Full wwPDB EM Validation Report ⓘ

Sep 22, 2026 – 07:28 pm BST

PDB ID	:	7ZE3 / pdb_00007ze3
EMDB ID	:	EMD-14682
Title	:	PucD-LH2 complex from Rps. palustris
Authors	:	Qian, P.; Cogdell, R.J.; Nguyen-Phan, T.C.
Deposited on	:	2022-03-30
Resolution	:	2.70 Å(reported)

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

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

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

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

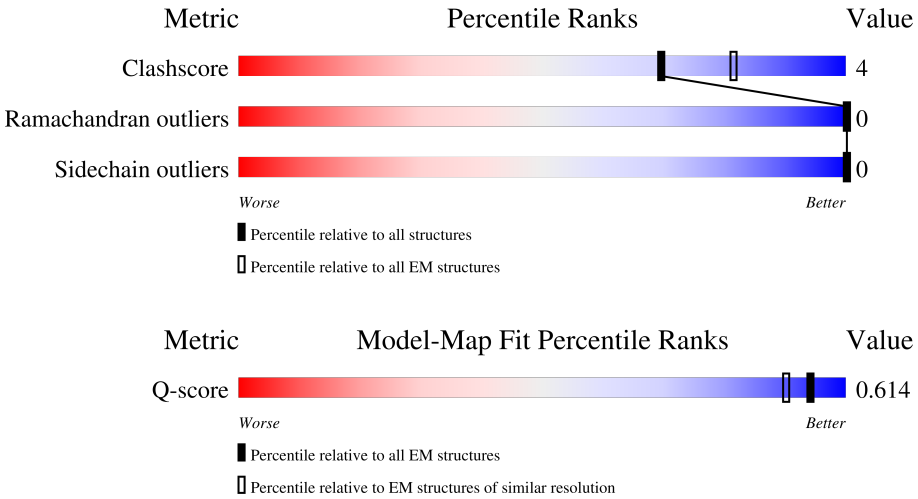
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	59	73% 7% • 19%
1	C	59	75% 7% 19%
1	E	59	75% 5% • 19%
1	G	59	71% 10% 19%

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Mol	Chain	Length	Quality of chain
1	I	59	68% 14% 19%
1	K	59	73% 8% 19%
1	M	59	69% 10% 19%
1	O	59	71% 10% 19%
1	Q	59	73% 7% 19%
2	B	51	86% 10%
2	D	51	94%
2	F	51	86% 10%
2	H	51	88% 8%
2	J	51	90% 6%
2	L	51	6% 90% 6%
2	N	51	86% 10%
2	P	51	88% 8%
2	R	51	90% 6%
3	S	97	26% 89% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10285 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
			377	252	63	59	3		
1	C	48	Total	C	N	O	S	0	0
			377	252	63	59	3		
1	E	48	Total	C	N	O	S	0	0
			377	252	63	59	3		
1	G	48	Total	C	N	O	S	0	0
			377	252	63	59	3		
1	I	48	Total	C	N	O	S	0	0
			377	252	63	59	3		
1	K	48	Total	C	N	O	S	0	0
			377	252	63	59	3		
1	M	48	Total	C	N	O	S	0	0
			377	252	63	59	3		
1	O	48	Total	C	N	O	S	0	0
			377	252	63	59	3		
1	Q	48	Total	C	N	O	S	0	0
			377	252	63	59	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	49	Total	C	N	O	0	0
			396	261	65	70		
2	D	49	Total	C	N	O	0	0
			396	261	65	70		
2	F	49	Total	C	N	O	0	0
			396	261	65	70		
2	H	49	Total	C	N	O	0	0
			396	261	65	70		
2	J	49	Total	C	N	O	0	0
			396	261	65	70		
2	L	49	Total	C	N	O	0	0
			396	261	65	70		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	49	Total 396	C 261	N 65	O 70	0	0
2	P	49	Total 396	C 261	N 65	O 70	0	0
2	R	49	Total 396	C 261	N 65	O 70	0	0

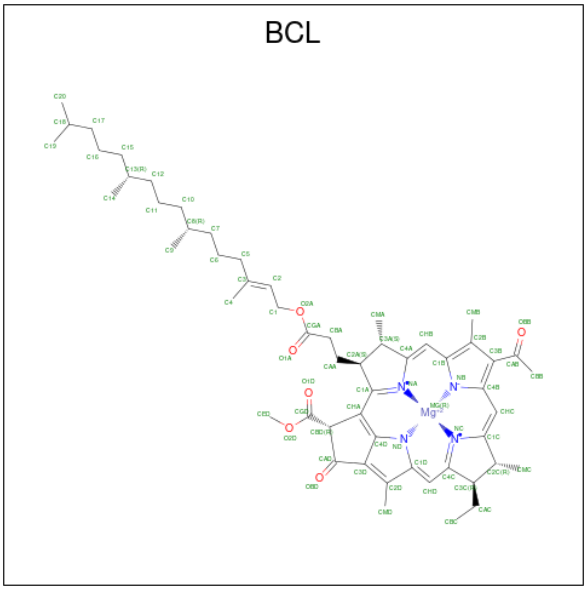
- Molecule 3 is a protein called PucA-LH2-gamma.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 66	C 55	Mg 1	N 4	O 6	0

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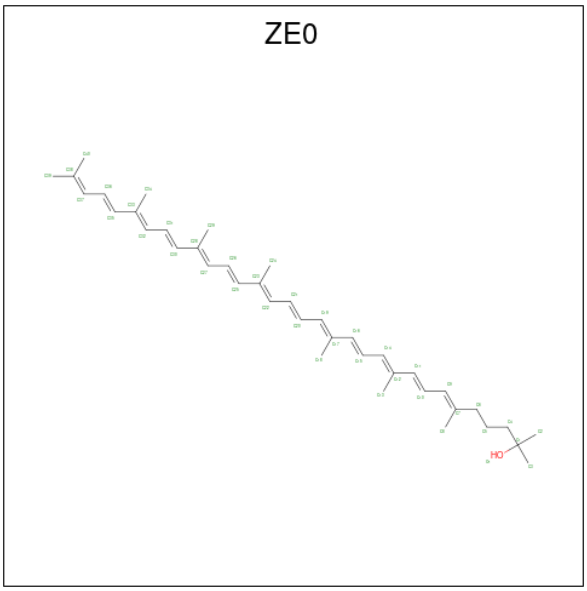
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
4	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 5 is (3'E)-3',4'-didehydro-1,2-dihydro-psi,psi-caroten-1-ol (CCD ID: ZE0) (formula: $C_{40}H_{56}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 41 40 1	0
5	B	1	Total C O 41 40 1	0
5	C	1	Total C O 41 40 1	0
5	E	1	Total C O 41 40 1	0
5	G	1	Total C O 41 40 1	0
5	I	1	Total C O 41 40 1	0
5	K	1	Total C O 41 40 1	0
5	M	1	Total C O 41 40 1	0
5	O	1	Total C O 41 40 1	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	3	Total O 3 3	0
6	B	1	Total O 1 1	0
6	C	3	Total O 3 3	0
6	D	1	Total O 1 1	0
6	E	3	Total O 3 3	0
6	F	1	Total O 1 1	0
6	G	3	Total O 3 3	0
6	H	1	Total O 1 1	0
6	I	2	Total O 2 2	0
6	J	2	Total O 2 2	0
6	K	3	Total O 3 3	0

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Mol	Chain	Residues	Atoms	AltConf
6	M	4	Total O 4 4	0
6	N	1	Total O 1 1	0
6	O	3	Total O 3 3	0
6	P	1	Total O 1 1	0
6	Q	4	Total O 4 4	0
6	R	1	Total O 1 1	0

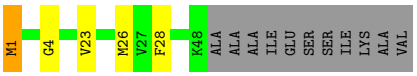
3 Residue-property plots (i)

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: Light-harvesting protein B-800-850 alpha chain

Chain A:

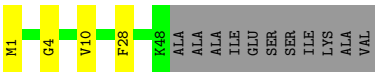




- Molecule 1: Light-harvesting protein B-800-850 alpha chain

Chain C:

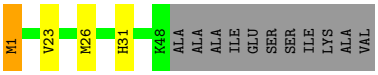




- Molecule 1: Light-harvesting protein B-800-850 alpha chain

Chain E:

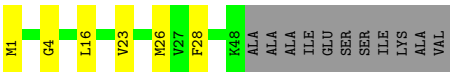




- Molecule 1: Light-harvesting protein B-800-850 alpha chain

Chain G:

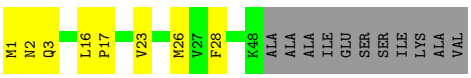




- Molecule 1: Light-harvesting protein B-800-850 alpha chain

Chain I:

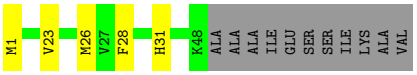




- Molecule 1: Light-harvesting protein B-800-850 alpha chain

Chain K:

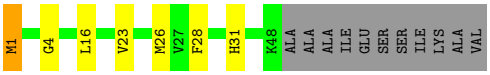




• Molecule 1: Light-harvesting protein B-800-850 alpha chain

Chain M:

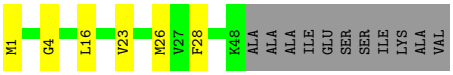




• Molecule 1: Light-harvesting protein B-800-850 alpha chain

Chain O:

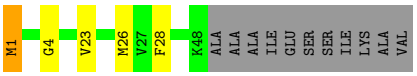




• Molecule 1: Light-harvesting protein B-800-850 alpha chain

Chain Q:

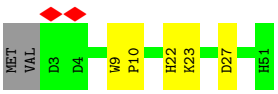




• Molecule 2: Light-harvesting protein B-800-850 beta chain

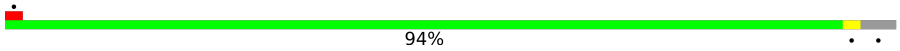
Chain B:

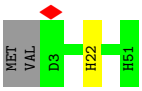




• Molecule 2: Light-harvesting protein B-800-850 beta chain

Chain D:





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

Chain F:

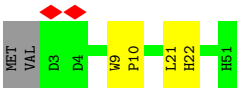




• Molecule 2: Light-harvesting protein B-800-850 beta chain

Chain H:

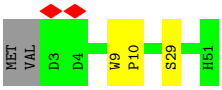




• Molecule 2: Light-harvesting protein B-800-850 beta chain

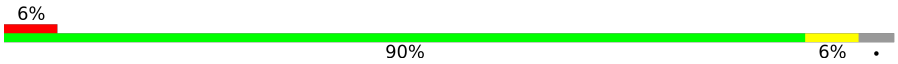
Chain J:

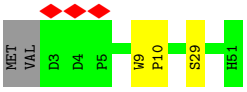




• Molecule 2: Light-harvesting protein B-800-850 beta chain

Chain L:

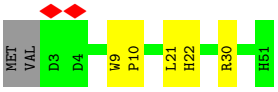




• Molecule 2: Light-harvesting protein B-800-850 beta chain

Chain N:

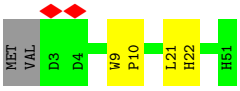




• Molecule 2: Light-harvesting protein B-800-850 beta chain

Chain P:

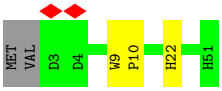




• Molecule 2: Light-harvesting protein B-800-850 beta chain

Chain R:

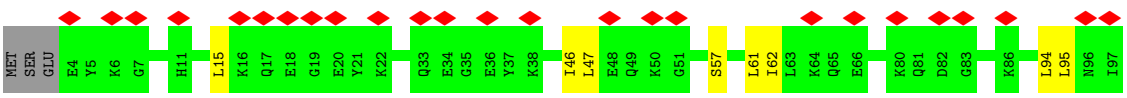




• Molecule 3: PucA-LH2-gamma

Chain S:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	809902	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.361	Depositor
Minimum map value	-0.217	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0347	Depositor
Map size (Å)	195.0, 195.0, 195.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CXM, BCL, ZE0

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	0.13	0/376	0.42	0/513
1	C	0.13	0/376	0.41	0/513
1	E	0.13	0/376	0.42	0/513
1	G	0.13	0/376	0.40	0/513
1	I	0.13	0/376	0.40	0/513
1	K	0.14	0/376	0.41	0/513
1	M	0.13	0/376	0.40	0/513
1	O	0.14	0/376	0.42	0/513
1	Q	0.13	0/376	0.40	0/513
2	B	0.14	0/410	0.46	0/561
2	D	0.13	0/410	0.43	0/561
2	F	0.13	0/410	0.43	0/561
2	H	0.13	0/410	0.44	0/561
2	J	0.13	0/410	0.44	0/561
2	L	0.13	0/410	0.42	0/561
2	N	0.13	0/410	0.43	0/561
2	P	0.14	0/410	0.43	0/561
2	R	0.13	0/410	0.45	0/561
3	S	0.12	0/763	0.38	0/1023
All	All	0.13	0/7837	0.42	0/10689

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	377	0	401	5	0
1	C	377	0	401	3	0
1	E	377	0	401	5	0
1	G	377	0	401	5	0
1	I	377	0	401	5	0
1	K	377	0	401	5	0
1	M	377	0	401	9	0
1	O	377	0	401	5	0
1	Q	377	0	401	6	0
2	B	396	0	383	4	0
2	D	396	0	383	1	0
2	F	396	0	383	4	0
2	H	396	0	383	3	0
2	J	396	0	383	2	0
2	L	396	0	383	2	0
2	N	396	0	383	5	0
2	P	396	0	383	3	0
2	R	396	0	383	2	0
3	S	744	0	730	9	0
4	A	132	0	148	2	0
4	B	66	0	74	2	0
4	C	132	0	148	2	0
4	D	66	0	74	2	0
4	E	132	0	148	3	0
4	F	66	0	74	2	0
4	G	132	0	148	2	0
4	H	66	0	74	1	0
4	I	132	0	148	1	0
4	J	66	0	74	1	0
4	K	132	0	148	1	0
4	L	66	0	74	2	0
4	M	198	0	222	3	0
4	O	132	0	148	1	0
4	P	66	0	74	1	0
4	Q	132	0	148	1	0
4	R	66	0	74	1	0
4	S	396	0	444	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	41	0	0	1	0
5	B	41	0	0	1	0
5	C	41	0	0	0	0
5	E	41	0	0	2	0
5	G	41	0	0	0	0
5	I	41	0	0	0	0
5	K	41	0	0	0	0
5	M	41	0	0	1	0
5	O	41	0	0	1	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	3	0	0	0	0
6	H	1	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	3	0	0	0	0
6	M	4	0	0	0	0
6	N	1	0	0	0	0
6	O	3	0	0	0	0
6	P	1	0	0	0	0
6	Q	4	0	0	0	0
6	R	1	0	0	0	0
All	All	10285	0	10228	73	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 4.

All (73) 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:23:LYS:HG2	3:S:61:LEU:HD23	1.79	0.65
1:A:23:VAL:HA	1:A:26:MET:HE2	1.80	0.62
1:K:23:VAL:HA	1:K:26:MET:HE2	1.81	0.61
2:B:27:ASP:HB2	3:S:61:LEU:HD21	1.83	0.60
1:A:1:CXM:HB2	3:S:62:ILE:HA	1.86	0.57
4:A:102:BCL:H42	4:B:101:BCL:H193	1.87	0.56
1:I:23:VAL:HA	1:I:26:MET:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:MET:HB2	1:G:28:PHE:CZ	2.42	0.54
4:M:102:BCL:HHC	4:M:102:BCL:HBB2	1.89	0.54
5:M:104:ZE0:C23	4:P:101:BCL:H43	2.38	0.54
1:Q:23:VAL:HA	1:Q:26:MET:HE2	1.90	0.53
4:I:101:BCL:HHC	4:I:101:BCL:HBB2	1.90	0.53
4:K:101:BCL:HBB2	4:K:101:BCL:HHC	1.91	0.53
1:A:26:MET:HB2	1:C:28:PHE:CZ	2.44	0.52
1:A:28:PHE:CZ	1:Q:26:MET:HB2	2.44	0.52
1:M:23:VAL:HA	1:M:26:MET:HE2	1.91	0.52
1:K:26:MET:HB2	1:M:28:PHE:CZ	2.45	0.52
4:A:102:BCL:HHC	4:A:102:BCL:HBB2	1.92	0.51
1:O:26:MET:HB2	1:Q:28:PHE:CZ	2.45	0.51
5:A:103:ZE0:C23	4:D:101:BCL:H43	2.41	0.51
2:J:29:SER:HB3	4:J:101:BCL:H41	1.92	0.51
1:G:23:VAL:HA	1:G:26:MET:HE2	1.91	0.51
4:C:102:BCL:HBB2	4:C:102:BCL:HHC	1.93	0.51
4:E:101:BCL:HBB2	4:E:101:BCL:HHC	1.93	0.50
4:O:102:BCL:HBB2	4:O:102:BCL:HHC	1.92	0.50
1:G:26:MET:HB2	1:I:28:PHE:CZ	2.47	0.50
1:I:26:MET:HB2	1:K:28:PHE:CZ	2.48	0.49
4:G:102:BCL:HBB2	4:G:102:BCL:HHC	1.94	0.49
4:C:102:BCL:H42	4:D:101:BCL:H193	1.94	0.49
5:O:103:ZE0:C23	4:R:101:BCL:H43	2.43	0.49
1:E:31:HIS:CE1	4:F:101:BCL:HMD3	2.47	0.48
1:E:23:VAL:HA	1:E:26:MET:HE2	1.95	0.48
4:Q:101:BCL:HHC	4:Q:101:BCL:HBB2	1.96	0.48
3:S:46:ILE:HA	1:Q:1:CXM:HB2	1.97	0.47
2:R:9:TRP:HB3	2:R:10:PRO:HD2	1.97	0.47
1:M:31:HIS:CE1	4:M:103:BCL:HMD3	2.49	0.46
5:E:103:ZE0:C23	4:H:101:BCL:H43	2.46	0.46
1:M:26:MET:HB2	1:O:28:PHE:CZ	2.51	0.46
1:A:4:GLY:HA2	2:B:22:HIS:CG	2.52	0.45
1:C:4:GLY:HA2	2:D:22:HIS:CG	2.52	0.45
3:S:95:LEU:HG	1:E:1:CXM:HE3	1.99	0.44
4:B:101:BCL:H43	5:B:102:ZE0:C23	2.47	0.44
1:M:1:CXM:ON2	2:N:22:HIS:NE2	2.47	0.44
2:J:9:TRP:HB3	2:J:10:PRO:HD2	2.00	0.43
1:M:4:GLY:HA2	2:N:22:HIS:CG	2.53	0.43
1:Q:4:GLY:HA2	2:R:22:HIS:CG	2.54	0.43
2:L:29:SER:HB3	4:L:101:BCL:H41	2.01	0.43
2:N:9:TRP:HB3	2:N:10:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:15:LEU:HG	1:M:1:CXM:HE3	2.00	0.43
1:K:31:HIS:CE1	4:L:101:BCL:HMD3	2.53	0.43
2:P:9:TRP:HB3	2:P:10:PRO:HD2	2.00	0.43
3:S:47:LEU:HG	1:Q:1:CXM:HE3	2.00	0.42
4:S:1703:BCL:HBB1	2:F:33:VAL:HG11	2.01	0.42
2:H:9:TRP:HB3	2:H:10:PRO:HD2	2.01	0.42
1:O:4:GLY:HA2	2:P:22:HIS:CG	2.54	0.42
1:C:10:VAL:HG11	4:E:102:BCL:H192	2.02	0.42
2:L:9:TRP:HB3	2:L:10:PRO:HD2	2.02	0.42
4:E:102:BCL:HMD3	2:F:40:HIS:CE1	2.54	0.42
1:M:16:LEU:HD11	2:N:21:LEU:HD21	2.02	0.42
1:M:1:CXM:SD	2:N:30:ARG:NH2	2.92	0.41
1:O:16:LEU:HD11	2:P:21:LEU:HD21	2.01	0.41
3:S:57:SER:HA	4:S:1701:BCL:C4C	2.51	0.41
2:F:9:TRP:HB3	2:F:10:PRO:HD2	2.01	0.41
5:E:103:ZE0:C24	4:G:102:BCL:HAA2	2.51	0.41
1:G:4:GLY:HA2	2:H:22:HIS:CG	2.56	0.41
1:K:26:MET:HE1	4:M:101:BCL:H93	2.02	0.41
1:I:2:ASN:OD1	1:I:3:GLN:NE2	2.54	0.41
1:O:23:VAL:HA	1:O:26:MET:HE2	2.03	0.41
2:F:29:SER:HB3	4:F:101:BCL:H41	2.01	0.41
1:G:16:LEU:HD11	2:H:21:LEU:HD21	2.03	0.41
2:B:9:TRP:HB3	2:B:10:PRO:HD2	2.03	0.40
3:S:94:LEU:HA	1:E:1:CXM:HB2	2.04	0.40
1:I:16:LEU:HB2	1:I:17:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	46/59 (78%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	46/59 (78%)	46 (100%)	0	0	100	100
1	E	46/59 (78%)	46 (100%)	0	0	100	100
1	G	46/59 (78%)	46 (100%)	0	0	100	100
1	I	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
1	K	46/59 (78%)	46 (100%)	0	0	100	100
1	M	46/59 (78%)	46 (100%)	0	0	100	100
1	O	46/59 (78%)	46 (100%)	0	0	100	100
1	Q	46/59 (78%)	46 (100%)	0	0	100	100
2	B	47/51 (92%)	47 (100%)	0	0	100	100
2	D	47/51 (92%)	47 (100%)	0	0	100	100
2	F	47/51 (92%)	45 (96%)	2 (4%)	0	100	100
2	H	47/51 (92%)	47 (100%)	0	0	100	100
2	J	47/51 (92%)	47 (100%)	0	0	100	100
2	L	47/51 (92%)	47 (100%)	0	0	100	100
2	N	47/51 (92%)	47 (100%)	0	0	100	100
2	P	47/51 (92%)	46 (98%)	1 (2%)	0	100	100
2	R	47/51 (92%)	46 (98%)	1 (2%)	0	100	100
3	S	92/97 (95%)	85 (92%)	7 (8%)	0	100	100
All	All	929/1087 (86%)	916 (99%)	13 (1%)	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	40/47 (85%)	40 (100%)	0	100	100
1	C	40/47 (85%)	40 (100%)	0	100	100
1	E	40/47 (85%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	40/47 (85%)	40 (100%)	0	100	100
1	I	40/47 (85%)	40 (100%)	0	100	100
1	K	40/47 (85%)	40 (100%)	0	100	100
1	M	40/47 (85%)	40 (100%)	0	100	100
1	O	40/47 (85%)	40 (100%)	0	100	100
1	Q	40/47 (85%)	40 (100%)	0	100	100
2	B	42/44 (96%)	42 (100%)	0	100	100
2	D	42/44 (96%)	42 (100%)	0	100	100
2	F	42/44 (96%)	42 (100%)	0	100	100
2	H	42/44 (96%)	42 (100%)	0	100	100
2	J	42/44 (96%)	42 (100%)	0	100	100
2	L	42/44 (96%)	42 (100%)	0	100	100
2	N	42/44 (96%)	42 (100%)	0	100	100
2	P	42/44 (96%)	42 (100%)	0	100	100
2	R	42/44 (96%)	42 (100%)	0	100	100
3	S	78/81 (96%)	78 (100%)	0	100	100
All	All	816/900 (91%)	816 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3	GLN
1	E	37	HIS
1	G	3	GLN
1	G	37	HIS
1	I	3	GLN
1	I	37	HIS
2	J	40	HIS
1	K	3	GLN
1	K	37	HIS
1	M	37	HIS
1	O	37	HIS
1	Q	3	GLN
1	Q	37	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CXM	K	1	4,1	8,10,11	2.14	2 (25%)	7,11,13	1.55	3 (42%)
1	CXM	E	1	4,1	8,10,11	2.13	2 (25%)	7,11,13	1.51	3 (42%)
1	CXM	A	1	4,1	8,10,11	2.15	2 (25%)	7,11,13	1.69	3 (42%)
1	CXM	I	1	4,1	8,10,11	2.16	2 (25%)	7,11,13	1.70	3 (42%)
1	CXM	M	1	4,1	8,10,11	2.15	2 (25%)	7,11,13	1.49	1 (14%)
1	CXM	G	1	4,1	8,10,11	2.15	2 (25%)	7,11,13	1.59	3 (42%)
1	CXM	O	1	4,1	8,10,11	2.15	2 (25%)	7,11,13	1.53	2 (28%)
1	CXM	C	1	4,1	8,10,11	2.14	2 (25%)	7,11,13	1.65	3 (42%)
1	CXM	Q	1	4,1	8,10,11	2.14	2 (25%)	7,11,13	1.59	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	K	1	4,1	-	4/9/10/12	-
1	CXM	E	1	4,1	-	2/9/10/12	-
1	CXM	A	1	4,1	-	4/9/10/12	-
1	CXM	I	1	4,1	-	4/9/10/12	-
1	CXM	M	1	4,1	-	2/9/10/12	-
1	CXM	G	1	4,1	-	3/9/10/12	-
1	CXM	O	1	4,1	-	2/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	C	1	4,1	-	4/9/10/12	-
1	CXM	Q	1	4,1	-	3/9/10/12	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1	CXM	CN-N	4.12	1.42	1.35
1	A	1	CXM	CN-N	4.11	1.42	1.35
1	G	1	CXM	CN-N	4.10	1.42	1.35
1	M	1	CXM	CN-N	4.08	1.42	1.35
1	K	1	CXM	CN-N	4.07	1.42	1.35
1	O	1	CXM	CN-N	4.07	1.42	1.35
1	C	1	CXM	CN-N	4.06	1.42	1.35
1	Q	1	CXM	CN-N	4.05	1.42	1.35
1	E	1	CXM	CN-N	4.04	1.42	1.35
1	I	1	CXM	ON1-CN	3.55	1.28	1.21
1	O	1	CXM	ON1-CN	3.53	1.28	1.21
1	M	1	CXM	ON1-CN	3.52	1.28	1.21
1	G	1	CXM	ON1-CN	3.50	1.28	1.21
1	C	1	CXM	ON1-CN	3.50	1.28	1.21
1	A	1	CXM	ON1-CN	3.50	1.28	1.21
1	Q	1	CXM	ON1-CN	3.50	1.28	1.21
1	E	1	CXM	ON1-CN	3.49	1.28	1.21
1	K	1	CXM	ON1-CN	3.48	1.28	1.21

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	1	CXM	C-CA-N	2.87	114.92	109.73
1	A	1	CXM	C-CA-N	2.78	114.75	109.73
1	Q	1	CXM	C-CA-N	2.56	114.34	109.73
1	M	1	CXM	ON1-CN-N	-2.54	120.69	124.85
1	C	1	CXM	ON1-CN-N	-2.53	120.69	124.85
1	C	1	CXM	C-CA-N	2.47	114.19	109.73
1	G	1	CXM	C-CA-N	2.44	114.14	109.73
1	A	1	CXM	ON1-CN-N	-2.44	120.84	124.85
1	K	1	CXM	ON1-CN-N	-2.44	120.85	124.85
1	G	1	CXM	ON1-CN-N	-2.42	120.88	124.85
1	E	1	CXM	ON1-CN-N	-2.41	120.90	124.85
1	O	1	CXM	ON1-CN-N	-2.39	120.93	124.85
1	Q	1	CXM	ON1-CN-N	-2.37	120.96	124.85
1	I	1	CXM	ON1-CN-N	-2.30	121.08	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	1	CXM	C-CA-N	2.29	113.86	109.73
1	K	1	CXM	C-CA-N	2.24	113.78	109.73
1	I	1	CXM	O-C-CA	-2.18	119.07	124.78
1	A	1	CXM	O-C-CA	-2.17	119.10	124.78
1	E	1	CXM	C-CA-N	2.15	113.62	109.73
1	G	1	CXM	O-C-CA	-2.12	119.23	124.78
1	C	1	CXM	O-C-CA	-2.10	119.27	124.78
1	E	1	CXM	O-C-CA	-2.07	119.35	124.78
1	K	1	CXM	O-C-CA	-2.06	119.37	124.78
1	Q	1	CXM	O-C-CA	-2.05	119.40	124.78

There are no chirality outliers.

