wwPDB EM Validation Summary Report (i)

Sep 22, 2026 – 07:24 pm BST

PDB ID	:	7PBW / pdb_00007pbw
EMDB ID	:	EMD-13307
Title	:	Cryo-EM structure of light harvesting complex 2 from Rba. sphaeroides.
Authors	:	Qian, P.; Swainsbury, D.J.K.; Croll, T.I.; Castro-Hartmann, P.; Sader, K.; Divitini, G.; Hunter, C.N.
Deposited on	:	2021-08-02
Resolution	:	2.10 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

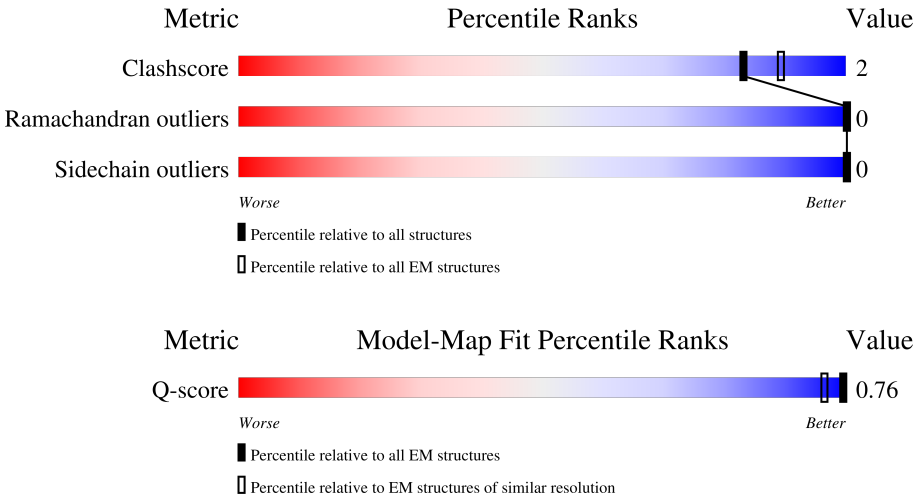
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 (i)

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

The reported resolution of this entry is 2.10 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	2317 (1.60 - 2.60)

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	AA	50	94% 6%
1	AB	50	94% 6%
1	AC	50	94% 6%
1	AD	50	94% 6%

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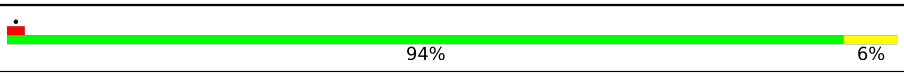
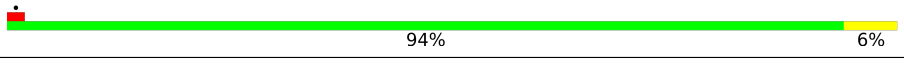
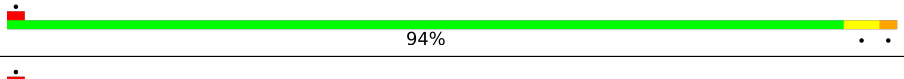
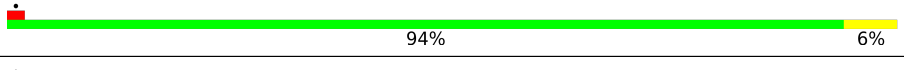
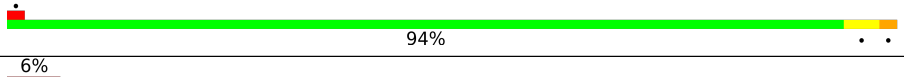
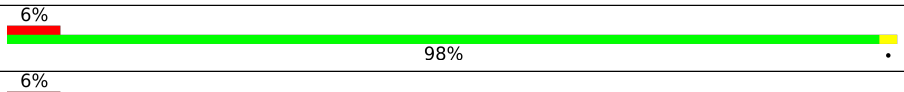
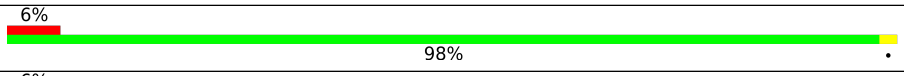
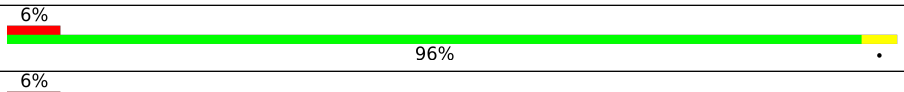
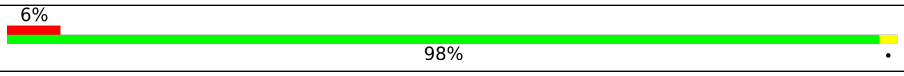
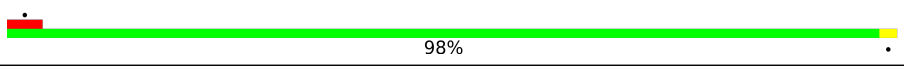
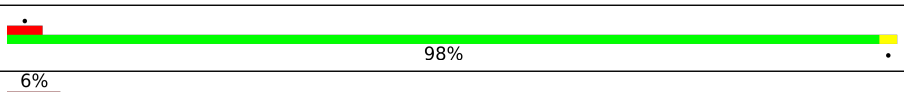
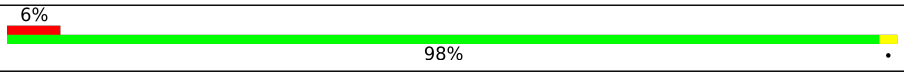
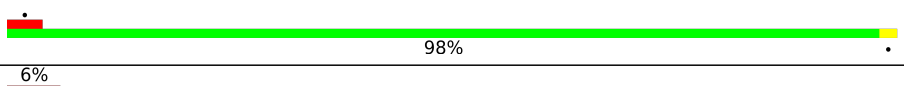
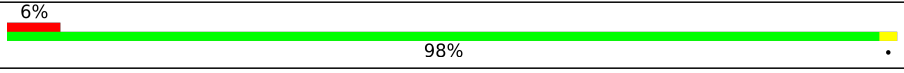
Mol	Chain	Length	Quality of chain
1	AE	50	
1	AF	50	
1	AG	50	
1	AH	50	
1	AI	50	
2	BA	47	
2	BB	47	
2	BC	47	
2	BD	47	
2	BE	47	
2	BF	47	
2	BG	47	
2	BH	47	
2	BI	47	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9500 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	AA	50	Total	C	N	O	S	0	0
			372	248	58	65	1		
1	AB	50	Total	C	N	O	S	0	0
			372	248	58	65	1		
1	AC	50	Total	C	N	O	S	0	0
			372	248	58	65	1		
1	AD	50	Total	C	N	O	S	0	0
			372	248	58	65	1		
1	AE	50	Total	C	N	O	S	0	0
			372	248	58	65	1		
1	AF	50	Total	C	N	O	S	0	0
			372	248	58	65	1		
1	AG	50	Total	C	N	O	S	0	0
			372	248	58	65	1		
1	AH	50	Total	C	N	O	S	0	0
			372	248	58	65	1		
1	AI	50	Total	C	N	O	S	0	0
			372	248	58	65	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	47	Total	C	N	O	S	0	0
			353	232	60	60	1		
2	BB	47	Total	C	N	O	S	0	0
			353	232	60	60	1		
2	BC	47	Total	C	N	O	S	0	0
			353	232	60	60	1		
2	BD	47	Total	C	N	O	S	0	0
			353	232	60	60	1		
2	BE	47	Total	C	N	O	S	0	0
			353	232	60	60	1		
2	BF	47	Total	C	N	O	S	0	0
			353	232	60	60	1		

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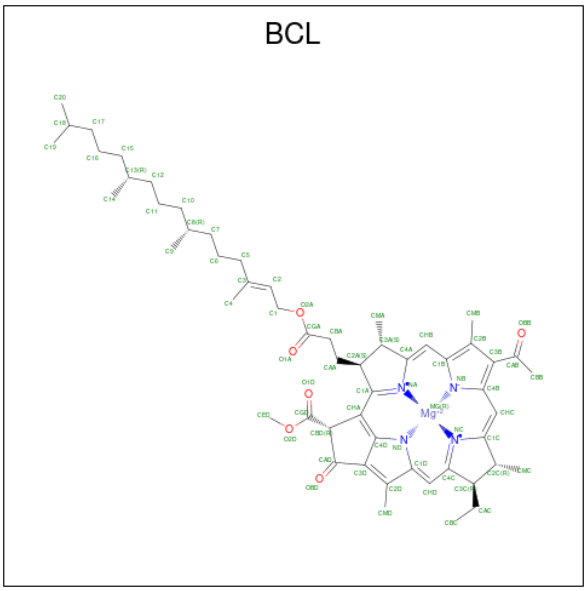
Mol	Chain	Residues	Atoms					AltConf	Trace
2	BG	47	Total	C	N	O	S	0	0
			353	232	60	60	1		
2	BH	47	Total	C	N	O	S	0	0
			353	232	60	60	1		
2	BI	47	Total	C	N	O	S	0	0
			353	232	60	60	1		

- Molecule 3 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
3	AA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AC	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AC	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AD	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AD	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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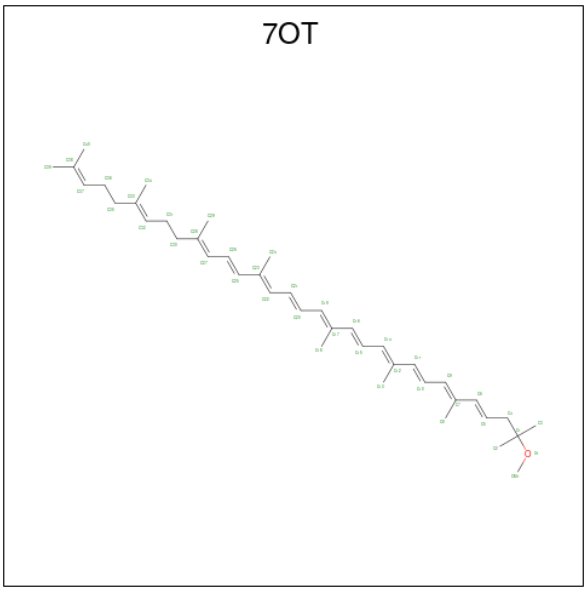
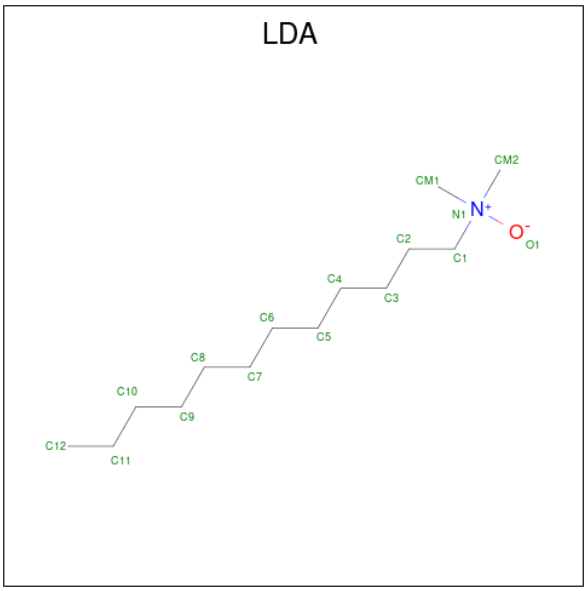
Mol	Chain	Residues	Atoms					AltConf
3	AE	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AE	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AF	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AF	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AG	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AG	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AH	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AH	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	AI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	BA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	BB	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	BC	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	BD	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	BE	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	BF	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	BG	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	BH	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	BI	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 4 is SPHEROIDENE (CCD ID: 7OT) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms	AltConf
4	AA	1	Total C O 42 41 1	0
4	AB	1	Total C O 42 41 1	0
4	AC	1	Total C O 42 41 1	0
4	AD	1	Total C O 42 41 1	0
4	AE	1	Total C O 42 41 1	0
4	AF	1	Total C O 42 41 1	0
4	AG	1	Total C O 42 41 1	0
4	AH	1	Total C O 42 41 1	0
4	AI	1	Total C O 42 41 1	0

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				AltConf
5	AA	1	Total	C	N	O	0
			16	14	1	1	
5	AA	1	Total	C	N	O	0
			16	14	1	1	
5	AA	1	Total	C	N	O	0
			16	14	1	1	
5	AB	1	Total	C	N	O	0
			16	14	1	1	
5	AB	1	Total	C	N	O	0
			16	14	1	1	
5	AC	1	Total	C	N	O	0
			16	14	1	1	
5	AC	1	Total	C	N	O	0
			16	14	1	1	
5	AD	1	Total	C	N	O	0
			16	14	1	1	
5	AD	1	Total	C	N	O	0
			16	14	1	1	
5	AD	1	Total	C	N	O	0
			16	14	1	1	
5	AE	1	Total	C	N	O	0
			16	14	1	1	
5	AE	1	Total	C	N	O	0
			16	14	1	1	
5	AF	1	Total	C	N	O	0
			16	14	1	1	
5	AF	1	Total	C	N	O	0
			16	14	1	1	

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Mol	Chain	Residues	Atoms				AltConf
5	AG	1	Total	C	N	O	0
			16	14	1	1	
5	AG	1	Total	C	N	O	0
			16	14	1	1	
5	AH	1	Total	C	N	O	0
			16	14	1	1	
5	AH	1	Total	C	N	O	0
			16	14	1	1	
5	AI	1	Total	C	N	O	0
			16	14	1	1	
5	BA	1	Total	C	N	O	0
			16	14	1	1	
5	BA	1	Total	C	N	O	0
			16	14	1	1	
5	BB	1	Total	C	N	O	0
			16	14	1	1	
5	BB	1	Total	C	N	O	0
			16	14	1	1	
5	BC	1	Total	C	N	O	0
			16	14	1	1	
5	BC	1	Total	C	N	O	0
			16	14	1	1	
5	BD	1	Total	C	N	O	0
			16	14	1	1	
5	BE	1	Total	C	N	O	0
			16	14	1	1	
5	BE	1	Total	C	N	O	0
			16	14	1	1	
5	BF	1	Total	C	N	O	0
			16	14	1	1	
5	BF	1	Total	C	N	O	0
			16	14	1	1	
5	BG	1	Total	C	N	O	0
			16	14	1	1	
5	BG	1	Total	C	N	O	0
			16	14	1	1	
5	BH	1	Total	C	N	O	0
			16	14	1	1	
5	BH	1	Total	C	N	O	0
			16	14	1	1	
5	BI	1	Total	C	N	O	0
			16	14	1	1	

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Mol	Chain	Residues	Atoms	AltConf
5	BI	1	Total C N O 16 14 1 1	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
6	BA	1	Total Ca 1 1	0
6	BB	1	Total Ca 1 1	0
6	BC	1	Total Ca 1 1	0
6	BD	1	Total Ca 1 1	0
6	BE	1	Total Ca 1 1	0
6	BF	1	Total Ca 1 1	0
6	BG	1	Total Ca 1 1	0
6	BH	1	Total Ca 1 1	0
6	BI	1	Total Ca 1 1	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	AltConf
7	AA	15	Total O 15 15	0
7	AB	12	Total O 12 12	0
7	AC	12	Total O 12 12	0
7	AD	13	Total O 13 13	0
7	AE	12	Total O 12 12	0
7	AF	9	Total O 9 9	0
7	AG	12	Total O 12 12	0

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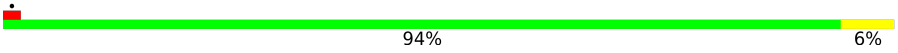
Mol	Chain	Residues	Atoms	AltConf
7	AH	13	Total O 13 13	0
7	AI	13	Total O 13 13	0
7	BA	11	Total O 11 11	0
7	BB	15	Total O 15 15	0
7	BC	15	Total O 15 15	0
7	BD	13	Total O 13 13	0
7	BE	13	Total O 13 13	0
7	BF	11	Total O 11 11	0
7	BG	14	Total O 14 14	0
7	BH	13	Total O 13 13	0
7	BI	14	Total O 14 14	0

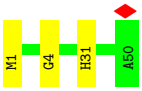
3 Residue-property plots (i)

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

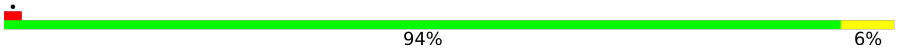
Chain AA:

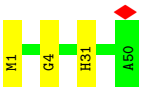




- Molecule 1: Light-harvesting protein B-800/850 alpha chain

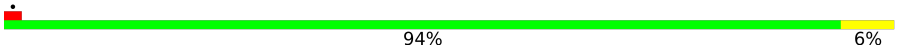
Chain AB:

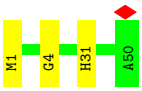




- Molecule 1: Light-harvesting protein B-800/850 alpha chain

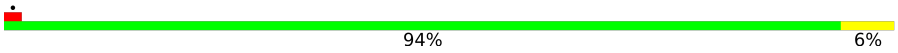
Chain AC:

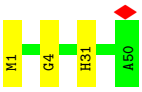




- Molecule 1: Light-harvesting protein B-800/850 alpha chain

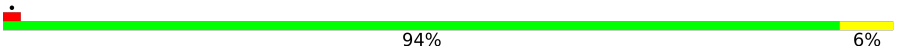
Chain AD:

