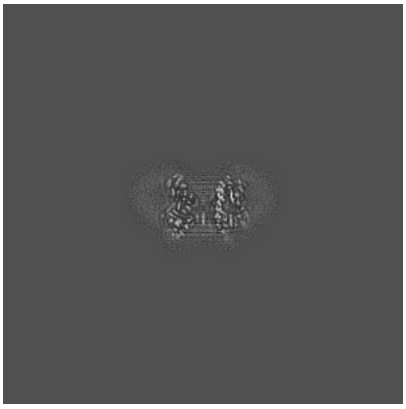


Z

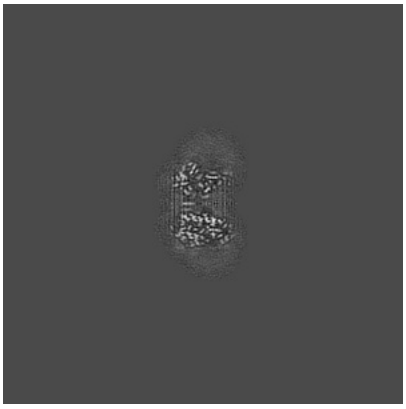
The images above show the map projected in three orthogonal directions.

6.2 Central slices

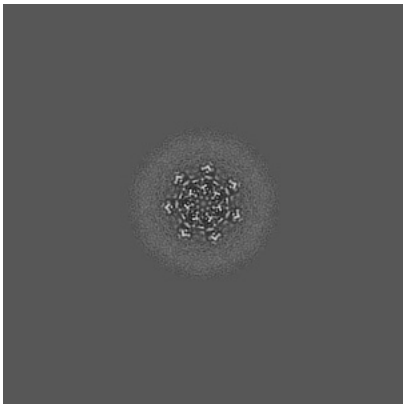
6.2.1 Primary map



X Index: 256



Y Index: 256

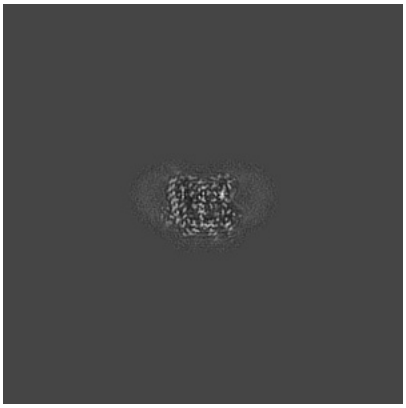


Z Index: 256

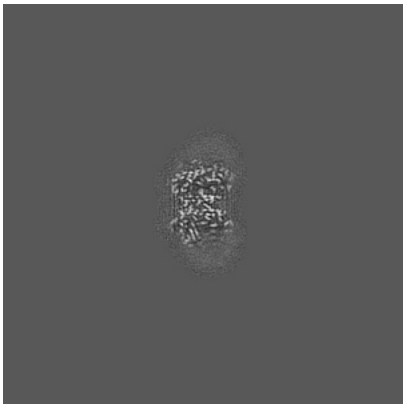
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

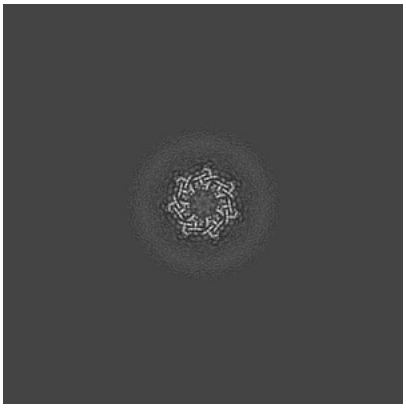
6.3.1 Primary map



X Index: 234



Y Index: 238



Z Index: 269

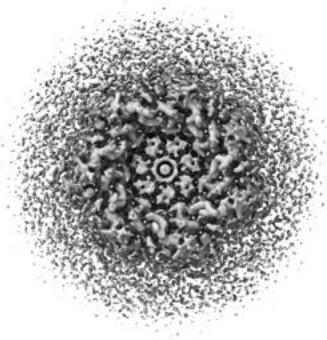
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0167. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