All (28) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	C	1	CXM	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	1	CXM	2	0
1	A	1	CXM	1	0
1	M	1	CXM	3	0
1	Q	1	CXM	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BCL	Q	102	1	69,74,74	1.14	4 (5%)	83,115,115	1.40	11 (13%)
4	BCL	G	102	1	69,74,74	1.15	5 (7%)	83,115,115	1.45	9 (10%)
4	BCL	S	1706	3	69,74,74	1.16	5 (7%)	83,115,115	1.45	11 (13%)
4	BCL	S	1705	3	69,74,74	1.17	5 (7%)	83,115,115	1.48	11 (13%)
4	BCL	S	1701	3	69,74,74	1.16	4 (5%)	83,115,115	1.53	13 (15%)
5	ZE0	B	102	-	40,40,40	1.32	3 (7%)	48,49,49	1.09	3 (6%)
5	ZE0	E	103	-	40,40,40	1.32	3 (7%)	48,49,49	1.02	3 (6%)
5	ZE0	A	103	-	40,40,40	1.31	3 (7%)	48,49,49	1.05	3 (6%)
4	BCL	S	1704	3	69,74,74	1.18	5 (7%)	83,115,115	1.48	12 (14%)
4	BCL	C	102	1	69,74,74	1.15	5 (7%)	83,115,115	1.46	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ZE0	M	104	-	40,40,40	1.31	3 (7%)	48,49,49	0.98	2 (4%)
4	BCL	S	1703	3	69,74,74	1.17	5 (7%)	83,115,115	1.48	11 (13%)
4	BCL	I	101	1	69,74,74	1.14	5 (7%)	83,115,115	1.42	10 (12%)
4	BCL	J	101	2	69,74,74	1.14	5 (7%)	83,115,115	1.44	9 (10%)
4	BCL	O	102	1	69,74,74	1.14	5 (7%)	83,115,115	1.42	9 (10%)
4	BCL	M	103	2	69,74,74	1.12	5 (7%)	83,115,115	1.44	10 (12%)
4	BCL	R	101	2	69,74,74	1.14	5 (7%)	83,115,115	1.47	11 (13%)
5	ZE0	C	103	-	40,40,40	1.31	3 (7%)	48,49,49	0.99	2 (4%)
4	BCL	K	102	1	69,74,74	1.13	4 (5%)	83,115,115	1.43	11 (13%)
4	BCL	S	1702	3	69,74,74	1.15	5 (7%)	83,115,115	1.48	12 (14%)
4	BCL	H	101	2	69,74,74	1.15	5 (7%)	83,115,115	1.49	13 (15%)
4	BCL	Q	101	1	69,74,74	1.15	5 (7%)	83,115,115	1.42	10 (12%)
4	BCL	C	101	1	69,74,74	1.13	4 (5%)	83,115,115	1.45	12 (14%)
4	BCL	I	102	1	69,74,74	1.13	5 (7%)	83,115,115	1.41	11 (13%)
4	BCL	M	102	1	69,74,74	1.13	5 (7%)	83,115,115	1.44	10 (12%)
5	ZE0	O	103	-	40,40,40	1.32	3 (7%)	48,49,49	1.06	3 (6%)
5	ZE0	K	103	-	40,40,40	1.31	3 (7%)	48,49,49	0.99	2 (4%)
4	BCL	E	102	1	69,74,74	1.14	4 (5%)	83,115,115	1.47	12 (14%)
4	BCL	E	101	1	69,74,74	1.15	5 (7%)	83,115,115	1.45	9 (10%)
4	BCL	B	101	2	69,74,74	1.16	5 (7%)	83,115,115	1.50	11 (13%)
4	BCL	F	101	2	69,74,74	1.14	5 (7%)	83,115,115	1.45	10 (12%)
5	ZE0	G	103	-	40,40,40	1.32	3 (7%)	48,49,49	1.05	3 (6%)
4	BCL	L	101	2	69,74,74	1.15	5 (7%)	83,115,115	1.44	10 (12%)
4	BCL	O	101	1	69,74,74	1.12	4 (5%)	83,115,115	1.43	11 (13%)
4	BCL	G	101	1	69,74,74	1.14	4 (5%)	83,115,115	1.41	11 (13%)
4	BCL	D	101	2	69,74,74	1.16	5 (7%)	83,115,115	1.50	13 (15%)
4	BCL	A	102	1	69,74,74	1.15	5 (7%)	83,115,115	1.50	10 (12%)
4	BCL	K	101	1	69,74,74	1.16	5 (7%)	83,115,115	1.45	9 (10%)
4	BCL	P	101	2	69,74,74	1.14	4 (5%)	83,115,115	1.47	11 (13%)
4	BCL	A	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.41	11 (13%)
5	ZE0	I	103	-	40,40,40	1.32	3 (7%)	48,49,49	1.02	3 (6%)
4	BCL	M	101	1	69,74,74	1.13	4 (5%)	83,115,115	1.43	11 (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
4	BCL	Q	102	1	-	1/41/137/137	-
4	BCL	G	102	1	-	5/41/137/137	-
4	BCL	S	1706	3	-	9/41/137/137	-
4	BCL	S	1705	3	-	9/41/137/137	-
4	BCL	S	1701	3	-	9/41/137/137	-
5	ZE0	B	102	-	-	3/44/44/44	-
5	ZE0	E	103	-	-	3/44/44/44	-
5	ZE0	A	103	-	-	4/44/44/44	-
4	BCL	S	1704	3	-	5/41/137/137	-
4	BCL	C	102	1	-	5/41/137/137	-
5	ZE0	M	104	-	-	3/44/44/44	-
4	BCL	S	1703	3	-	4/41/137/137	-
4	BCL	I	101	1	-	4/41/137/137	-
4	BCL	J	101	2	-	7/41/137/137	-
4	BCL	O	102	1	-	8/41/137/137	-
4	BCL	M	103	2	-	3/41/137/137	-
4	BCL	R	101	2	-	3/41/137/137	-
5	ZE0	C	103	-	-	3/44/44/44	-
4	BCL	K	102	1	-	0/41/137/137	-
4	BCL	S	1702	3	-	5/41/137/137	-
4	BCL	H	101	2	-	4/41/137/137	-
4	BCL	Q	101	1	-	4/41/137/137	-
4	BCL	C	101	1	-	1/41/137/137	-
4	BCL	I	102	1	-	1/41/137/137	-
4	BCL	M	102	1	-	11/41/137/137	-
5	ZE0	O	103	-	-	3/44/44/44	-
5	ZE0	K	103	-	-	3/44/44/44	-
4	BCL	E	102	1	-	2/41/137/137	-
4	BCL	E	101	1	-	6/41/137/137	-
4	BCL	B	101	2	-	3/41/137/137	-
4	BCL	F	101	2	-	4/41/137/137	-
5	ZE0	G	103	-	-	3/44/44/44	-
4	BCL	L	101	2	-	6/41/137/137	-
4	BCL	O	101	1	-	1/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	G	101	1	-	0/41/137/137	-
4	BCL	D	101	2	-	3/41/137/137	-
4	BCL	A	102	1	-	9/41/137/137	-
4	BCL	K	101	1	-	4/41/137/137	-
4	BCL	P	101	2	-	3/41/137/137	-
4	BCL	A	101	1	-	0/41/137/137	-
5	ZE0	I	103	-	-	3/44/44/44	-
4	BCL	M	101	1	-	1/41/137/137	-

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	102	ZE0	C36-C35	7.47	1.53	1.34
5	O	103	ZE0	C36-C35	7.47	1.53	1.34
5	I	103	ZE0	C36-C35	7.46	1.53	1.34
5	E	103	ZE0	C36-C35	7.45	1.53	1.34
5	G	103	ZE0	C36-C35	7.45	1.53	1.34
5	A	103	ZE0	C36-C35	7.42	1.53	1.34
5	M	104	ZE0	C36-C35	7.42	1.53	1.34
5	K	103	ZE0	C36-C35	7.41	1.53	1.34
5	C	103	ZE0	C36-C35	7.41	1.53	1.34
4	S	1704	BCL	MG-NA	5.20	2.18	2.06
4	S	1701	BCL	MG-NA	5.09	2.18	2.06
4	L	101	BCL	MG-NA	5.07	2.18	2.06
4	B	101	BCL	MG-NA	5.06	2.18	2.06
4	S	1705	BCL	MG-NA	5.05	2.18	2.06
4	Q	102	BCL	MG-NA	5.01	2.18	2.06
4	D	101	BCL	MG-NA	5.00	2.18	2.06
4	S	1702	BCL	MG-NA	5.00	2.18	2.06
4	G	101	BCL	MG-NA	4.99	2.18	2.06
4	I	102	BCL	MG-NA	4.99	2.18	2.06
4	S	1703	BCL	MG-NA	4.98	2.18	2.06
4	R	101	BCL	MG-NA	4.98	2.18	2.06
4	E	102	BCL	MG-NA	4.98	2.18	2.06
4	H	101	BCL	MG-NA	4.97	2.18	2.06
4	J	101	BCL	MG-NA	4.97	2.18	2.06
4	P	101	BCL	MG-NA	4.97	2.18	2.06
4	O	101	BCL	MG-NA	4.96	2.18	2.06
4	K	102	BCL	MG-NA	4.95	2.18	2.06
4	C	101	BCL	MG-NA	4.94	2.18	2.06
4	F	101	BCL	MG-NA	4.94	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	102	BCL	MG-NA	4.93	2.18	2.06
4	S	1706	BCL	MG-NA	4.93	2.18	2.06
4	A	101	BCL	MG-NA	4.93	2.18	2.06
4	M	101	BCL	MG-NA	4.91	2.17	2.06
4	A	102	BCL	MG-NA	4.87	2.17	2.06
4	K	101	BCL	MG-NA	4.85	2.17	2.06
4	Q	101	BCL	MG-NA	4.82	2.17	2.06
4	O	102	BCL	MG-NA	4.82	2.17	2.06
4	G	102	BCL	MG-NA	4.78	2.17	2.06
4	E	101	BCL	MG-NA	4.78	2.17	2.06
4	M	102	BCL	MG-NA	4.77	2.17	2.06
4	M	103	BCL	MG-NA	4.74	2.17	2.06
4	I	101	BCL	MG-NA	4.72	2.17	2.06
4	J	101	BCL	MG-NC	3.87	2.15	2.06
4	L	101	BCL	MG-NC	3.81	2.15	2.06
4	B	101	BCL	MG-NC	3.80	2.15	2.06
4	D	101	BCL	MG-NC	3.78	2.15	2.06
4	S	1704	BCL	MG-NC	3.73	2.15	2.06
4	R	101	BCL	MG-NC	3.73	2.15	2.06
4	P	101	BCL	MG-NC	3.72	2.15	2.06
4	F	101	BCL	MG-NC	3.68	2.15	2.06
4	S	1705	BCL	MG-NC	3.66	2.15	2.06
4	H	101	BCL	MG-NC	3.64	2.14	2.06
4	S	1703	BCL	MG-NC	3.64	2.14	2.06
4	S	1706	BCL	MG-NC	3.61	2.14	2.06
4	S	1701	BCL	MG-NC	3.58	2.14	2.06
4	M	101	BCL	MG-NC	3.56	2.14	2.06
4	G	101	BCL	MG-NC	3.54	2.14	2.06
4	E	102	BCL	MG-NC	3.53	2.14	2.06
4	C	101	BCL	MG-NC	3.51	2.14	2.06
4	Q	102	BCL	MG-NC	3.51	2.14	2.06
4	S	1702	BCL	MG-NC	3.50	2.14	2.06
4	K	102	BCL	MG-NC	3.50	2.14	2.06
4	Q	101	BCL	MG-NC	3.50	2.14	2.06
4	I	102	BCL	MG-NC	3.49	2.14	2.06
4	O	101	BCL	MG-NC	3.48	2.14	2.06
4	C	102	BCL	MG-NC	3.47	2.14	2.06
4	O	102	BCL	MG-NC	3.45	2.14	2.06
4	A	102	BCL	MG-NC	3.44	2.14	2.06
4	E	101	BCL	MG-NC	3.44	2.14	2.06
4	G	102	BCL	MG-NC	3.42	2.14	2.06
4	K	101	BCL	MG-NC	3.42	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	103	BCL	MG-NC	3.40	2.14	2.06
4	A	101	BCL	MG-NC	3.40	2.14	2.06
4	M	102	BCL	MG-NC	3.37	2.14	2.06
4	I	101	BCL	MG-NC	3.37	2.14	2.06
4	E	101	BCL	C3B-C4B	3.25	1.47	1.41
4	G	102	BCL	C3B-C4B	3.24	1.47	1.41
4	I	101	BCL	C3B-C4B	3.22	1.47	1.41
4	M	102	BCL	C3B-C4B	3.22	1.47	1.41
4	A	102	BCL	C3B-C4B	3.22	1.47	1.41
4	C	102	BCL	C3B-C4B	3.20	1.47	1.41
4	O	102	BCL	C3B-C4B	3.18	1.47	1.41
4	K	101	BCL	C3B-C4B	3.16	1.47	1.41
4	Q	101	BCL	C3B-C4B	3.15	1.46	1.41
4	S	1704	BCL	C3B-C4B	3.05	1.46	1.41
4	S	1701	BCL	C3B-C4B	2.97	1.46	1.41
4	S	1703	BCL	C3B-C4B	2.97	1.46	1.41
4	S	1705	BCL	C3B-C4B	2.96	1.46	1.41
4	S	1706	BCL	C3B-C4B	2.94	1.46	1.41
4	S	1702	BCL	C3B-C4B	2.91	1.46	1.41
4	A	101	BCL	C3B-C4B	2.86	1.46	1.41
4	Q	102	BCL	C3B-C4B	2.86	1.46	1.41
4	H	101	BCL	C3B-C4B	2.84	1.46	1.41
4	I	102	BCL	C3B-C4B	2.84	1.46	1.41
4	K	102	BCL	C3B-C4B	2.82	1.46	1.41
4	C	101	BCL	C3B-C4B	2.81	1.46	1.41
4	G	101	BCL	C3B-C4B	2.81	1.46	1.41
4	B	101	BCL	C3B-C4B	2.76	1.46	1.41
4	M	101	BCL	C3B-C4B	2.76	1.46	1.41
4	L	101	BCL	C3B-C4B	2.76	1.46	1.41
4	E	102	BCL	C3B-C4B	2.76	1.46	1.41
4	D	101	BCL	C3B-C4B	2.73	1.46	1.41
4	F	101	BCL	C3B-C4B	2.72	1.46	1.41
4	O	101	BCL	C3B-C4B	2.71	1.46	1.41
4	P	101	BCL	C3B-C4B	2.70	1.46	1.41
4	J	101	BCL	C3B-C4B	2.65	1.46	1.41
4	R	101	BCL	C3B-C4B	2.64	1.46	1.41
4	M	103	BCL	C3B-C4B	2.60	1.45	1.41
4	M	103	BCL	CHD-C1D	2.48	1.43	1.38
4	S	1702	BCL	CHD-C1D	2.45	1.43	1.38
4	S	1703	BCL	CHD-C1D	2.43	1.43	1.38
5	I	103	ZE0	C35-C33	2.41	1.51	1.45
5	M	104	ZE0	C35-C33	2.41	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	103	ZE0	C35-C33	2.40	1.51	1.45
5	B	102	ZE0	C35-C33	2.40	1.51	1.45
5	E	103	ZE0	C35-C33	2.40	1.51	1.45
5	A	103	ZE0	C35-C33	2.40	1.51	1.45
5	G	103	ZE0	C35-C33	2.39	1.51	1.45
5	K	103	ZE0	C35-C33	2.38	1.51	1.45
4	S	1706	BCL	CHD-C1D	2.38	1.43	1.38
5	C	103	ZE0	C35-C33	2.36	1.51	1.45
4	C	102	BCL	CHD-C1D	2.36	1.43	1.38
4	S	1705	BCL	CHD-C1D	2.36	1.43	1.38
4	O	102	BCL	CHD-C1D	2.35	1.43	1.38
4	S	1701	BCL	CHD-C1D	2.33	1.42	1.38
4	M	102	BCL	CHD-C1D	2.32	1.42	1.38
4	K	101	BCL	CHD-C1D	2.32	1.42	1.38
4	A	102	BCL	CHD-C1D	2.31	1.42	1.38
4	I	101	BCL	CHD-C1D	2.30	1.42	1.38
4	G	102	BCL	CHD-C1D	2.30	1.42	1.38
4	Q	101	BCL	CHD-C1D	2.30	1.42	1.38
4	E	101	BCL	CHD-C1D	2.29	1.42	1.38
4	S	1704	BCL	CHD-C1D	2.29	1.42	1.38
4	L	101	BCL	CHD-C1D	2.28	1.42	1.38
4	A	101	BCL	CHD-C1D	2.27	1.42	1.38
4	D	101	BCL	CHD-C1D	2.26	1.42	1.38
4	K	102	BCL	CHD-C1D	2.24	1.42	1.38
4	B	101	BCL	CHD-C1D	2.24	1.42	1.38
4	C	101	BCL	CHD-C1D	2.23	1.42	1.38
4	I	102	BCL	CHD-C1D	2.22	1.42	1.38
5	A	103	ZE0	C36-C37	2.21	1.50	1.43
5	M	104	ZE0	C36-C37	2.21	1.50	1.43
5	I	103	ZE0	C36-C37	2.21	1.50	1.43
5	E	103	ZE0	C36-C37	2.20	1.50	1.43
5	K	103	ZE0	C36-C37	2.20	1.50	1.43
5	B	102	ZE0	C36-C37	2.20	1.50	1.43
5	O	103	ZE0	C36-C37	2.19	1.50	1.43
5	C	103	ZE0	C36-C37	2.19	1.50	1.43
4	E	102	BCL	CHD-C1D	2.19	1.42	1.38
4	M	101	BCL	CHD-C1D	2.18	1.42	1.38
5	G	103	ZE0	C36-C37	2.18	1.50	1.43
4	S	1702	BCL	C1D-ND	2.18	1.40	1.37
4	Q	102	BCL	CHD-C1D	2.17	1.42	1.38
4	G	101	BCL	CHD-C1D	2.17	1.42	1.38
4	J	101	BCL	CHD-C1D	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	101	BCL	CHD-C1D	2.15	1.42	1.38
4	H	101	BCL	CHD-C1D	2.14	1.42	1.38
4	O	101	BCL	CHD-C1D	2.14	1.42	1.38
4	F	101	BCL	CHD-C1D	2.12	1.42	1.38
4	E	101	BCL	C3D-C4D	-2.11	1.39	1.44
4	G	102	BCL	C3D-C4D	-2.11	1.39	1.44
4	P	101	BCL	CHD-C1D	2.10	1.42	1.38
4	C	102	BCL	C3D-C4D	-2.09	1.39	1.44
4	O	102	BCL	C3D-C4D	-2.08	1.39	1.44
4	S	1706	BCL	C1D-ND	2.07	1.40	1.37
4	S	1703	BCL	C1D-ND	2.07	1.40	1.37
4	K	101	BCL	C3D-C4D	-2.06	1.39	1.44
4	Q	101	BCL	C3D-C4D	-2.06	1.39	1.44
4	S	1704	BCL	C1D-ND	2.05	1.40	1.37
4	S	1705	BCL	C1D-ND	2.05	1.40	1.37
4	H	101	BCL	C1D-ND	2.04	1.40	1.37
4	M	103	BCL	C3D-C4D	-2.04	1.39	1.44
4	J	101	BCL	C1D-ND	2.04	1.40	1.37
4	A	102	BCL	C3D-C4D	-2.03	1.39	1.44
4	D	101	BCL	C3D-C4D	-2.02	1.39	1.44
4	A	101	BCL	C3D-C4D	-2.02	1.39	1.44
4	L	101	BCL	C1D-ND	2.02	1.40	1.37
4	B	101	BCL	C1D-ND	2.02	1.40	1.37
4	M	102	BCL	C3D-C4D	-2.01	1.39	1.44
4	R	101	BCL	C1D-ND	2.01	1.40	1.37
4	I	101	BCL	C3D-C4D	-2.01	1.39	1.44
4	I	102	BCL	C3D-C4D	-2.00	1.39	1.44
4	F	101	BCL	C1D-ND	2.00	1.40	1.37