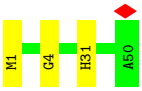




- Molecule 1: Light-harvesting protein B-800/850 alpha chain

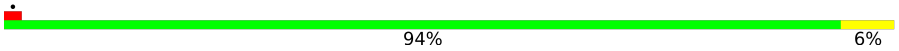
Chain AE:

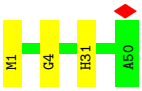




• Molecule 1: Light-harvesting protein B-800/850 alpha chain

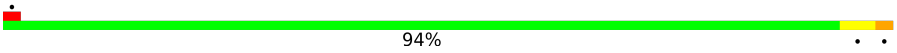
Chain AF:

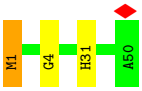




• Molecule 1: Light-harvesting protein B-800/850 alpha chain

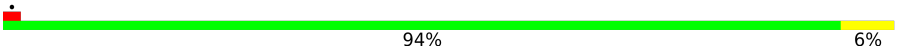
Chain AG:

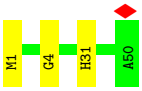




• Molecule 1: Light-harvesting protein B-800/850 alpha chain

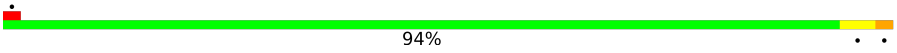
Chain AH:

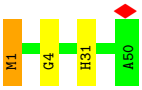




• Molecule 1: Light-harvesting protein B-800/850 alpha chain

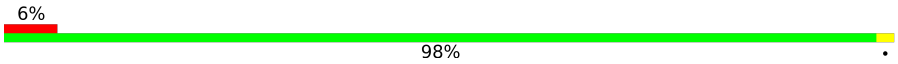
Chain AI:

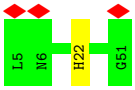




• Molecule 2: Light-harvesting protein B-800/850 beta chain

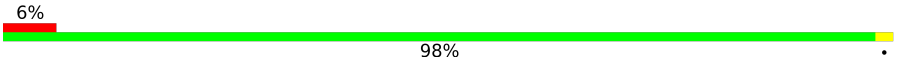
Chain BA:

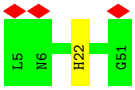




• Molecule 2: Light-harvesting protein B-800/850 beta chain

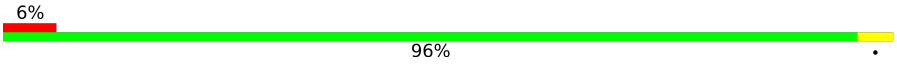
Chain BB:

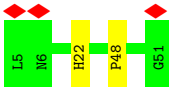




• Molecule 2: Light-harvesting protein B-800/850 beta chain

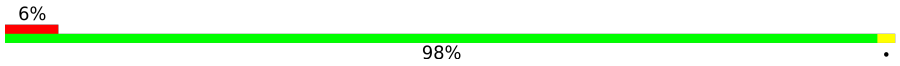
Chain BC:

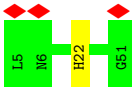




• Molecule 2: Light-harvesting protein B-800/850 beta chain

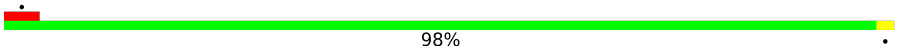
Chain BD:

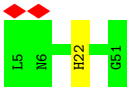




• Molecule 2: Light-harvesting protein B-800/850 beta chain

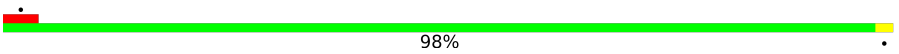
Chain BE:

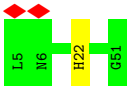




• Molecule 2: Light-harvesting protein B-800/850 beta chain

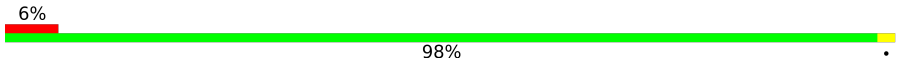
Chain BF:

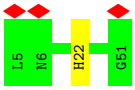




• Molecule 2: Light-harvesting protein B-800/850 beta chain

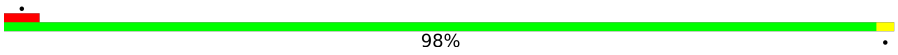
Chain BG:

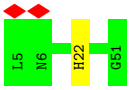




• Molecule 2: Light-harvesting protein B-800/850 beta chain

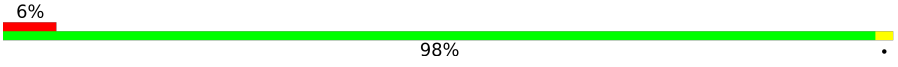
Chain BH:

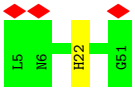




• Molecule 2: Light-harvesting protein B-800/850 beta chain

Chain BI:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C9	Depositor
Number of particles used	835641	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.158	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0305	Depositor
Map size (Å)	250.8, 250.8, 250.8	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7OT, BCL, CXM, LDA, CA

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	AA	0.17	0/371	0.45	0/514
1	AB	0.16	0/371	0.45	0/514
1	AC	0.15	0/371	0.44	0/514
1	AD	0.16	0/371	0.46	0/514
1	AE	0.16	0/371	0.45	0/514
1	AF	0.16	0/371	0.45	0/514
1	AG	0.16	0/371	0.45	0/514
1	AH	0.16	0/371	0.46	0/514
1	AI	0.16	0/371	0.45	0/514
2	BA	0.14	0/362	0.37	0/492
2	BB	0.14	0/362	0.38	0/492
2	BC	0.15	0/362	0.38	0/492
2	BD	0.15	0/362	0.38	0/492
2	BE	0.14	0/362	0.40	0/492
2	BF	0.14	0/362	0.38	0/492
2	BG	0.15	0/362	0.39	0/492
2	BH	0.15	0/362	0.39	0/492
2	BI	0.15	0/362	0.39	0/492
All	All	0.15	0/6597	0.42	0/9054

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	372	0	390	3	0
1	AB	372	0	390	3	0
1	AC	372	0	390	3	0
1	AD	372	0	390	3	0
1	AE	372	0	390	3	0
1	AF	372	0	390	3	0
1	AG	372	0	390	4	0
1	AH	372	0	390	3	0
1	AI	372	0	390	4	0
2	BA	353	0	361	1	0
2	BB	353	0	361	1	0
2	BC	353	0	361	2	0
2	BD	353	0	361	1	0
2	BE	353	0	361	1	0
2	BF	353	0	361	1	0
2	BG	353	0	361	2	0
2	BH	353	0	361	1	0
2	BI	353	0	361	2	0
3	AA	132	0	148	1	0
3	AB	132	0	148	1	0
3	AC	132	0	148	1	0
3	AD	132	0	148	1	0
3	AE	132	0	148	2	0
3	AF	132	0	148	1	0
3	AG	132	0	148	1	0
3	AH	132	0	148	1	0
3	AI	132	0	148	1	0
3	BA	66	0	74	1	0
3	BB	66	0	74	1	0
3	BC	66	0	74	1	0
3	BD	66	0	74	1	0
3	BE	66	0	74	1	0
3	BF	66	0	74	1	0
3	BG	66	0	74	1	0
3	BH	66	0	74	1	0
3	BI	66	0	74	1	0
4	AA	42	0	0	1	0
4	AB	42	0	0	1	0
4	AC	42	0	0	1	0
4	AD	42	0	0	1	0
4	AE	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AF	42	0	0	1	0
4	AG	42	0	0	1	0
4	AH	42	0	0	1	0
4	AI	42	0	0	1	0
5	AA	48	0	93	0	0
5	AB	32	0	62	0	0
5	AC	32	0	62	0	0
5	AD	48	0	93	1	0
5	AE	32	0	62	1	0
5	AF	32	0	62	1	0
5	AG	32	0	62	0	0
5	AH	32	0	62	1	0
5	AI	16	0	31	0	0
5	BA	32	0	62	0	0
5	BB	32	0	62	0	0
5	BC	32	0	62	2	0
5	BD	16	0	31	1	0
5	BE	32	0	62	0	0
5	BF	32	0	62	0	0
5	BG	32	0	62	0	0
5	BH	32	0	62	0	0
5	BI	32	0	62	0	0
6	BA	1	0	0	0	0
6	BB	1	0	0	0	0
6	BC	1	0	0	0	0
6	BD	1	0	0	0	0
6	BE	1	0	0	0	0
6	BF	1	0	0	0	0
6	BG	1	0	0	0	0
6	BH	1	0	0	0	0
6	BI	1	0	0	0	0
7	AA	15	0	0	0	0
7	AB	12	0	0	0	0
7	AC	12	0	0	0	0
7	AD	13	0	0	0	0
7	AE	12	0	0	0	0
7	AF	9	0	0	0	0
7	AG	12	0	0	0	0
7	AH	13	0	0	0	0
7	AI	13	0	0	0	0
7	BA	11	0	0	0	0
7	BB	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BC	15	0	0	0	0
7	BD	13	0	0	0	0
7	BE	13	0	0	0	0
7	BF	11	0	0	0	0
7	BG	14	0	0	0	0
7	BH	13	0	0	0	0
7	BI	14	0	0	0	0
All	All	9500	0	9873	45	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 2.

The worst 5 of 45 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:31:HIS:CE1	3:BH:101:BCL:HMD3	2.41	0.56
1:AB:31:HIS:CE1	3:BB:101:BCL:HMD3	2.40	0.56
1:AC:31:HIS:CE1	3:BC:101:BCL:HMD3	2.41	0.56
1:AF:31:HIS:CE1	3:BF:101:BCL:HMD3	2.41	0.55
1:AA:31:HIS:CE1	3:BA:101:BCL:HMD3	2.41	0.55

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	AA	48/50 (96%)	48 (100%)	0	0	100	100
1	AB	48/50 (96%)	48 (100%)	0	0	100	100
1	AC	48/50 (96%)	48 (100%)	0	0	100	100
1	AD	48/50 (96%)	48 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AE	48/50 (96%)	48 (100%)	0	0	100	100
1	AF	48/50 (96%)	48 (100%)	0	0	100	100
1	AG	48/50 (96%)	48 (100%)	0	0	100	100
1	AH	48/50 (96%)	48 (100%)	0	0	100	100
1	AI	48/50 (96%)	48 (100%)	0	0	100	100
2	BA	45/47 (96%)	45 (100%)	0	0	100	100
2	BB	45/47 (96%)	45 (100%)	0	0	100	100
2	BC	45/47 (96%)	45 (100%)	0	0	100	100
2	BD	45/47 (96%)	45 (100%)	0	0	100	100
2	BE	45/47 (96%)	45 (100%)	0	0	100	100
2	BF	45/47 (96%)	45 (100%)	0	0	100	100
2	BG	45/47 (96%)	45 (100%)	0	0	100	100
2	BH	45/47 (96%)	45 (100%)	0	0	100	100
2	BI	45/47 (96%)	45 (100%)	0	0	100	100
All	All	837/873 (96%)	837 (100%)	0	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	AA	38/38 (100%)	38 (100%)	0	100	100
1	AB	38/38 (100%)	38 (100%)	0	100	100
1	AC	38/38 (100%)	38 (100%)	0	100	100
1	AD	38/38 (100%)	38 (100%)	0	100	100
1	AE	38/38 (100%)	38 (100%)	0	100	100
1	AF	38/38 (100%)	38 (100%)	0	100	100
1	AG	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AH	38/38 (100%)	38 (100%)	0	100	100
1	AI	38/38 (100%)	38 (100%)	0	100	100
2	BA	34/34 (100%)	34 (100%)	0	100	100
2	BB	34/34 (100%)	34 (100%)	0	100	100
2	BC	34/34 (100%)	34 (100%)	0	100	100
2	BD	34/34 (100%)	34 (100%)	0	100	100
2	BE	34/34 (100%)	34 (100%)	0	100	100
2	BF	34/34 (100%)	34 (100%)	0	100	100
2	BG	34/34 (100%)	34 (100%)	0	100	100
2	BH	34/34 (100%)	34 (100%)	0	100	100
2	BI	34/34 (100%)	34 (100%)	0	100	100
All	All	648/648 (100%)	648 (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. There are no such sidechains identified.

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	AC	1	3,1	8,10,11	2.05	2 (25%)	7,11,13	2.44	3 (42%)
1	CXM	AH	1	3,1	8,10,11	2.05	2 (25%)	7,11,13	2.44	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CXM	AB	1	3,1	8,10,11	2.04	2 (25%)	7,11,13	2.37	3 (42%)
1	CXM	AA	1	3,1	8,10,11	2.05	2 (25%)	7,11,13	2.45	3 (42%)
1	CXM	AG	1	3,1	8,10,11	2.05	2 (25%)	7,11,13	2.44	3 (42%)
1	CXM	AE	1	3,1	8,10,11	2.05	2 (25%)	7,11,13	2.41	3 (42%)
1	CXM	AD	1	3,1	8,10,11	2.05	2 (25%)	7,11,13	2.39	3 (42%)
1	CXM	AF	1	3,1	8,10,11	2.05	2 (25%)	7,11,13	2.42	3 (42%)
1	CXM	AI	1	3,1	8,10,11	2.05	2 (25%)	7,11,13	2.44	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	AC	1	3,1	-	4/9/10/12	-
1	CXM	AH	1	3,1	-	4/9/10/12	-
1	CXM	AB	1	3,1	-	4/9/10/12	-
1	CXM	AA	1	3,1	-	3/9/10/12	-
1	CXM	AG	1	3,1	-	4/9/10/12	-
1	CXM	AE	1	3,1	-	3/9/10/12	-
1	CXM	AD	1	3,1	-	3/9/10/12	-
1	CXM	AF	1	3,1	-	4/9/10/12	-
1	CXM	AI	1	3,1	-	3/9/10/12	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AG	1	CXM	CN-N	3.96	1.42	1.35
1	AD	1	CXM	CN-N	3.95	1.42	1.35
1	AF	1	CXM	CN-N	3.95	1.42	1.35
1	AA	1	CXM	CN-N	3.95	1.42	1.35
1	AI	1	CXM	CN-N	3.94	1.42	1.35

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AH	1	CXM	ON1-CN-N	-4.96	116.71	124.85
1	AI	1	CXM	ON1-CN-N	-4.95	116.73	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AE	1	CXM	ON1-CN-N	-4.95	116.73	124.85
1	AA	1	CXM	ON1-CN-N	-4.93	116.76	124.85
1	AD	1	CXM	ON1-CN-N	-4.93	116.76	124.85