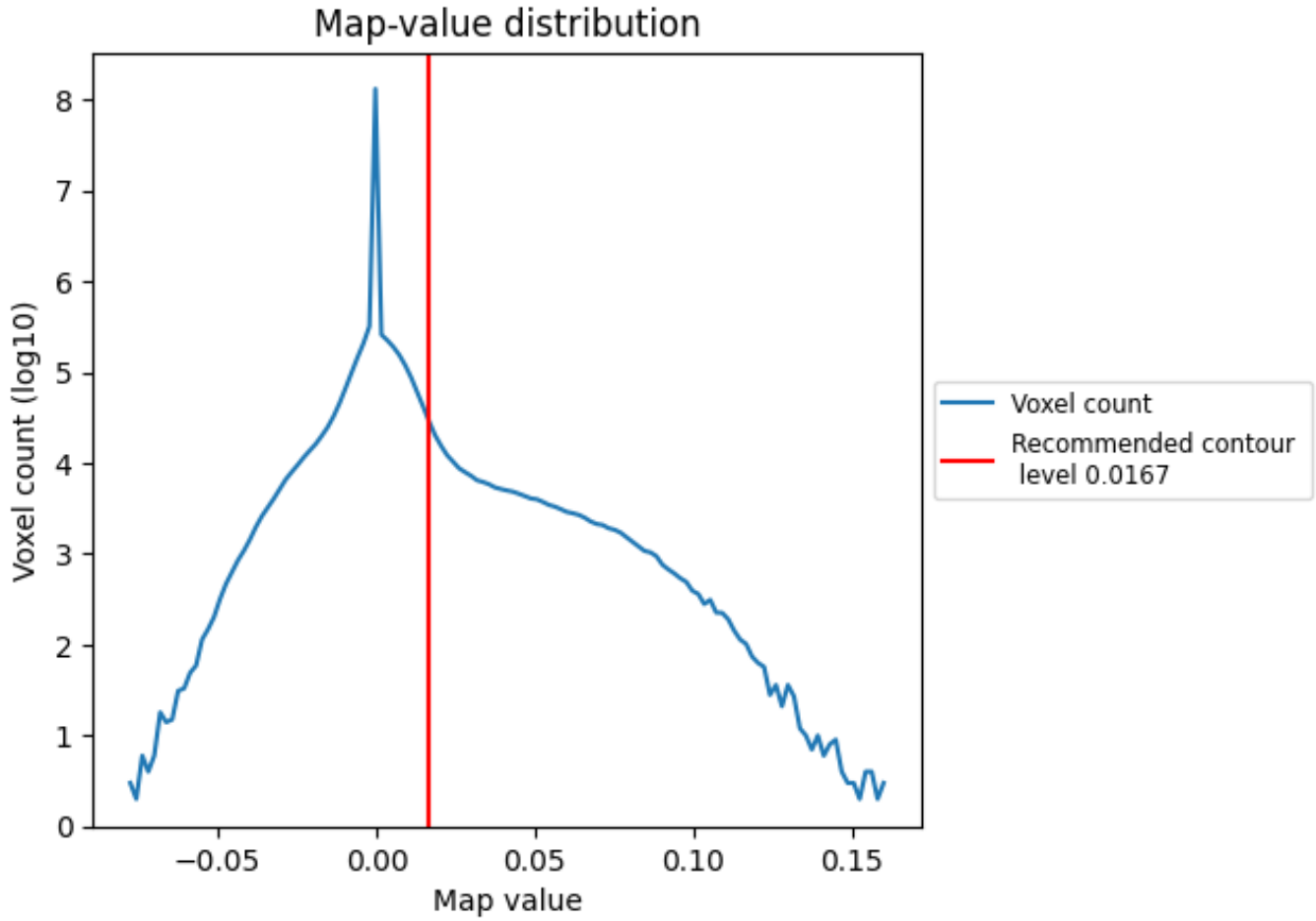
6.5 Mask visualisation (i)