All (379) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	1705	BCL	CHD-C1D-ND	-5.48	119.42	124.45
4	S	1701	BCL	CHD-C1D-ND	-5.47	119.42	124.45
4	S	1706	BCL	CHD-C1D-ND	-5.43	119.47	124.45
4	S	1704	BCL	CHD-C1D-ND	-5.42	119.47	124.45
4	J	101	BCL	CHD-C1D-ND	-5.36	119.53	124.45
4	S	1703	BCL	CHD-C1D-ND	-5.26	119.62	124.45
4	G	102	BCL	CHD-C1D-ND	-5.24	119.64	124.45
4	E	101	BCL	CHD-C1D-ND	-5.21	119.67	124.45
4	I	101	BCL	C4D-CHA-C1A	5.19	127.57	121.25
4	I	101	BCL	CHD-C1D-ND	-5.17	119.70	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	103	BCL	C4D-CHA-C1A	5.17	127.54	121.25
4	B	101	BCL	CHD-C1D-ND	-5.16	119.71	124.45
4	O	102	BCL	CHD-C1D-ND	-5.16	119.71	124.45
4	K	101	BCL	C4D-CHA-C1A	5.14	127.51	121.25
4	O	102	BCL	C4D-CHA-C1A	5.14	127.51	121.25
4	S	1701	BCL	C4D-CHA-C1A	5.14	127.51	121.25
4	S	1703	BCL	C4D-CHA-C1A	5.14	127.51	121.25
4	M	102	BCL	C4D-CHA-C1A	5.14	127.50	121.25
4	G	102	BCL	C4D-CHA-C1A	5.13	127.49	121.25
4	S	1702	BCL	CHD-C1D-ND	-5.13	119.74	124.45
4	E	101	BCL	C4D-CHA-C1A	5.12	127.48	121.25
4	A	102	BCL	CHD-C1D-ND	-5.10	119.77	124.45
4	Q	101	BCL	C4D-CHA-C1A	5.10	127.46	121.25
4	K	101	BCL	CHD-C1D-ND	-5.10	119.77	124.45
4	A	102	BCL	C4D-CHA-C1A	5.09	127.44	121.25
4	Q	101	BCL	CHD-C1D-ND	-5.09	119.78	124.45
4	M	102	BCL	CHD-C1D-ND	-5.07	119.80	124.45
4	R	101	BCL	CHD-C1D-ND	-5.06	119.80	124.45
4	H	101	BCL	CHD-C1D-ND	-5.00	119.86	124.45
4	D	101	BCL	CHD-C1D-ND	-4.97	119.88	124.45
4	C	102	BCL	CHD-C1D-ND	-4.95	119.91	124.45
4	S	1705	BCL	C4D-CHA-C1A	4.94	127.26	121.25
4	P	101	BCL	CHD-C1D-ND	-4.94	119.92	124.45
4	L	101	BCL	CHD-C1D-ND	-4.93	119.92	124.45
4	S	1702	BCL	C4D-CHA-C1A	4.90	127.21	121.25
4	F	101	BCL	CHD-C1D-ND	-4.90	119.95	124.45
4	H	101	BCL	C4D-CHA-C1A	4.89	127.20	121.25
4	S	1706	BCL	C4D-CHA-C1A	4.88	127.19	121.25
4	C	102	BCL	C4D-CHA-C1A	4.88	127.18	121.25
4	E	102	BCL	C4D-CHA-C1A	4.87	127.17	121.25
4	O	101	BCL	C4D-CHA-C1A	4.86	127.17	121.25
4	M	103	BCL	CHD-C1D-ND	-4.84	120.01	124.45
4	D	101	BCL	C4D-CHA-C1A	4.83	127.13	121.25
4	M	101	BCL	C4D-CHA-C1A	4.82	127.12	121.25
5	G	103	ZE0	C36-C35-C33	-4.78	112.98	126.42
5	B	102	ZE0	C36-C35-C33	-4.78	113.00	126.42
4	B	101	BCL	C4D-CHA-C1A	4.77	127.06	121.25
4	I	102	BCL	CHD-C1D-ND	-4.77	120.07	124.45
4	C	101	BCL	C4D-CHA-C1A	4.76	127.04	121.25
4	C	101	BCL	CHD-C1D-ND	-4.75	120.09	124.45
4	Q	102	BCL	CHD-C1D-ND	-4.74	120.10	124.45
4	S	1704	BCL	C4D-CHA-C1A	4.74	127.01	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	101	BCL	C4D-CHA-C1A	4.72	127.00	121.25
4	R	101	BCL	C4D-CHA-C1A	4.71	126.98	121.25
4	M	101	BCL	CHD-C1D-ND	-4.71	120.13	124.45
4	K	102	BCL	CHD-C1D-ND	-4.70	120.14	124.45
4	G	101	BCL	C4D-CHA-C1A	4.69	126.96	121.25
4	Q	102	BCL	C4D-CHA-C1A	4.68	126.94	121.25
4	O	101	BCL	CHD-C1D-ND	-4.68	120.16	124.45
4	G	101	BCL	CHD-C1D-ND	-4.67	120.16	124.45
4	E	102	BCL	CHD-C1D-ND	-4.67	120.16	124.45
4	A	101	BCL	CHD-C1D-ND	-4.67	120.16	124.45
4	K	102	BCL	C4D-CHA-C1A	4.66	126.92	121.25
4	P	101	BCL	C4D-CHA-C1A	4.65	126.91	121.25
4	L	101	BCL	C4D-CHA-C1A	4.64	126.89	121.25
5	I	103	ZE0	C36-C35-C33	-4.63	113.42	126.42
5	O	103	ZE0	C36-C35-C33	-4.61	113.47	126.42
4	J	101	BCL	C4D-CHA-C1A	4.57	126.81	121.25
4	A	101	BCL	C4D-CHA-C1A	4.56	126.80	121.25
5	A	103	ZE0	C36-C35-C33	-4.54	113.67	126.42
5	E	103	ZE0	C36-C35-C33	-4.47	113.87	126.42
4	I	102	BCL	C4D-CHA-C1A	4.43	126.64	121.25
5	K	103	ZE0	C36-C35-C33	-4.36	114.16	126.42
5	C	103	ZE0	C36-C35-C33	-4.26	114.44	126.42
5	M	104	ZE0	C36-C35-C33	-4.18	114.68	126.42
5	C	103	ZE0	C37-C36-C35	-4.14	110.29	123.22
5	M	104	ZE0	C37-C36-C35	-4.09	110.47	123.22
5	K	103	ZE0	C37-C36-C35	-4.07	110.50	123.22
5	E	103	ZE0	C37-C36-C35	-4.04	110.59	123.22
5	O	103	ZE0	C37-C36-C35	-4.04	110.62	123.22
4	A	102	BCL	C1-C2-C3	4.00	132.97	126.04
5	G	103	ZE0	C37-C36-C35	-4.00	110.73	123.22
5	A	103	ZE0	C37-C36-C35	-3.99	110.76	123.22
5	I	103	ZE0	C37-C36-C35	-3.96	110.85	123.22
5	B	102	ZE0	C37-C36-C35	-3.96	110.85	123.22
4	G	102	BCL	C1D-ND-C4D	-3.92	103.55	106.33
4	G	102	BCL	C4A-NA-C1A	3.88	108.45	106.71
4	O	102	BCL	C1D-ND-C4D	-3.81	103.63	106.33
4	Q	101	BCL	C1D-ND-C4D	-3.80	103.64	106.33
4	K	101	BCL	C4A-NA-C1A	3.79	108.41	106.71
4	I	101	BCL	C1D-ND-C4D	-3.77	103.66	106.33
4	E	101	BCL	C1D-ND-C4D	-3.76	103.67	106.33
4	K	101	BCL	C1D-ND-C4D	-3.75	103.67	106.33
4	A	102	BCL	C4A-NA-C1A	3.73	108.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	102	BCL	C1D-ND-C4D	-3.72	103.69	106.33
4	A	102	BCL	C1D-ND-C4D	-3.72	103.69	106.33
4	C	102	BCL	C1D-ND-C4D	-3.67	103.73	106.33
4	K	102	BCL	C4A-NA-C1A	3.66	108.35	106.71
4	C	101	BCL	C4A-NA-C1A	3.66	108.35	106.71
4	C	102	BCL	C4A-NA-C1A	3.66	108.35	106.71
4	O	101	BCL	C4A-NA-C1A	3.63	108.34	106.71
4	M	102	BCL	C4A-NA-C1A	3.63	108.34	106.71
4	S	1702	BCL	C4A-NA-C1A	3.62	108.33	106.71
4	E	101	BCL	C4A-NA-C1A	3.61	108.33	106.71
4	C	102	BCL	C1-C2-C3	3.61	132.28	126.04
4	O	102	BCL	C4A-NA-C1A	3.60	108.33	106.71
4	E	102	BCL	C4A-NA-C1A	3.60	108.32	106.71
4	M	101	BCL	C4A-NA-C1A	3.57	108.31	106.71
4	S	1702	BCL	C1D-ND-C4D	-3.52	103.83	106.33
4	A	101	BCL	C4A-NA-C1A	3.50	108.28	106.71
4	S	1703	BCL	C4A-NA-C1A	3.50	108.28	106.71
4	S	1706	BCL	C1D-ND-C4D	-3.44	103.89	106.33
4	S	1701	BCL	C1D-ND-C4D	-3.42	103.90	106.33
4	S	1703	BCL	C1D-ND-C4D	-3.42	103.90	106.33
4	S	1705	BCL	C1D-ND-C4D	-3.42	103.91	106.33
4	G	101	BCL	C4A-NA-C1A	3.40	108.23	106.71
4	I	101	BCL	C4A-NA-C1A	3.40	108.23	106.71
4	I	102	BCL	C4A-NA-C1A	3.40	108.23	106.71
4	Q	101	BCL	C4A-NA-C1A	3.38	108.22	106.71
4	O	101	BCL	C1D-ND-C4D	-3.38	103.94	106.33
4	F	101	BCL	C4A-NA-C1A	3.36	108.22	106.71
4	J	101	BCL	C1D-ND-C4D	-3.35	103.95	106.33
4	M	103	BCL	C4A-NA-C1A	3.34	108.21	106.71
4	S	1704	BCL	C1D-ND-C4D	-3.34	103.96	106.33
4	D	101	BCL	C1D-ND-C4D	-3.33	103.97	106.33
4	M	101	BCL	C1D-ND-C4D	-3.33	103.97	106.33
4	Q	102	BCL	C4A-NA-C1A	3.33	108.20	106.71
4	F	101	BCL	C1D-ND-C4D	-3.31	103.98	106.33
4	Q	102	BCL	C1D-ND-C4D	-3.29	104.00	106.33
4	H	101	BCL	C1D-ND-C4D	-3.28	104.00	106.33
4	B	101	BCL	C1D-ND-C4D	-3.28	104.01	106.33
4	C	101	BCL	C1D-ND-C4D	-3.27	104.01	106.33
4	E	102	BCL	C1D-ND-C4D	-3.26	104.02	106.33
4	G	101	BCL	C1D-ND-C4D	-3.26	104.02	106.33
4	L	101	BCL	C1D-ND-C4D	-3.26	104.02	106.33
4	R	101	BCL	C1D-ND-C4D	-3.26	104.02	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	101	BCL	CHA-C1A-NA	-3.26	118.94	126.40
4	P	101	BCL	C1D-ND-C4D	-3.26	104.02	106.33
4	I	102	BCL	CHA-C1A-NA	-3.26	118.94	126.40
4	S	1701	BCL	C4A-NA-C1A	3.25	108.17	106.71
4	S	1706	BCL	C4A-NA-C1A	3.24	108.16	106.71
4	E	102	BCL	CHA-C1A-NA	-3.23	119.00	126.40
4	K	102	BCL	CHA-C1A-NA	-3.22	119.02	126.40
4	C	101	BCL	CHA-C1A-NA	-3.20	119.08	126.40
4	I	102	BCL	C1D-ND-C4D	-3.19	104.07	106.33
4	K	102	BCL	C1D-ND-C4D	-3.19	104.07	106.33
4	M	101	BCL	CHA-C1A-NA	-3.19	119.10	126.40
4	I	102	BCL	C2A-C1A-CHA	3.18	129.42	123.86
4	G	101	BCL	CHA-C1A-NA	-3.17	119.15	126.40
4	Q	102	BCL	CHA-C1A-NA	-3.17	119.15	126.40
4	A	101	BCL	C2A-C1A-CHA	3.15	129.37	123.86
4	M	101	BCL	C2A-C1A-CHA	3.15	129.37	123.86
4	O	101	BCL	CHA-C1A-NA	-3.14	119.22	126.40
4	S	1705	BCL	C4A-NA-C1A	3.13	108.11	106.71
4	M	103	BCL	C1D-ND-C4D	-3.12	104.12	106.33
4	C	101	BCL	C2A-C1A-CHA	3.12	129.31	123.86
4	A	101	BCL	C1D-ND-C4D	-3.12	104.12	106.33
4	Q	102	BCL	C2A-C1A-CHA	3.12	129.31	123.86
4	G	101	BCL	C2A-C1A-CHA	3.11	129.30	123.86
4	K	102	BCL	C2A-C1A-CHA	3.10	129.28	123.86
4	P	101	BCL	C4A-NA-C1A	3.09	108.09	106.71
4	E	102	BCL	C2A-C1A-CHA	3.08	129.24	123.86
4	O	101	BCL	C2A-C1A-CHA	3.05	129.19	123.86
4	H	101	BCL	C4A-NA-C1A	3.05	108.08	106.71
4	S	1704	BCL	C4A-NA-C1A	3.03	108.07	106.71
4	S	1704	BCL	CHA-C1A-NA	-3.03	119.46	126.40
5	B	102	ZE0	C31-C32-C33	-3.02	123.00	127.31
4	S	1701	BCL	CHA-C1A-NA	-2.96	119.63	126.40
4	L	101	BCL	C4A-NA-C1A	2.95	108.03	106.71
4	C	101	BCL	CAB-C3B-C2B	2.95	132.76	128.34
4	S	1704	BCL	CAB-C3B-C2B	2.94	132.75	128.34
4	H	101	BCL	CAB-C3B-C2B	2.94	132.74	128.34
4	E	102	BCL	CAB-C3B-C2B	2.93	132.73	128.34
4	K	102	BCL	CAB-C3B-C2B	2.93	132.73	128.34
4	S	1706	BCL	C2A-C1A-CHA	2.93	128.99	123.86
4	E	102	BCL	C1-C2-C3	-2.93	120.97	126.04
4	Q	101	BCL	CHA-C1A-NA	-2.93	119.69	126.40
4	S	1705	BCL	CHA-C1A-NA	-2.92	119.72	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	101	BCL	C1-C2-C3	-2.91	121.01	126.04
4	S	1702	BCL	CHA-C1A-NA	-2.90	119.75	126.40
4	S	1703	BCL	CHA-C1A-NA	-2.90	119.75	126.40
4	H	101	BCL	CHA-C1A-NA	-2.90	119.75	126.40
4	C	102	BCL	CHA-C1A-NA	-2.90	119.76	126.40
4	M	103	BCL	CHA-C1A-NA	-2.89	119.77	126.40
4	I	102	BCL	CAB-C3B-C2B	2.88	132.65	128.34
4	B	101	BCL	CHA-C1A-NA	-2.88	119.81	126.40
4	S	1706	BCL	CHA-C1A-NA	-2.87	119.82	126.40
4	M	102	BCL	CHA-C1A-NA	-2.87	119.83	126.40
4	I	101	BCL	CHA-C1A-NA	-2.87	119.83	126.40
4	S	1701	BCL	CAB-C3B-C2B	2.87	132.64	128.34
4	L	101	BCL	CHA-C1A-NA	-2.87	119.83	126.40
4	S	1705	BCL	CAB-C3B-C2B	2.87	132.63	128.34
4	A	102	BCL	CHA-C1A-NA	-2.87	119.84	126.40
4	O	102	BCL	CHA-C1A-NA	-2.86	119.84	126.40
4	M	101	BCL	CAB-C3B-C2B	2.85	132.61	128.34
4	O	101	BCL	CAB-C3B-C2B	2.85	132.61	128.34
4	S	1703	BCL	CAB-C3B-C2B	2.85	132.61	128.34
4	P	101	BCL	CHA-C1A-NA	-2.84	119.89	126.40
4	F	101	BCL	CAB-C3B-C2B	2.84	132.60	128.34
4	F	101	BCL	CHA-C1A-NA	-2.84	119.89	126.40
4	G	102	BCL	CHA-C1A-NA	-2.84	119.90	126.40
4	K	101	BCL	CHA-C1A-NA	-2.84	119.90	126.40
4	E	101	BCL	CHA-C1A-NA	-2.84	119.90	126.40
4	J	101	BCL	C4A-NA-C1A	2.83	107.98	106.71
4	D	101	BCL	C4A-NA-C1A	2.83	107.98	106.71
4	D	101	BCL	CHA-C1A-NA	-2.82	119.94	126.40
4	R	101	BCL	CHA-C1A-NA	-2.82	119.94	126.40
4	A	101	BCL	CAB-C3B-C2B	2.82	132.56	128.34
4	B	101	BCL	C4A-NA-C1A	2.81	107.97	106.71
4	S	1702	BCL	CAB-C3B-C2B	2.81	132.55	128.34
4	R	101	BCL	C4A-NA-C1A	2.79	107.96	106.71
4	Q	102	BCL	CAB-C3B-C2B	2.79	132.52	128.34
4	L	101	BCL	CAB-C3B-C2B	2.79	132.51	128.34
4	G	101	BCL	CAB-C3B-C2B	2.78	132.51	128.34
4	J	101	BCL	CHA-C1A-NA	-2.78	120.04	126.40
4	S	1702	BCL	C2A-C1A-CHA	2.77	128.70	123.86
4	J	101	BCL	CAB-C3B-C2B	2.76	132.47	128.34
5	A	103	ZE0	C31-C32-C33	-2.75	123.38	127.31
4	B	101	BCL	CAB-C3B-C2B	2.75	132.46	128.34
4	S	1703	BCL	C2A-C1A-CHA	2.75	128.67	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	1701	BCL	C1-C2-C3	2.75	130.79	126.04
4	I	102	BCL	CHC-C4B-NB	-2.74	121.36	124.26
4	L	101	BCL	CHC-C4B-NB	-2.74	121.36	124.26
4	D	101	BCL	CAB-C3B-C2B	2.74	132.44	128.34
4	D	101	BCL	CHC-C4B-NB	-2.74	121.36	124.26
4	A	101	BCL	CHC-C4B-NB	-2.72	121.38	124.26
4	P	101	BCL	CAB-C3B-C2B	2.71	132.41	128.34
4	S	1706	BCL	CAB-C3B-C2B	2.71	132.40	128.34
4	M	102	BCL	C2A-C1A-CHA	2.71	128.60	123.86
4	Q	101	BCL	CHC-C4B-NB	-2.71	121.39	124.26
4	K	102	BCL	CHC-C4B-NB	-2.70	121.39	124.26
4	F	101	BCL	CHC-C4B-NB	-2.70	121.40	124.26
4	B	101	BCL	C2A-C1A-CHA	2.69	128.56	123.86
4	R	101	BCL	CAB-C3B-C2B	2.67	132.34	128.34
4	Q	101	BCL	C2A-C1A-CHA	2.66	128.51	123.86
4	M	103	BCL	CAB-C3B-C2B	2.65	132.32	128.34
4	Q	102	BCL	CHC-C4B-NB	-2.65	121.45	124.26
4	J	101	BCL	CHC-C4B-NB	-2.65	121.45	124.26
4	L	101	BCL	C2A-C1A-CHA	2.65	128.48	123.86
4	S	1705	BCL	C2A-C1A-CHA	2.64	128.47	123.86
4	R	101	BCL	C2A-C1A-CHA	2.63	128.46	123.86
4	G	102	BCL	CHC-C4B-NB	-2.63	121.47	124.26
4	C	102	BCL	C2A-C1A-CHA	2.63	128.45	123.86
4	E	101	BCL	CHC-C4B-NB	-2.61	121.49	124.26
4	S	1704	BCL	C2A-C1A-CHA	2.61	128.43	123.86
4	J	101	BCL	C2A-C1A-CHA	2.61	128.43	123.86
4	E	102	BCL	CHC-C4B-NB	-2.61	121.49	124.26
4	C	102	BCL	CHC-C4B-NB	-2.61	121.50	124.26
4	S	1701	BCL	C2A-C1A-CHA	2.61	128.42	123.86
4	C	101	BCL	CHC-C4B-NB	-2.61	121.50	124.26
4	M	101	BCL	CHC-C4B-NB	-2.60	121.51	124.26
4	O	102	BCL	C2A-C1A-CHA	2.59	128.39	123.86
4	S	1703	BCL	CHC-C4B-NB	-2.58	121.52	124.26
4	A	102	BCL	C2A-C1A-CHA	2.58	128.38	123.86
4	G	101	BCL	CHC-C4B-NB	-2.58	121.52	124.26
4	O	102	BCL	CHC-C4B-NB	-2.58	121.53	124.26
4	B	101	BCL	CHC-C4B-NB	-2.57	121.53	124.26
4	S	1702	BCL	CHC-C4B-NB	-2.57	121.54	124.26
4	E	101	BCL	C2A-C1A-CHA	2.57	128.35	123.86
4	A	102	BCL	CHC-C4B-NB	-2.57	121.54	124.26
4	H	101	BCL	C2A-C1A-CHA	2.57	128.35	123.86
4	I	101	BCL	C2A-C1A-CHA	2.55	128.32	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	101	BCL	CHC-C4B-NB	-2.55	121.56	124.26
4	K	101	BCL	CHC-C4B-NB	-2.54	121.57	124.26
4	O	101	BCL	CHC-C4B-NB	-2.53	121.58	124.26
4	H	101	BCL	CHC-C4B-NB	-2.52	121.58	124.26
4	G	102	BCL	C2A-C1A-CHA	2.52	128.26	123.86
4	R	101	BCL	CHC-C4B-NB	-2.52	121.59	124.26
4	P	101	BCL	CHC-C4B-NB	-2.51	121.59	124.26
4	M	102	BCL	CHC-C4B-NB	-2.51	121.60	124.26
4	B	101	BCL	C1-C2-C3	-2.49	121.75	126.04
4	D	101	BCL	C2A-C1A-CHA	2.46	128.16	123.86
4	S	1705	BCL	CHC-C4B-NB	-2.46	121.65	124.26
5	O	103	ZE0	C31-C32-C33	-2.46	123.80	127.31
4	S	1704	BCL	CHC-C4B-NB	-2.45	121.66	124.26
4	K	101	BCL	C2A-C1A-CHA	2.45	128.14	123.86
4	M	103	BCL	CHC-C4B-NB	-2.44	121.68	124.26
4	P	101	BCL	C2A-C1A-CHA	2.42	128.09	123.86
4	M	103	BCL	C2A-C1A-CHA	2.40	128.05	123.86
4	S	1706	BCL	CHC-C4B-NB	-2.37	121.74	124.26
5	G	103	ZE0	C31-C32-C33	-2.32	124.00	127.31
4	I	102	BCL	C4B-C3B-C2B	-2.31	104.64	108.36
4	S	1701	BCL	CHC-C4B-NB	-2.31	121.81	124.26
4	K	102	BCL	C4B-C3B-C2B	-2.30	104.66	108.36
4	Q	102	BCL	C4B-C3B-C2B	-2.30	104.67	108.36
4	A	101	BCL	C4B-C3B-C2B	-2.29	104.67	108.36
4	S	1704	BCL	C4B-C3B-C2B	-2.29	104.67	108.36
4	S	1703	BCL	C4B-C3B-C2B	-2.28	104.69	108.36
4	H	101	BCL	C4B-C3B-C2B	-2.28	104.70	108.36
4	Q	101	BCL	C1-C2-C3	2.28	129.98	126.04
4	F	101	BCL	C2A-C1A-CHA	2.28	127.84	123.86
4	S	1702	BCL	C4B-C3B-C2B	-2.27	104.70	108.36
4	E	102	BCL	C4B-C3B-C2B	-2.27	104.71	108.36
4	G	101	BCL	C4B-C3B-C2B	-2.26	104.72	108.36
4	O	101	BCL	C4B-C3B-C2B	-2.26	104.72	108.36
4	M	101	BCL	C4B-C3B-C2B	-2.26	104.72	108.36
4	S	1701	BCL	C4B-C3B-C2B	-2.26	104.73	108.36
4	C	101	BCL	C4B-C3B-C2B	-2.26	104.73	108.36
4	S	1705	BCL	C4B-C3B-C2B	-2.25	104.73	108.36
4	H	101	BCL	C1-C2-C3	-2.25	122.15	126.04
4	S	1704	BCL	OBB-CAB-CBB	-2.24	114.76	119.73
4	H	101	BCL	OBB-CAB-CBB	-2.24	114.76	119.73
4	G	101	BCL	OBB-CAB-CBB	-2.23	114.78	119.73
4	F	101	BCL	C4B-C3B-C2B	-2.23	104.77	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	101	BCL	OBB-CAB-CBB	-2.23	114.80	119.73
4	K	102	BCL	OBB-CAB-CBB	-2.22	114.81	119.73
4	Q	102	BCL	OBB-CAB-CBB	-2.22	114.81	119.73
4	Q	101	BCL	C4B-C3B-C2B	-2.22	104.78	108.36
4	C	102	BCL	C4B-C3B-C2B	-2.22	104.79	108.36
4	M	101	BCL	OBB-CAB-CBB	-2.21	114.83	119.73
4	S	1706	BCL	C4B-C3B-C2B	-2.21	104.80	108.36
4	E	102	BCL	OBB-CAB-CBB	-2.21	114.83	119.73
4	I	102	BCL	OBB-CAB-CBB	-2.21	114.83	119.73
4	E	101	BCL	C4B-C3B-C2B	-2.21	104.81	108.36
4	D	101	BCL	C4B-C3B-C2B	-2.20	104.82	108.36
4	I	101	BCL	C4B-C3B-C2B	-2.20	104.83	108.36
4	S	1701	BCL	OBB-CAB-CBB	-2.20	114.86	119.73
4	S	1703	BCL	CMB-C2B-C1B	-2.19	122.03	125.37
4	S	1705	BCL	OBB-CAB-CBB	-2.19	114.88	119.73
4	P	101	BCL	C4B-C3B-C2B	-2.18	104.85	108.36
4	S	1702	BCL	OBB-CAB-CBB	-2.18	114.90	119.73
4	O	102	BCL	C4B-C3B-C2B	-2.18	104.86	108.36
4	S	1702	BCL	C1-O2A-CGA	2.18	122.16	116.44
4	A	101	BCL	CMB-C2B-C1B	-2.18	122.05	125.37
4	L	101	BCL	C4B-C3B-C2B	-2.18	104.86	108.36
4	A	102	BCL	C4B-C3B-C2B	-2.17	104.86	108.36
4	K	101	BCL	C4B-C3B-C2B	-2.17	104.87	108.36
4	M	102	BCL	C4B-C3B-C2B	-2.17	104.87	108.36
4	G	102	BCL	C4B-C3B-C2B	-2.17	104.87	108.36
4	S	1704	BCL	C17-C16-C15	2.16	123.19	113.24
4	Q	102	BCL	CMB-C2B-C1B	-2.16	122.08	125.37
4	B	101	BCL	C4B-C3B-C2B	-2.15	104.89	108.36
4	H	101	BCL	C11-C10-C8	2.15	122.88	115.92
4	E	101	BCL	OBB-CAB-CBB	-2.15	114.97	119.73
4	R	101	BCL	C4B-C3B-C2B	-2.14	104.91	108.36
4	C	101	BCL	OBB-CAB-CBB	-2.14	114.98	119.73
4	I	102	BCL	CMB-C2B-C1B	-2.14	122.11	125.37
4	Q	101	BCL	OBB-CAB-CBB	-2.14	115.00	119.73
4	S	1701	BCL	CMB-C2B-C1B	-2.13	122.12	125.37
4	K	102	BCL	CMB-C2B-C1B	-2.13	122.12	125.37
4	S	1703	BCL	OBB-CAB-CBB	-2.13	115.01	119.73
4	J	101	BCL	C4B-C3B-C2B	-2.13	104.93	108.36
4	A	101	BCL	OBB-CAB-CBB	-2.13	115.01	119.73
4	C	102	BCL	OBB-CAB-CBB	-2.13	115.01	119.73
4	S	1704	BCL	CMB-C2B-C1B	-2.12	122.14	125.37
4	M	101	BCL	CMB-C2B-C1B	-2.12	122.14	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	101	BCL	C1-C2-C3	-2.11	122.39	126.04
4	R	101	BCL	C4-C3-C5	-2.11	111.72	115.27
4	K	101	BCL	OBB-CAB-CBB	-2.11	115.05	119.73
4	S	1705	BCL	CMB-C2B-C1B	-2.11	122.16	125.37
4	I	101	BCL	OBB-CAB-CBB	-2.11	115.06	119.73
4	D	101	BCL	C11-C10-C8	2.10	122.72	115.92
4	S	1706	BCL	CMB-C2B-C1B	-2.10	122.17	125.37
4	F	101	BCL	OBB-CAB-CBB	-2.09	115.10	119.73
4	M	103	BCL	C4B-C3B-C2B	-2.09	105.00	108.36
4	S	1702	BCL	CMB-C2B-C1B	-2.09	122.19	125.37
4	O	101	BCL	CMB-C2B-C1B	-2.09	122.19	125.37
5	E	103	ZE0	C31-C32-C33	-2.08	124.33	127.31
4	E	102	BCL	CMB-C2B-C1B	-2.08	122.19	125.37
4	S	1706	BCL	OBB-CAB-CBB	-2.08	115.12	119.73
4	M	102	BCL	C1C-NC-C4C	2.08	107.64	106.71
4	C	101	BCL	CMB-C2B-C1B	-2.08	122.20	125.37
4	G	102	BCL	OBB-CAB-CBB	-2.07	115.13	119.73
4	A	102	BCL	OBB-CAB-CBB	-2.07	115.14	119.73
4	D	101	BCL	OBB-CAB-CBB	-2.07	115.15	119.73
4	P	101	BCL	OBB-CAB-CBB	-2.05	115.18	119.73
4	O	102	BCL	OBB-CAB-CBB	-2.05	115.19	119.73
4	S	1701	BCL	C1-O2A-CGA	2.05	121.82	116.44
4	G	101	BCL	CMB-C2B-C1B	-2.04	122.26	125.37
4	M	103	BCL	C1C-NC-C4C	2.04	107.62	106.71
4	H	101	BCL	CMB-C2B-C1B	-2.03	122.27	125.37
4	B	101	BCL	OBB-CAB-CBB	-2.03	115.23	119.73
4	M	102	BCL	OBB-CAB-CBB	-2.03	115.23	119.73
4	D	101	BCL	C1-C2-C3	-2.03	122.53	126.04
5	I	103	ZE0	C31-C32-C33	-2.02	124.43	127.31
4	R	101	BCL	OBB-CAB-CBB	-2.02	115.26	119.73
4	I	101	BCL	C1C-NC-C4C	2.01	107.61	106.71
4	L	101	BCL	OBB-CAB-CBB	-2.01	115.28	119.73
4	D	101	BCL	C4-C3-C5	-2.01	111.89	115.27

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	1701	BCL	O2A-C1-C2-C3
4	S	1702	BCL	CHA-CBD-CGD-O1D
4	S	1702	BCL	CHA-CBD-CGD-O2D
5	A	103	ZE0	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
5	A	103	ZE0	C34-C33-C35-C36
5	B	102	ZE0	C32-C33-C35-C36
5	B	102	ZE0	C34-C33-C35-C36
5	C	103	ZE0	C32-C33-C35-C36
5	C	103	ZE0	C34-C33-C35-C36
5	E	103	ZE0	C34-C33-C35-C36
5	G	103	ZE0	C34-C33-C35-C36
5	I	103	ZE0	C32-C33-C35-C36
5	I	103	ZE0	C34-C33-C35-C36
5	K	103	ZE0	C34-C33-C35-C36
5	M	104	ZE0	C32-C33-C35-C36
5	M	104	ZE0	C34-C33-C35-C36
5	O	103	ZE0	C32-C33-C35-C36
5	O	103	ZE0	C34-C33-C35-C36
5	A	103	ZE0	C35-C36-C37-C38
5	K	103	ZE0	C35-C36-C37-C38
5	C	103	ZE0	C35-C36-C37-C38
5	E	103	ZE0	C32-C33-C35-C36
5	G	103	ZE0	C32-C33-C35-C36
5	K	103	ZE0	C32-C33-C35-C36
4	S	1706	BCL	C6-C7-C8-C10
4	M	102	BCL	C11-C10-C8-C7
5	M	104	ZE0	C35-C36-C37-C38
4	J	101	BCL	C13-C15-C16-C17
4	L	101	BCL	C13-C15-C16-C17
4	S	1701	BCL	C2A-CAA-CBA-CGA
4	S	1705	BCL	C2A-CAA-CBA-CGA
4	K	101	BCL	C5-C6-C7-C8
4	S	1701	BCL	C4-C3-C5-C6
4	J	101	BCL	C4-C3-C5-C6
4	L	101	BCL	C2-C3-C5-C6
4	S	1703	BCL	O2A-C1-C2-C3
4	S	1706	BCL	O2A-C1-C2-C3
4	M	102	BCL	C4-C3-C5-C6
4	G	102	BCL	C2-C3-C5-C6
4	M	102	BCL	C2-C3-C5-C6
4	L	101	BCL	C4-C3-C5-C6
4	S	1705	BCL	C6-C7-C8-C10
4	F	101	BCL	C4-C3-C5-C6
4	G	102	BCL	C4-C3-C5-C6
4	S	1705	BCL	C6-C7-C8-C9
4	S	1706	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	H	101	BCL	C14-C13-C15-C16
4	M	102	BCL	C11-C10-C8-C9
5	B	102	ZE0	C35-C36-C37-C38
4	S	1702	BCL	C15-C16-C17-C18
4	F	101	BCL	C10-C11-C12-C13
4	O	102	BCL	C4-C3-C5-C6
4	D	101	BCL	C14-C13-C15-C16
4	P	101	BCL	C14-C13-C15-C16
4	Q	101	BCL	C4-C3-C5-C6
4	F	101	BCL	C2-C3-C5-C6
4	O	102	BCL	C2-C3-C5-C6
4	Q	101	BCL	C2-C3-C5-C6
5	E	103	ZE0	C35-C36-C37-C38
4	S	1702	BCL	O2A-C1-C2-C3
4	S	1701	BCL	C2-C3-C5-C6
4	B	101	BCL	C14-C13-C15-C16
4	R	101	BCL	C14-C13-C15-C16
5	I	103	ZE0	C35-C36-C37-C38
5	O	103	ZE0	C35-C36-C37-C38
4	S	1704	BCL	C2A-CAA-CBA-CGA
4	A	102	BCL	C4-C3-C5-C6
4	C	102	BCL	C4-C3-C5-C6
4	O	102	BCL	C3-C5-C6-C7
4	A	102	BCL	CHA-CBD-CGD-O1D
4	S	1705	BCL	CHA-CBD-CGD-O1D
4	S	1705	BCL	CHA-CBD-CGD-O2D
4	S	1706	BCL	CHA-CBD-CGD-O1D
4	S	1706	BCL	CHA-CBD-CGD-O2D
4	C	102	BCL	CHA-CBD-CGD-O1D
4	C	102	BCL	CHA-CBD-CGD-O2D
4	E	101	BCL	CHA-CBD-CGD-O1D
4	E	101	BCL	CHA-CBD-CGD-O2D
4	I	101	BCL	CHA-CBD-CGD-O1D
4	K	101	BCL	CHA-CBD-CGD-O1D
4	K	101	BCL	CHA-CBD-CGD-O2D
4	M	102	BCL	CHA-CBD-CGD-O1D
4	O	102	BCL	CHA-CBD-CGD-O1D
4	A	102	BCL	C2-C3-C5-C6
4	C	102	BCL	C2-C3-C5-C6
4	J	101	BCL	C2-C3-C5-C6
4	S	1706	BCL	C2A-CAA-CBA-CGA
4	A	102	BCL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
4	S	1702	BCL	CAD-CBD-CGD-O1D
4	S	1705	BCL	CAD-CBD-CGD-O1D
4	S	1706	BCL	CAD-CBD-CGD-O1D
4	C	102	BCL	CAD-CBD-CGD-O1D
4	E	101	BCL	CAD-CBD-CGD-O1D
4	G	102	BCL	CAD-CBD-CGD-O1D
4	I	101	BCL	CAD-CBD-CGD-O1D
4	K	101	BCL	CAD-CBD-CGD-O1D
4	M	102	BCL	CAD-CBD-CGD-O1D
4	O	102	BCL	CAD-CBD-CGD-O1D
4	Q	101	BCL	CAD-CBD-CGD-O1D
4	S	1701	BCL	C6-C7-C8-C10
4	J	101	BCL	C6-C7-C8-C10
4	L	101	BCL	C6-C7-C8-C10
4	D	101	BCL	C8-C10-C11-C12
4	S	1704	BCL	C16-C17-C18-C19
4	B	101	BCL	C2A-CAA-CBA-CGA
4	E	101	BCL	C4-C3-C5-C6
4	M	103	BCL	C5-C6-C7-C8
4	S	1701	BCL	C16-C17-C18-C19
4	S	1705	BCL	C16-C17-C18-C19
4	J	101	BCL	C10-C11-C12-C13
4	L	101	BCL	C6-C7-C8-C9
4	S	1706	BCL	C16-C17-C18-C19
4	S	1703	BCL	C16-C17-C18-C19
4	P	101	BCL	C8-C10-C11-C12
4	D	101	BCL	C2A-CAA-CBA-CGA
4	M	103	BCL	C10-C11-C12-C13
4	F	101	BCL	C2A-CAA-CBA-CGA
4	S	1704	BCL	C16-C17-C18-C20
4	S	1705	BCL	O2A-C1-C2-C3
4	E	101	BCL	C10-C11-C12-C13
4	L	101	BCL	C2A-CAA-CBA-CGA
5	A	103	ZE0	C2-C1-C4-C5
4	E	101	BCL	C2-C3-C5-C6
4	S	1706	BCL	C16-C17-C18-C20
5	G	103	ZE0	C35-C36-C37-C38
4	S	1704	BCL	C4-C3-C5-C6
4	A	102	BCL	C4C-C3C-CAC-CBC
4	M	102	BCL	C4C-C3C-CAC-CBC
4	S	1705	BCL	C16-C17-C18-C20
4	O	101	BCL	C2A-CAA-CBA-CGA

Continued on next page...

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Mol	Chain	Res	Type	Atoms
4	J	101	BCL	C2A-CAA-CBA-CGA
4	R	101	BCL	C2A-CAA-CBA-CGA
4	S	1703	BCL	C16-C17-C18-C20
4	S	1701	BCL	C6-C7-C8-C9
4	J	101	BCL	C6-C7-C8-C9
4	S	1703	BCL	CAD-CBD-CGD-O2D
4	S	1701	BCL	C16-C17-C18-C20
4	A	102	BCL	C2B-C3B-CAB-CBB
4	M	102	BCL	C2B-C3B-CAB-CBB
4	O	102	BCL	C2B-C3B-CAB-CBB
4	R	101	BCL	C8-C10-C11-C12
4	S	1704	BCL	O2A-C1-C2-C3
4	A	102	BCL	CHA-CBD-CGD-O2D
4	G	102	BCL	CHA-CBD-CGD-O1D
4	H	101	BCL	CHA-CBD-CGD-O1D
4	H	101	BCL	CHA-CBD-CGD-O2D
4	I	101	BCL	CHA-CBD-CGD-O2D
4	M	102	BCL	CHA-CBD-CGD-O2D
4	O	102	BCL	CHA-CBD-CGD-O2D
4	Q	101	BCL	CHA-CBD-CGD-O1D
4	A	102	BCL	C13-C15-C16-C17
4	M	103	BCL	C2A-CAA-CBA-CGA
4	E	102	BCL	CAA-CBA-CGA-O2A
4	B	101	BCL	C8-C10-C11-C12
4	P	101	BCL	C2A-CAA-CBA-CGA
4	E	102	BCL	CAA-CBA-CGA-O1A
4	H	101	BCL	C2A-CAA-CBA-CGA
4	I	101	BCL	C4-C3-C5-C6
4	S	1701	BCL	CAD-CBD-CGD-O1D
4	Q	102	BCL	CAD-CBD-CGD-O1D
4	I	102	BCL	C8-C10-C11-C12
4	A	102	BCL	C2B-C3B-CAB-OBB
4	G	102	BCL	C2B-C3B-CAB-OBB
4	M	102	BCL	C2B-C3B-CAB-OBB
4	O	102	BCL	C2B-C3B-CAB-OBB
4	C	101	BCL	CAA-CBA-CGA-O2A
4	M	101	BCL	C8-C10-C11-C12
4	M	102	BCL	C13-C15-C16-C17

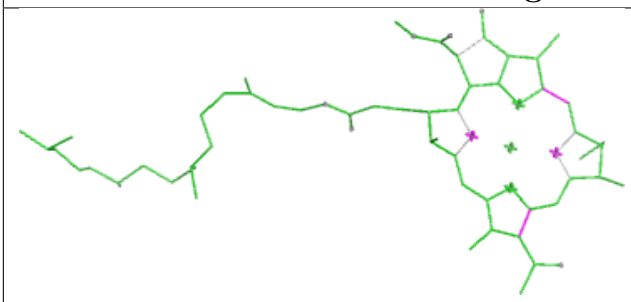
There are no ring outliers.