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AB	1	CXM	O-C-CA-CB
1	AC	1	CXM	O-C-CA-CB
1	AF	1	CXM	O-C-CA-CB
1	AG	1	CXM	O-C-CA-CB
1	AH	1	CXM	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AG	1	CXM	1	0
1	AI	1	CXM	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 81 ligands modelled in this entry, 9 are monoatomic - leaving 72 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BCL	BD	101	2	69,74,74	1.21	6 (8%)	83,115,115	1.44	11 (13%)
3	BCL	AA	101	1	69,74,74	1.19	6 (8%)	83,115,115	1.45	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BCL	BE	101	2	69,74,74	1.21	6 (8%)	83,115,115	1.44	11 (13%)
3	BCL	BF	101	2	69,74,74	1.21	6 (8%)	83,115,115	1.45	11 (13%)
4	7OT	AE	103	-	40,41,41	0.20	0	47,50,50	0.45	0
5	LDA	BA	103	-	12,15,15	2.08	1 (8%)	14,17,17	0.90	1 (7%)
5	LDA	BG	103	-	12,15,15	2.06	1 (8%)	14,17,17	0.44	0
5	LDA	BI	103	-	12,15,15	2.06	1 (8%)	14,17,17	0.96	1 (7%)
3	BCL	AI	101	1	69,74,74	1.17	5 (7%)	83,115,115	1.39	9 (10%)
5	LDA	AC	104	-	12,15,15	2.06	1 (8%)	14,17,17	0.50	0
5	LDA	BG	104	-	12,15,15	2.08	1 (8%)	14,17,17	0.42	0
3	BCL	BB	101	2	69,74,74	1.22	6 (8%)	83,115,115	1.45	11 (13%)
5	LDA	AD	106	-	12,15,15	2.08	1 (8%)	14,17,17	0.54	0
3	BCL	AE	102	1	69,74,74	1.16	5 (7%)	83,115,115	1.41	10 (12%)
3	BCL	BH	101	2	69,74,74	1.21	6 (8%)	83,115,115	1.44	9 (10%)
3	BCL	AC	101	1	69,74,74	1.19	6 (8%)	83,115,115	1.44	12 (14%)
4	7OT	AA	103	-	40,41,41	0.20	0	47,50,50	0.45	0
5	LDA	AE	105	-	12,15,15	2.07	1 (8%)	14,17,17	0.54	0
3	BCL	BA	101	2	69,74,74	1.21	6 (8%)	83,115,115	1.44	11 (13%)
3	BCL	AC	102	1	69,74,74	1.16	5 (7%)	83,115,115	1.39	9 (10%)
5	LDA	AD	105	-	12,15,15	2.07	1 (8%)	14,17,17	0.43	0
3	BCL	AG	102	1	69,74,74	1.17	5 (7%)	83,115,115	1.35	9 (10%)
4	7OT	AH	103	-	40,41,41	0.21	0	47,50,50	0.45	0
4	7OT	AI	103	-	40,41,41	0.21	0	47,50,50	0.47	0
5	LDA	AD	104	-	12,15,15	2.07	1 (8%)	14,17,17	0.36	0
5	LDA	AG	104	-	12,15,15	2.08	1 (8%)	14,17,17	0.95	1 (7%)
5	LDA	AB	105	-	12,15,15	2.06	1 (8%)	14,17,17	0.54	0
5	LDA	BI	104	-	12,15,15	2.06	1 (8%)	14,17,17	0.36	0
3	BCL	BG	101	2	69,74,74	1.21	6 (8%)	83,115,115	1.45	11 (13%)
5	LDA	AA	106	-	12,15,15	2.08	1 (8%)	14,17,17	0.99	1 (7%)
5	LDA	AH	104	-	12,15,15	2.09	1 (8%)	14,17,17	0.50	0
3	BCL	AD	102	1	69,74,74	1.16	5 (7%)	83,115,115	1.38	9 (10%)
5	LDA	AH	105	-	12,15,15	2.06	1 (8%)	14,17,17	0.56	0
5	LDA	AB	104	-	12,15,15	2.08	1 (8%)	14,17,17	0.68	0
5	LDA	BF	103	-	12,15,15	2.08	1 (8%)	14,17,17	0.35	0
5	LDA	AF	105	-	12,15,15	2.07	1 (8%)	14,17,17	0.45	0
3	BCL	AG	101	1	69,74,74	1.18	6 (8%)	83,115,115	1.44	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BCL	AH	102	1	69,74,74	1.17	5 (7%)	83,115,115	1.43	9 (10%)
3	BCL	AI	102	1	69,74,74	1.17	6 (8%)	83,115,115	1.46	12 (14%)
3	BCL	AB	102	1	69,74,74	1.17	5 (7%)	83,115,115	1.39	9 (10%)
5	LDA	BB	104	-	12,15,15	2.08	1 (8%)	14,17,17	0.43	0
3	BCL	BC	101	2	69,74,74	1.22	6 (8%)	83,115,115	1.44	11 (13%)
5	LDA	BF	104	-	12,15,15	2.09	1 (8%)	14,17,17	0.43	0
3	BCL	BI	101	2	69,74,74	1.21	6 (8%)	83,115,115	1.44	11 (13%)
4	7OT	AG	103	-	40,41,41	0.22	0	47,50,50	0.46	1 (2%)
5	LDA	BD	103	-	12,15,15	2.08	1 (8%)	14,17,17	0.42	0
3	BCL	AE	101	1	69,74,74	1.19	6 (8%)	83,115,115	1.45	12 (14%)
5	LDA	AA	104	-	12,15,15	2.08	1 (8%)	14,17,17	0.50	0
4	7OT	AD	103	-	40,41,41	0.20	0	47,50,50	0.46	0
5	LDA	BA	104	-	12,15,15	2.07	1 (8%)	14,17,17	0.47	0
5	LDA	BC	103	-	12,15,15	2.06	1 (8%)	14,17,17	0.87	0
4	7OT	AB	103	-	40,41,41	0.20	0	47,50,50	0.45	1 (2%)
5	LDA	AC	105	-	12,15,15	2.08	1 (8%)	14,17,17	0.43	0
4	7OT	AF	103	-	40,41,41	0.20	0	47,50,50	0.45	1 (2%)
5	LDA	BE	104	-	12,15,15	2.09	1 (8%)	14,17,17	0.46	0
5	LDA	AF	104	-	12,15,15	2.08	1 (8%)	14,17,17	0.57	0
5	LDA	BC	104	-	12,15,15	2.08	1 (8%)	14,17,17	0.48	0
5	LDA	BE	103	-	12,15,15	2.06	1 (8%)	14,17,17	0.45	0
5	LDA	AG	105	-	12,15,15	2.07	1 (8%)	14,17,17	0.89	0
5	LDA	AI	104	-	12,15,15	2.08	1 (8%)	14,17,17	0.44	0
5	LDA	BH	103	-	12,15,15	2.07	1 (8%)	14,17,17	0.45	0
5	LDA	AA	105	-	12,15,15	2.10	1 (8%)	14,17,17	0.87	1 (7%)
3	BCL	AA	102	1	69,74,74	1.16	5 (7%)	83,115,115	1.39	9 (10%)
3	BCL	AD	101	1	69,74,74	1.18	6 (8%)	83,115,115	1.44	12 (14%)
5	LDA	AE	104	-	12,15,15	2.07	1 (8%)	14,17,17	0.49	0
4	7OT	AC	103	-	40,41,41	0.21	0	47,50,50	0.46	1 (2%)
3	BCL	AF	101	1	69,74,74	1.19	6 (8%)	83,115,115	1.45	12 (14%)
3	BCL	AF	102	1	69,74,74	1.16	5 (7%)	83,115,115	1.40	9 (10%)
3	BCL	AB	101	1	69,74,74	1.18	6 (8%)	83,115,115	1.45	12 (14%)
3	BCL	AH	101	1	69,74,74	1.19	6 (8%)	83,115,115	1.44	12 (14%)
5	LDA	BH	104	-	12,15,15	2.09	1 (8%)	14,17,17	0.44	0
5	LDA	BB	103	-	12,15,15	2.08	1 (8%)	14,17,17	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BCL	BD	101	2	-	1/41/137/137	-
3	BCL	AA	101	1	-	0/41/137/137	-
3	BCL	BE	101	2	-	1/41/137/137	-
3	BCL	BF	101	2	-	1/41/137/137	-
4	7OT	AE	103	-	-	0/47/47/47	-
5	LDA	BA	103	-	-	4/13/13/13	-
5	LDA	BG	103	-	-	0/13/13/13	-
5	LDA	BI	103	-	-	2/13/13/13	-
3	BCL	AI	101	1	-	4/41/137/137	-
5	LDA	AC	104	-	-	5/13/13/13	-
5	LDA	BG	104	-	-	0/13/13/13	-
3	BCL	BB	101	2	-	1/41/137/137	-
5	LDA	AD	106	-	-	1/13/13/13	-
3	BCL	AE	102	1	-	6/41/137/137	-
3	BCL	BH	101	2	-	7/41/137/137	-
3	BCL	AC	101	1	-	0/41/137/137	-
4	7OT	AA	103	-	-	0/47/47/47	-
5	LDA	AE	105	-	-	0/13/13/13	-
3	BCL	BA	101	2	-	1/41/137/137	-
3	BCL	AC	102	1	-	2/41/137/137	-
5	LDA	AD	105	-	-	1/13/13/13	-
3	BCL	AG	102	1	-	2/41/137/137	-
4	7OT	AH	103	-	-	0/47/47/47	-
4	7OT	AI	103	-	-	1/47/47/47	-
5	LDA	AD	104	-	-	1/13/13/13	-
5	LDA	AG	104	-	-	2/13/13/13	-
5	LDA	AB	105	-	-	4/13/13/13	-
5	LDA	BI	104	-	-	0/13/13/13	-
3	BCL	BG	101	2	-	4/41/137/137	-
5	LDA	AA	106	-	-	1/13/13/13	-
5	LDA	AH	104	-	-	1/13/13/13	-
3	BCL	AD	102	1	-	3/41/137/137	-
5	LDA	AH	105	-	-	0/13/13/13	-
5	LDA	AB	104	-	-	7/13/13/13	-
5	LDA	BF	103	-	-	3/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LDA	AF	105	-	-	2/13/13/13	-
3	BCL	AG	101	1	-	0/41/137/137	-
3	BCL	AH	102	1	-	5/41/137/137	-
3	BCL	AI	102	1	-	0/41/137/137	-
3	BCL	AB	102	1	-	4/41/137/137	-
5	LDA	BB	104	-	-	0/13/13/13	-
3	BCL	BC	101	2	-	1/41/137/137	-
5	LDA	BF	104	-	-	0/13/13/13	-
3	BCL	BI	101	2	-	1/41/137/137	-
4	7OT	AG	103	-	-	0/47/47/47	-
5	LDA	BD	103	-	-	0/13/13/13	-
3	BCL	AE	101	1	-	1/41/137/137	-
5	LDA	AA	104	-	-	0/13/13/13	-
4	7OT	AD	103	-	-	0/47/47/47	-
5	LDA	BA	104	-	-	0/13/13/13	-
5	LDA	BC	103	-	-	3/13/13/13	-
4	7OT	AB	103	-	-	0/47/47/47	-
5	LDA	AC	105	-	-	3/13/13/13	-
4	7OT	AF	103	-	-	0/47/47/47	-
5	LDA	BE	104	-	-	0/13/13/13	-
5	LDA	AF	104	-	-	3/13/13/13	-
5	LDA	BC	104	-	-	0/13/13/13	-
5	LDA	BE	103	-	-	2/13/13/13	-
5	LDA	AG	105	-	-	5/13/13/13	-
5	LDA	AI	104	-	-	1/13/13/13	-
5	LDA	BH	103	-	-	1/13/13/13	-
5	LDA	AA	105	-	-	2/13/13/13	-
3	BCL	AA	102	1	-	5/41/137/137	-
3	BCL	AD	101	1	-	0/41/137/137	-
5	LDA	AE	104	-	-	1/13/13/13	-
4	7OT	AC	103	-	-	0/47/47/47	-
3	BCL	AF	101	1	-	0/41/137/137	-
3	BCL	AF	102	1	-	3/41/137/137	-
3	BCL	AB	101	1	-	0/41/137/137	-
3	BCL	AH	101	1	-	0/41/137/137	-
5	LDA	BH	104	-	-	0/13/13/13	-
5	LDA	BB	103	-	-	3/13/13/13	-

The worst 5 of 189 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AA	105	LDA	O1-N1	-7.21	1.25	1.42
5	AH	104	LDA	O1-N1	-7.20	1.25	1.42
5	AA	104	LDA	O1-N1	-7.17	1.25	1.42
5	BH	104	LDA	O1-N1	-7.16	1.25	1.42
5	BE	104	LDA	O1-N1	-7.16	1.25	1.42

The worst 5 of 296 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AF	102	BCL	C4D-CHA-C1A	5.54	127.99	121.25
3	AG	102	BCL	C4D-CHA-C1A	5.53	127.98	121.25
3	AE	102	BCL	C4D-CHA-C1A	5.52	127.97	121.25
3	AC	102	BCL	C4D-CHA-C1A	5.52	127.97	121.25
3	AA	102	BCL	C4D-CHA-C1A	5.51	127.96	121.25

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AH	102	BCL	C6-C7-C8-C9
5	AA	105	LDA	N1-C1-C2-C3
5	AA	106	LDA	N1-C1-C2-C3
5	AB	104	LDA	C2-C1-N1-CM2
5	AB	105	LDA	C2-C1-N1-O1

There are no ring outliers.

34 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BD	101	BCL	1	0
3	BE	101	BCL	1	0
3	BF	101	BCL	1	0
4	AE	103	7OT	1	0
3	AI	101	BCL	1	0
3	BB	101	BCL	1	0
3	AE	102	BCL	1	0
3	BH	101	BCL	1	0
4	AA	103	7OT	1	0
5	AE	105	LDA	1	0
3	BA	101	BCL	1	0
3	AC	102	BCL	1	0
5	AD	105	LDA	1	0

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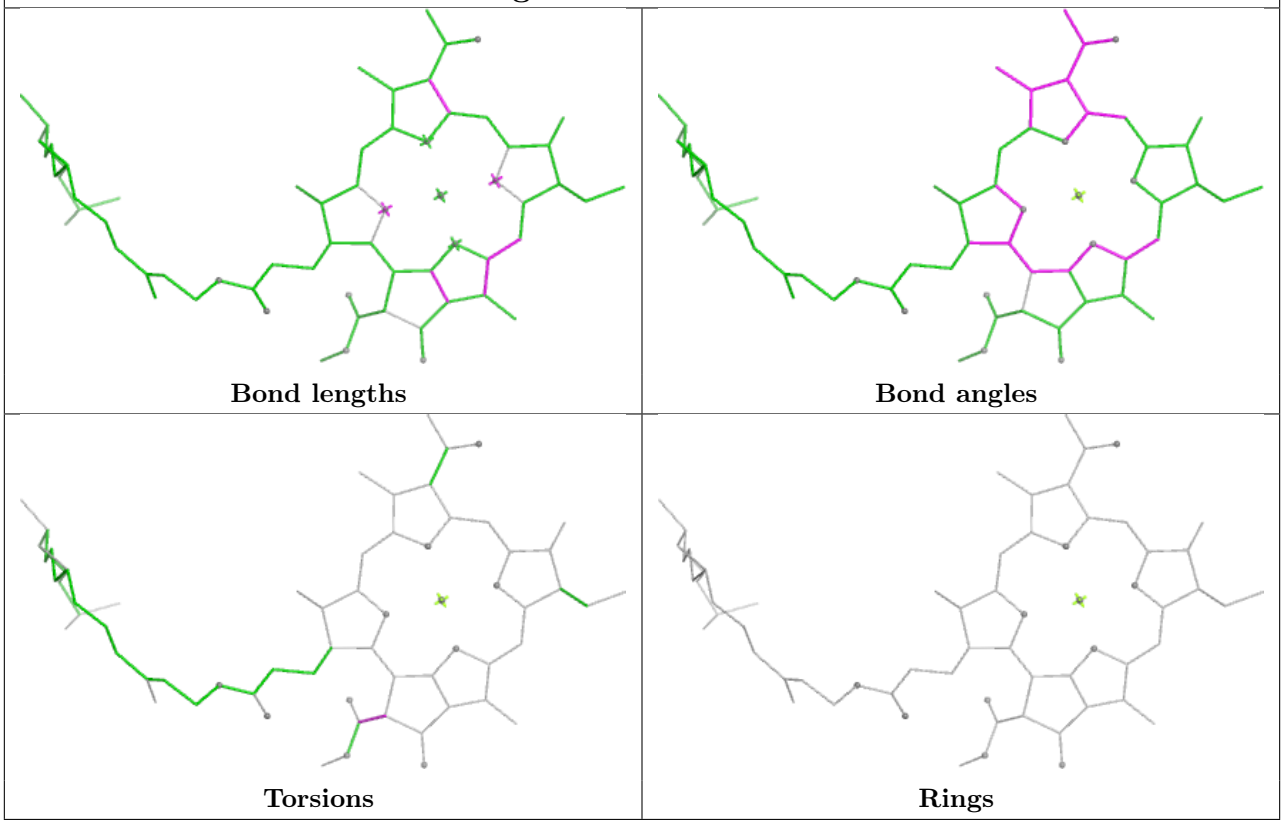
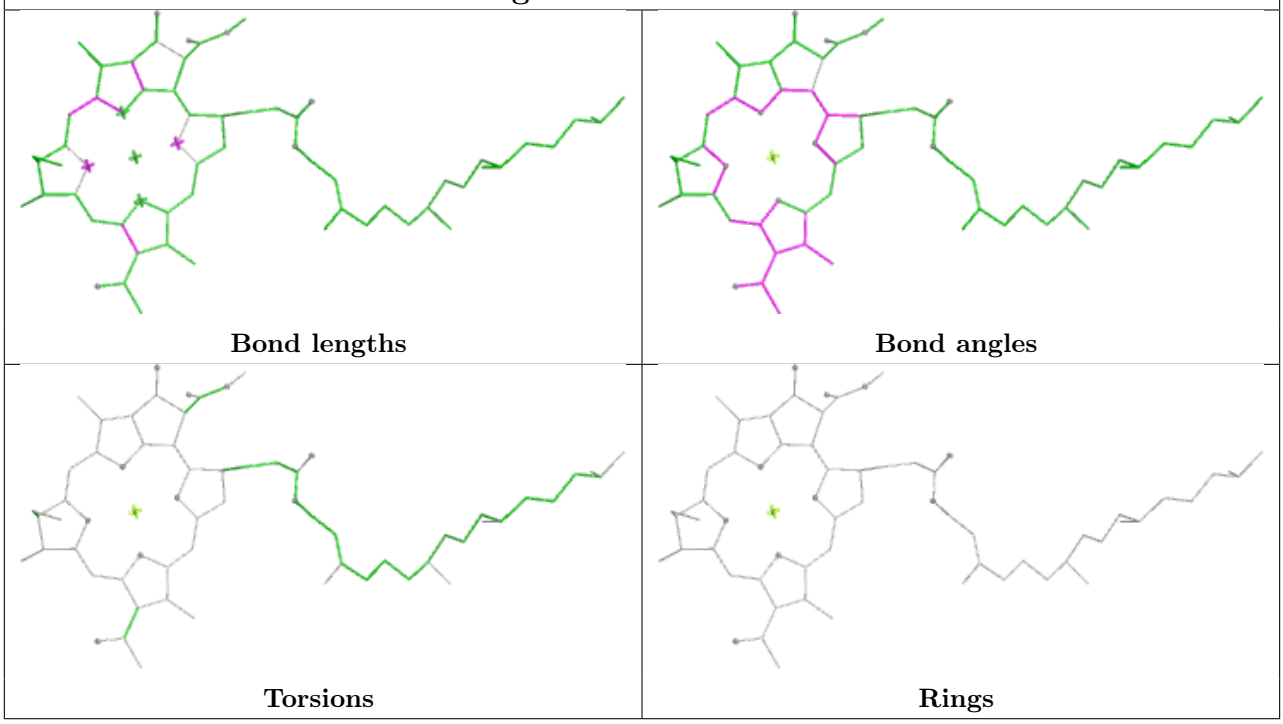
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AG	102	BCL	1	0
4	AH	103	7OT	1	0
4	AI	103	7OT	1	0
3	BG	101	BCL	1	0
3	AD	102	BCL	1	0
5	AH	105	LDA	1	0
5	AF	105	LDA	1	0
3	AH	102	BCL	1	0
3	AB	102	BCL	1	0
3	BC	101	BCL	1	0
3	BI	101	BCL	1	0
4	AG	103	7OT	1	0
5	BD	103	LDA	1	0
3	AE	101	BCL	1	0
4	AD	103	7OT	1	0
5	BC	103	LDA	2	0
4	AB	103	7OT	1	0
4	AF	103	7OT	1	0
3	AA	102	BCL	1	0
4	AC	103	7OT	1	0
3	AF	102	BCL	1	0