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

7 Map analysis

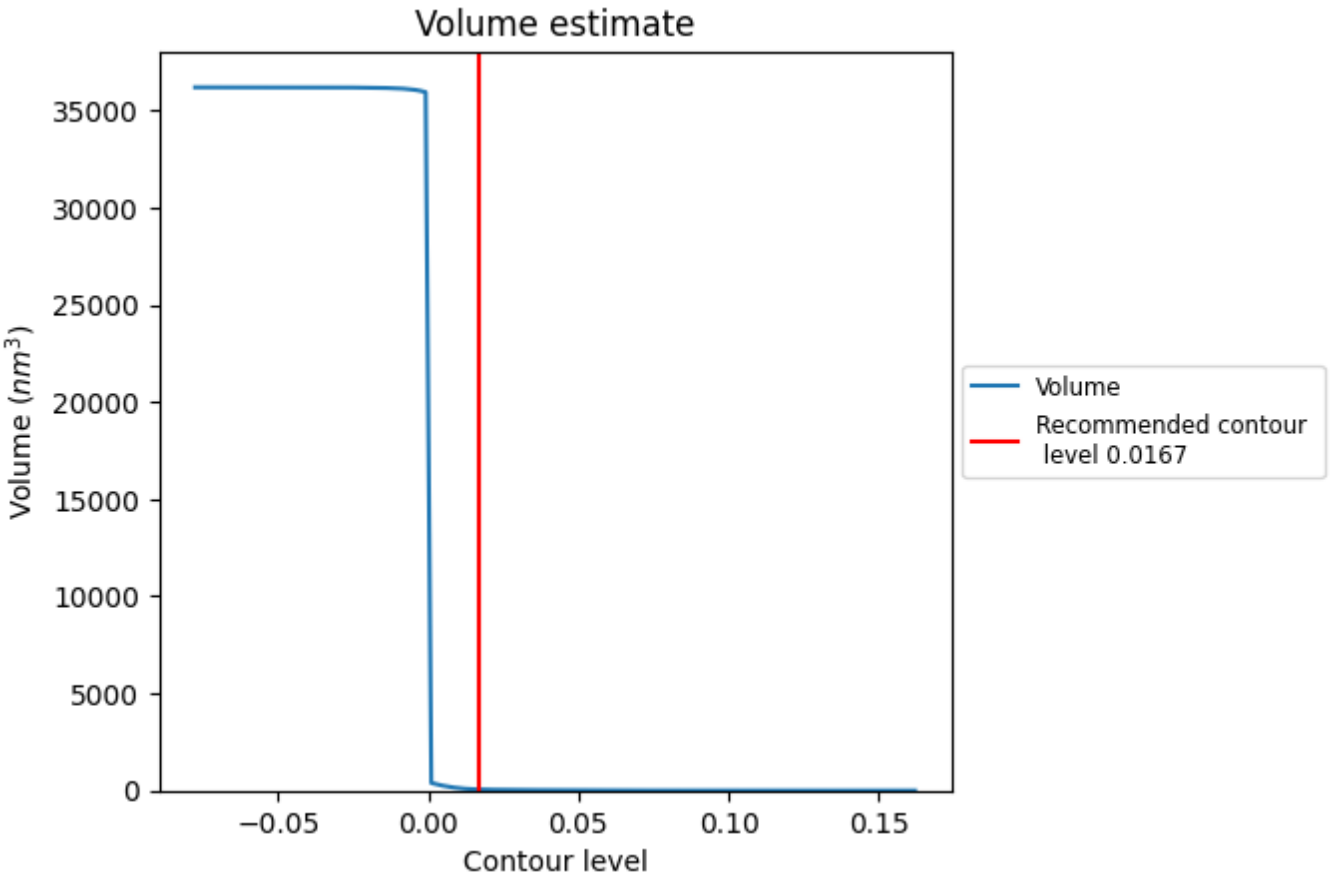
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