27 monomers are involved in 28 short contacts:

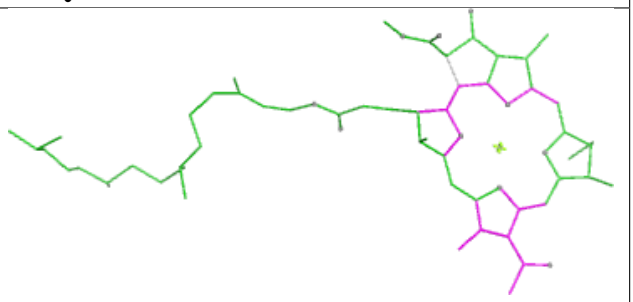
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	102	BCL	2	0
4	S	1701	BCL	1	0
5	B	102	ZE0	1	0
5	E	103	ZE0	2	0
5	A	103	ZE0	1	0
4	C	102	BCL	2	0
5	M	104	ZE0	1	0
4	S	1703	BCL	1	0
4	I	101	BCL	1	0
4	J	101	BCL	1	0
4	O	102	BCL	1	0
4	M	103	BCL	1	0
4	R	101	BCL	1	0
4	H	101	BCL	1	0
4	Q	101	BCL	1	0
4	M	102	BCL	1	0
5	O	103	ZE0	1	0
4	E	102	BCL	2	0
4	E	101	BCL	1	0
4	B	101	BCL	2	0
4	F	101	BCL	2	0
4	L	101	BCL	2	0
4	D	101	BCL	2	0
4	A	102	BCL	2	0
4	K	101	BCL	1	0
4	P	101	BCL	1	0
4	M	101	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.

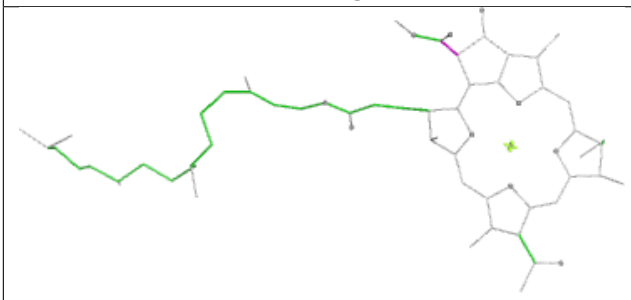
Ligand BCL Q 102



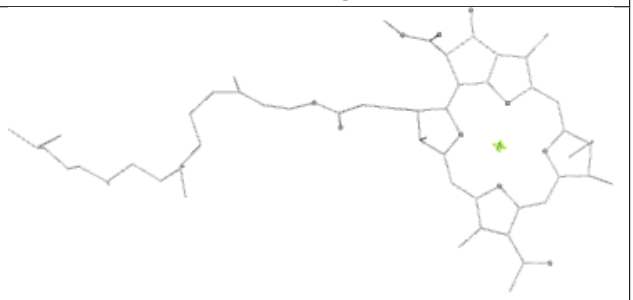
Bond lengths



Bond angles



Torsions

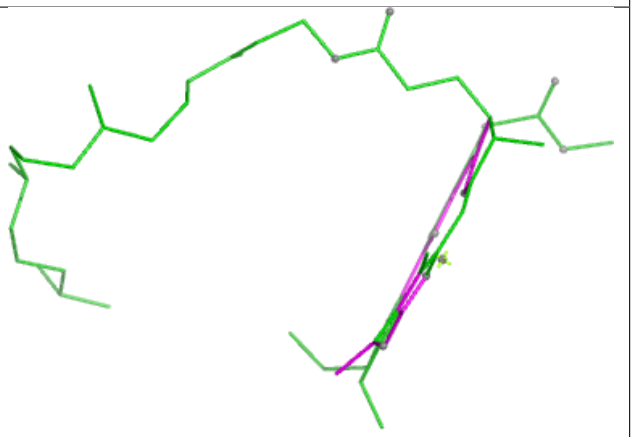


Rings

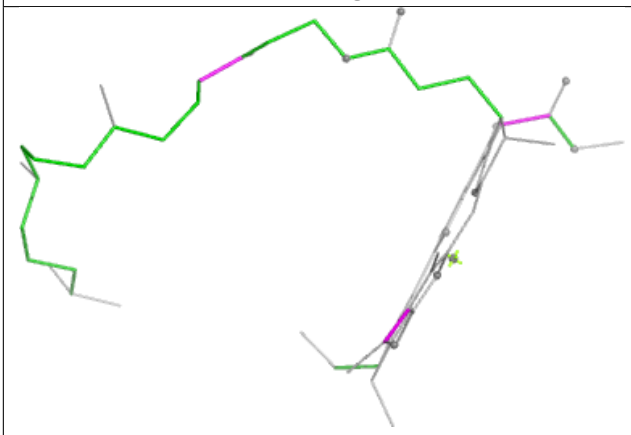
Ligand BCL G 102



Bond lengths



Bond angles

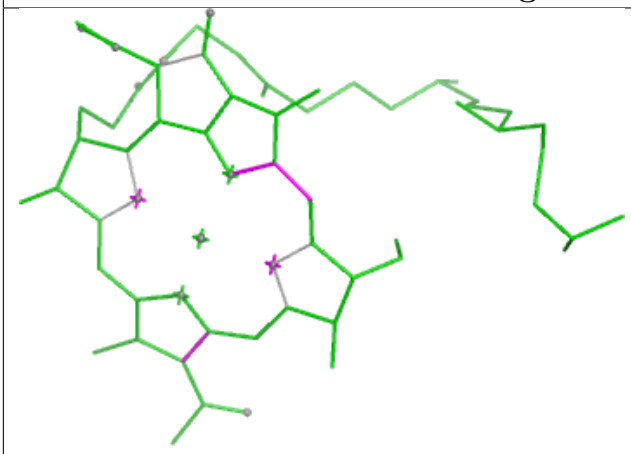


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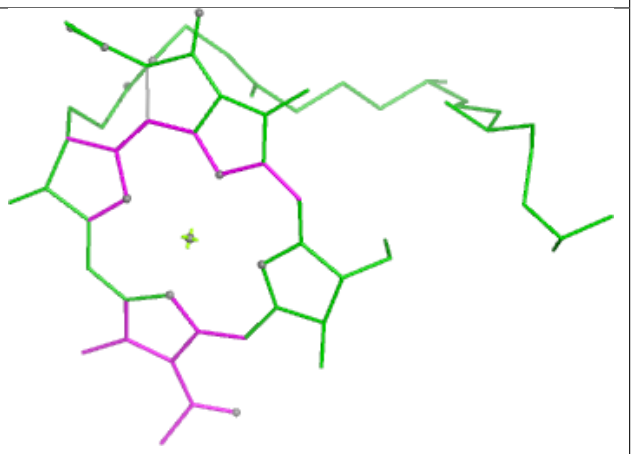


Rings

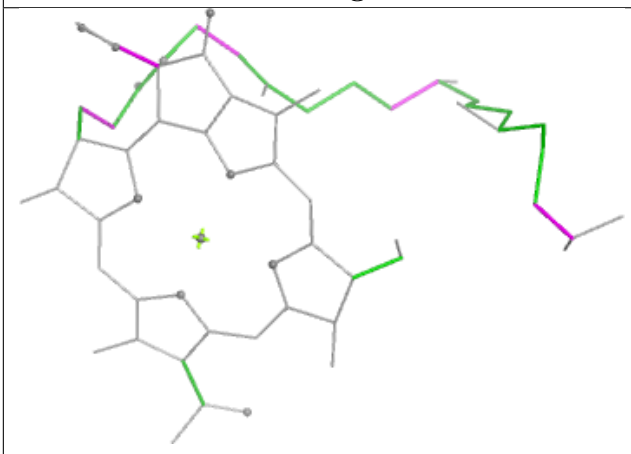
Ligand BCL S 1706



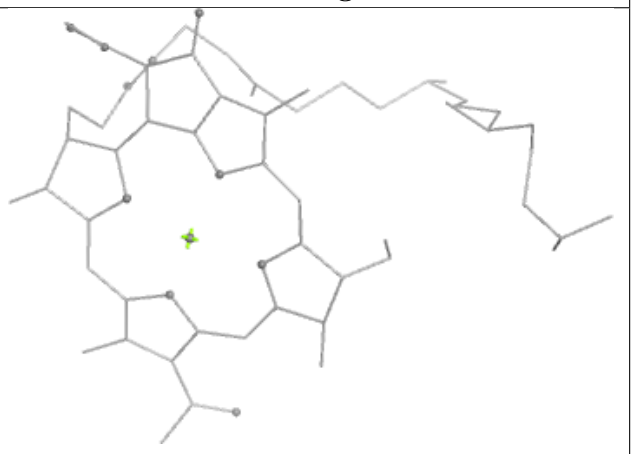
Bond lengths



Bond angles

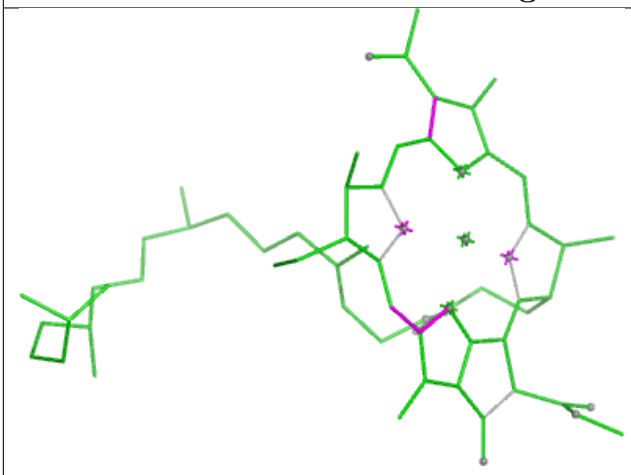


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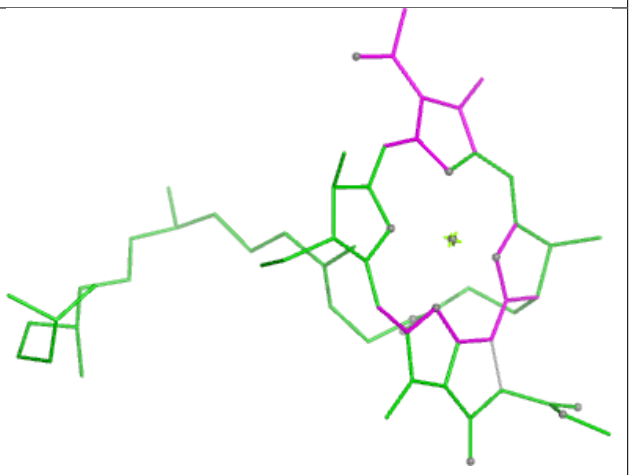


Rings

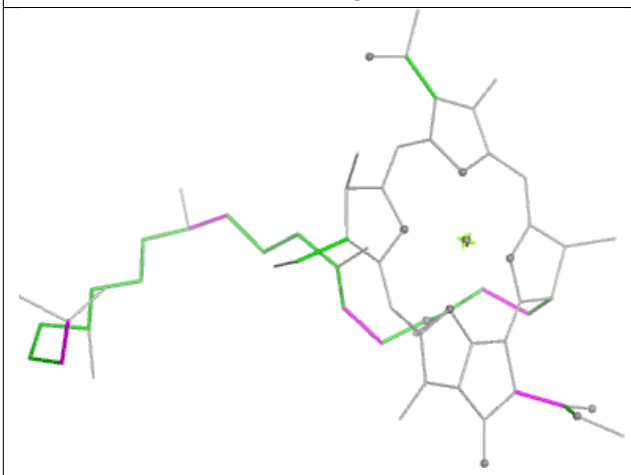
Ligand BCL S 1705



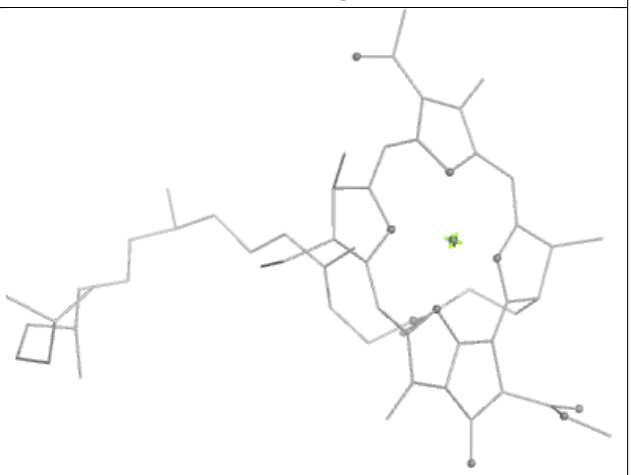
Bond lengths



Bond angles

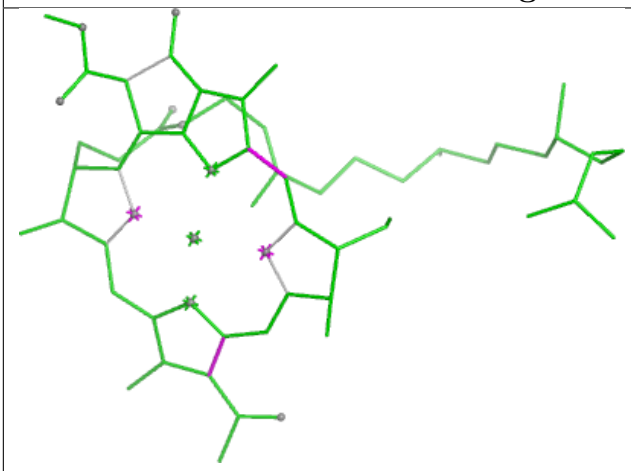


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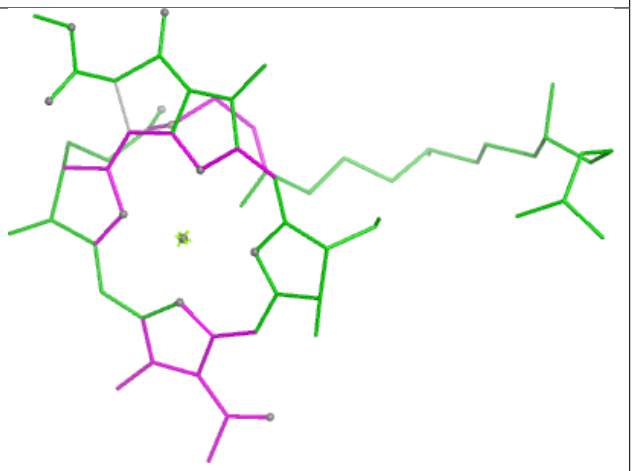


Rings

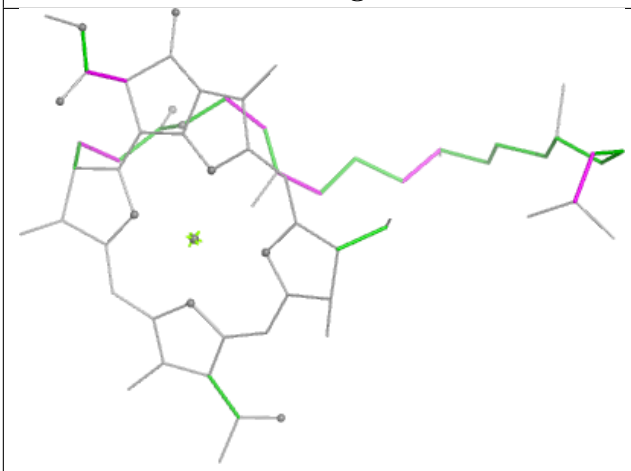
Ligand BCL S 1701



Bond lengths



Bond angles



Torsions



Rings

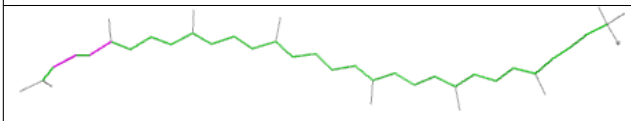
Ligand ZE0 B 102



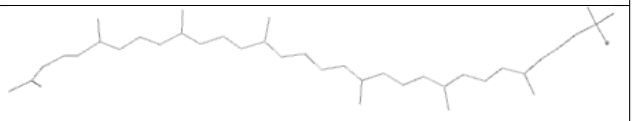
Bond lengths



Bond angles



Torsions



Rings

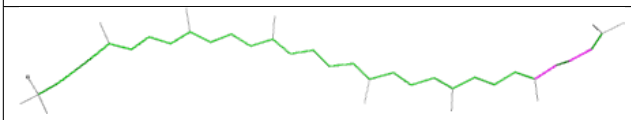
Ligand ZE0 E 103



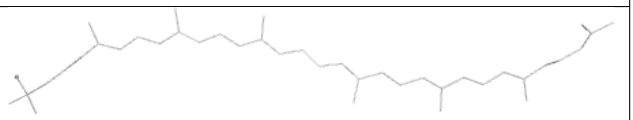
Bond lengths



Bond angles

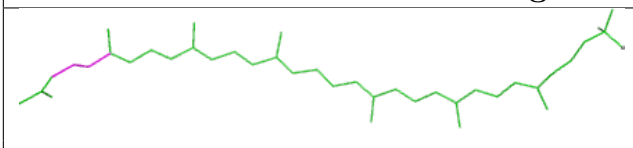


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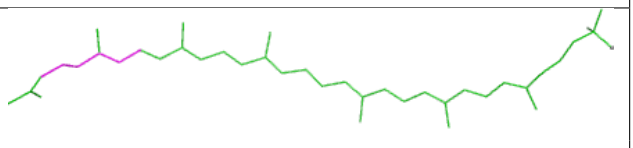


Rings

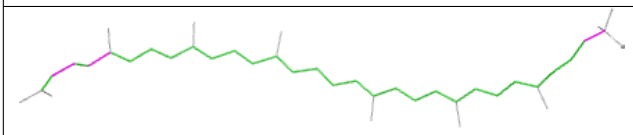
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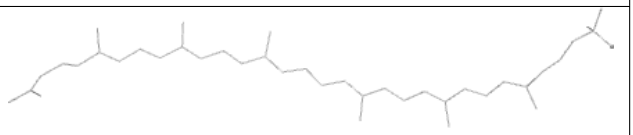
Bond lengths



Bond angles

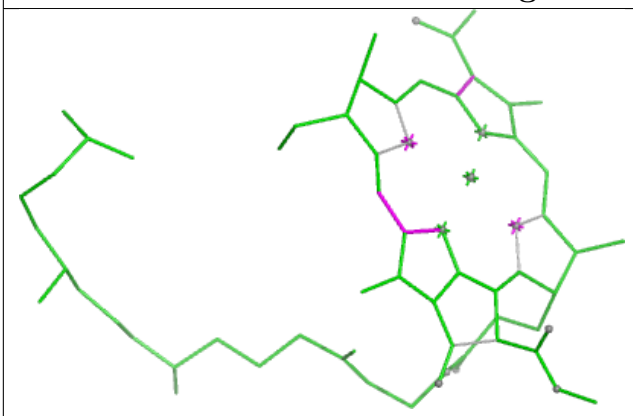


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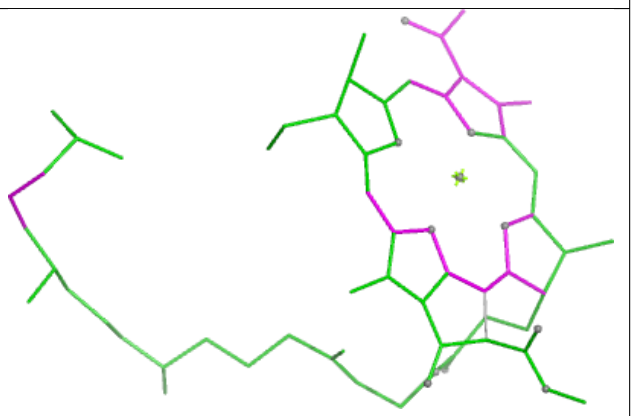


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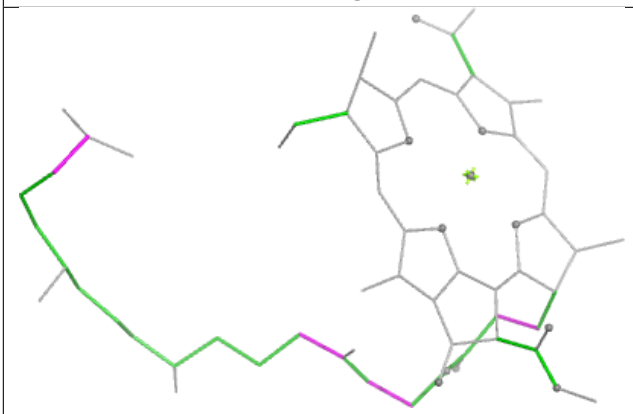
Ligand BCL S 1704



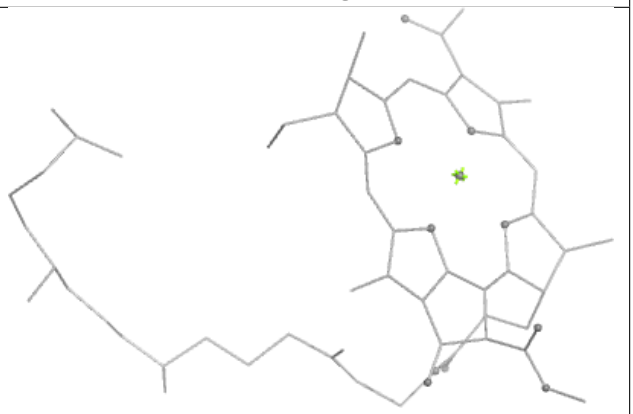
Bond lengths



Bond angles

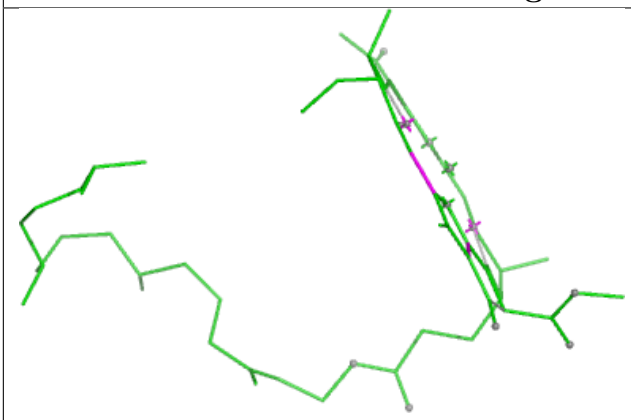


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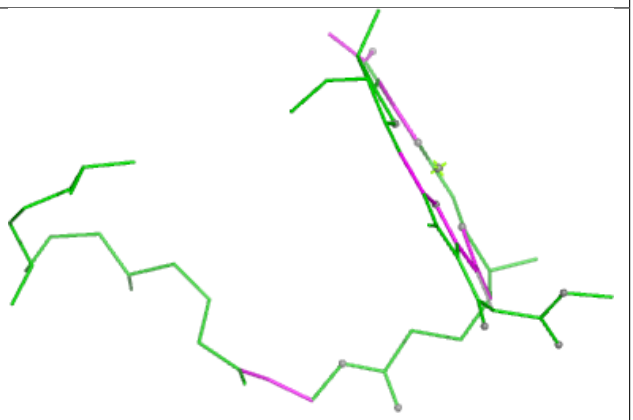


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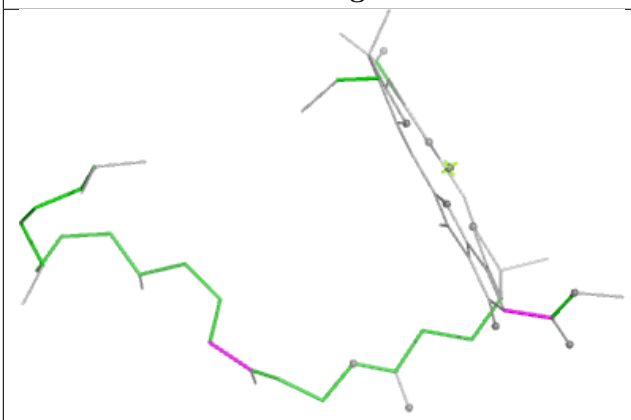
Ligand BCL C 102



Bond lengths



Bond angles

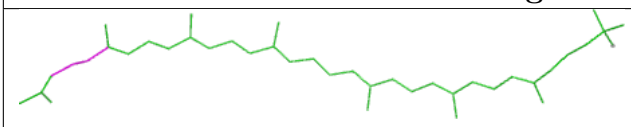


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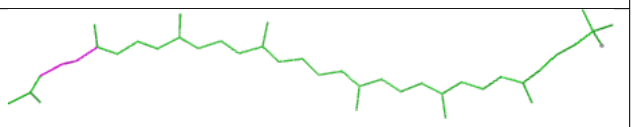


Rings

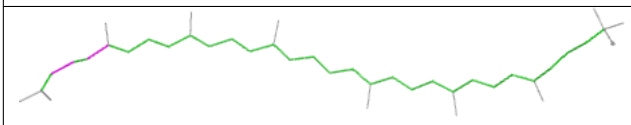
Ligand ZE0 M 104



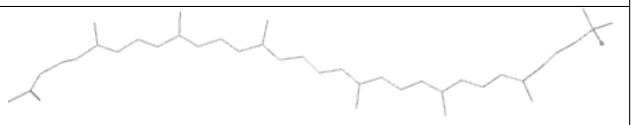
Bond lengths



Bond angles

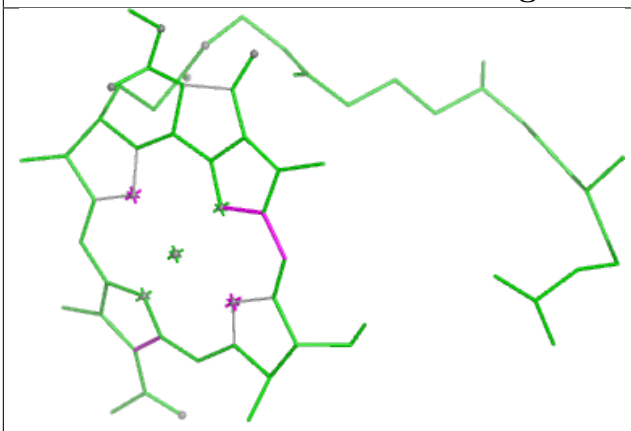


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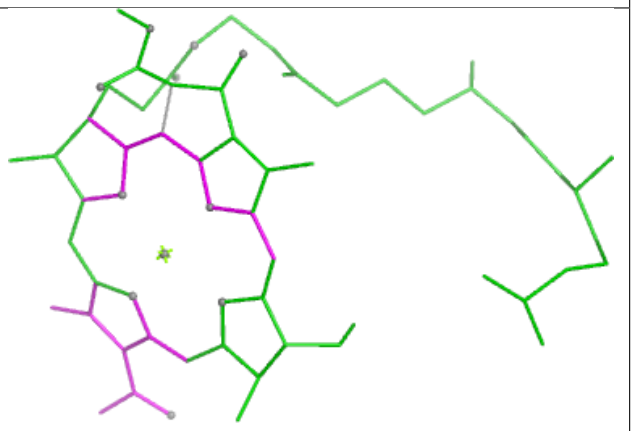