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

Ligand BCL BD 101



Ligand BCL AA 101



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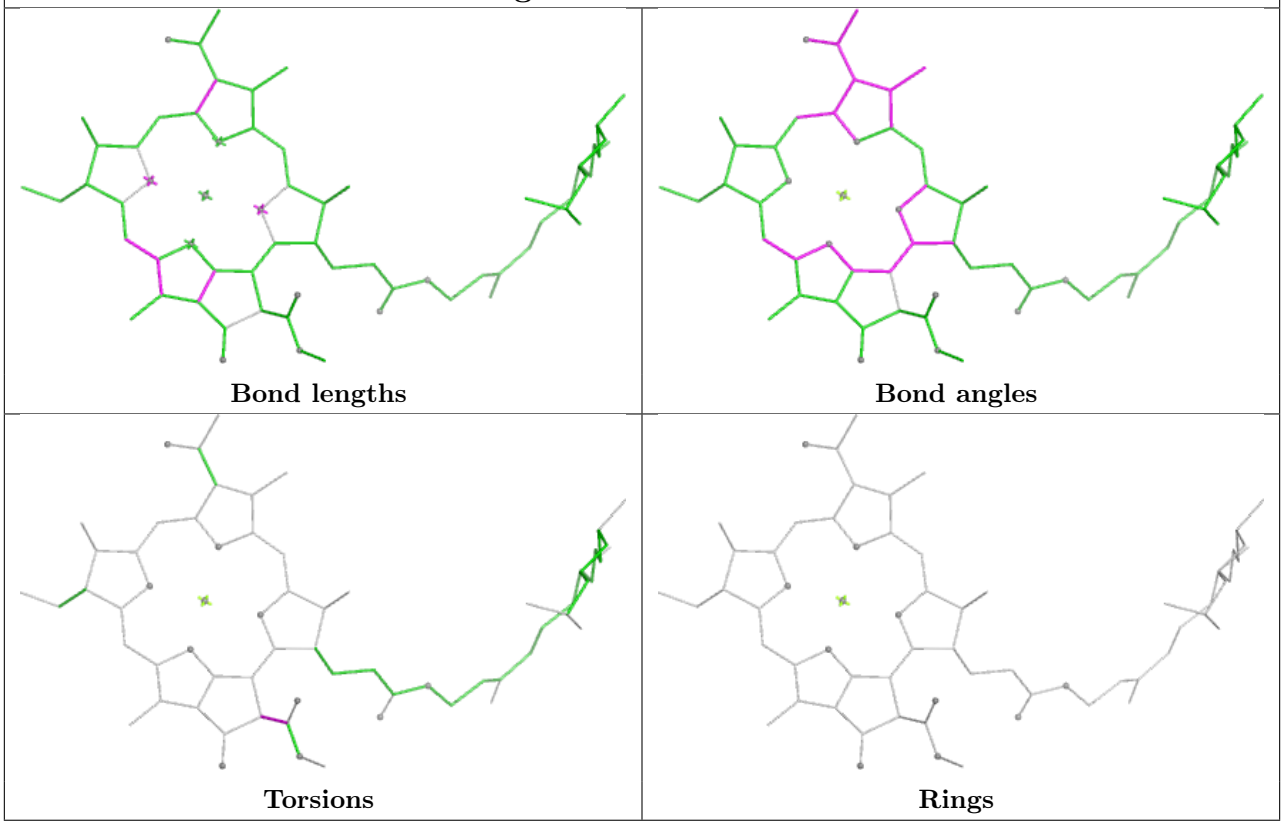

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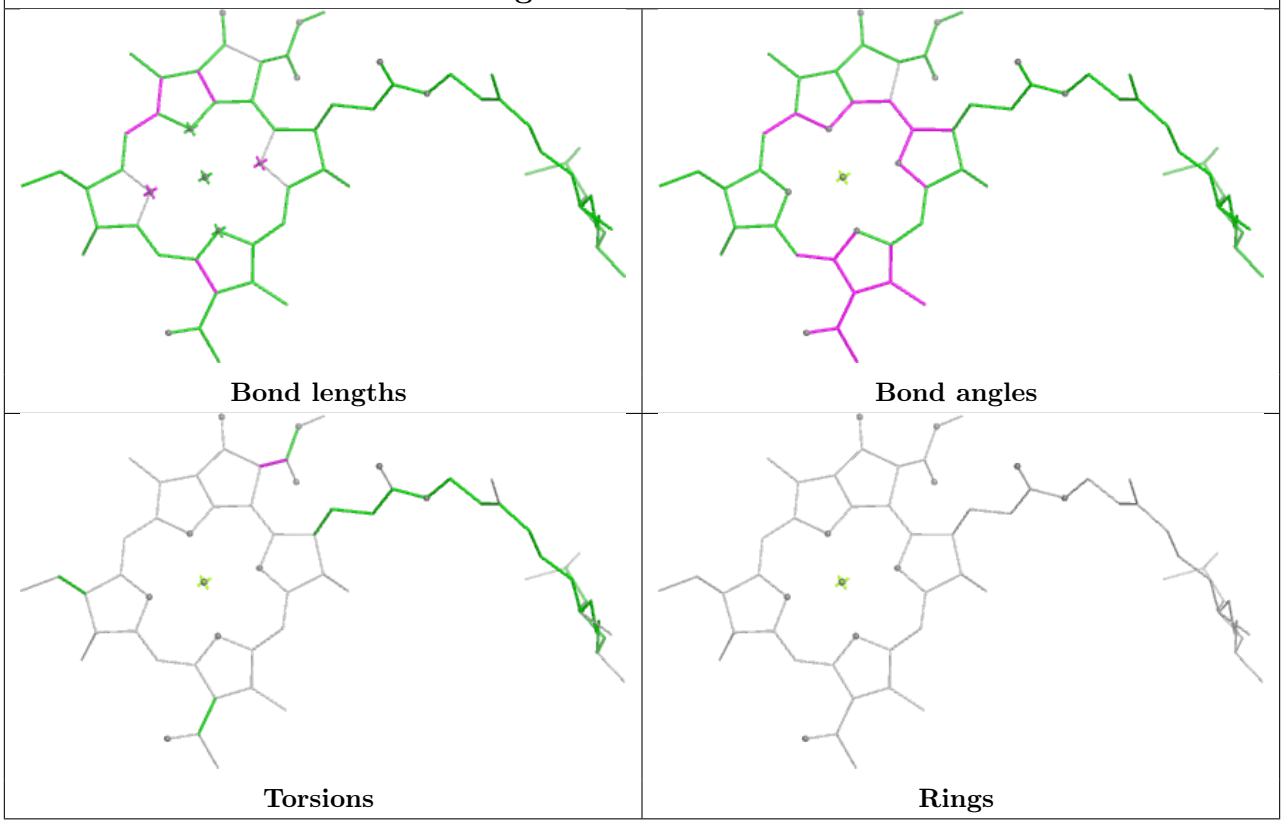

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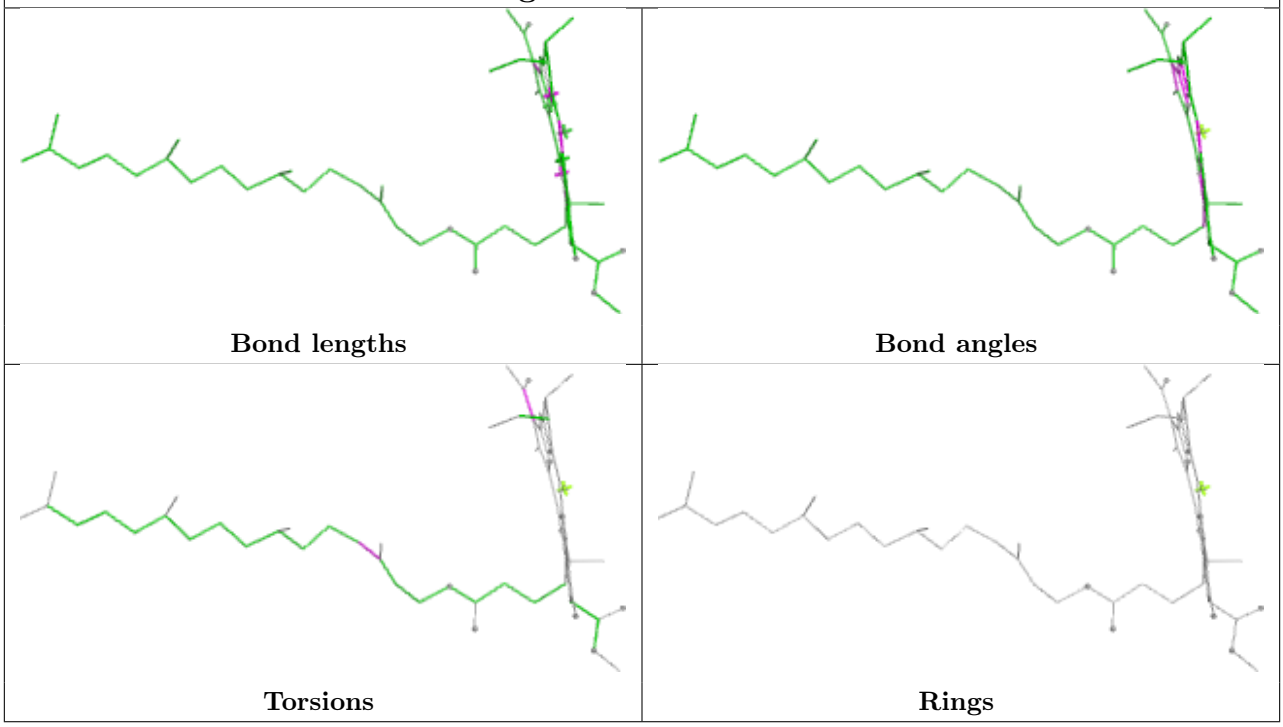

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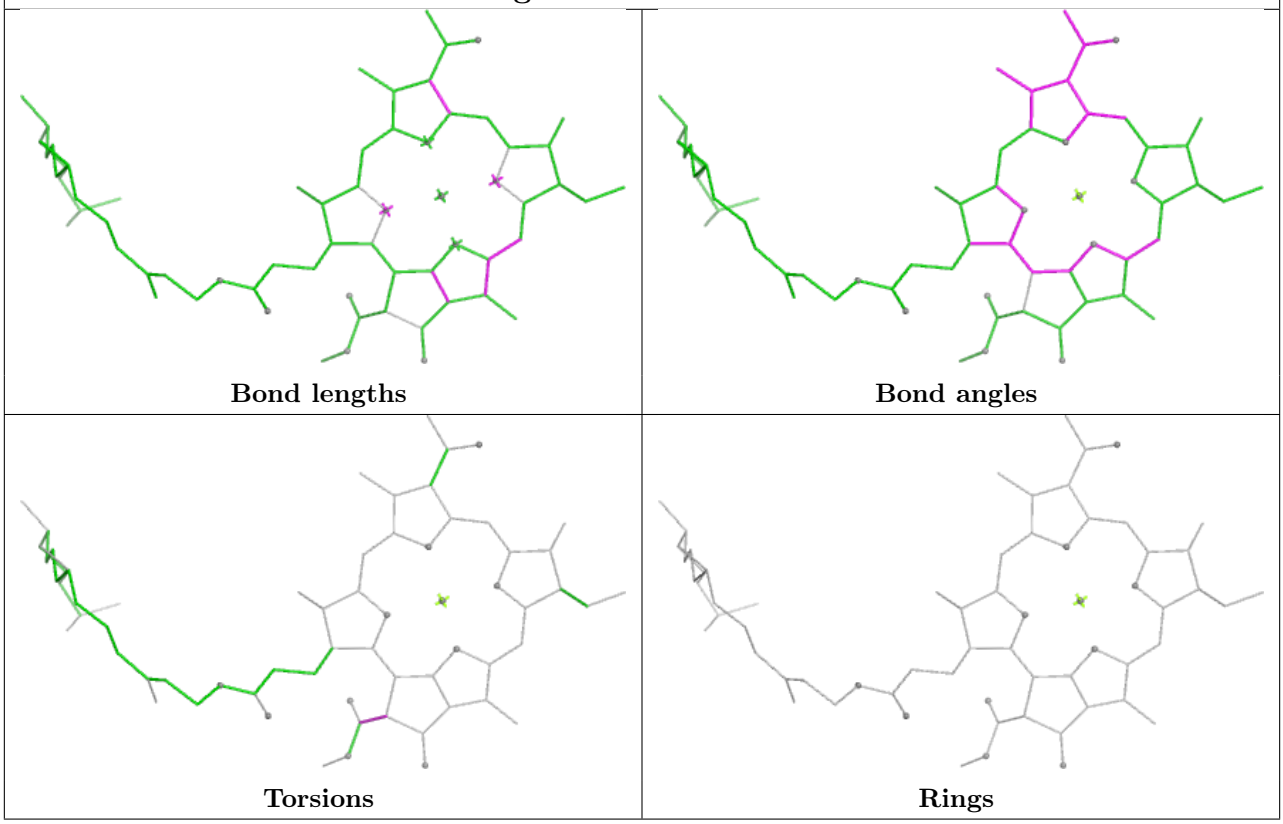

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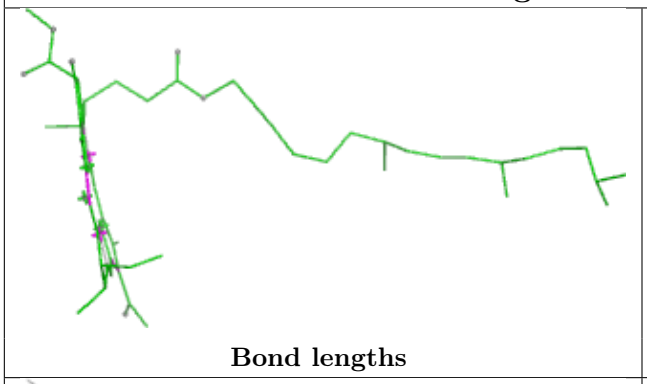
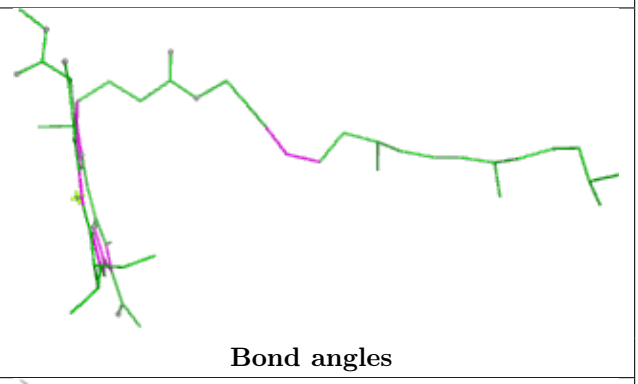
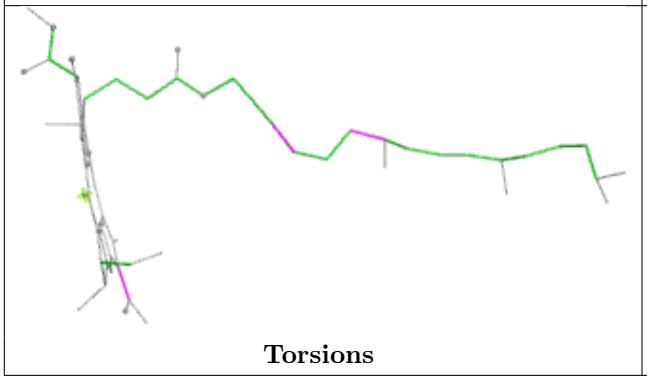