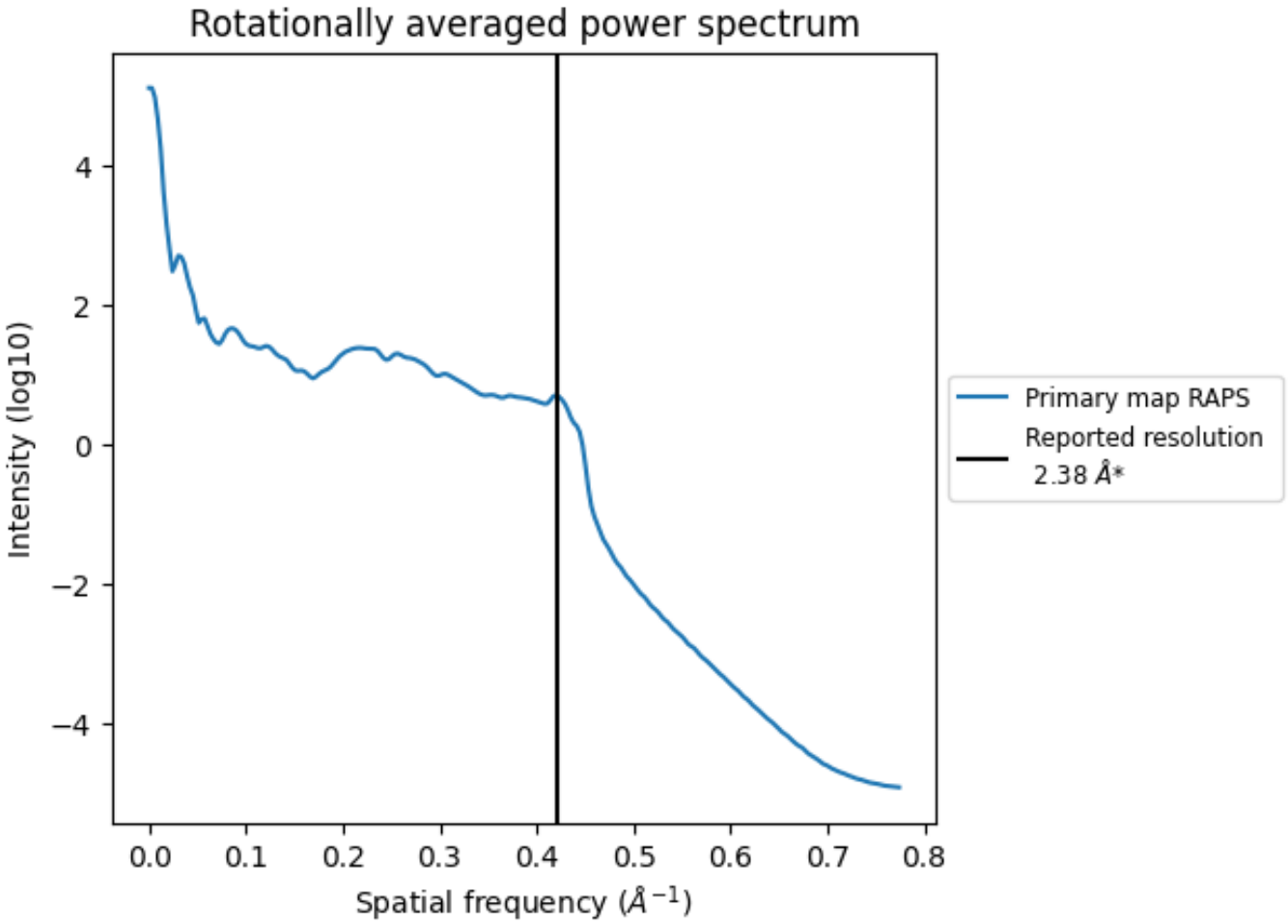
7.2 Volume estimate



The volume at the recommended contour level is 59 nm^3; this corresponds to an approximate mass of 53 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