Rings

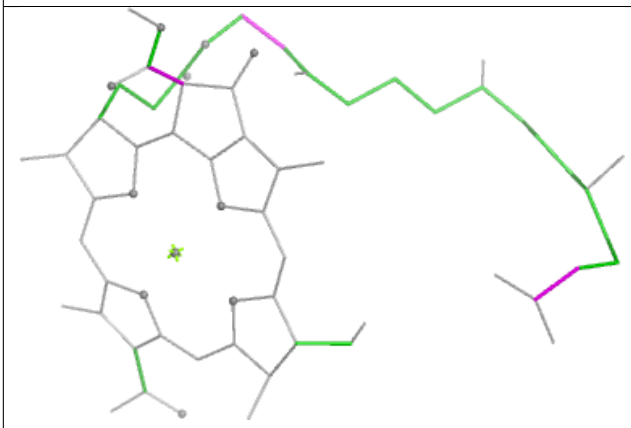
Ligand BCL S 1703



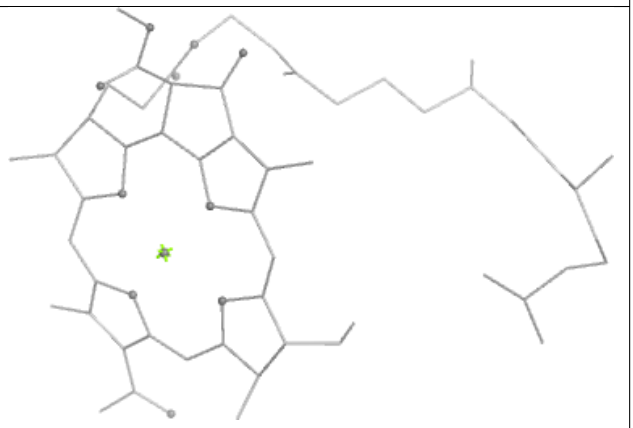
Bond lengths



Bond angles

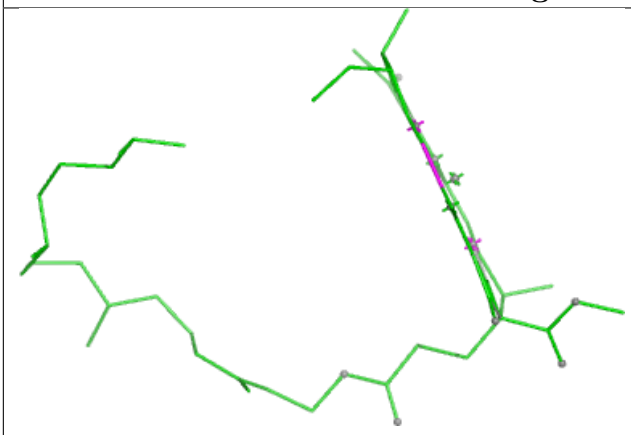


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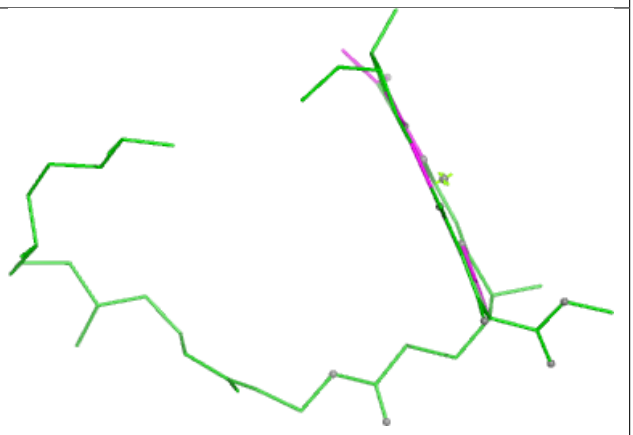


Rings

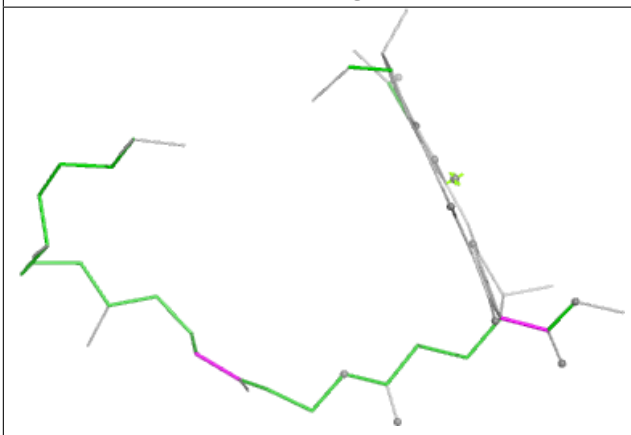
Ligand BCL I 101



Bond lengths



Bond angles

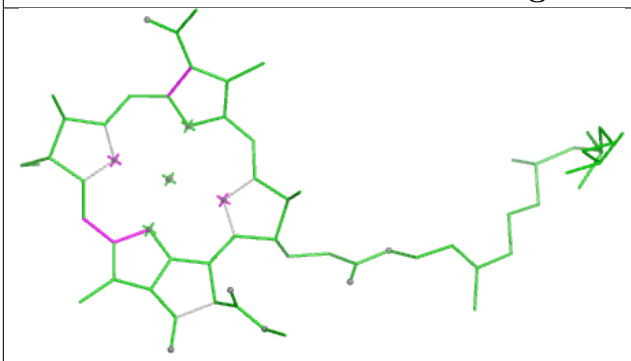


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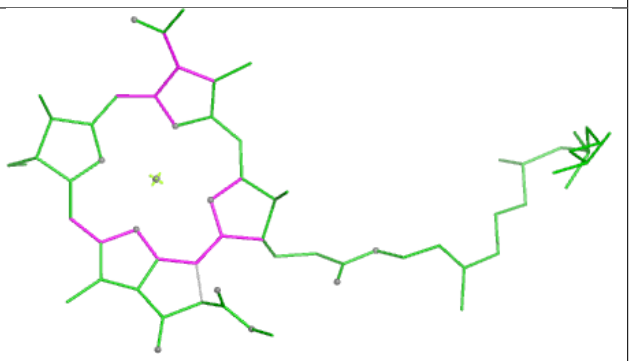


Rings

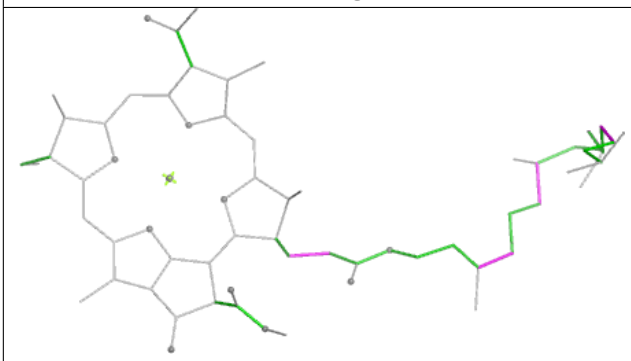
Ligand BCL J 101



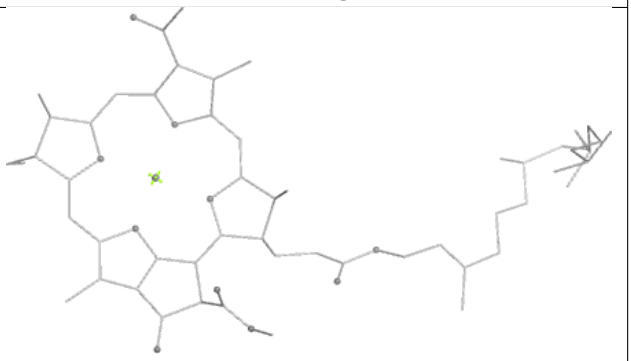
Bond lengths



Bond angles

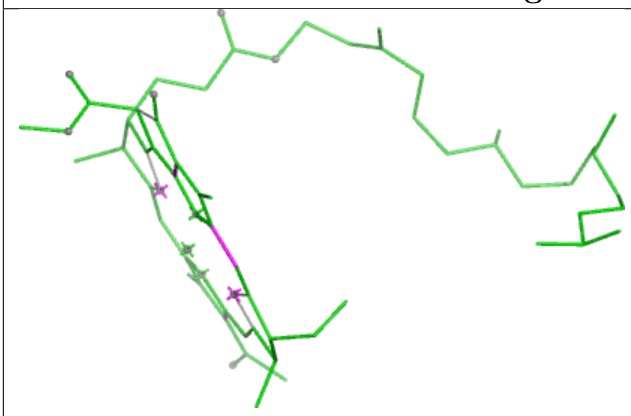


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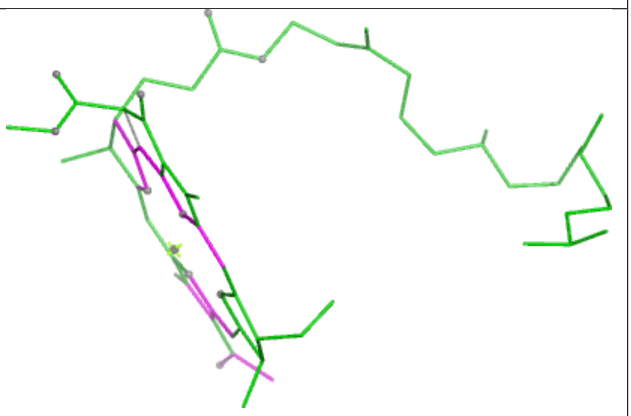


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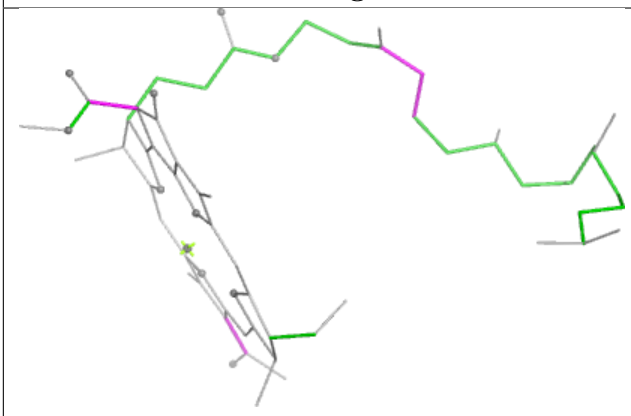
Ligand BCL O 102



Bond lengths



Bond angles

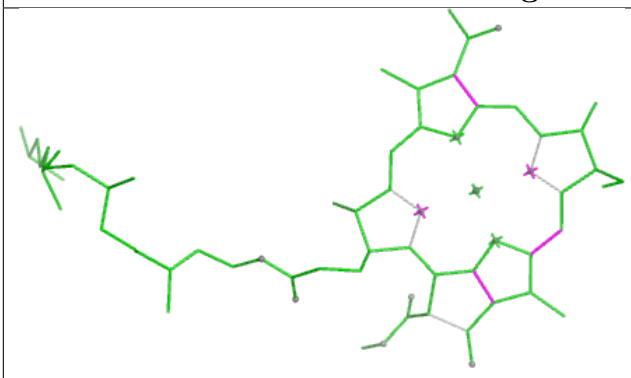


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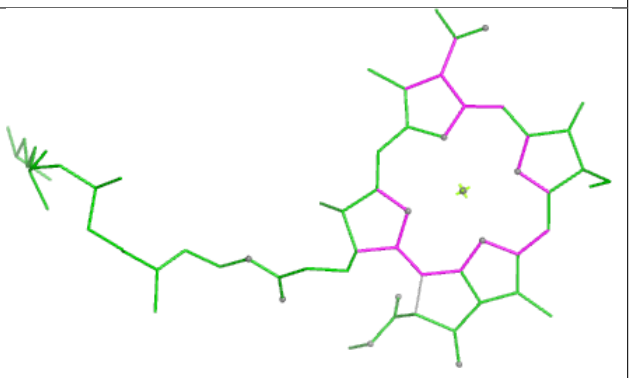


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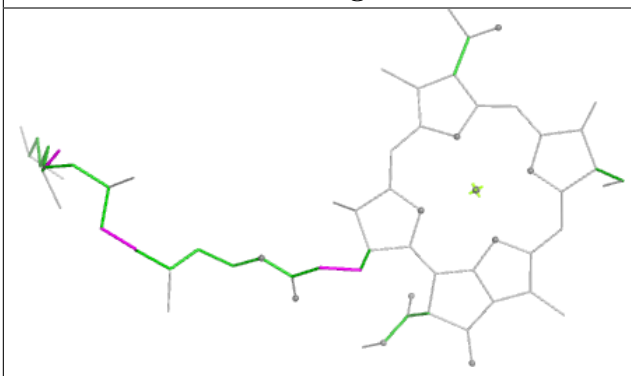
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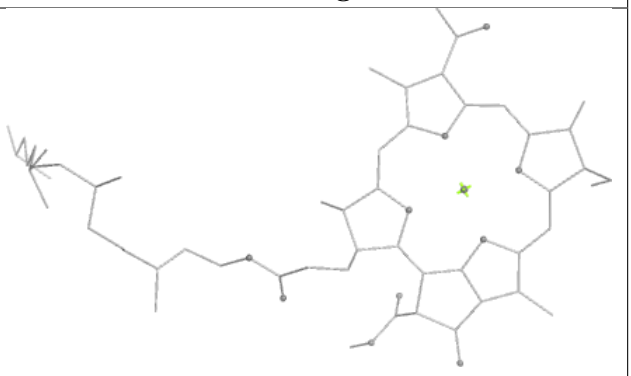
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Bond angles

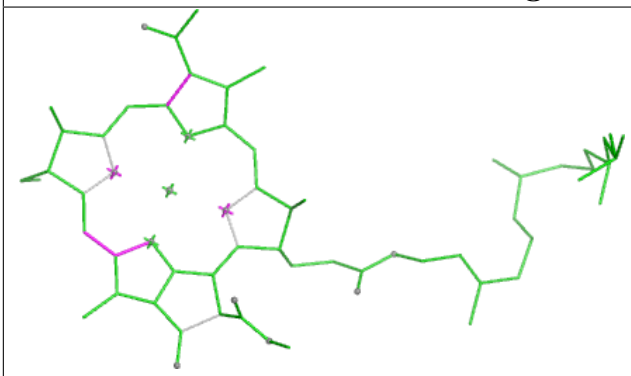


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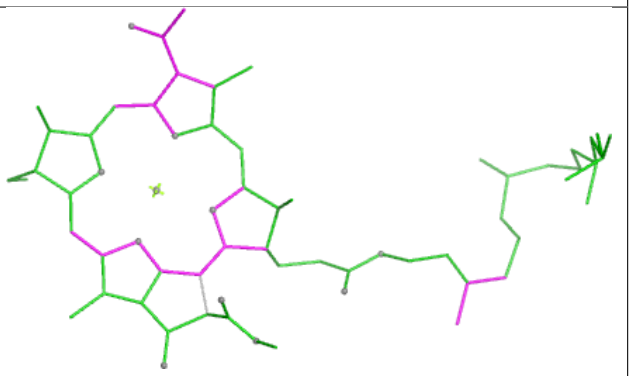


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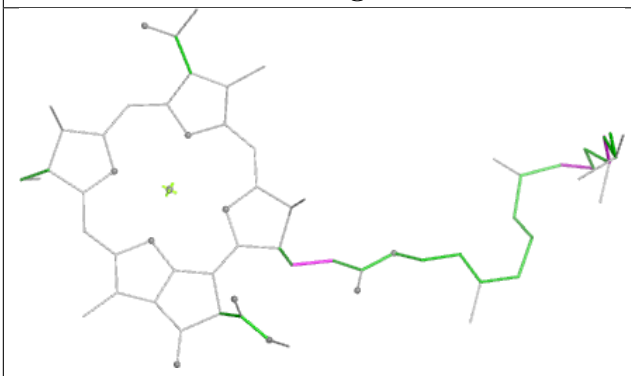
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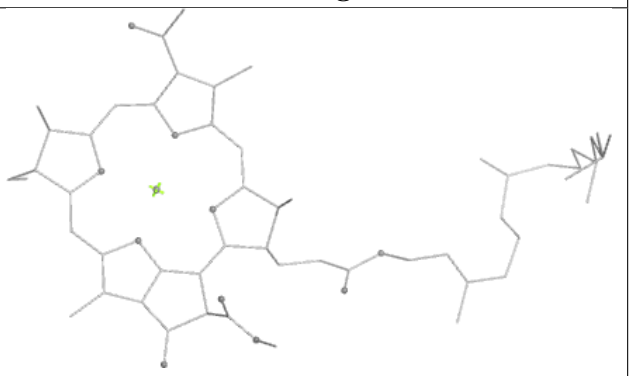
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Bond angles

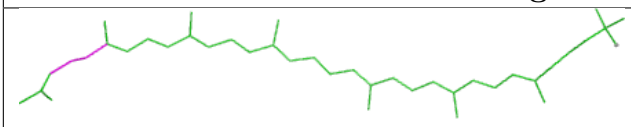


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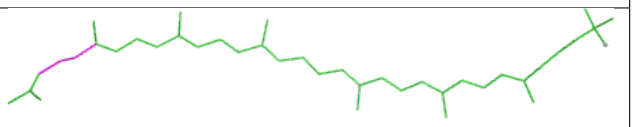


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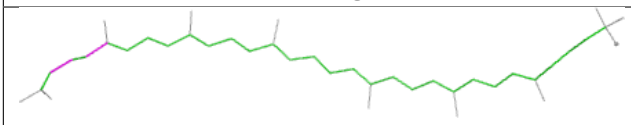
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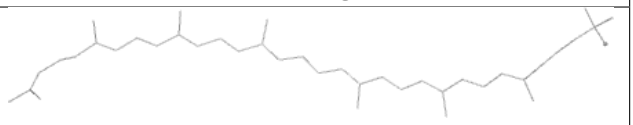
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Bond angles

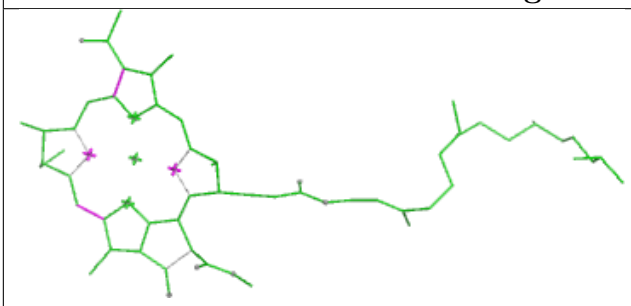


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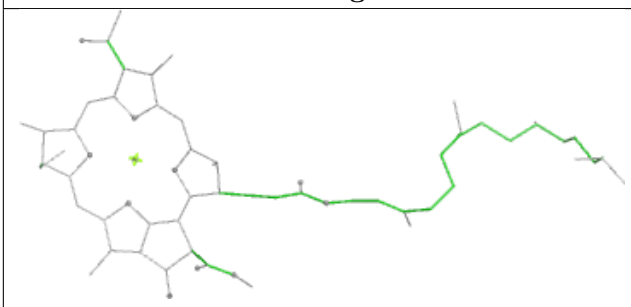
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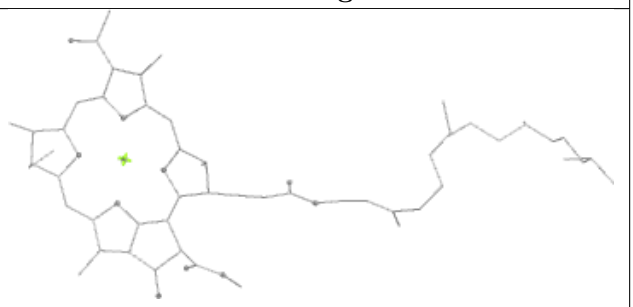
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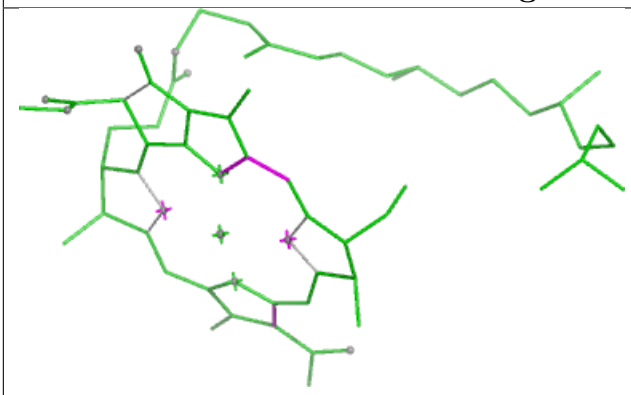


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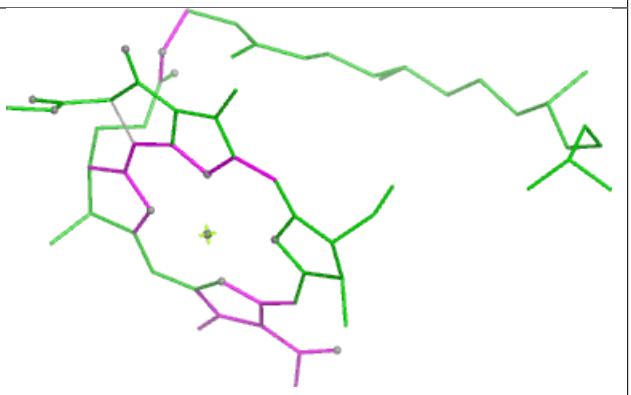


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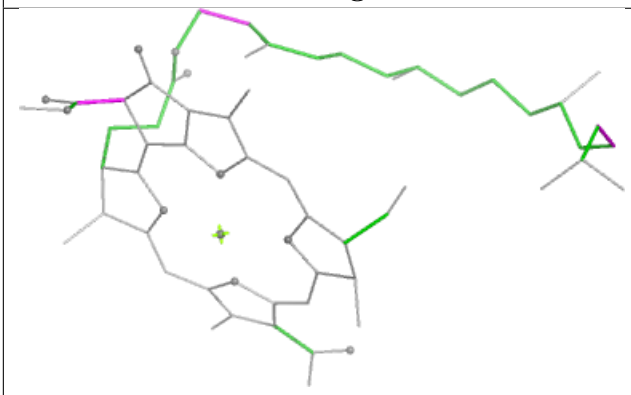
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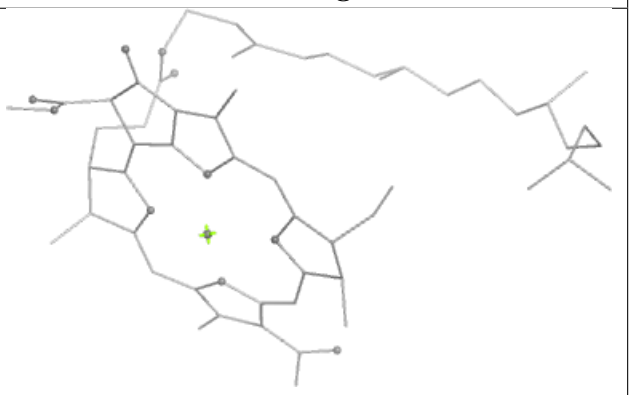
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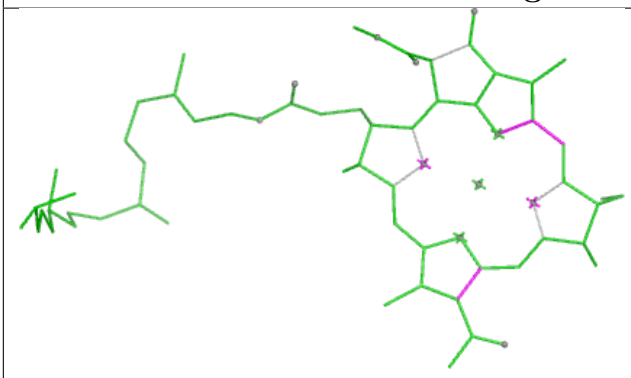


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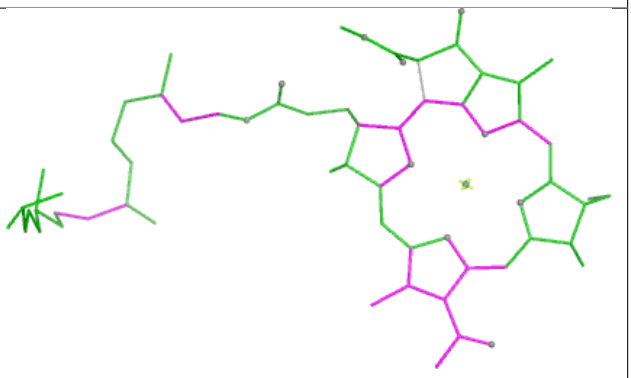


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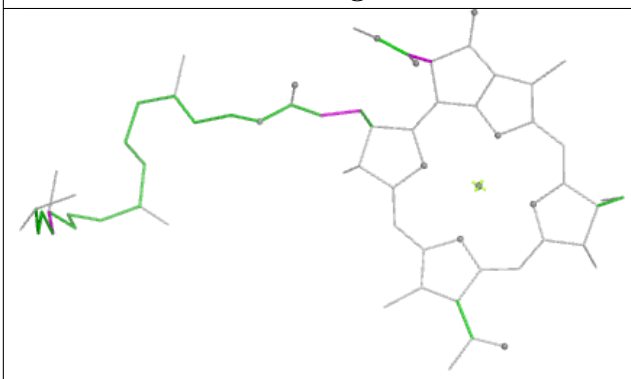
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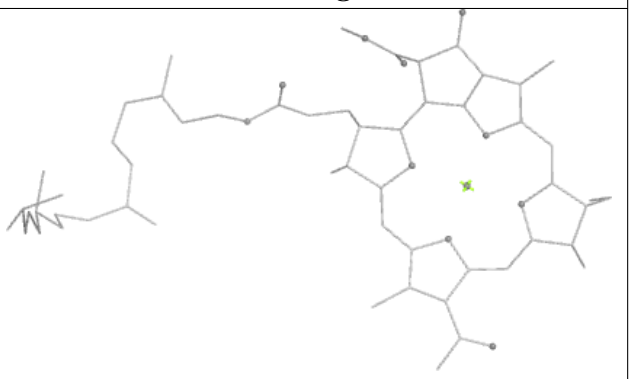
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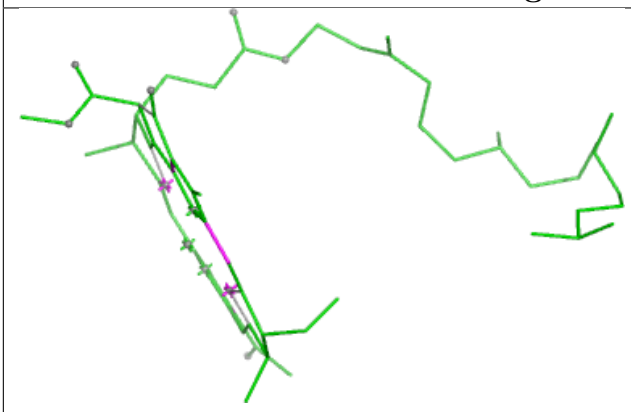


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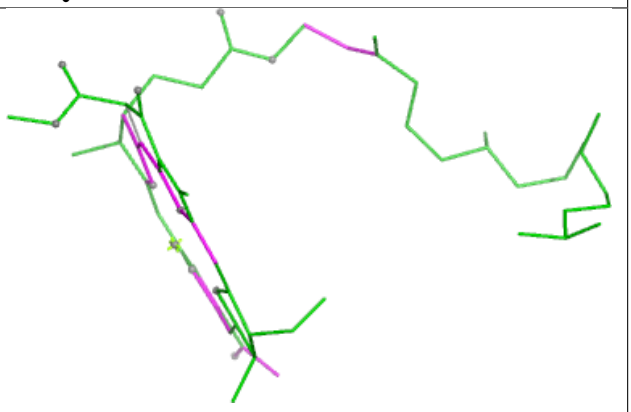


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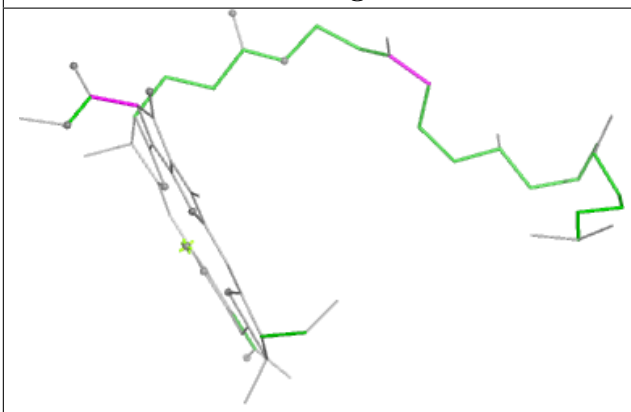
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Bond lengths



Bond angles

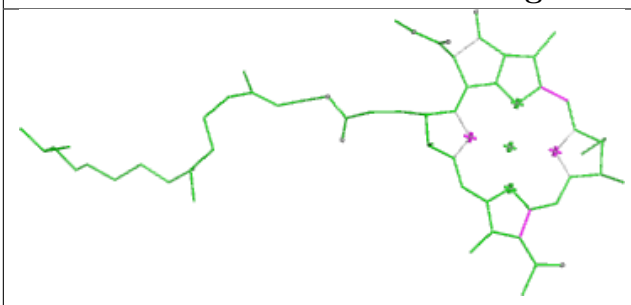


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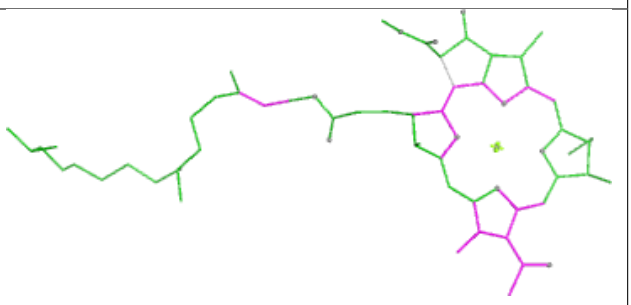