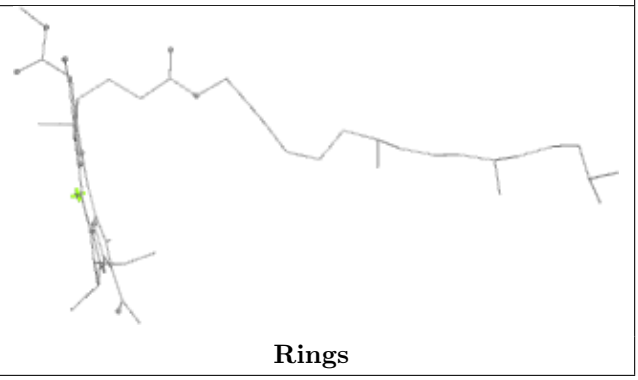
Bond lengths



Bond angles

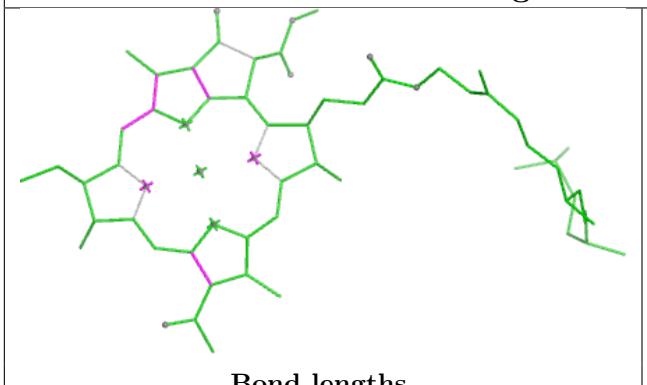


Torsions



Rings

Ligand BCL BH 101



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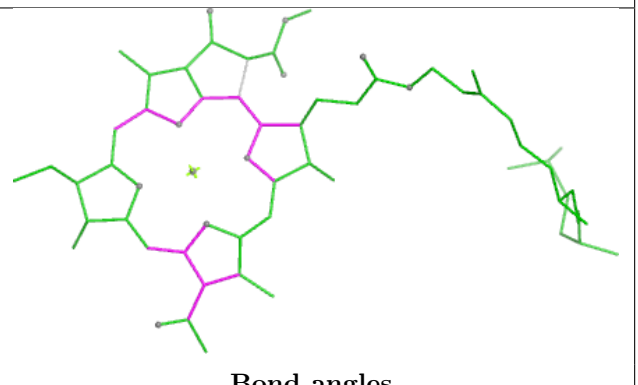
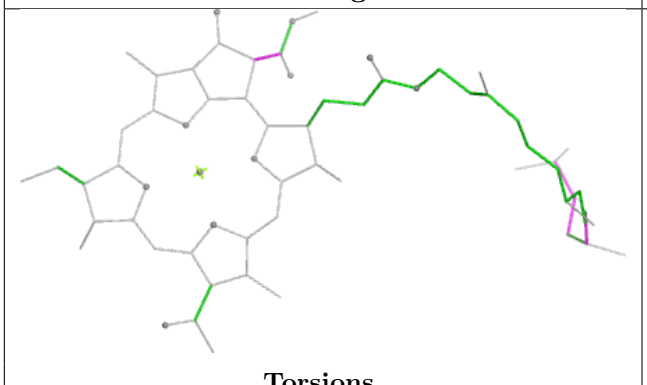


Bond angles



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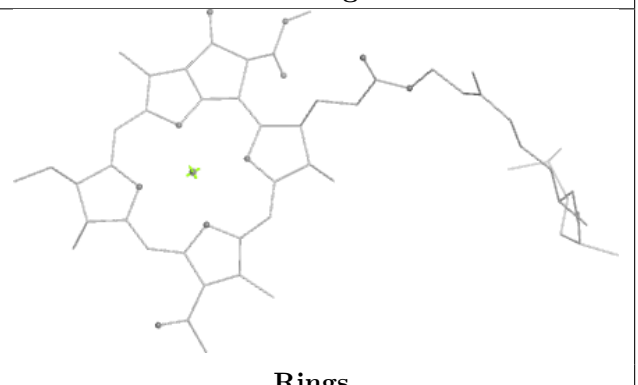
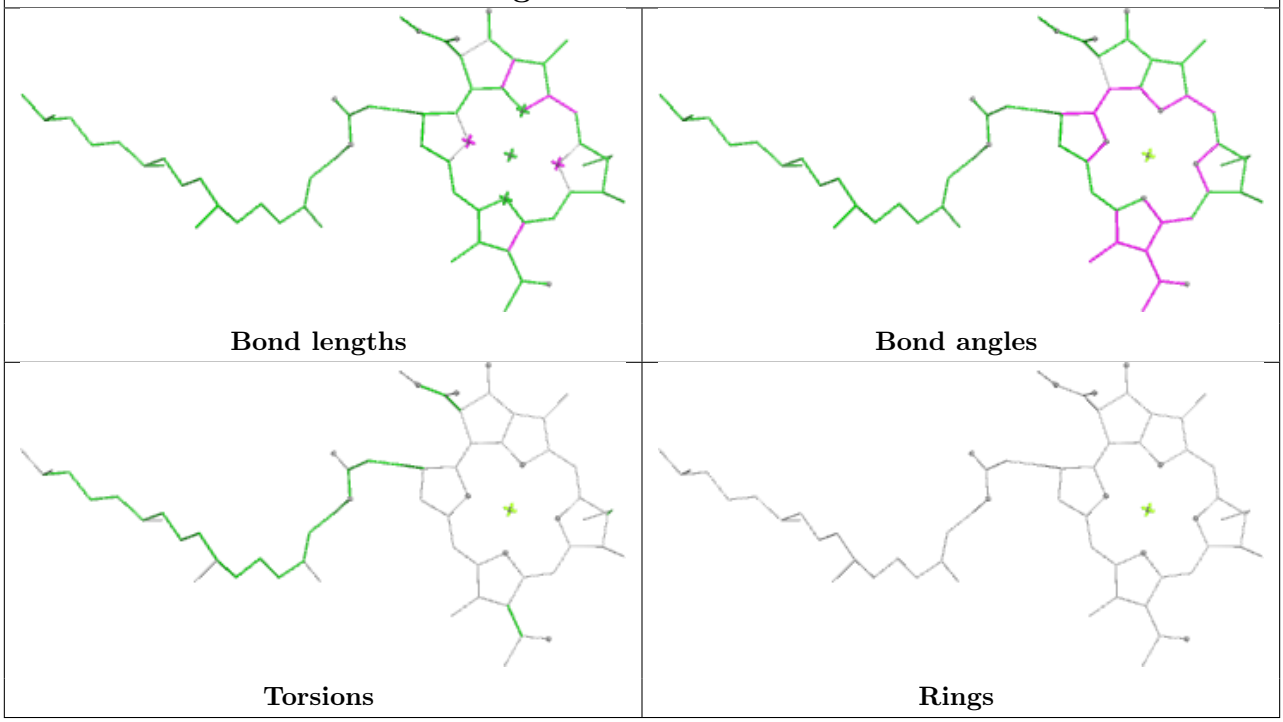
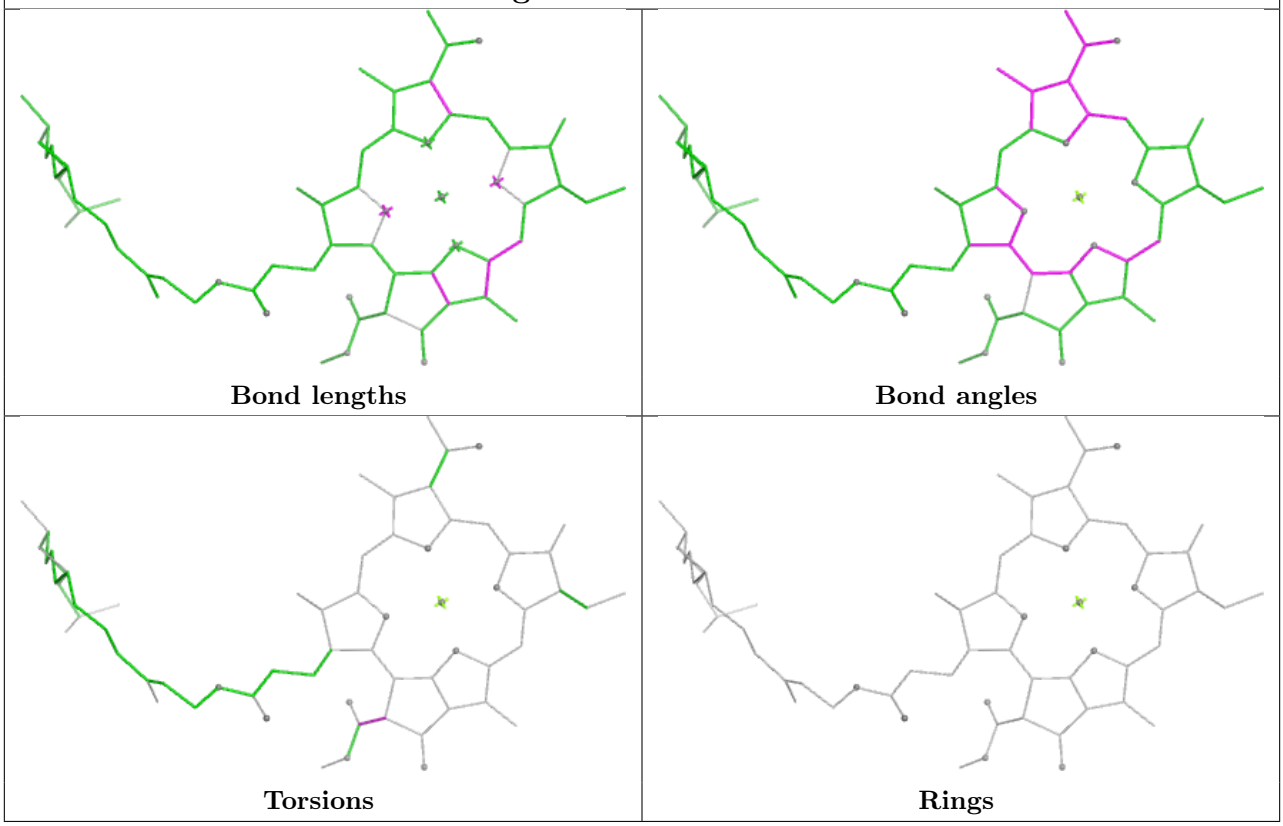


Rings

Ligand BCL AC 101



Ligand BCL BA 101



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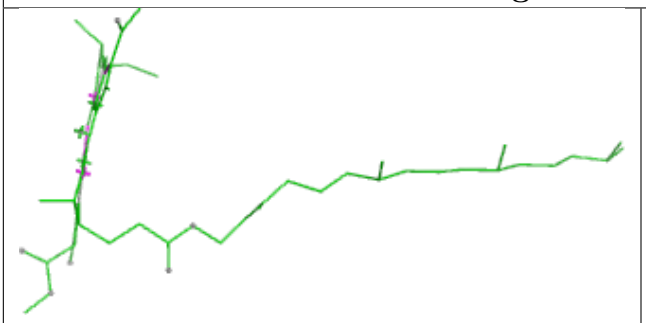

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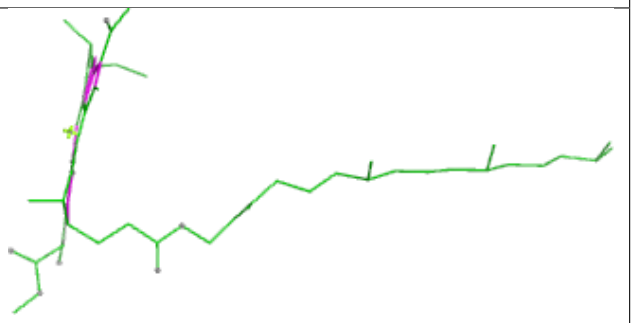


Bond angles

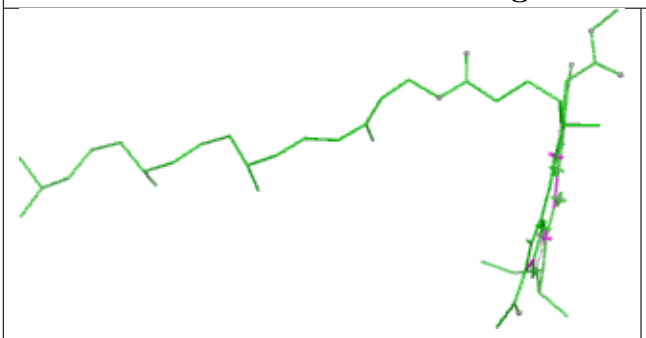


Torsions



Rings

Ligand BCL AG 102



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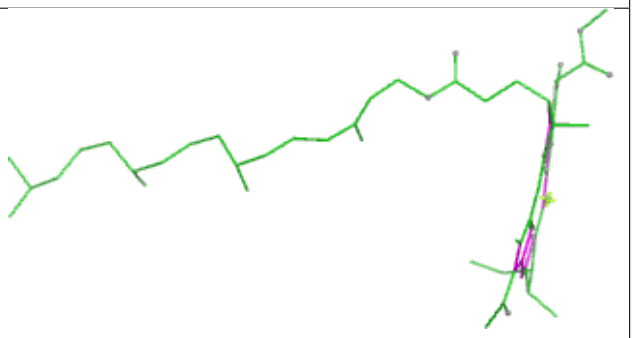
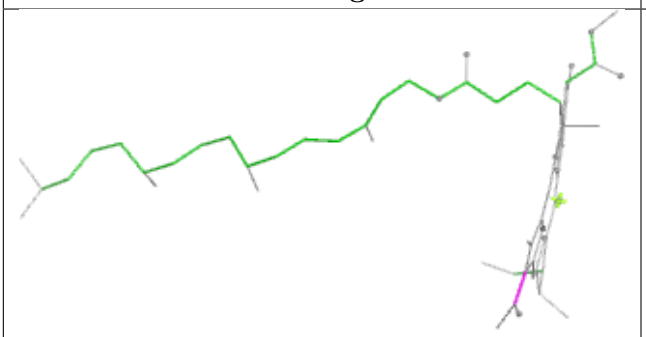


Bond angles



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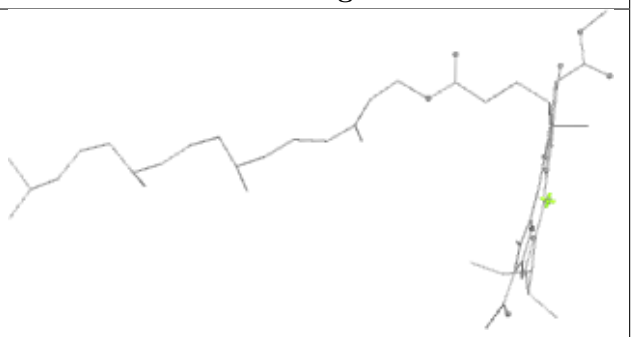
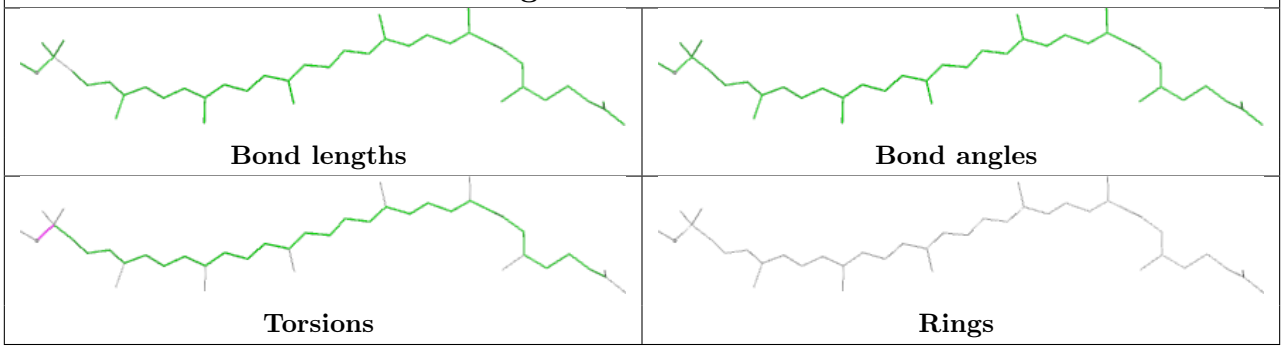


Rings

Ligand 7OT AI 103



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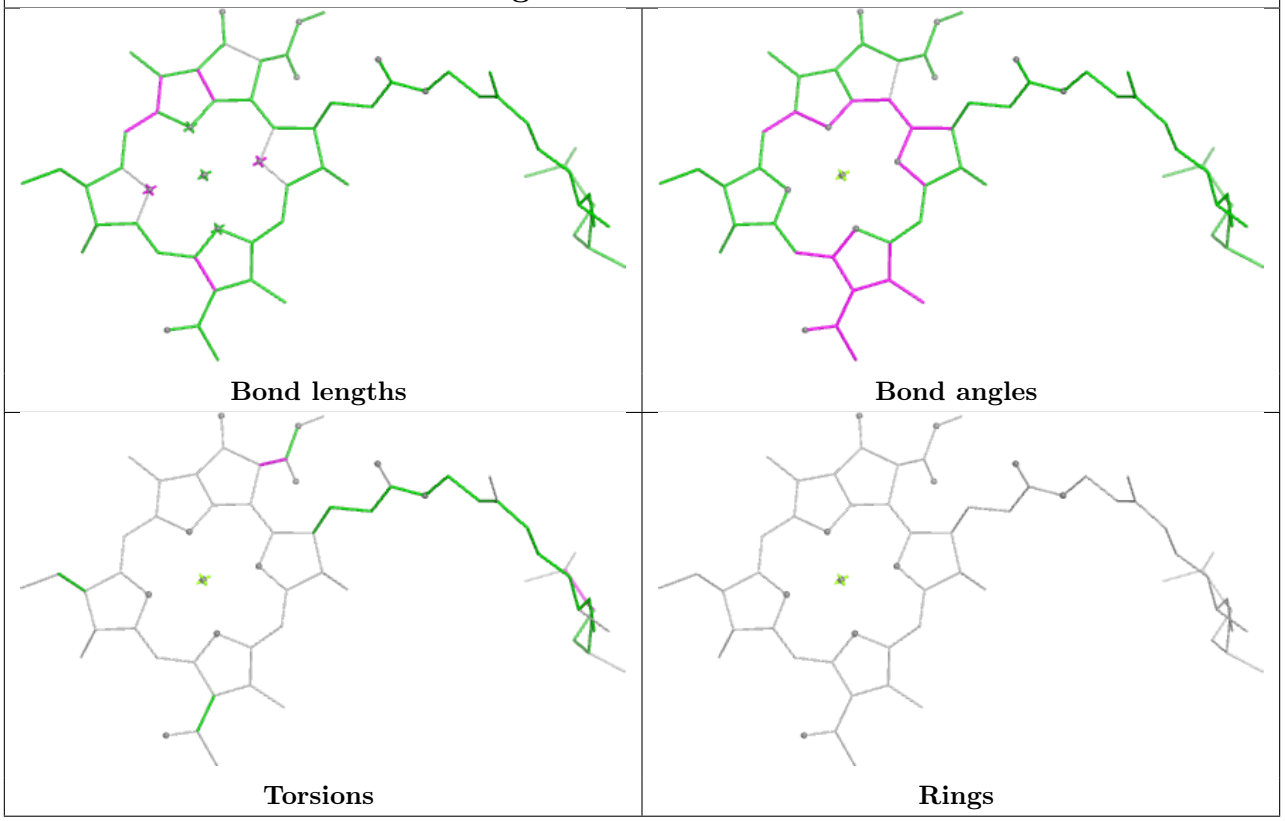