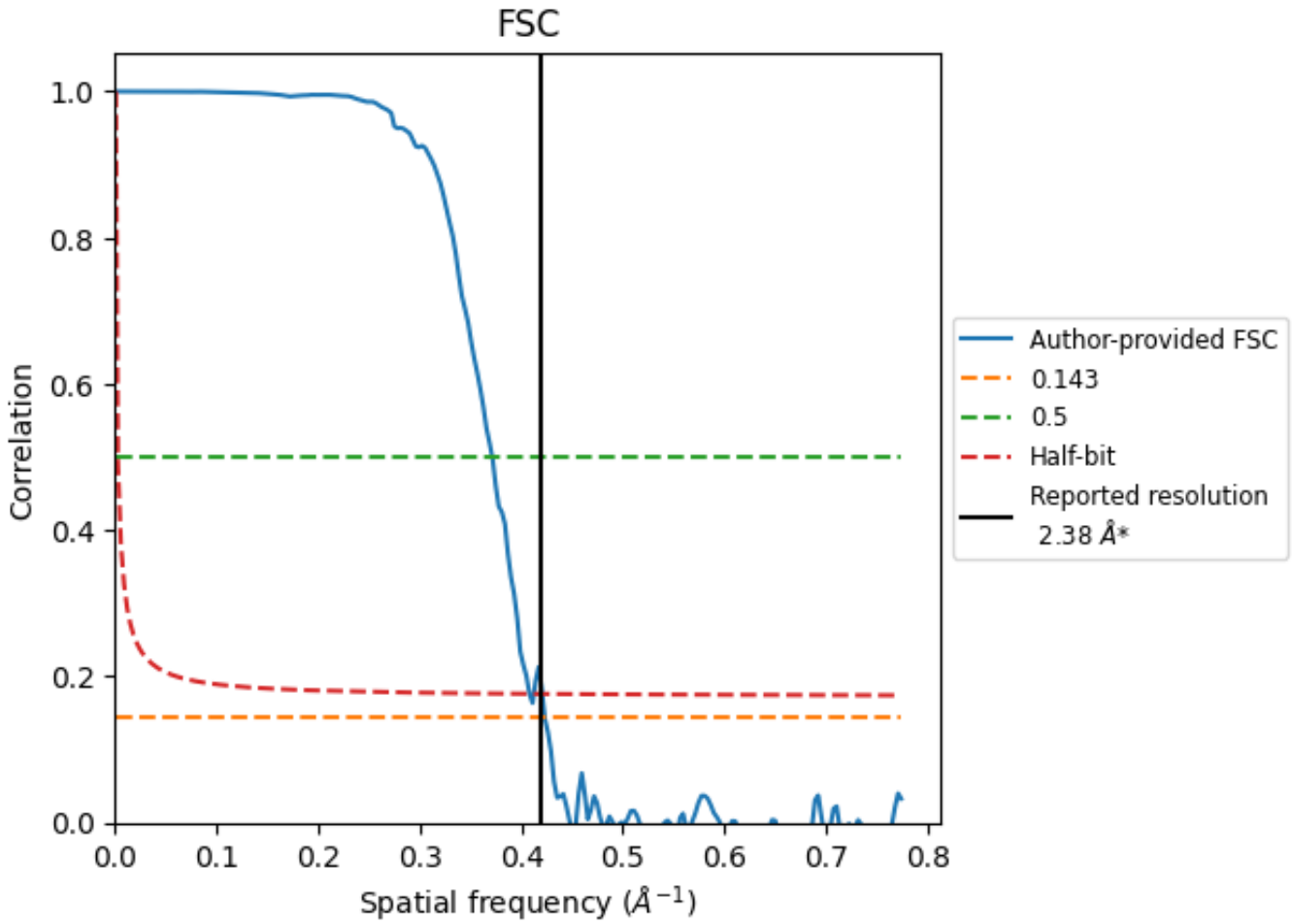


*Reported resolution corresponds to spatial frequency of 0.420 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.420 Å^{-1}

8.2 Resolution estimates (i)

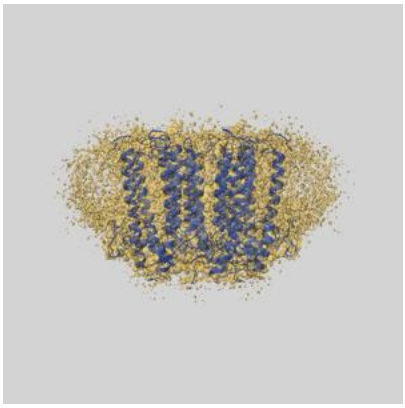
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.38	-	-
Author-provided FSC curve	2.36	2.69	2.45
Unmasked-calculated*	-	-	-

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

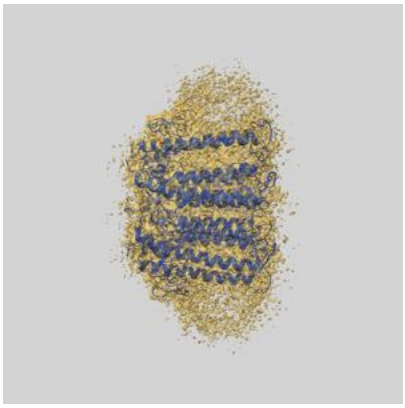
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11516 and PDB model 6ZXA. Per-residue inclusion information can be found in section 3 on page 8.