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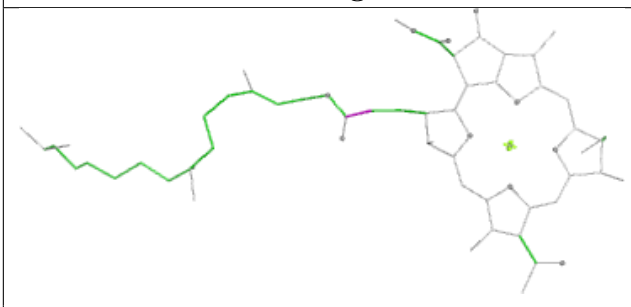
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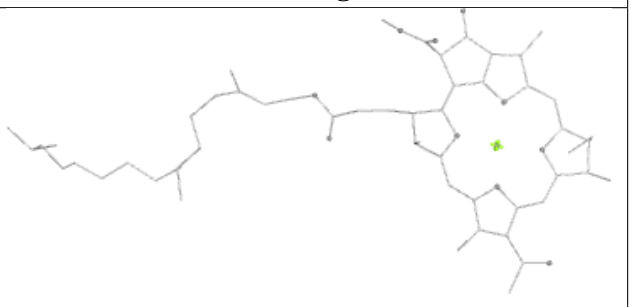
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Bond angles

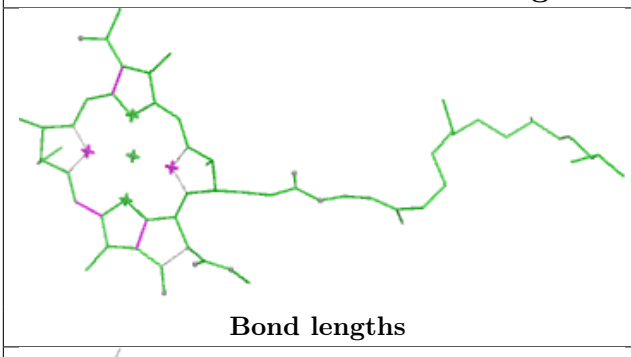


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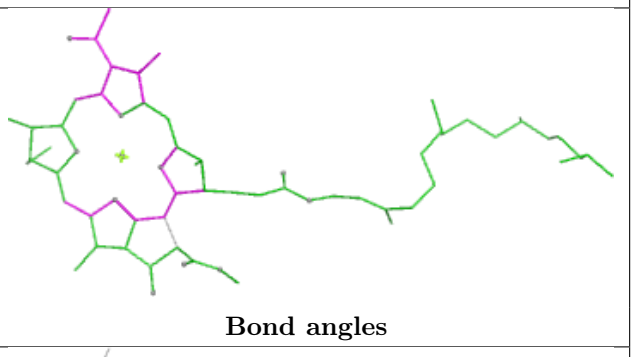


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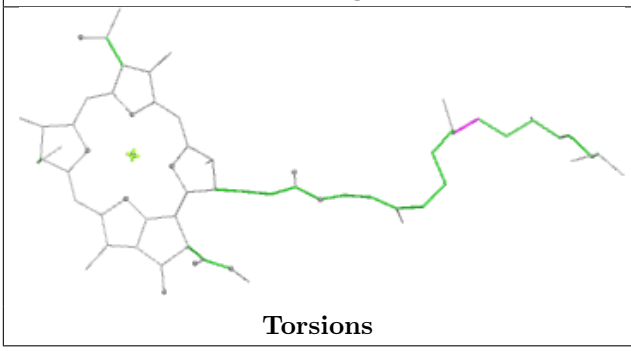
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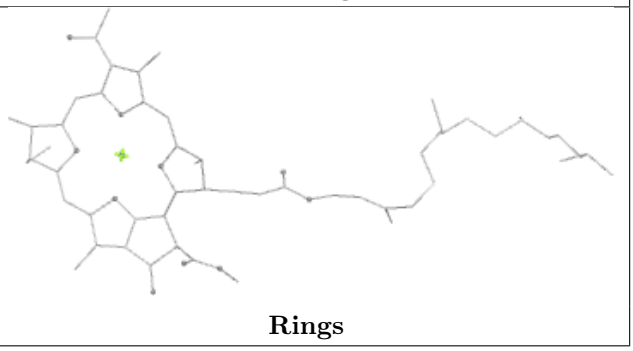
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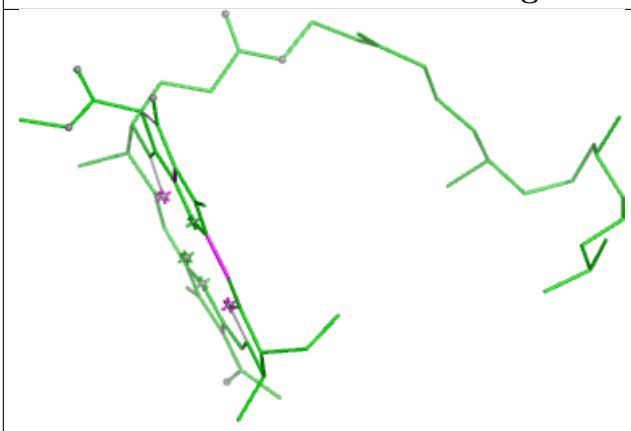


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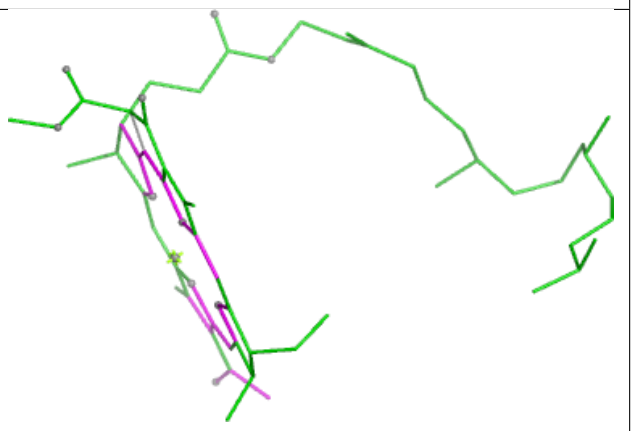


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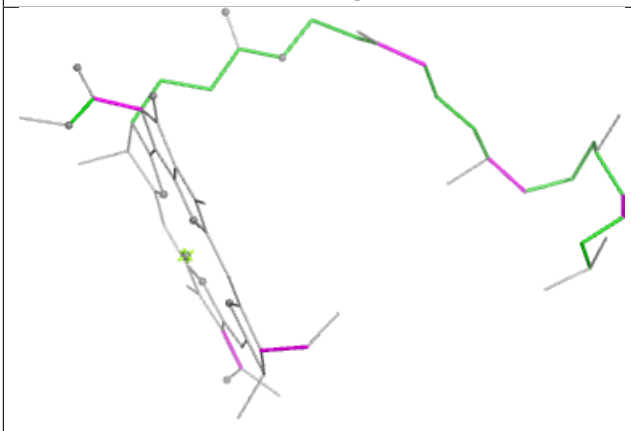
Ligand BCL M 102



Bond lengths



Bond angles

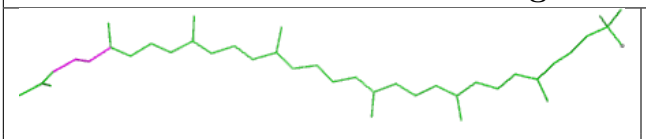


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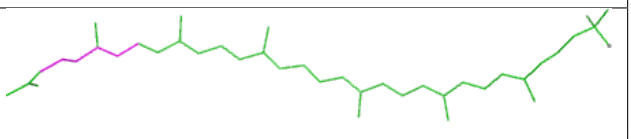


Rings

Ligand ZE0 O 103



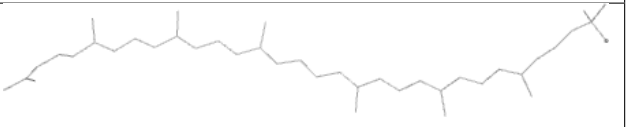
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Bond angles

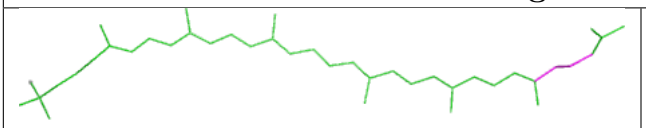


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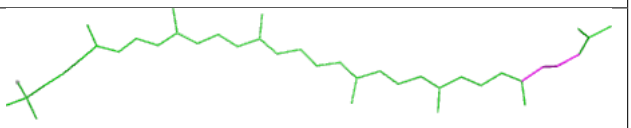


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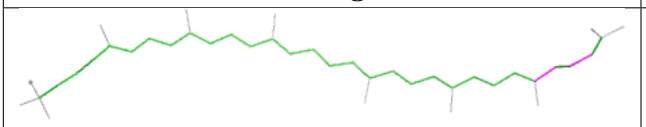
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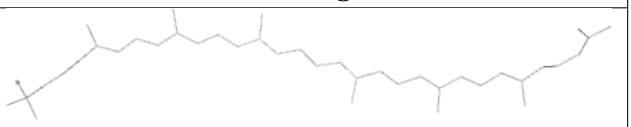
Bond lengths



Bond angles

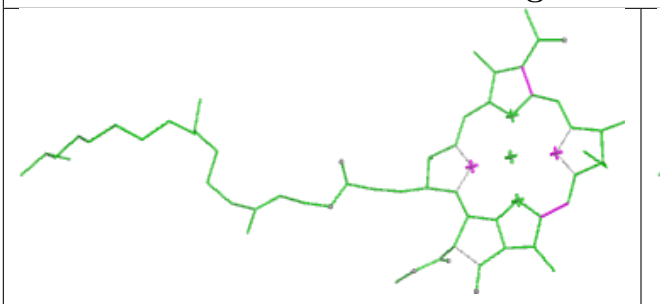


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Rings

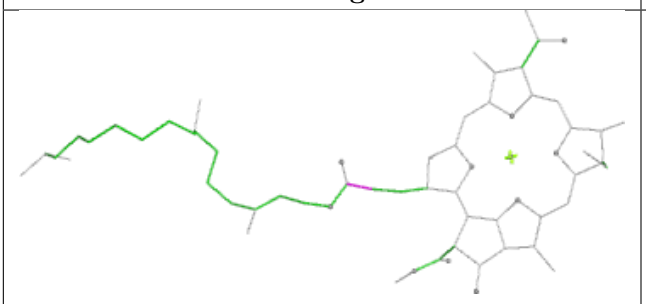
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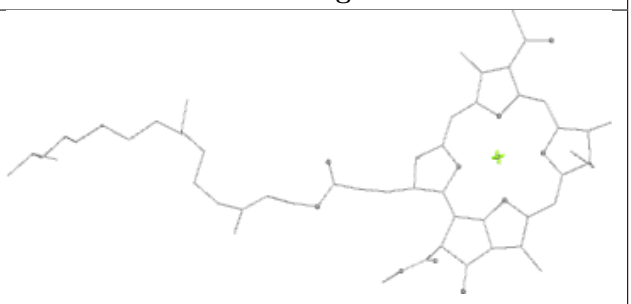
Bond lengths



Bond angles

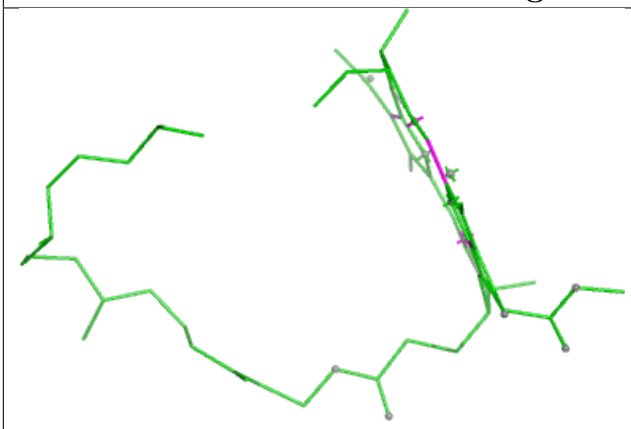


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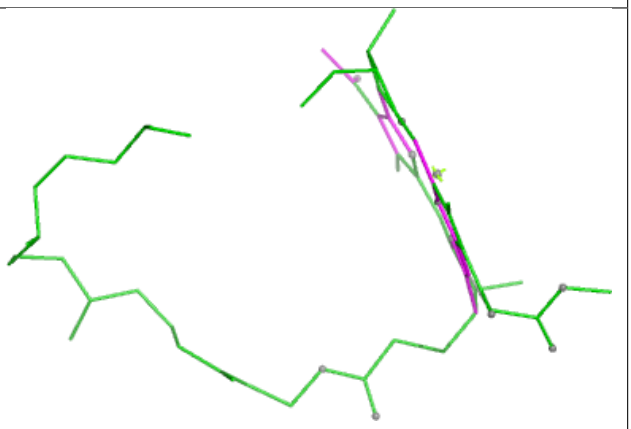


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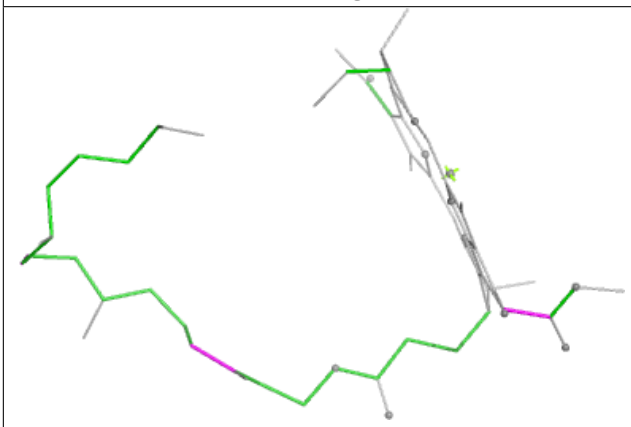
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Bond lengths



Bond angles

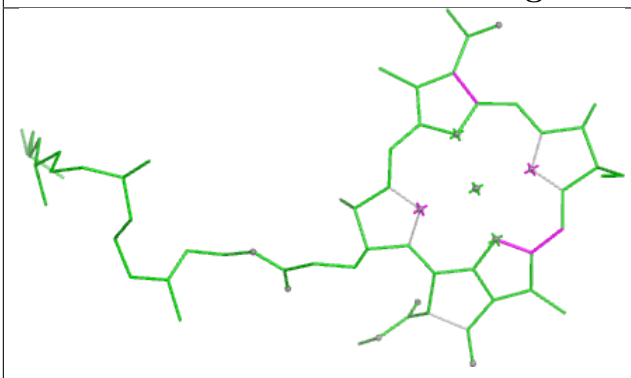


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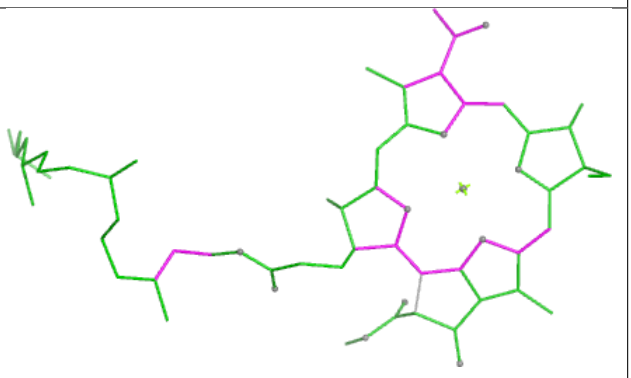


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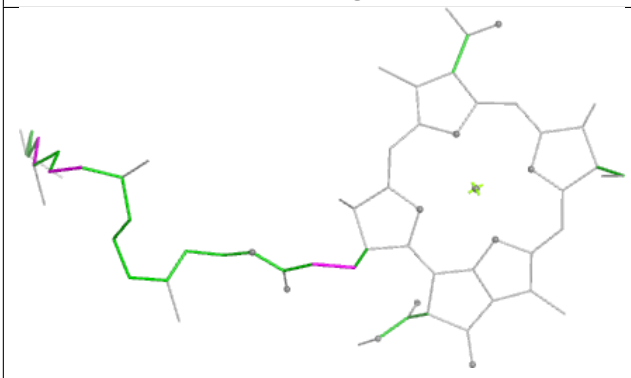
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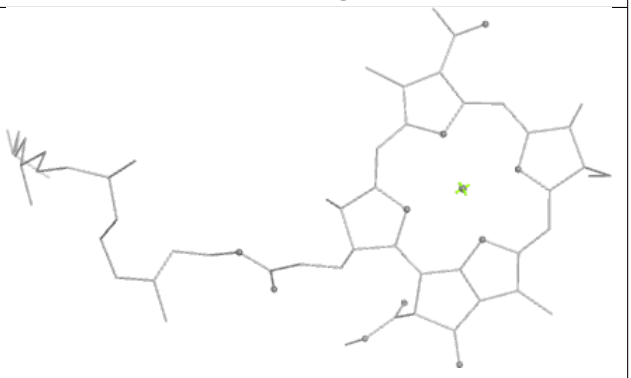
Bond lengths