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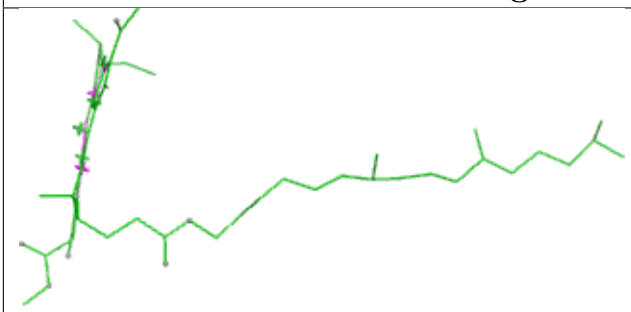

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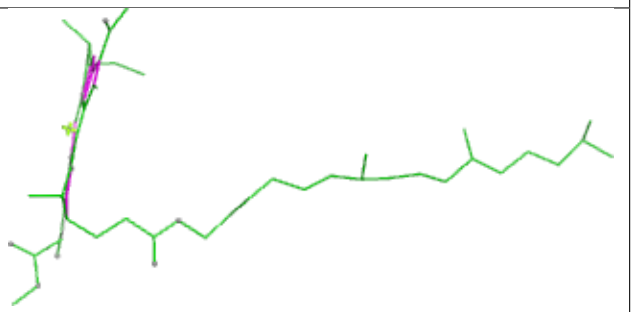
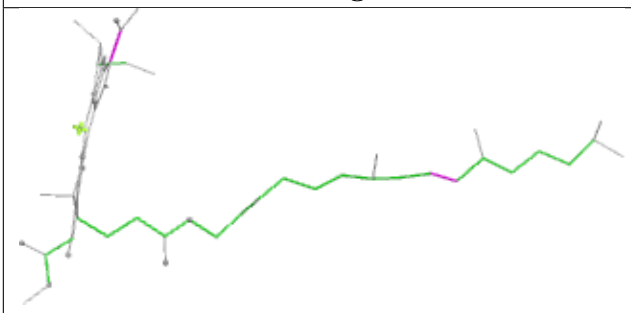


Bond angles



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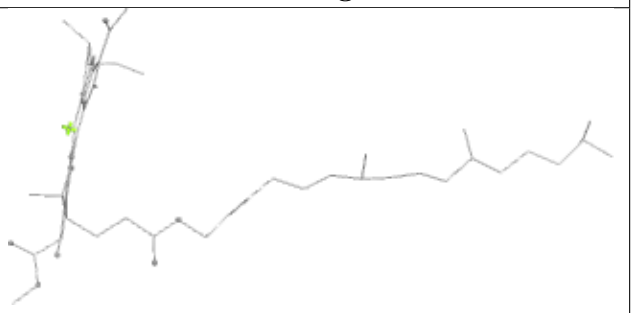
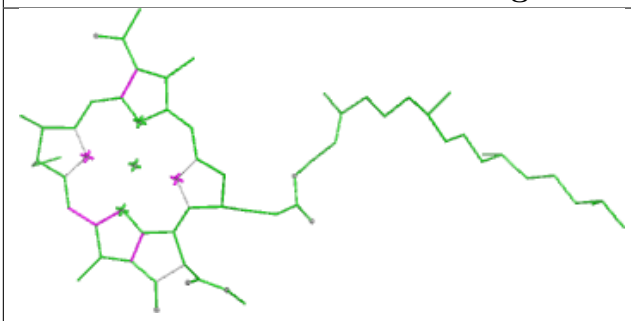


Rings

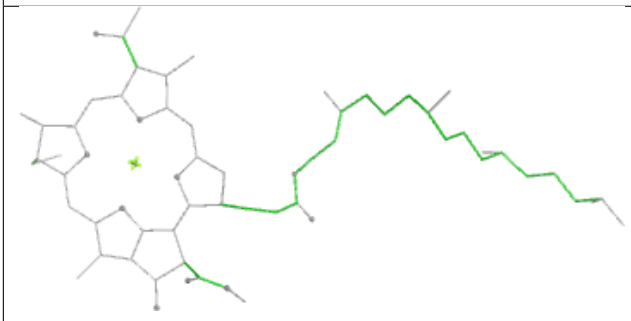
Ligand BCL AG 101



Bond lengths



Bond angles



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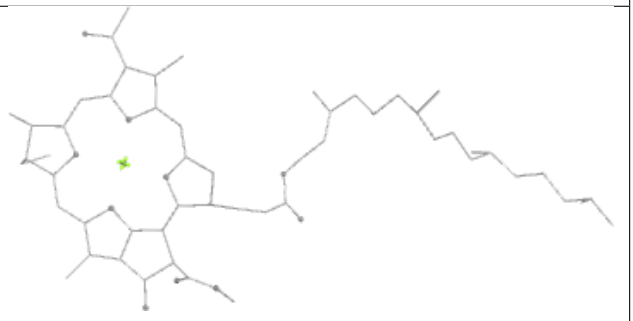
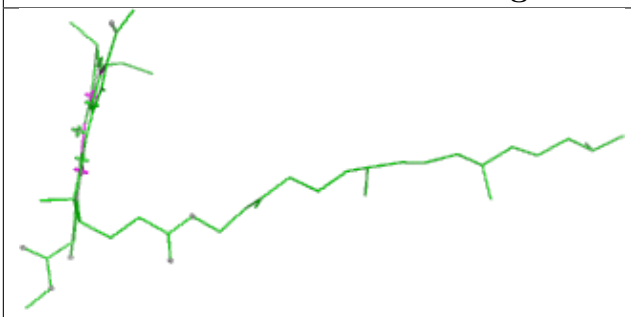


Rings

Ligand BCL AH 102



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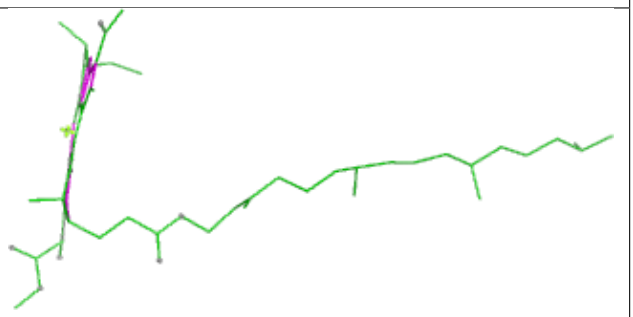
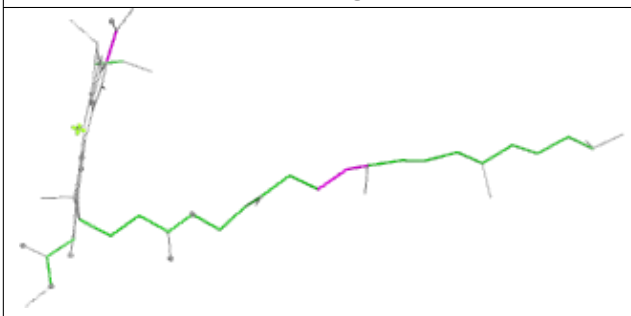


Bond angles



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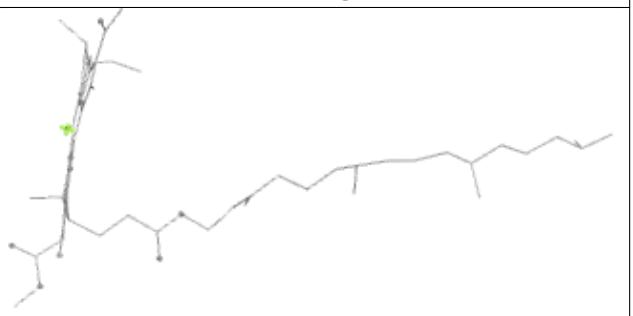
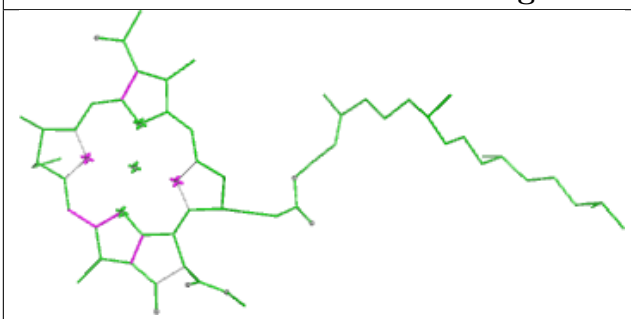


Rings

Ligand BCL AI 102



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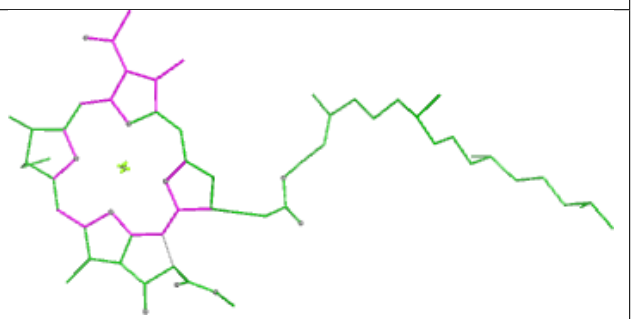
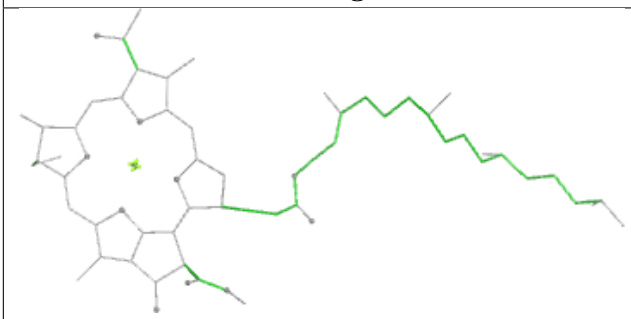


Bond angles



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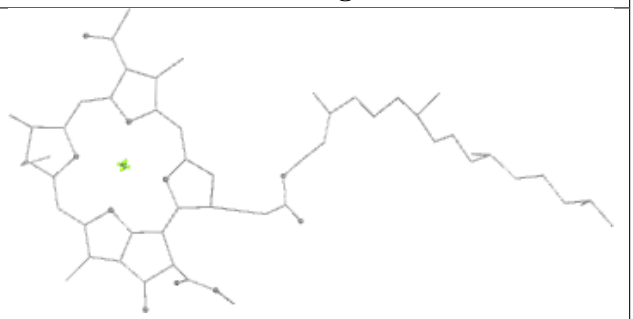
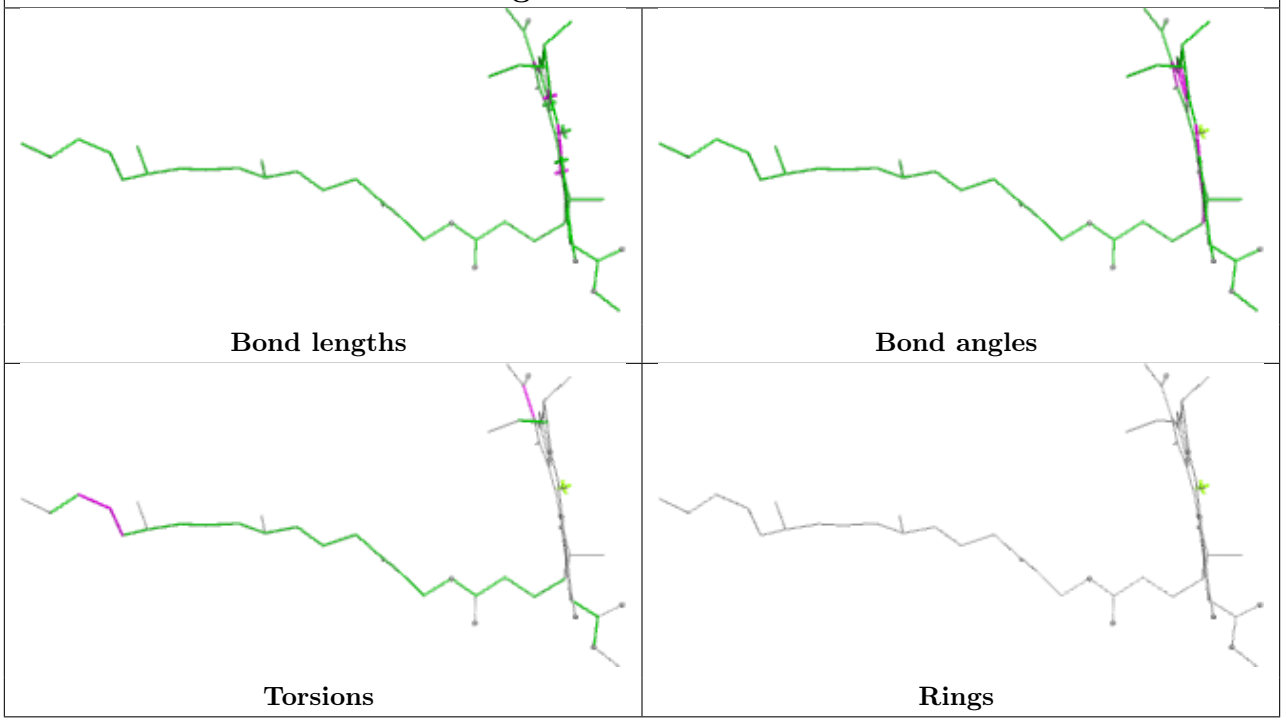


Rings

Ligand BCL AB 102



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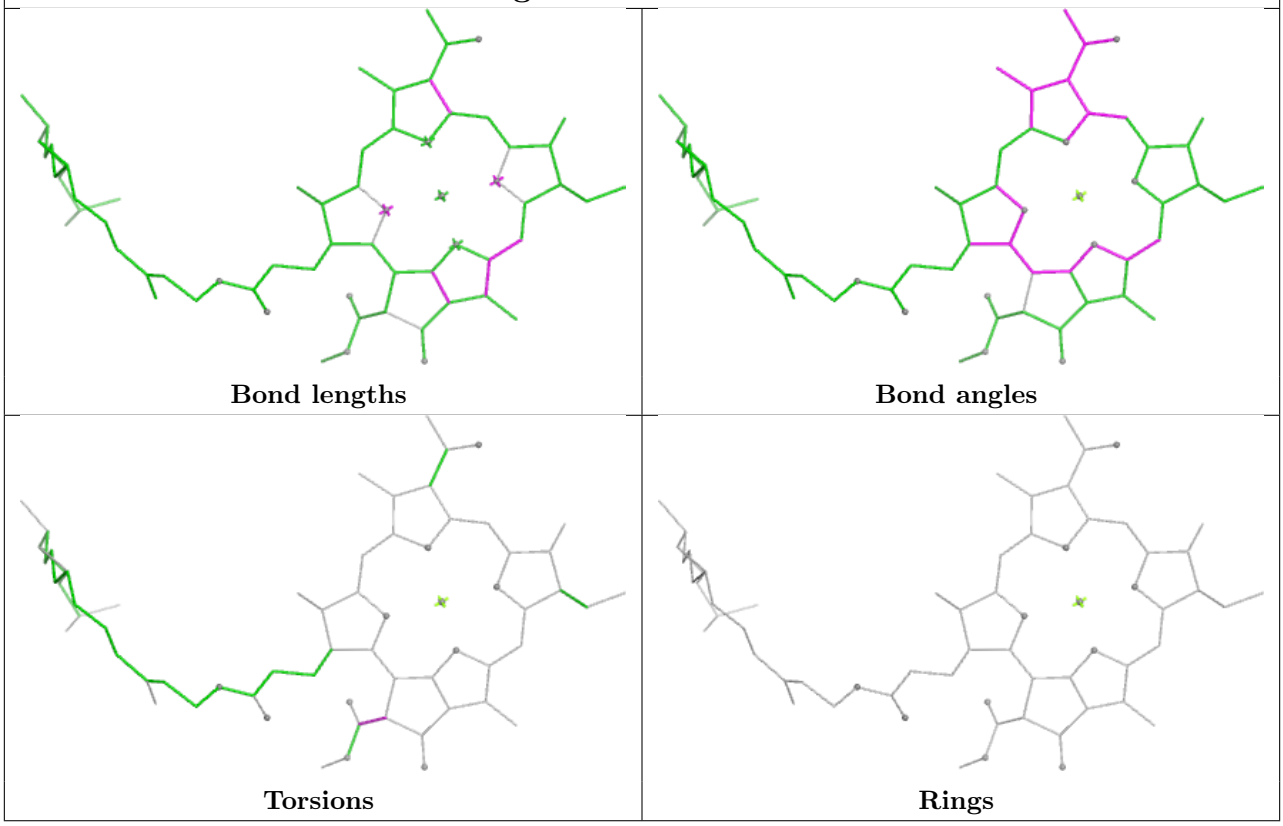