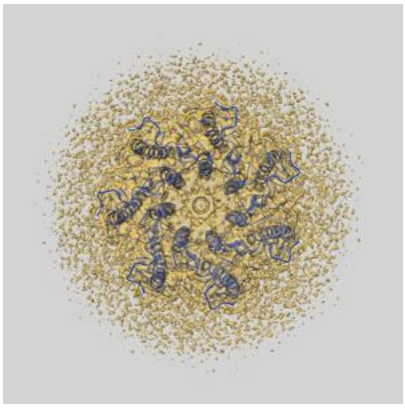
9.1 Map-model overlay



X



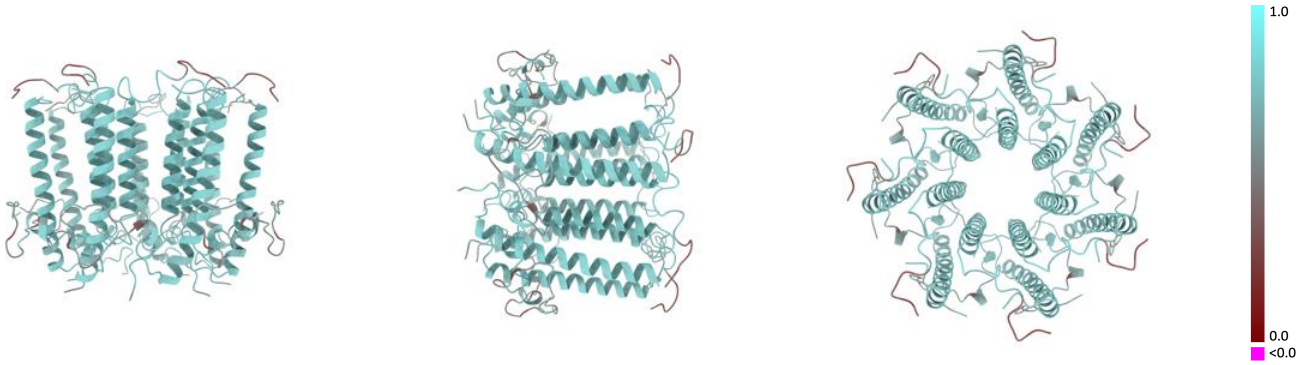
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0167 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.

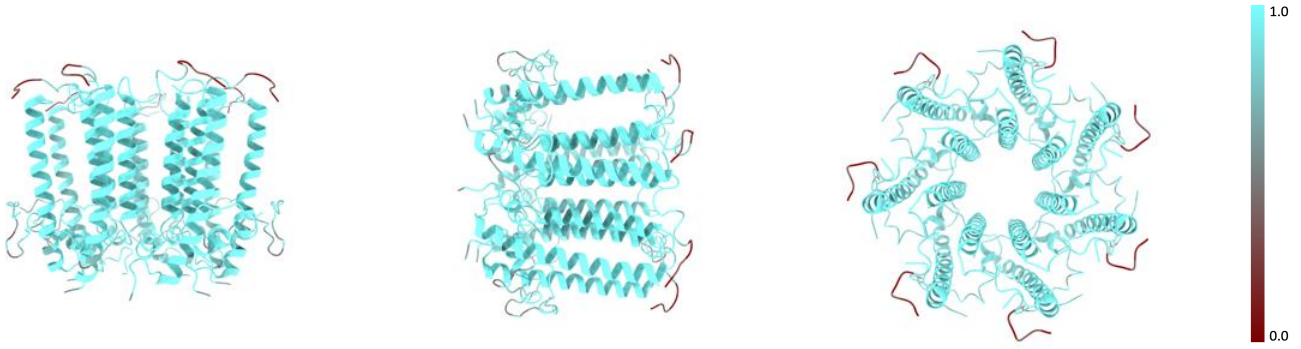
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