Bond angles

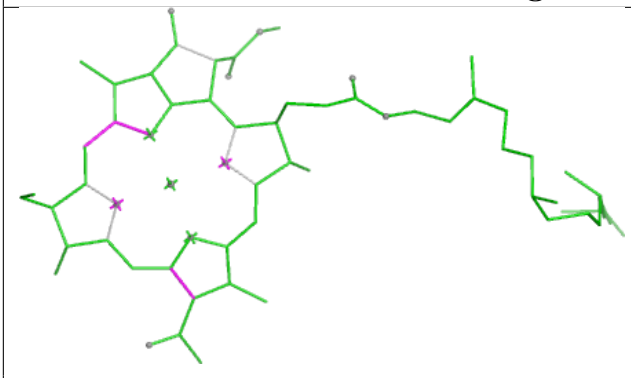


Torsions

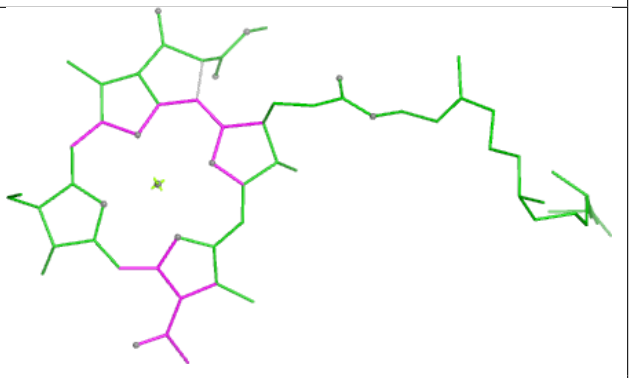


Rings

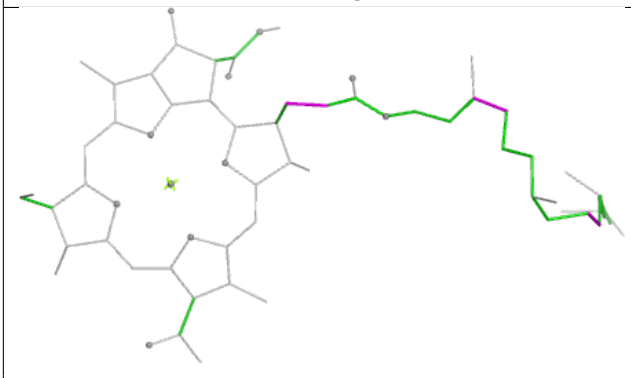
Ligand BCL F 101



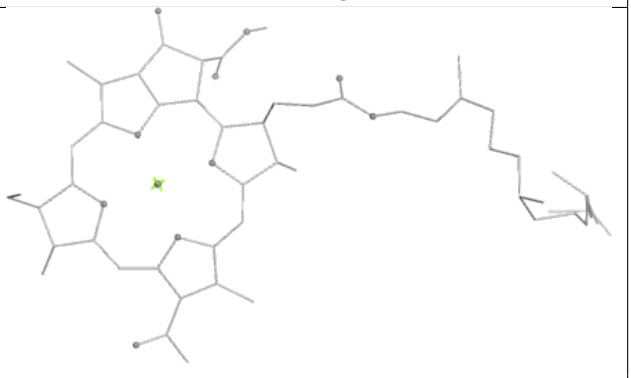
Bond lengths



Bond angles

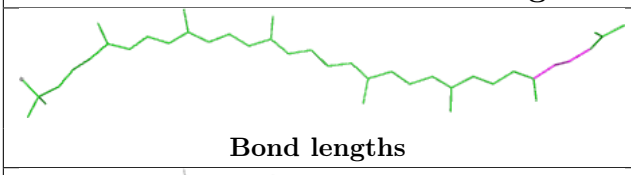


Torsions

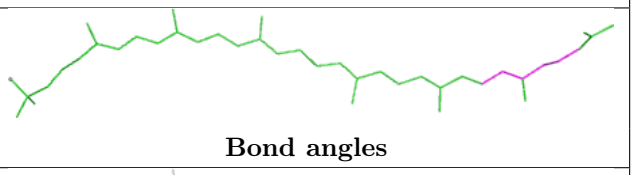


Rings

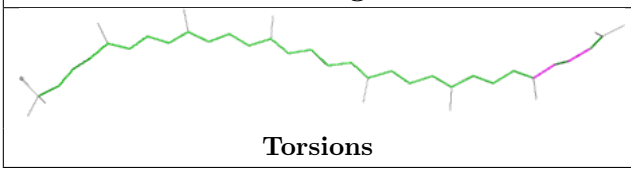
Ligand ZE0 G 103



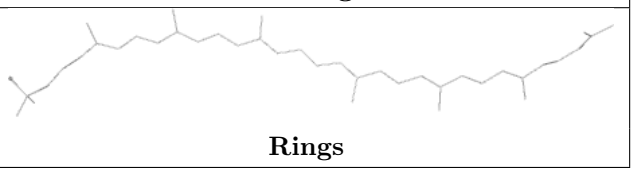
Bond lengths



Bond angles

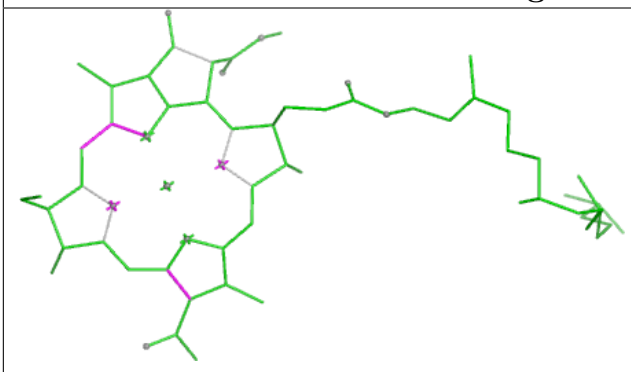


Torsions

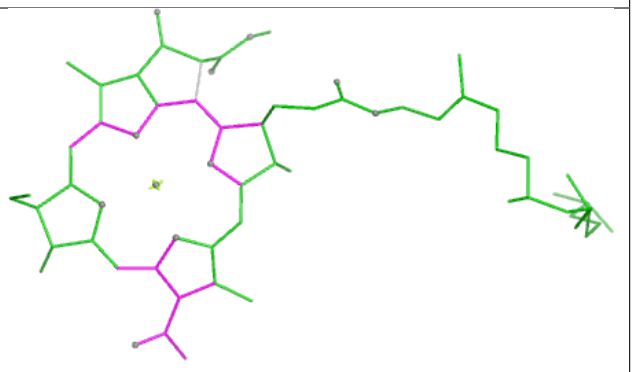


Rings

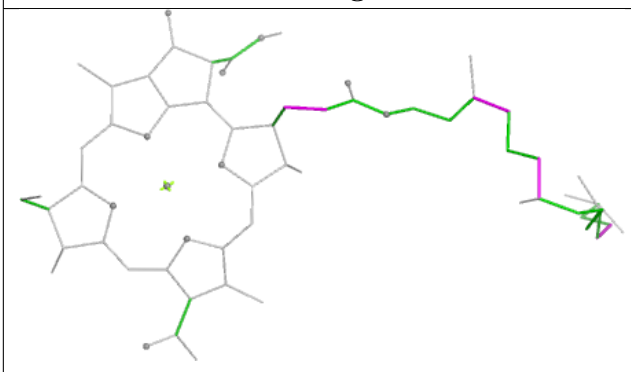
Ligand BCL L 101



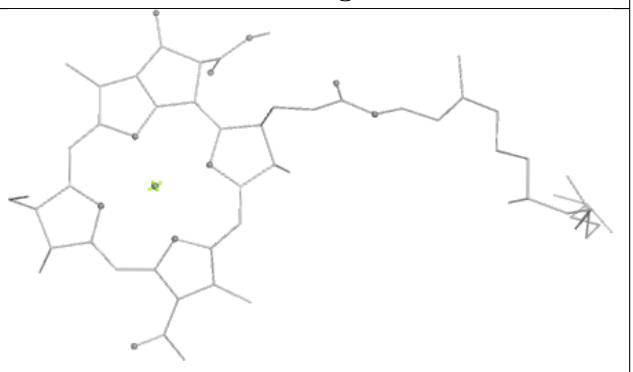
Bond lengths



Bond angles

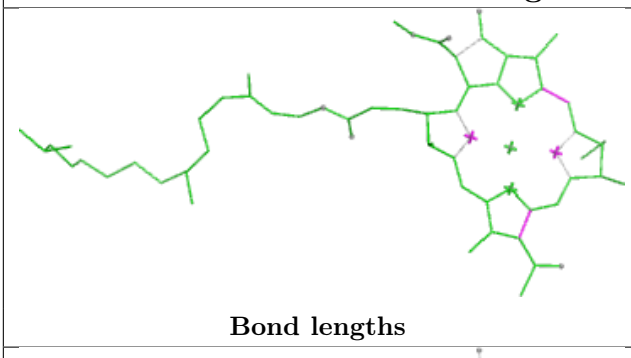


Torsions

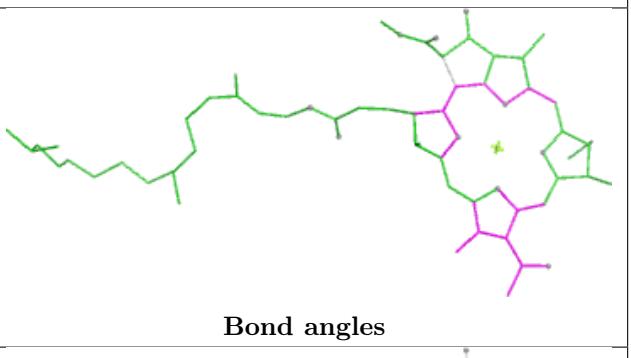


Rings

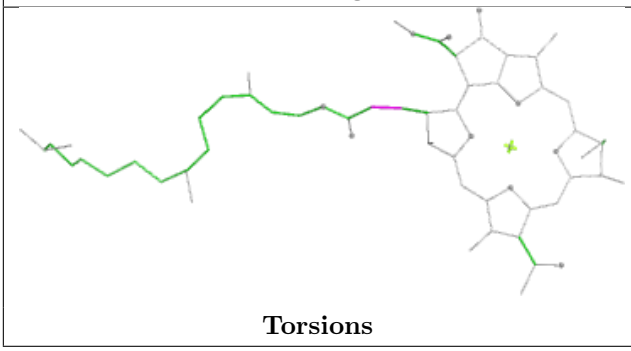
Ligand BCL O 101



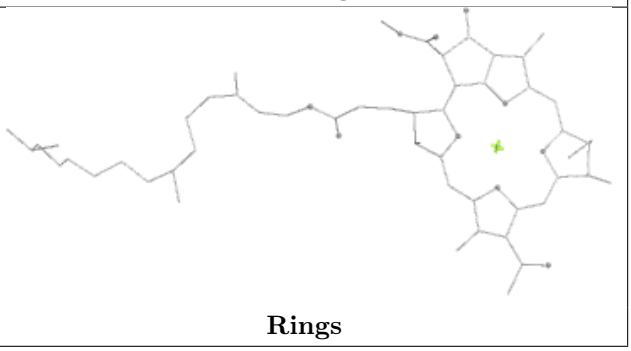
Bond lengths



Bond angles

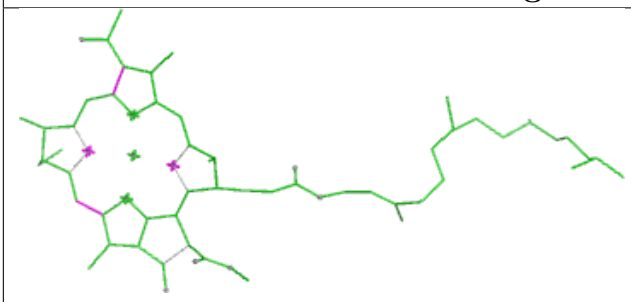


Torsions



Rings

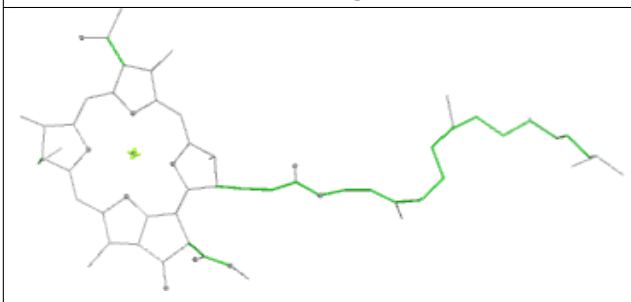
Ligand BCL G 101



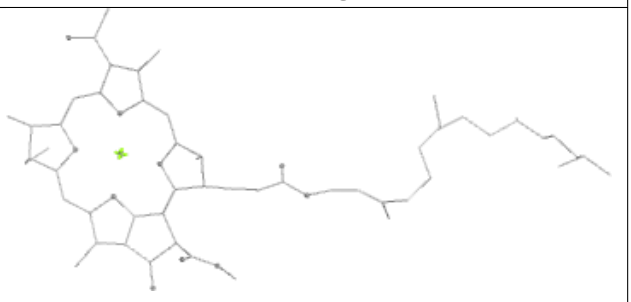
Bond lengths



Bond angles

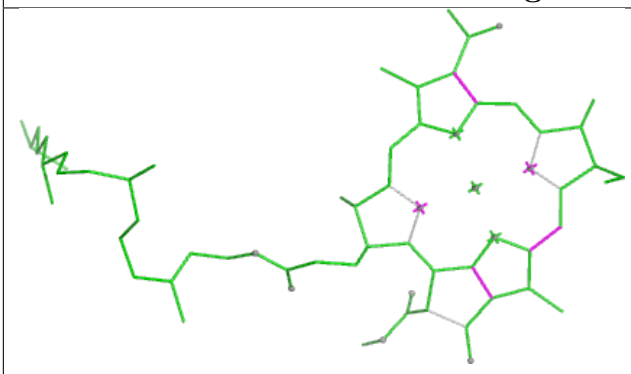


Torsions

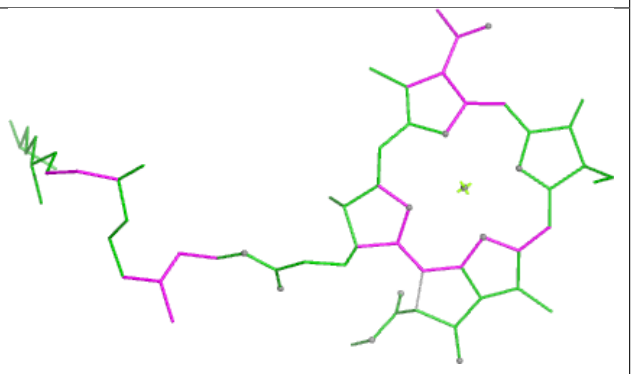


Rings

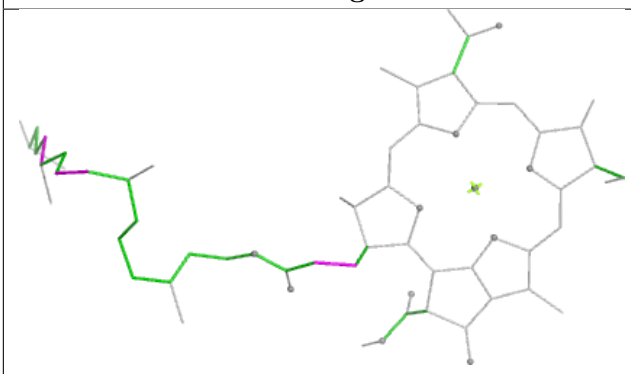
Ligand BCL D 101



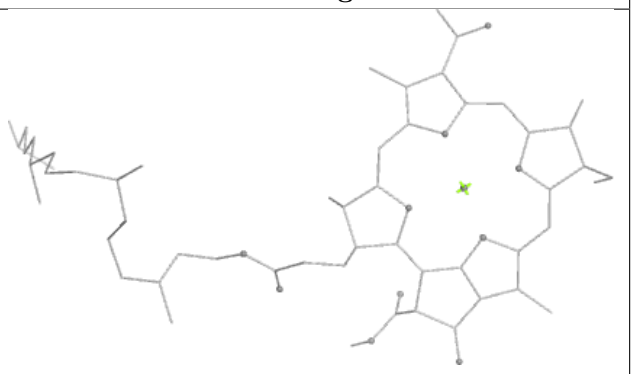
Bond lengths



Bond angles



Torsions

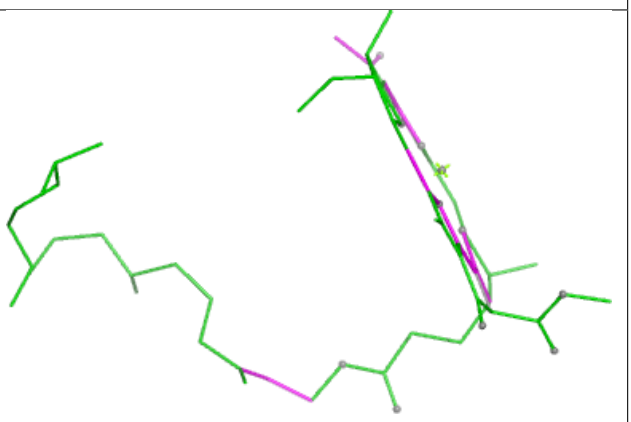


Rings

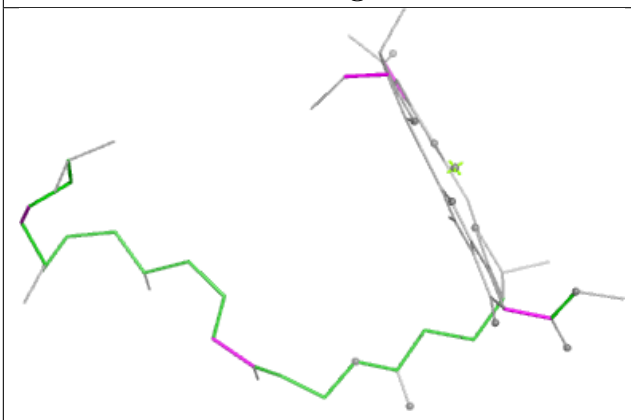
Ligand BCL A 102



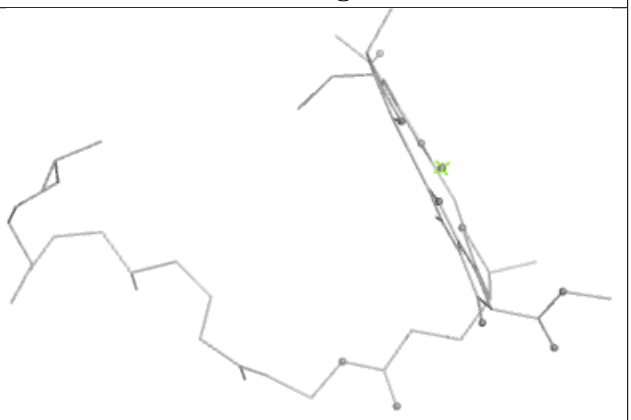
Bond lengths



Bond angles

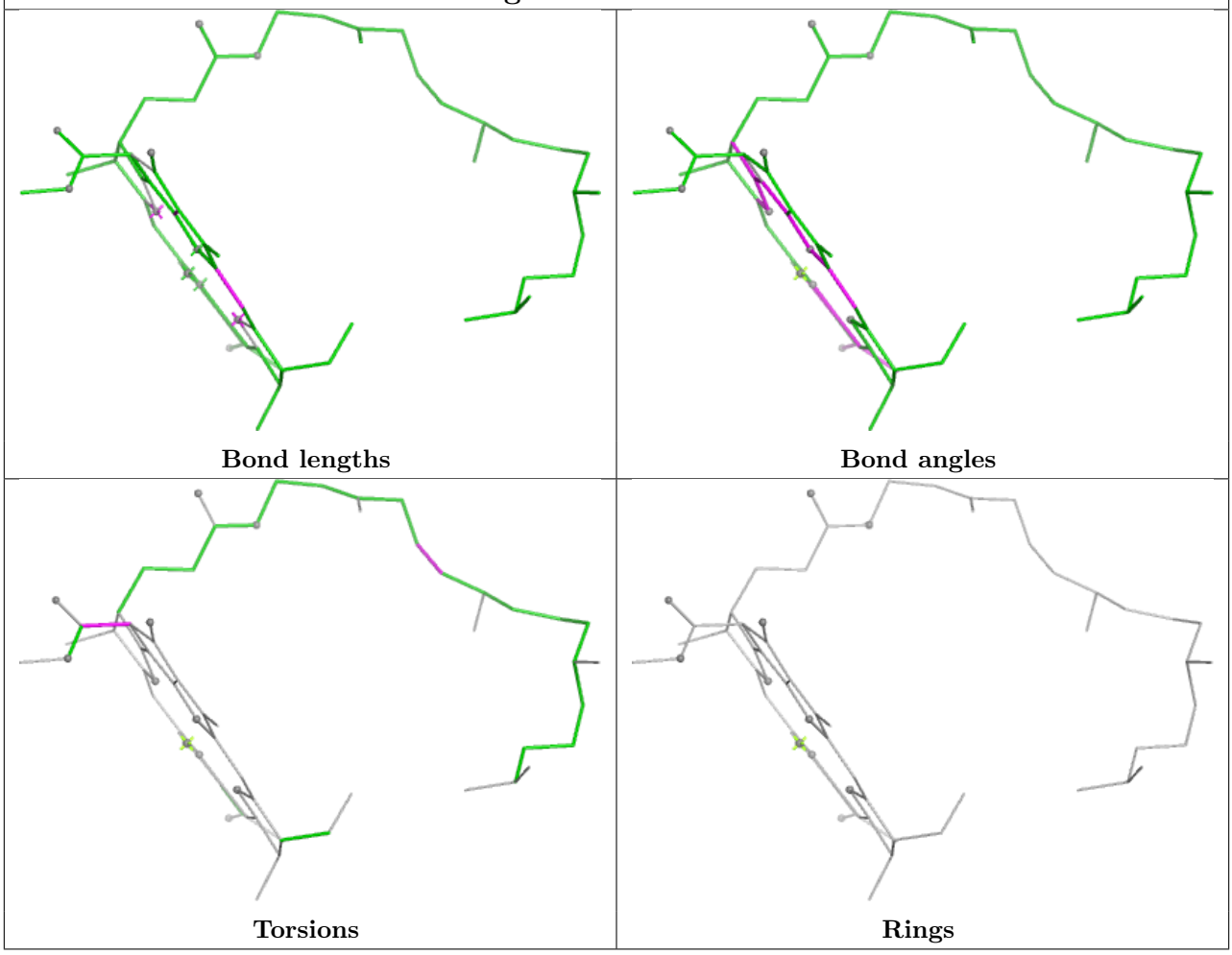


Torsions



Rings

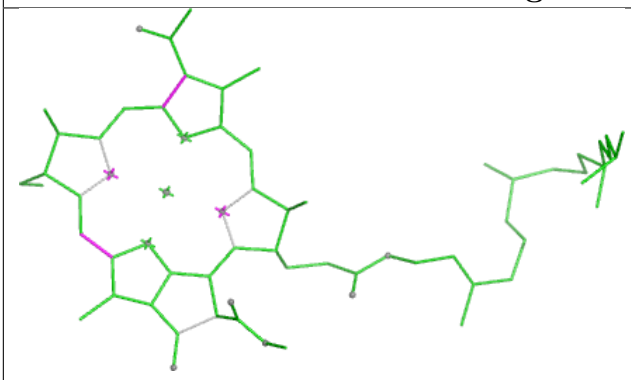
Ligand BCL K 101



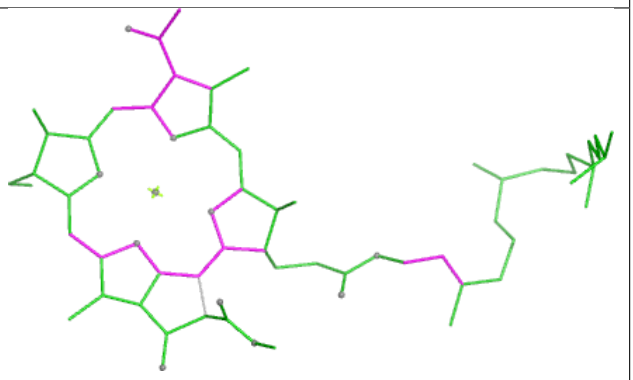
Bond lengths | **Bond angles**

Torsions | **Rings**

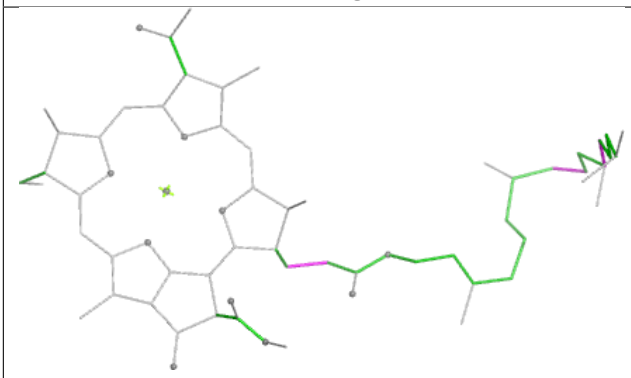
Ligand BCL P 101



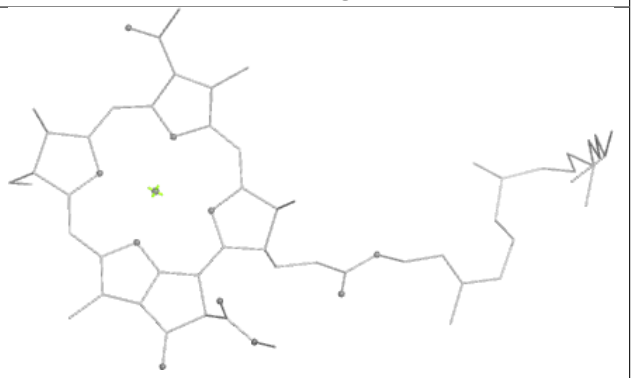
Bond lengths



Bond angles

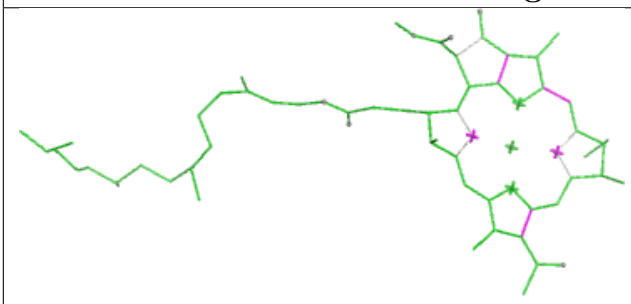


Torsions

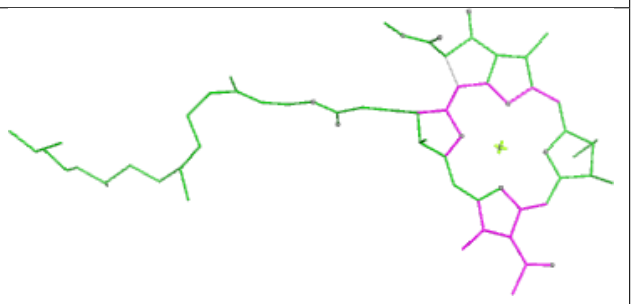


Rings

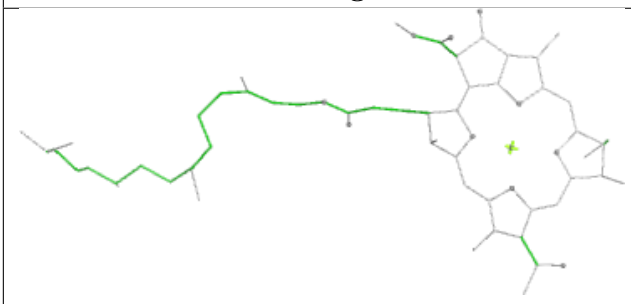
Ligand BCL A 101



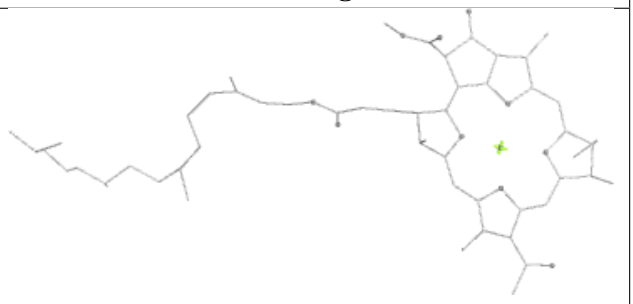
Bond lengths



Bond angles

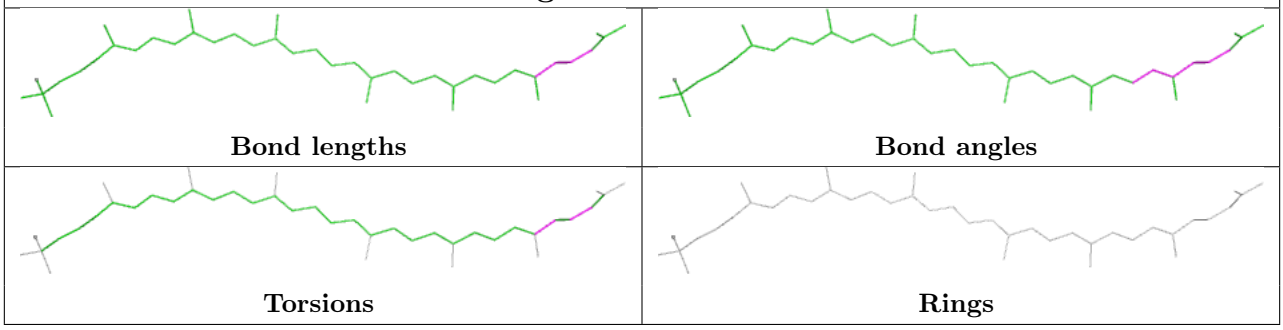


Torsions

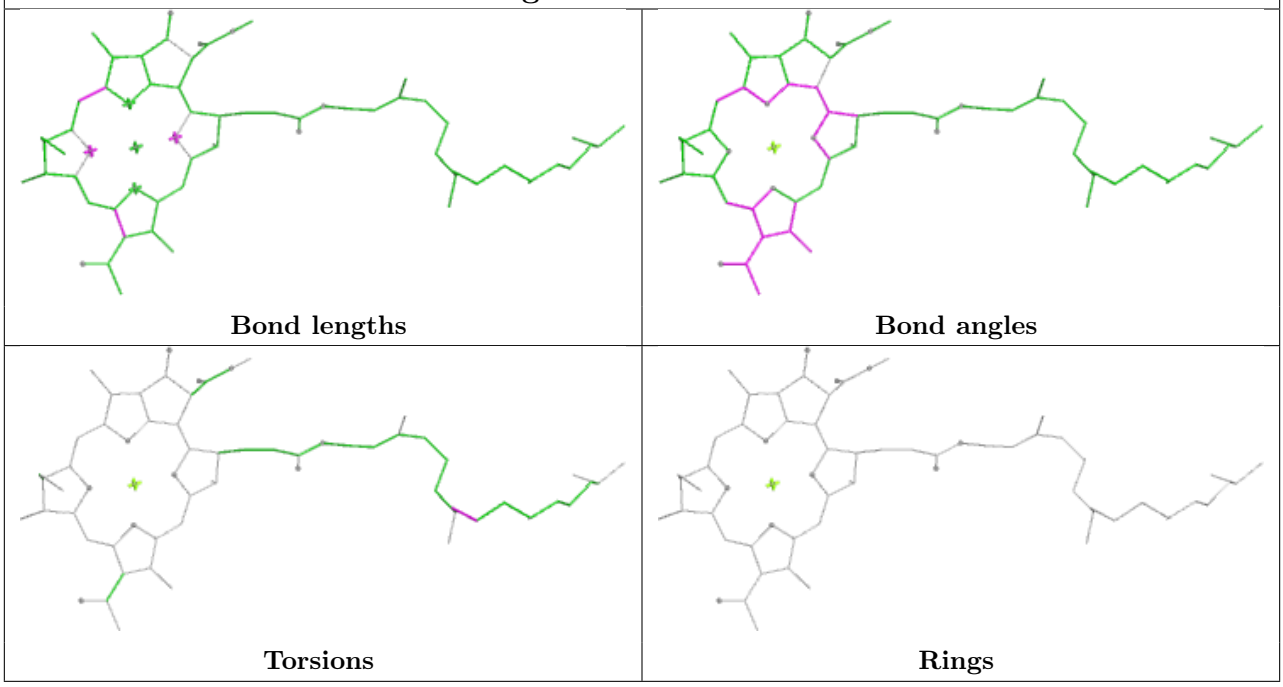


Rings

Ligand ZE0 I 103



Ligand BCL M 101



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.

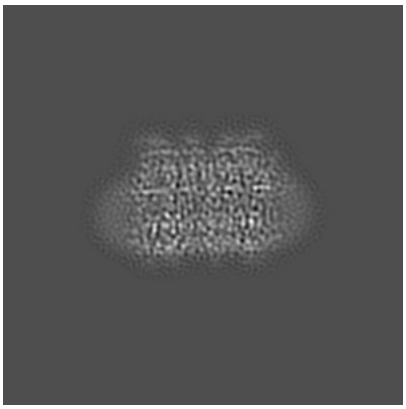
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14682. These allow visual inspection of the internal detail of the map and identification of artifacts.

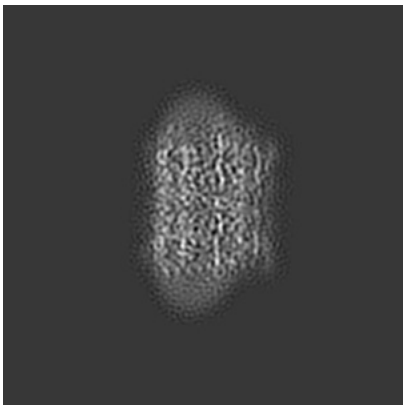
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

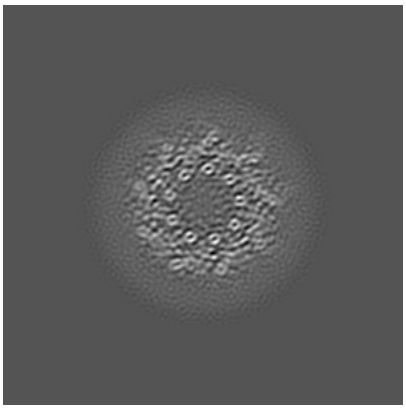
6.1.1 Primary map



X

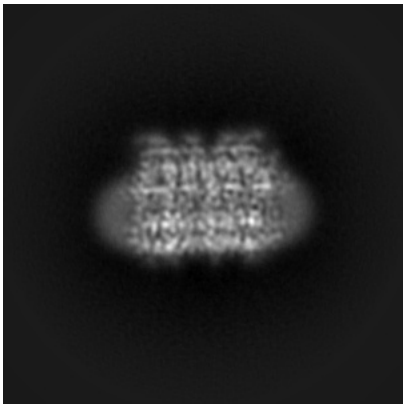


Y

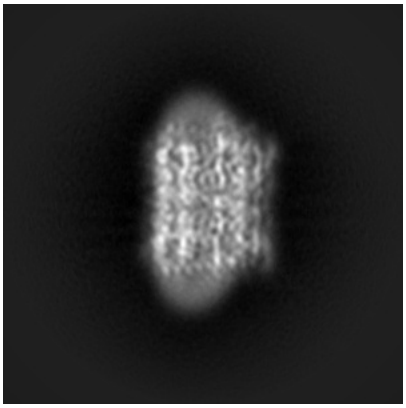


Z

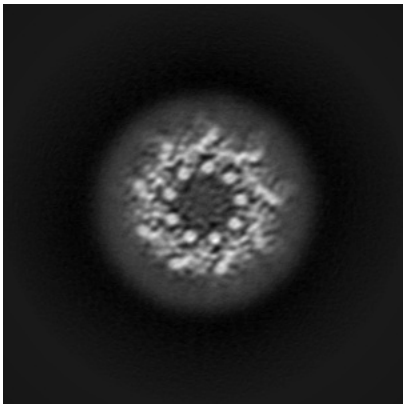
6.1.2 Raw map



X



Y

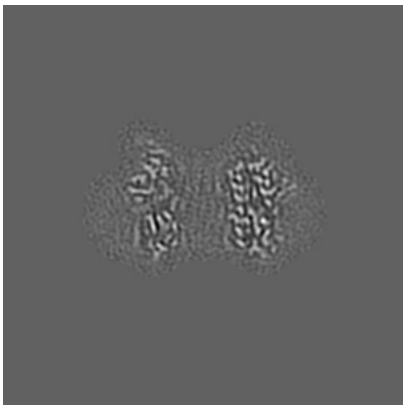


Z

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

6.2 Central slices (i)

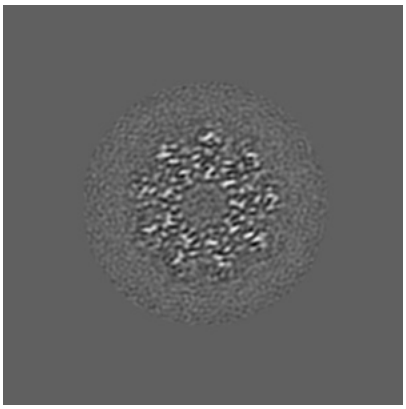
6.2.1 Primary map



X Index: 150

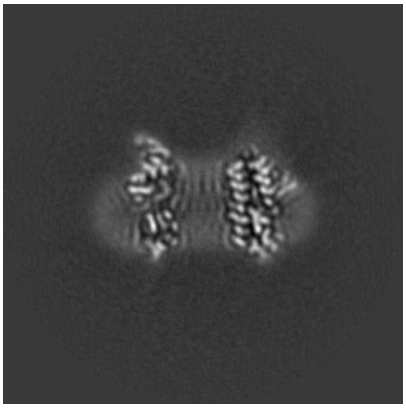


Y Index: 150

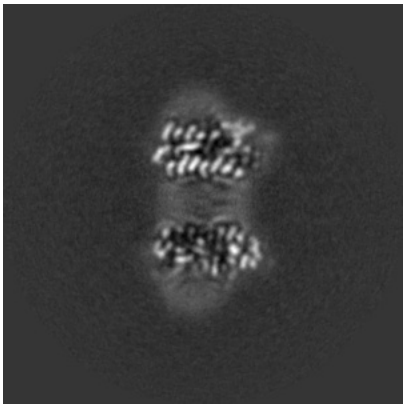


Z Index: 150

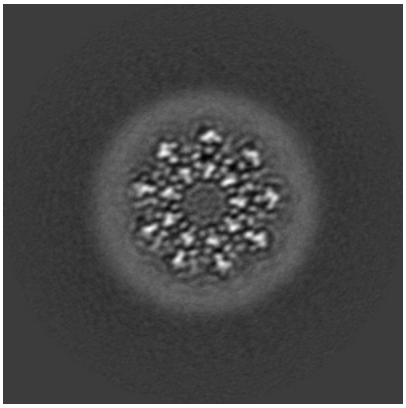
6.2.2 Raw map



X Index: 150



Y Index: 150

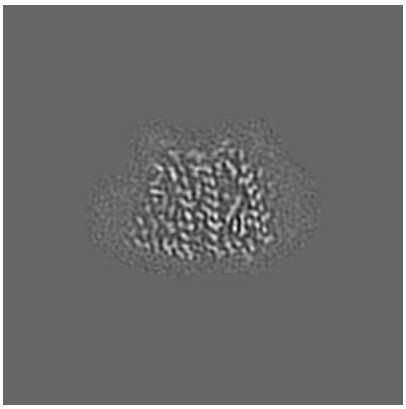


Z Index: 150

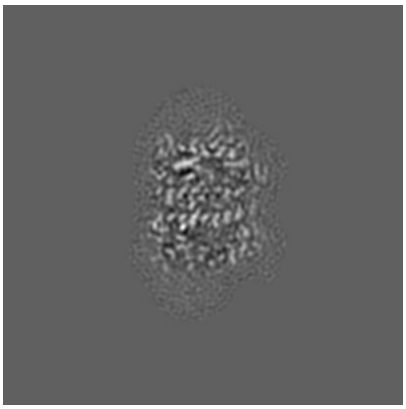
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

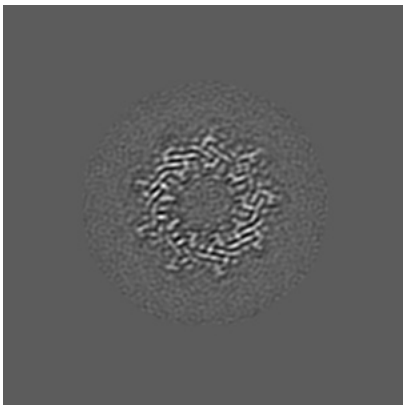
6.3.1 Primary map



X Index: 123

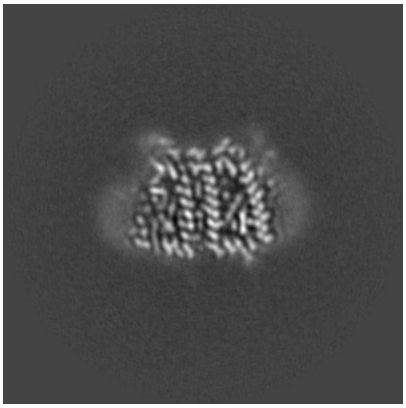


Y Index: 123

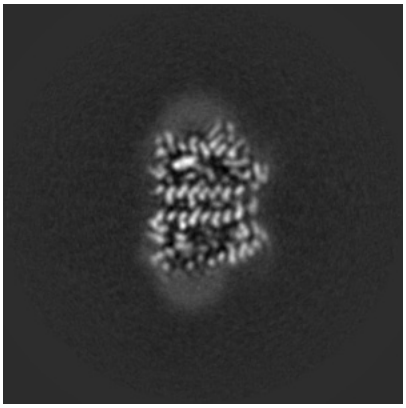


Z Index: 136

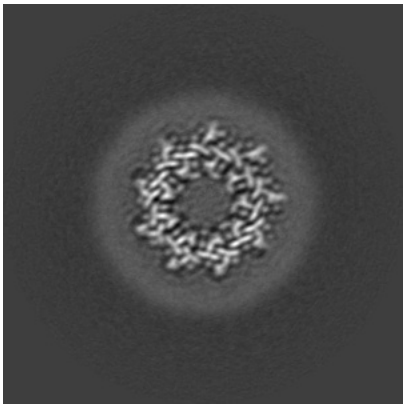
6.3.2 Raw map



X Index: 123



Y Index: 123

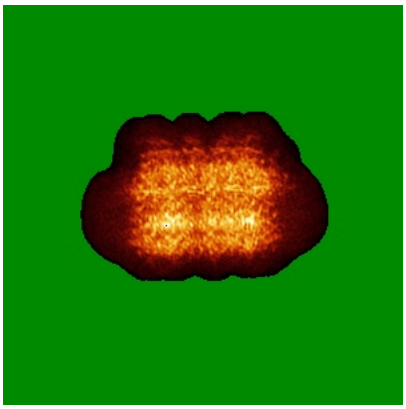


Z Index: 135

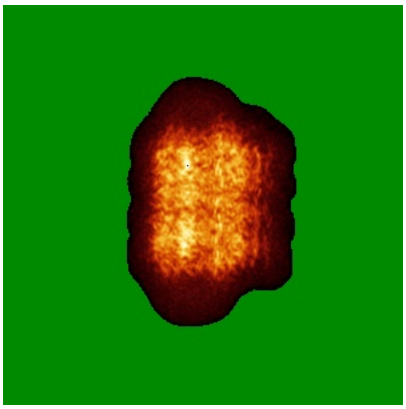
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