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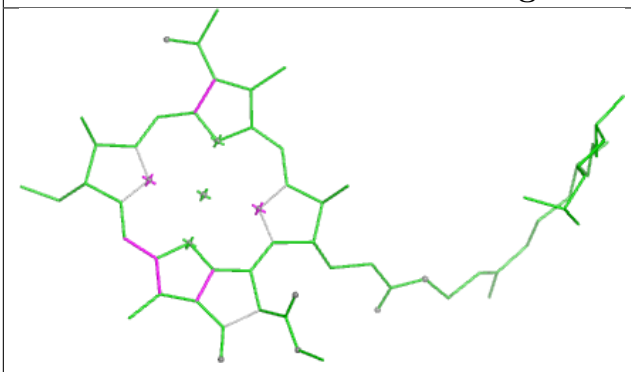

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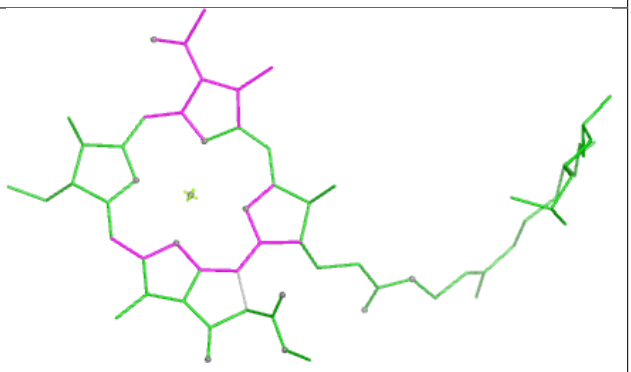
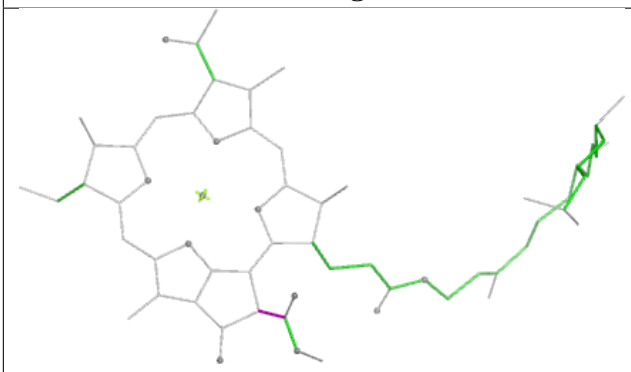


Bond angles



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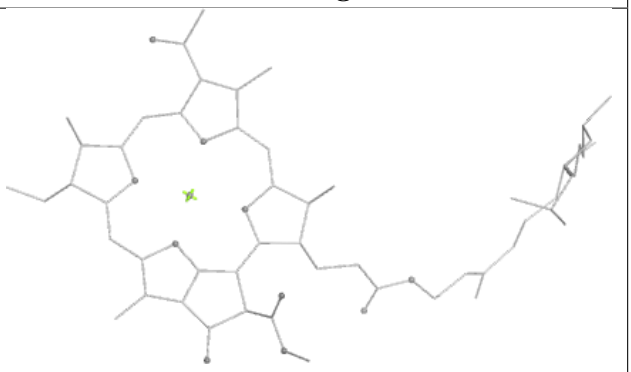
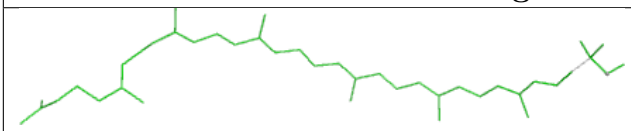


Rings

Ligand 7OT AG 103



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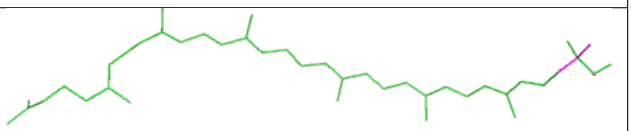
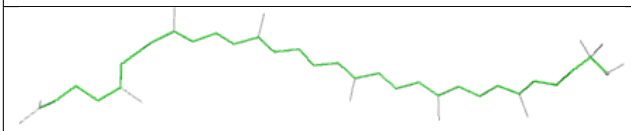


Bond angles

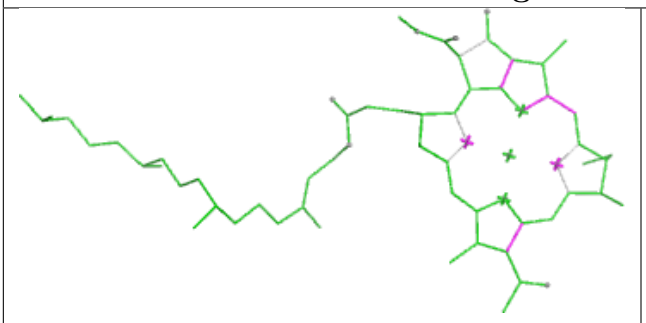


Torsions



Rings

Ligand BCL AE 101



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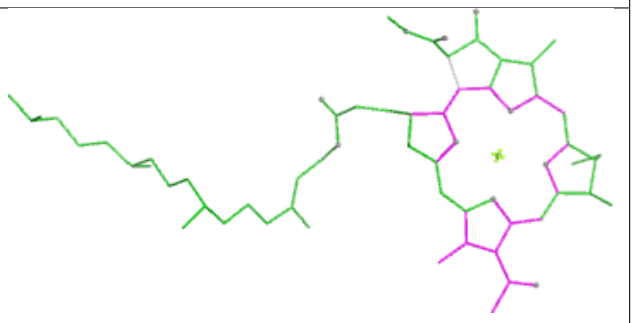
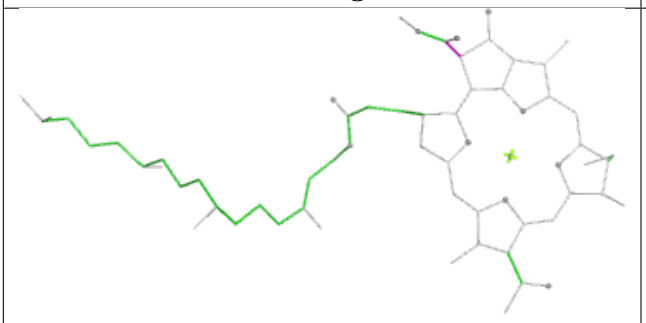
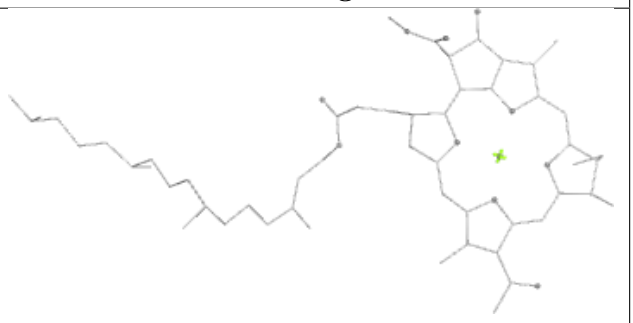


Bond angles

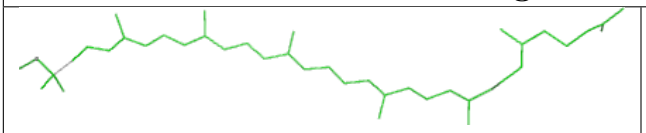


Torsions

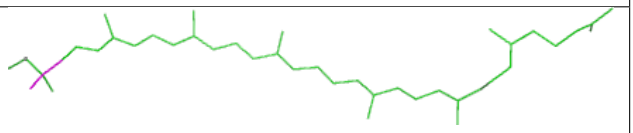


Rings

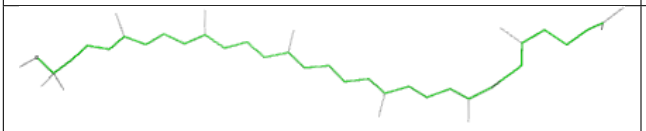
Ligand 7OT AB 103



Bond lengths



Bond angles



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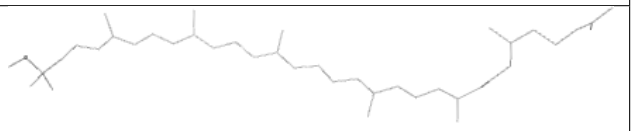