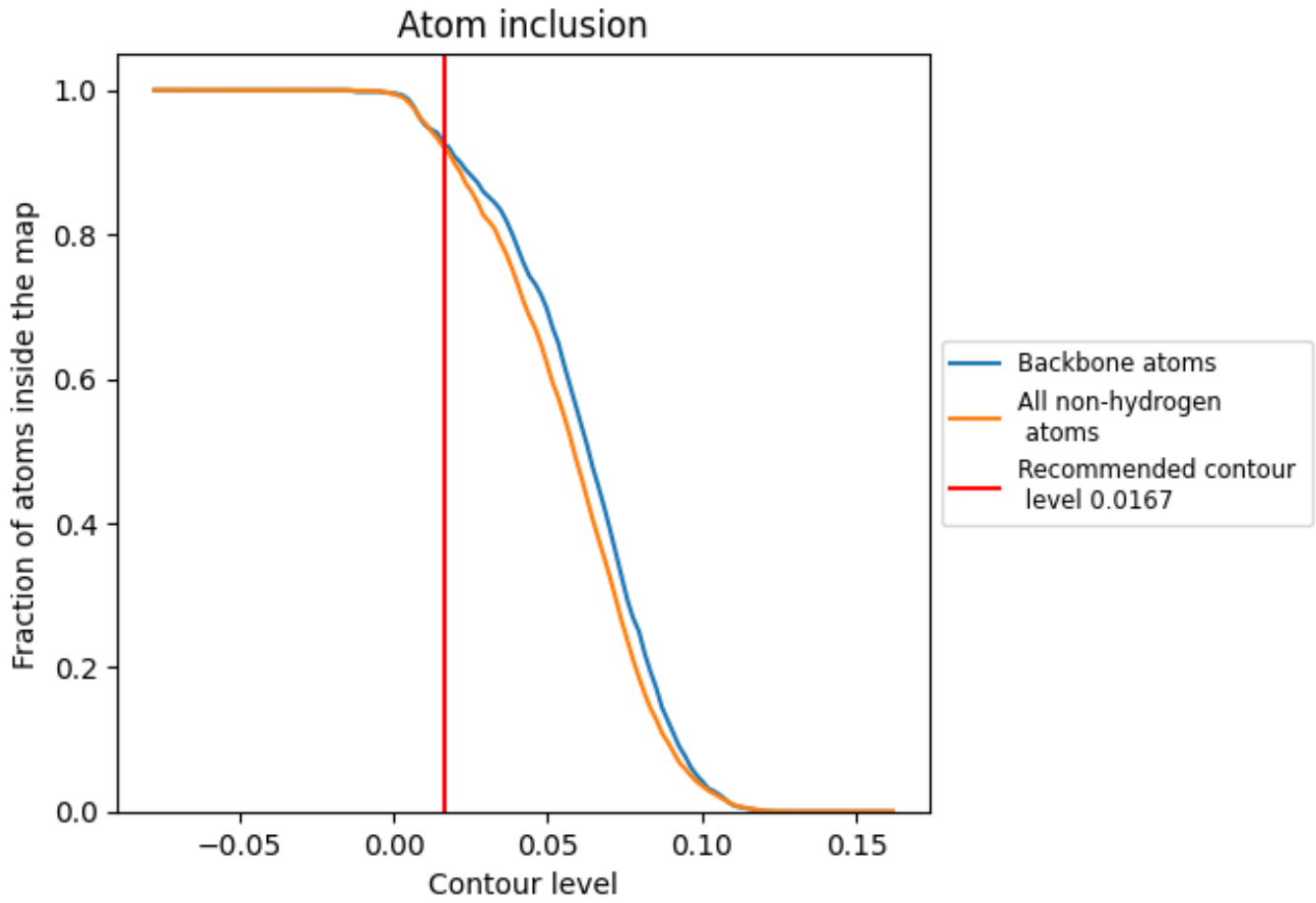
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0167).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.0167) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9185	0.6750
A	0.8821	0.6490
B	0.9564	0.7020
C	0.8836	0.6550
D	0.9628	0.7070
E	0.8879	0.6530
F	0.9639	0.7080
G	0.8806	0.6490
H	0.9639	0.7080
I	0.8836	0.6490
J	0.9658	0.7080
K	0.8806	0.6480
L	0.9628	0.7060
M	0.8908	0.6530
N	0.9639	0.7070