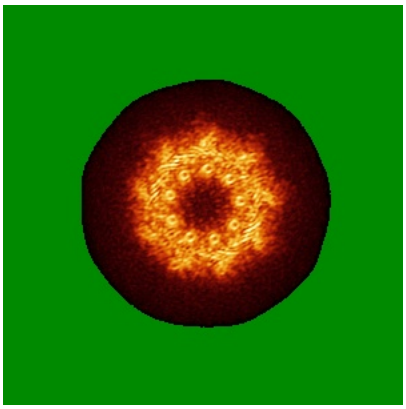
6.4.1 Primary map



X

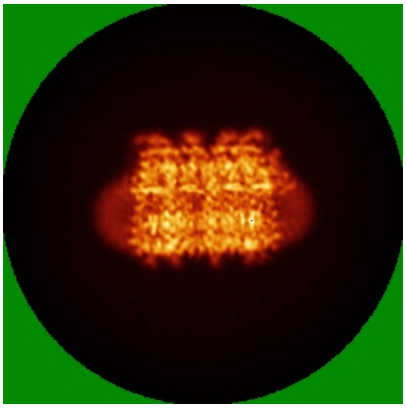


Y

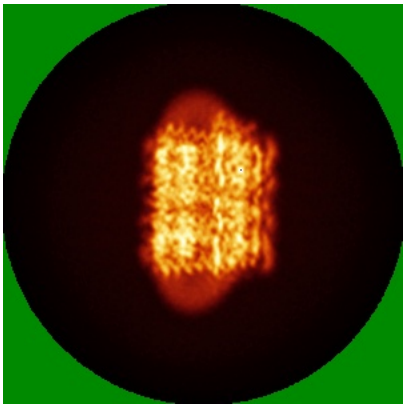


Z

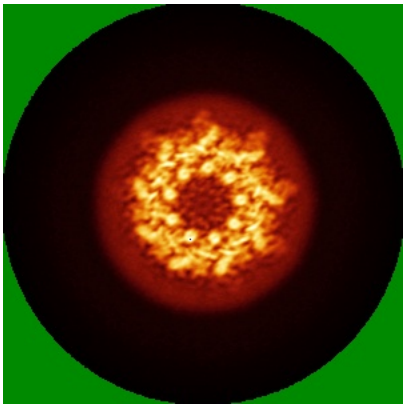
6.4.2 Raw map



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)

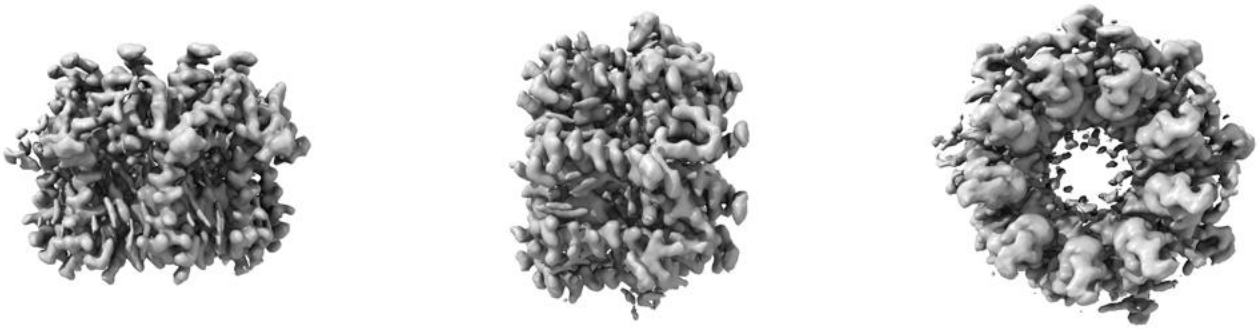
6.5.1 Primary map



X Y Z

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

6.5.2 Raw map



X Y Z

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.

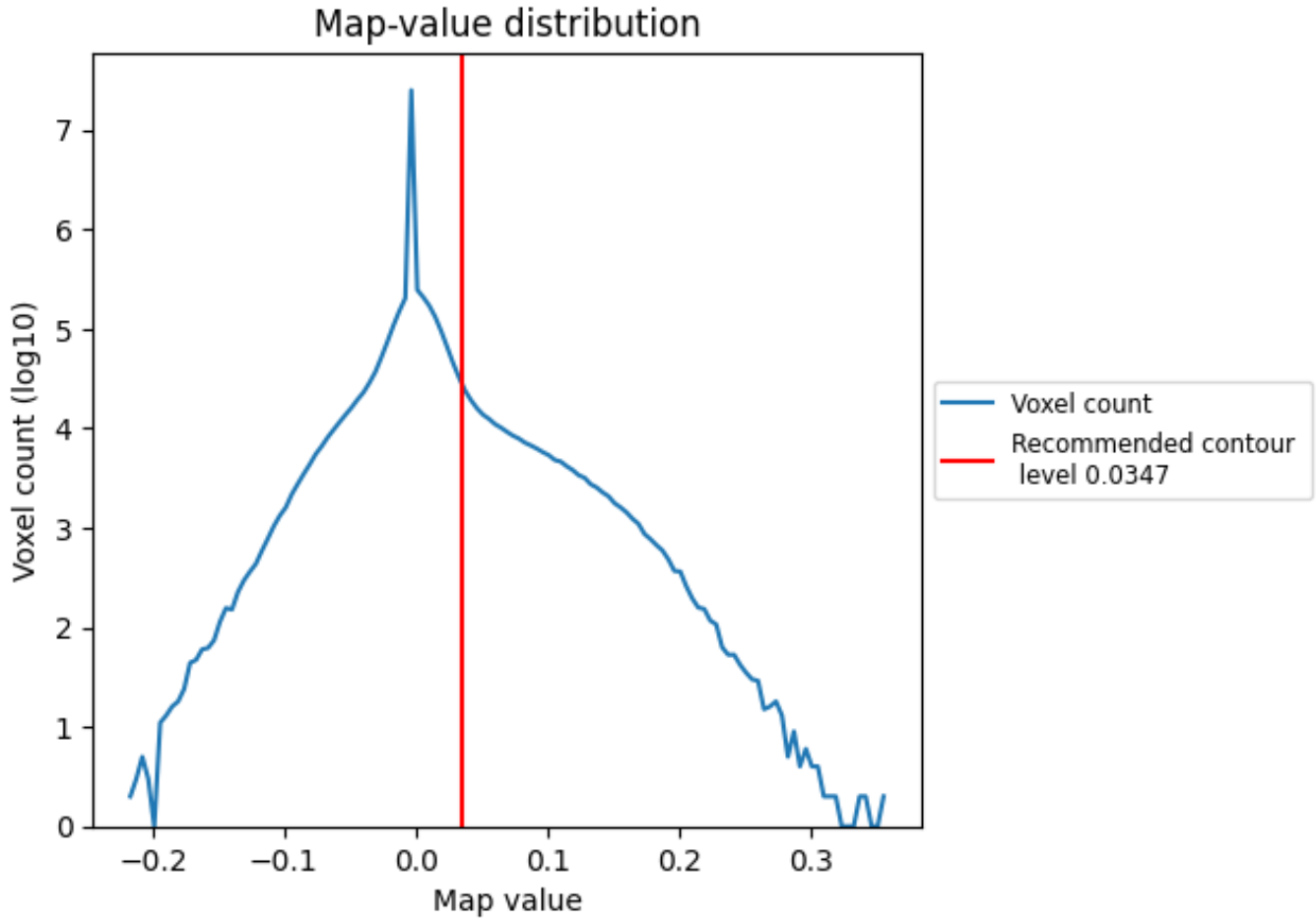
6.6 Mask visualisation (i)

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

7 Map analysis

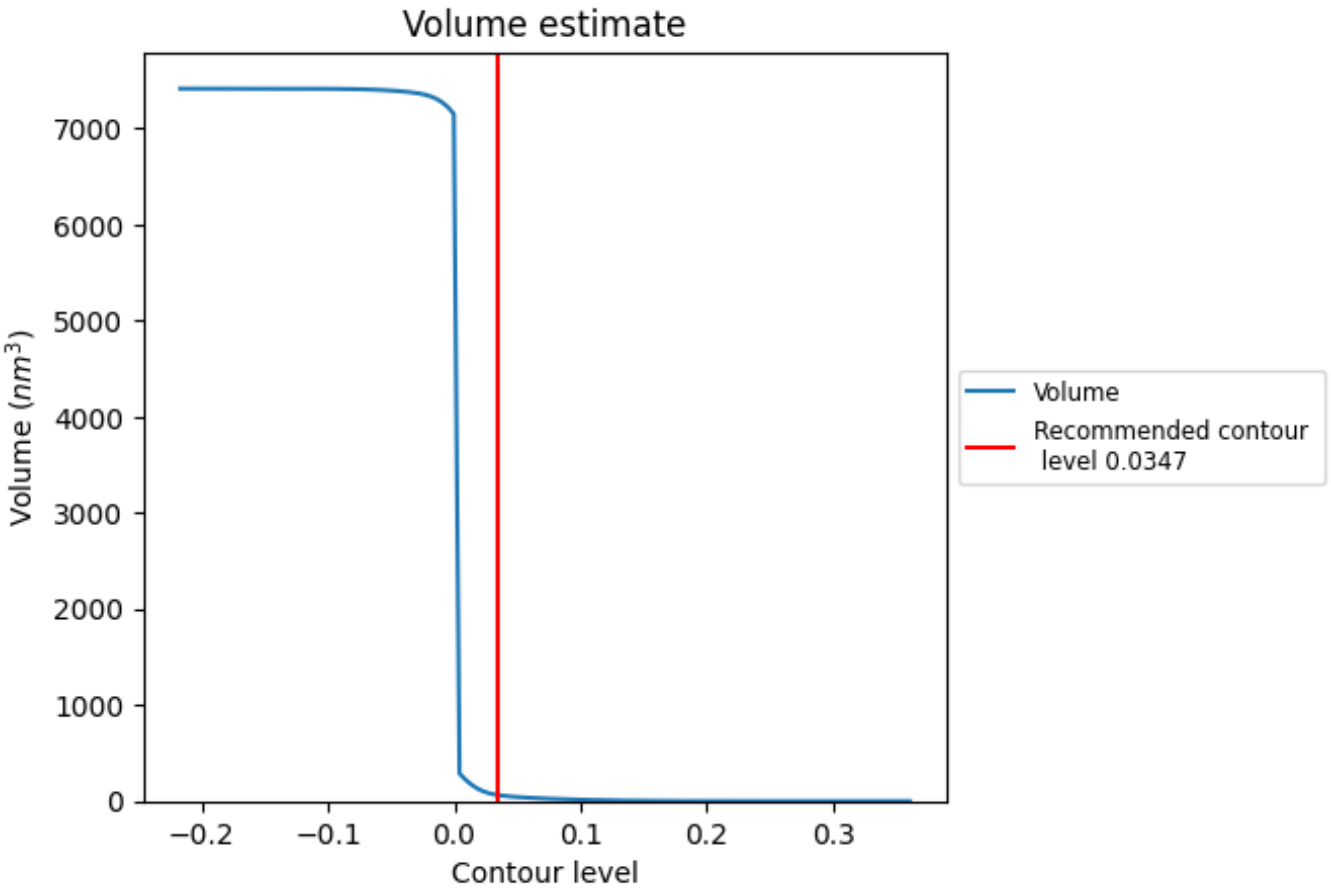
This section contains the results of statistical analysis of the map.

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.

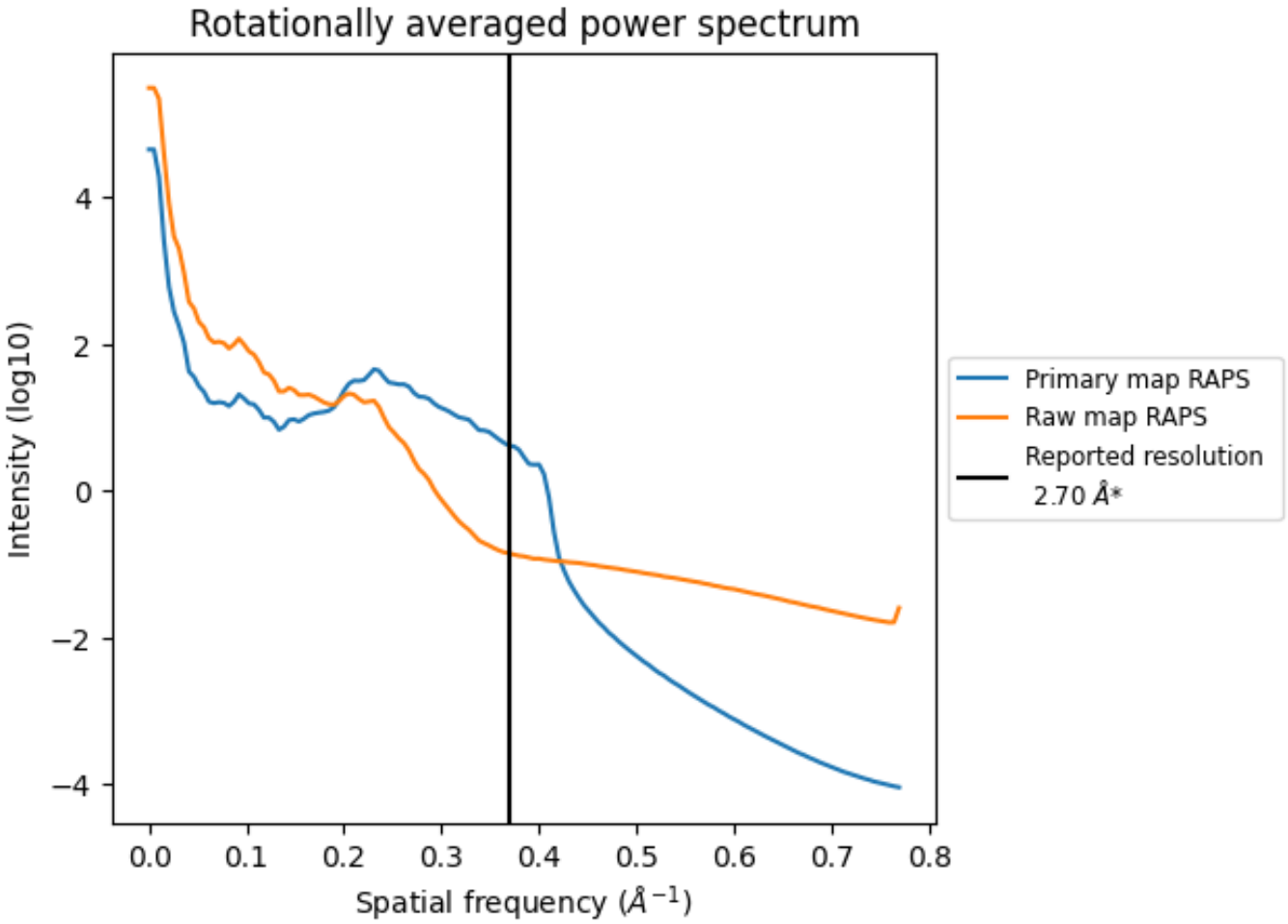
7.2 Volume estimate



The volume at the recommended contour level is 63 nm^3; this corresponds to an approximate mass of 57 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)

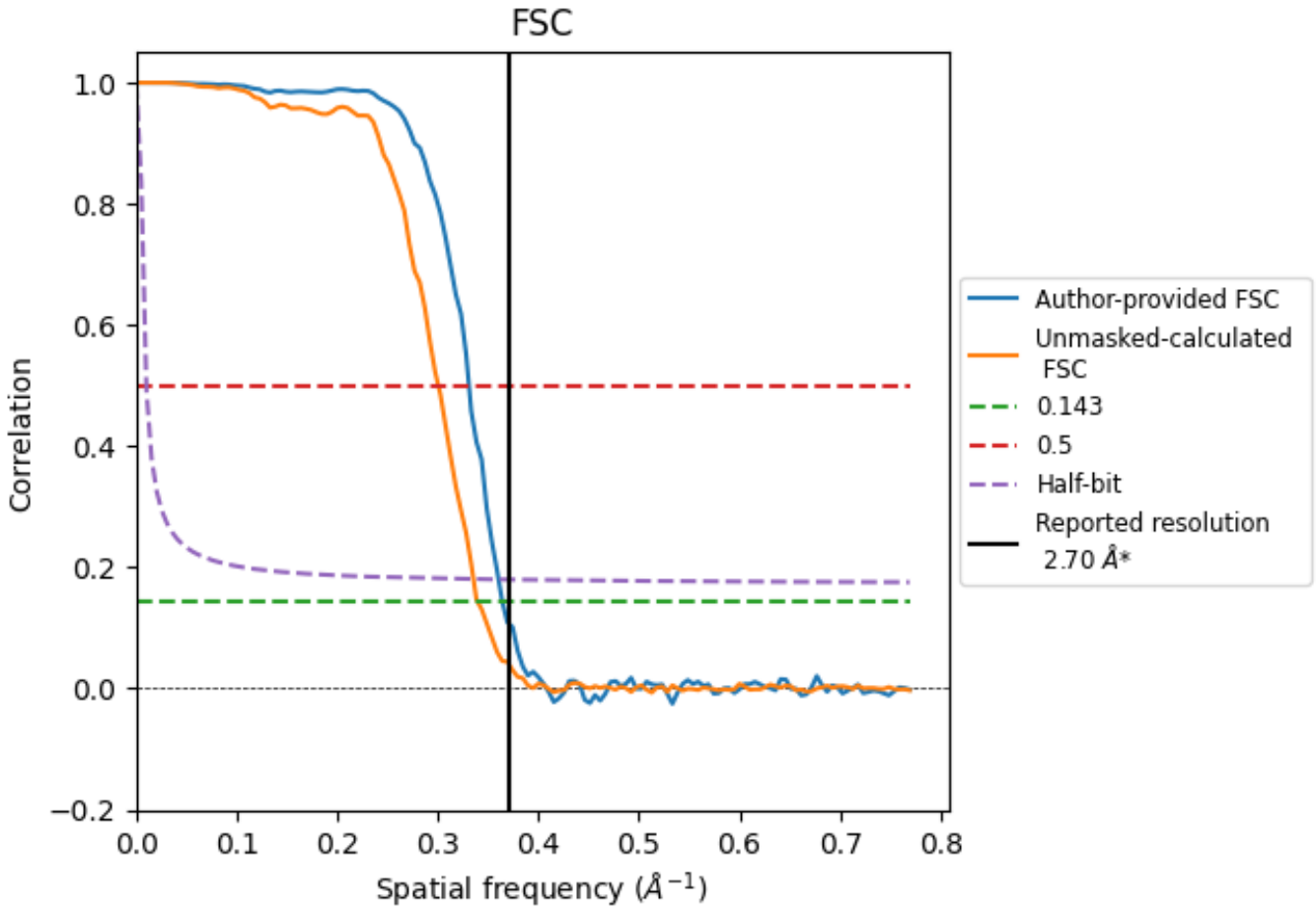


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

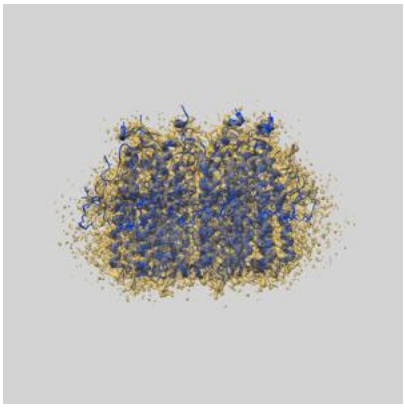
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.75	3.02	2.77
Unmasked-calculated*	2.94	3.33	2.98

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

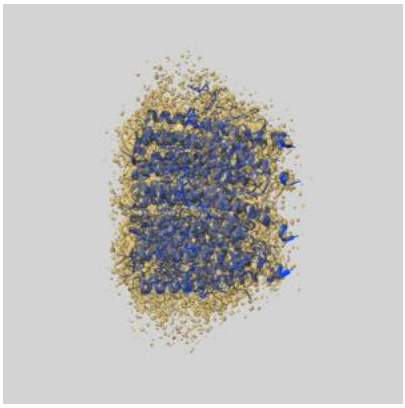
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14682 and PDB model 7ZE3. Per-residue inclusion information can be found in section 3 on page 10.

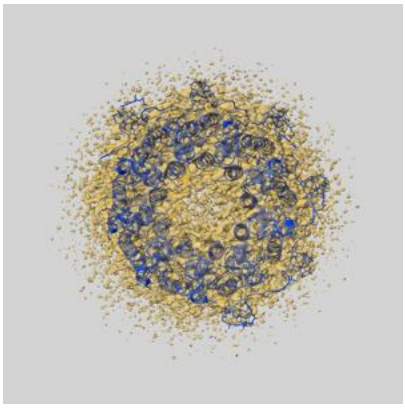
9.1 Map-model overlay



X



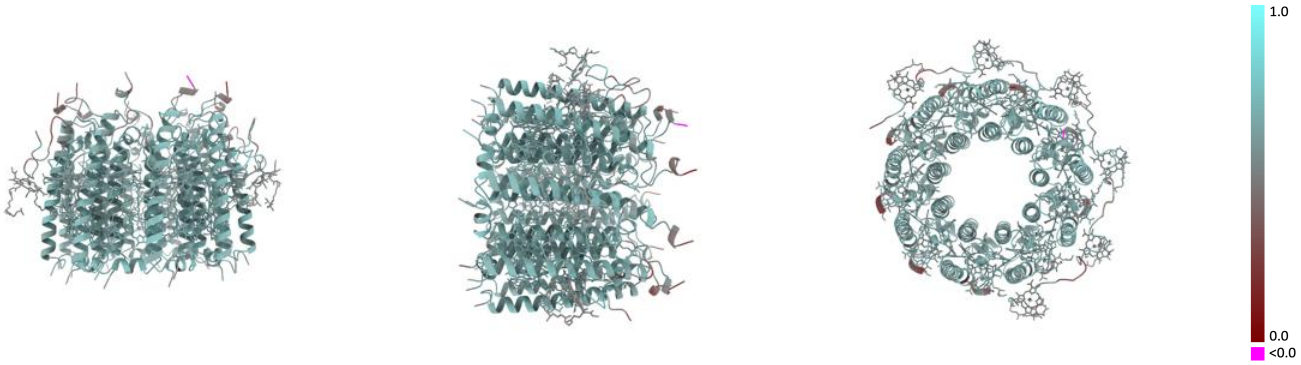
Y



Z

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

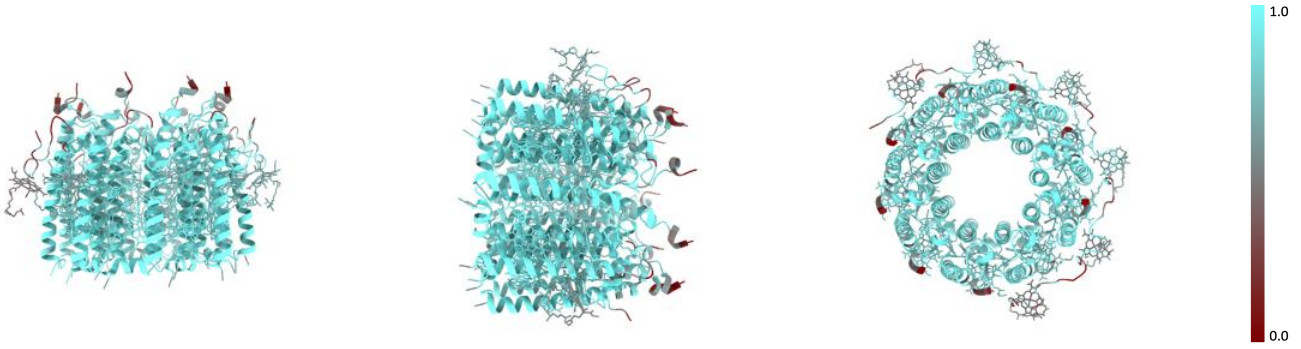
9.2 Q-score mapped to coordinate model (i)



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.

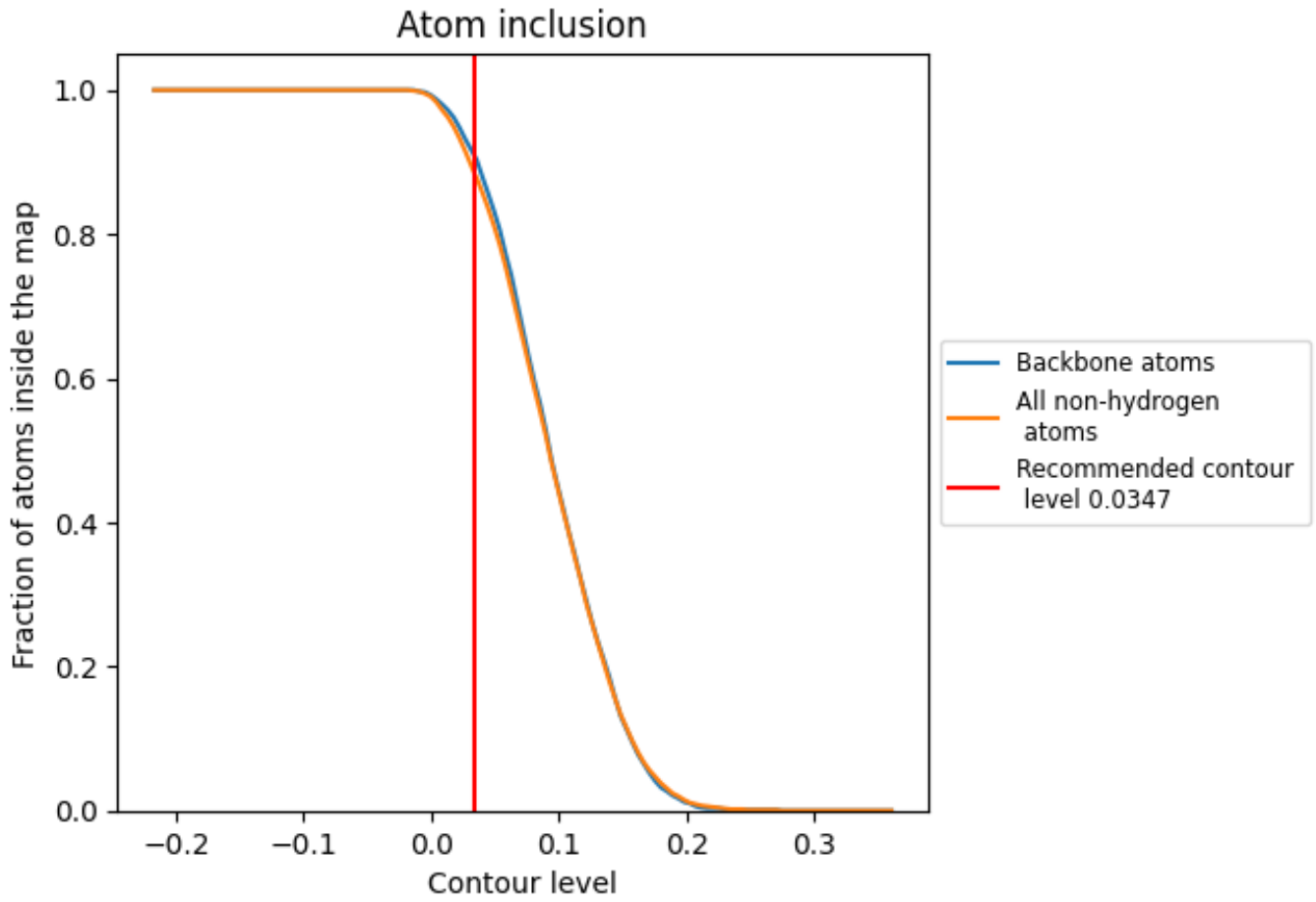
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0347).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0347) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.6140
A	0.9540	0.6390
B	0.9050	0.6220
C	0.9350	0.6510
D	0.9090	0.6180
E	0.9370	0.6360
F	0.8830	0.6160
G	0.9420	0.6360
H	0.8580	0.5980
I	0.9350	0.6370
J	0.8470	0.5990
K	0.9370	0.6360
L	0.8980	0.6060
M	0.9420	0.6330
N	0.8950	0.6080
O	0.9540	0.6370
P	0.8800	0.6200
Q	0.9560	0.6440
R	0.8890	0.6150
S	0.6140	0.5160