Rings

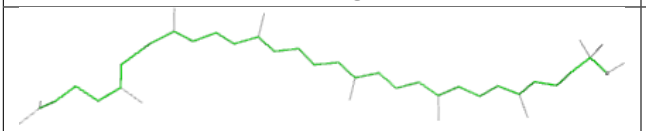
Ligand 7OT AF 103



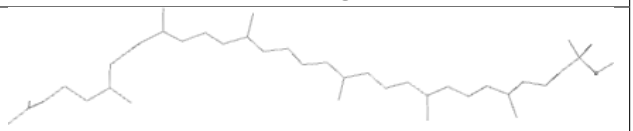
Bond lengths



Bond angles

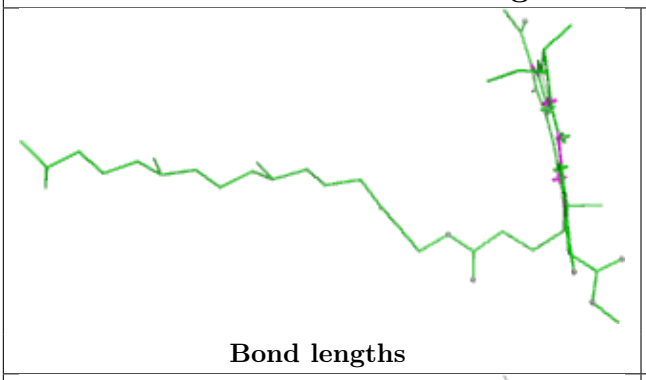


Torsions

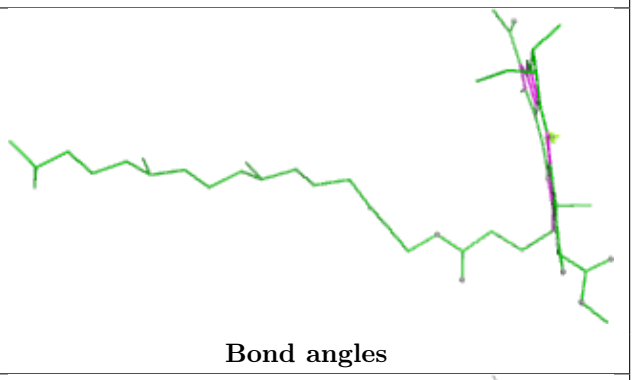


Rings

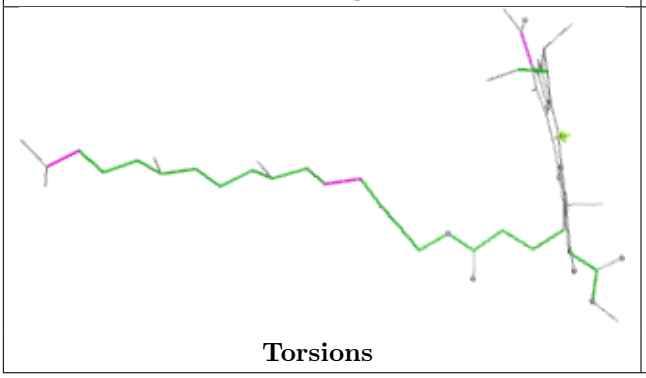
Ligand BCL AA 102



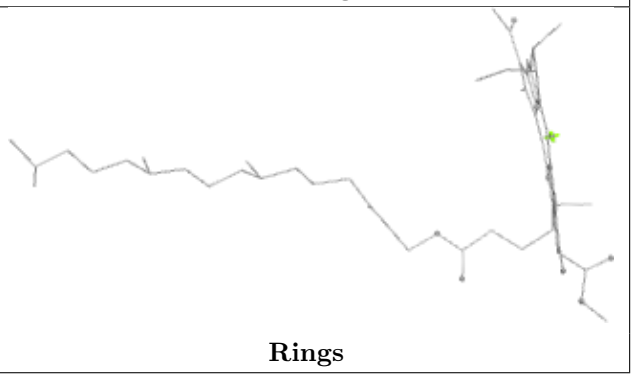
Bond lengths



Bond angles

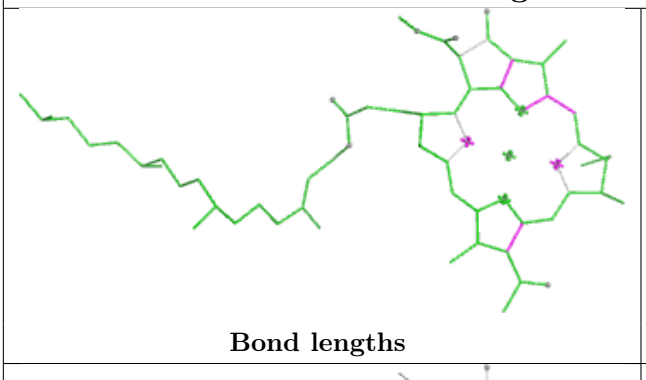


Torsions

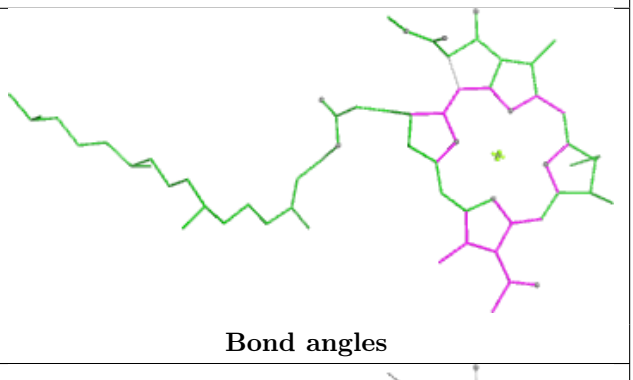


Rings

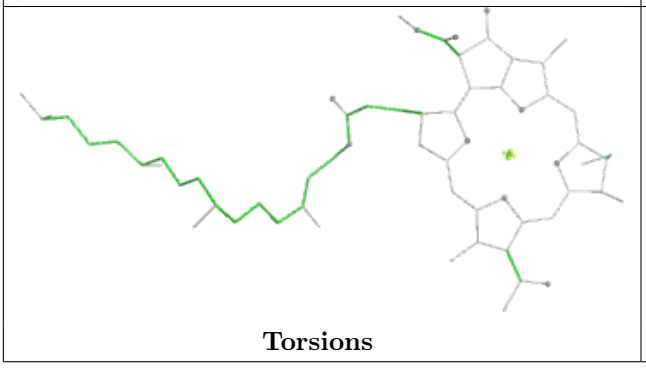
Ligand BCL AD 101



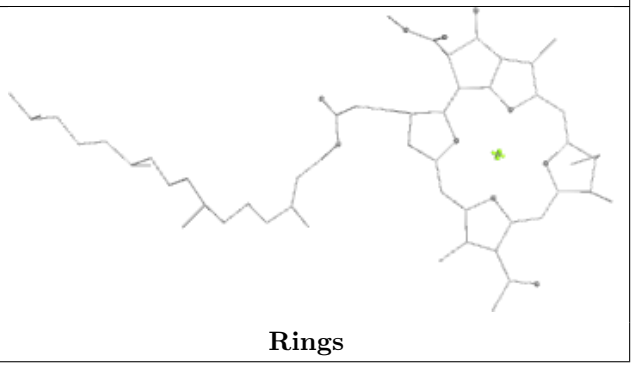
Bond lengths



Bond angles

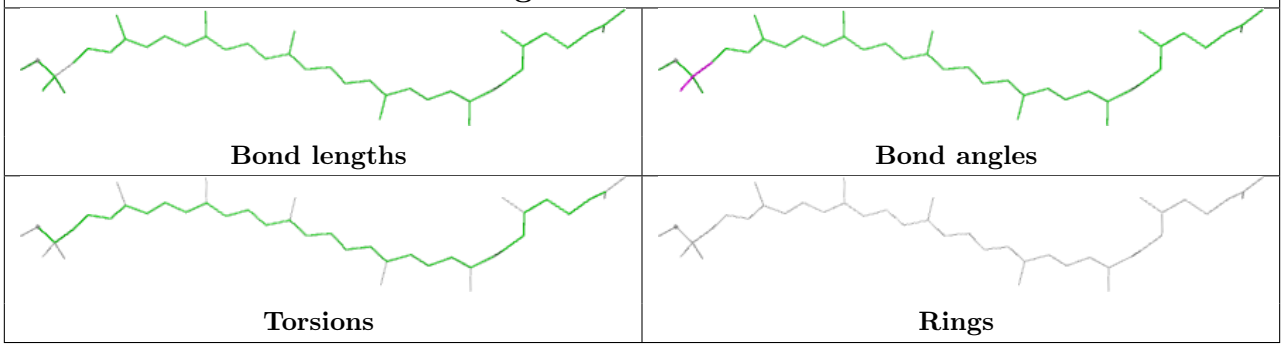


Torsions

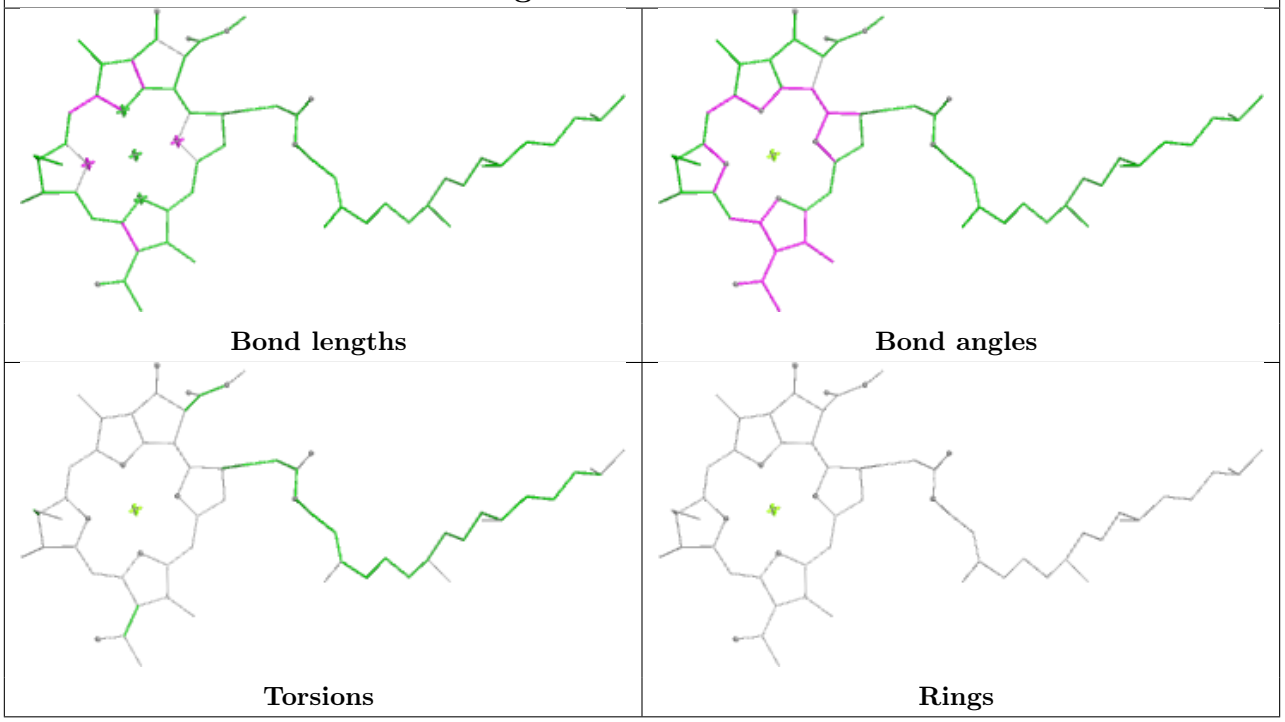


Rings

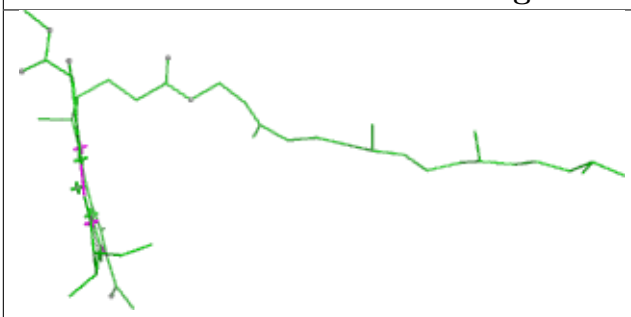
Ligand 7OT AC 103



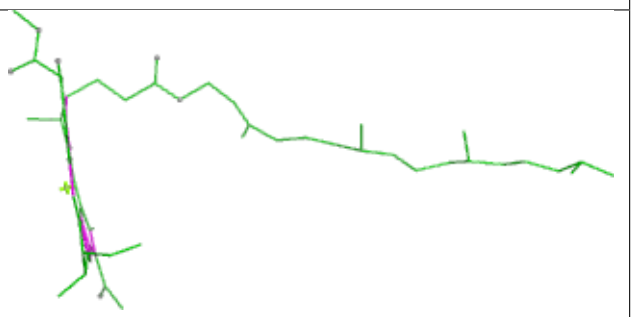
Ligand BCL AF 101



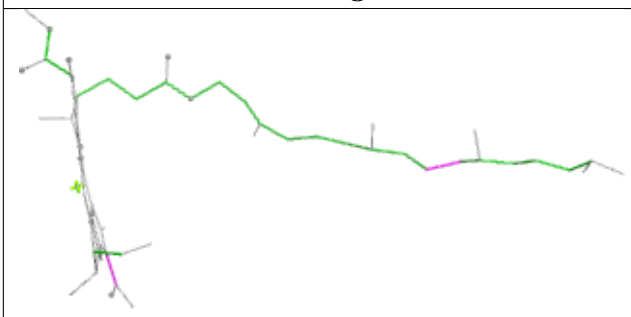
Ligand BCL AF 102



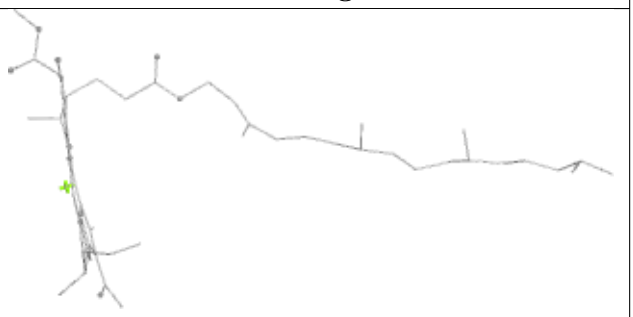
Bond lengths



Bond angles

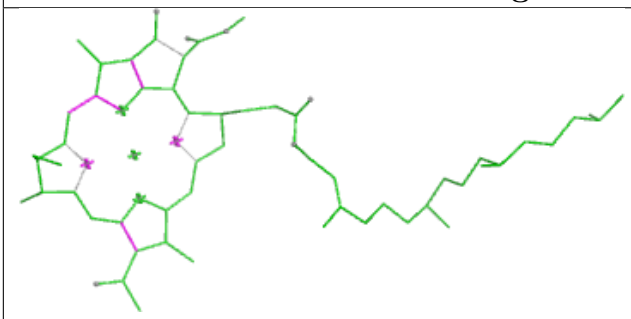


Torsions

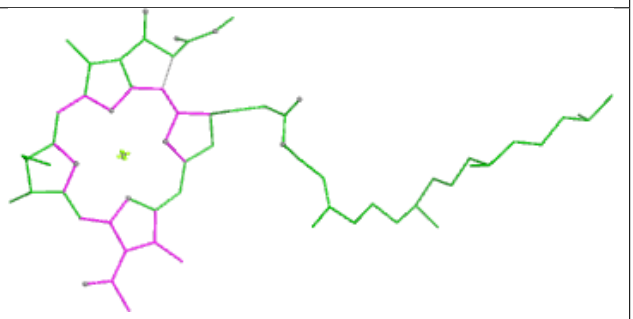


Rings

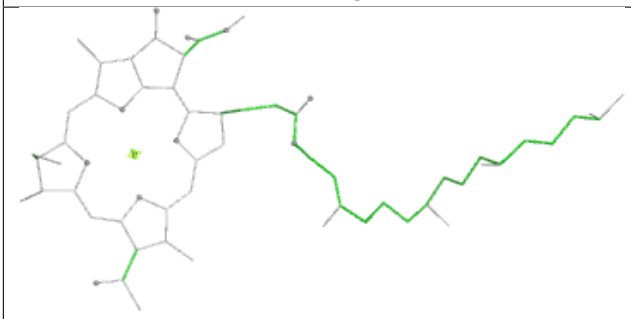
Ligand BCL AB 101



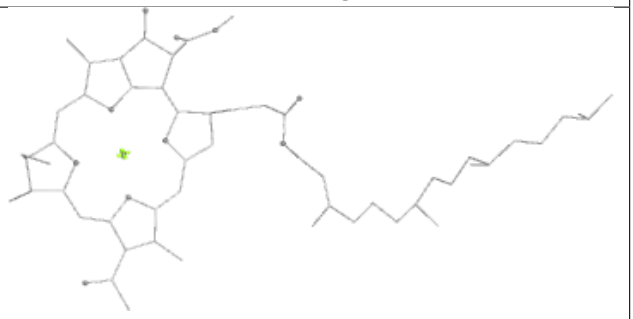
Bond lengths



Bond angles

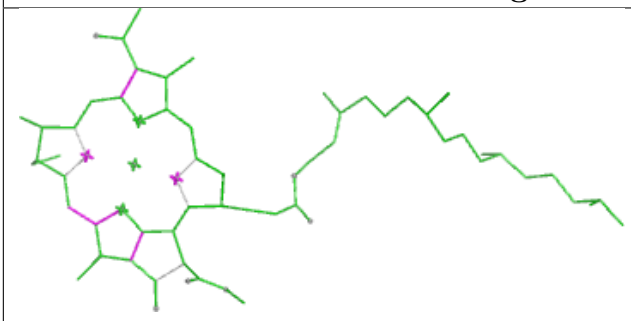


Torsions

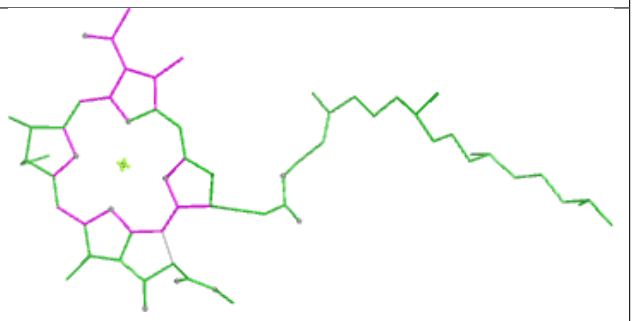


Rings

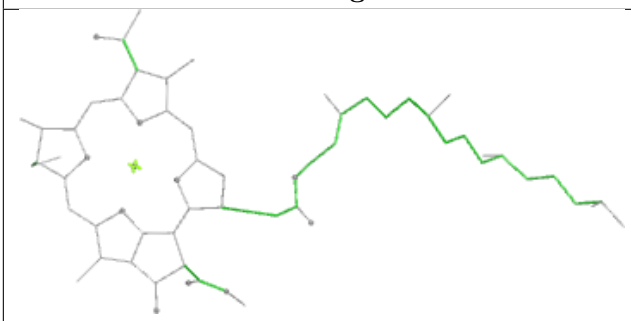
Ligand BCL AH 101



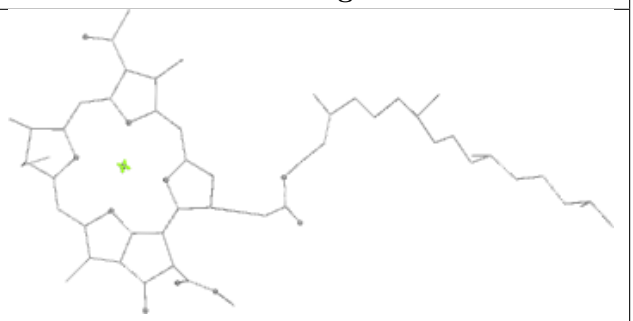
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

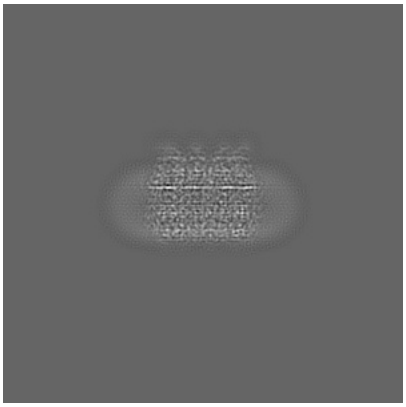
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13307. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

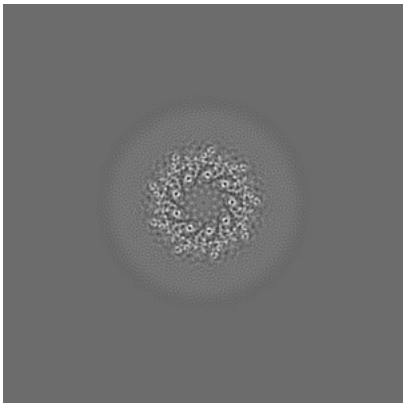
6.1.1 Primary map



X



Y

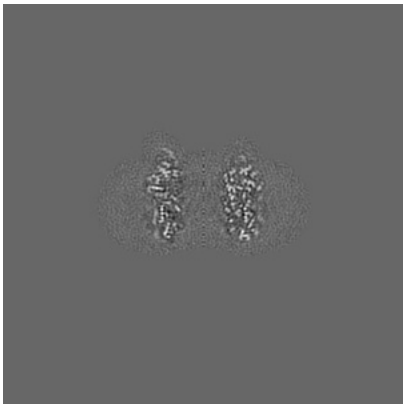


Z

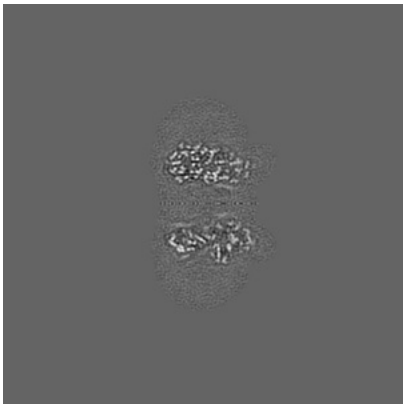
The images above show the map projected in three orthogonal directions.

6.2 Central slices

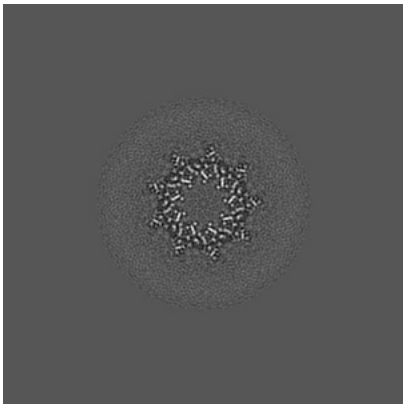
6.2.1 Primary map



X Index: 190



Y Index: 190

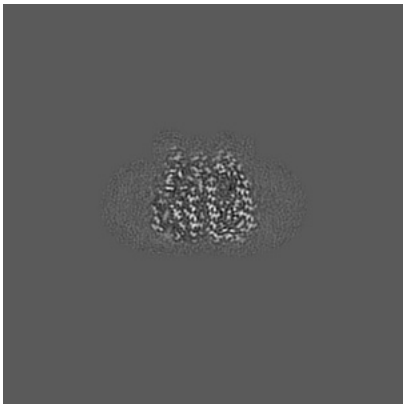


Z Index: 190

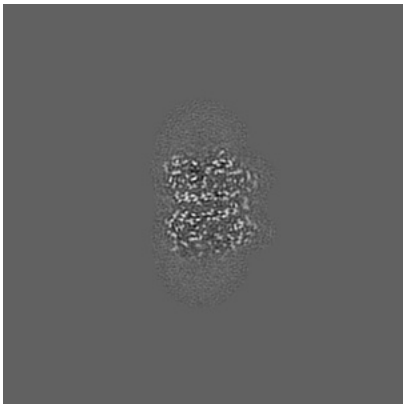
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

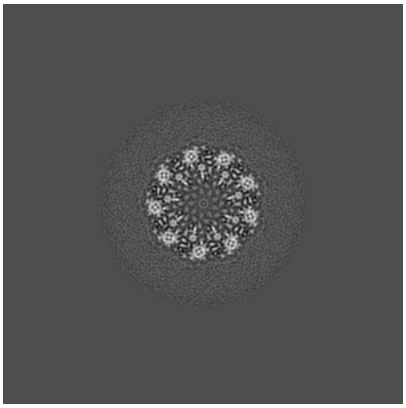
6.3.1 Primary map



X Index: 162



Y Index: 165

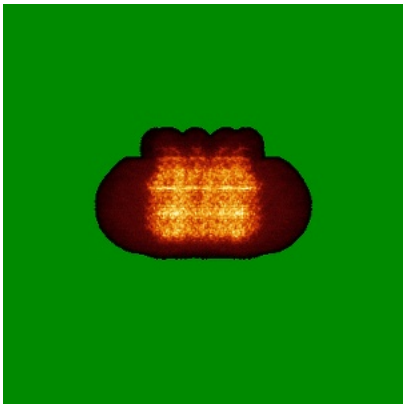


Z Index: 205

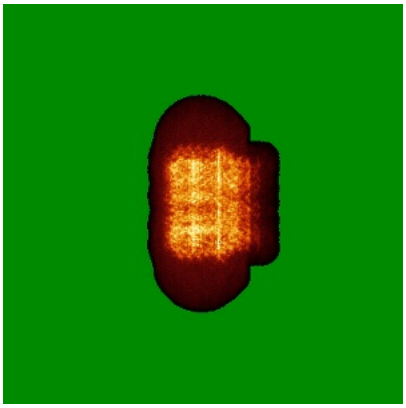
The images above show the largest variance slices of the map in three orthogonal directions.

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

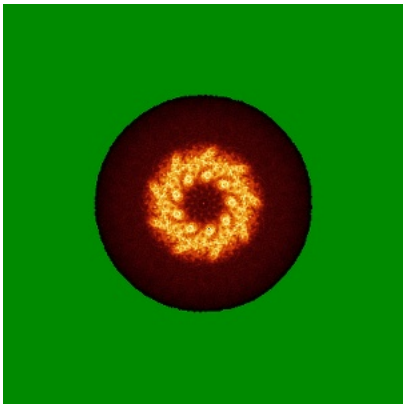
6.4.1 Primary map



X



Y

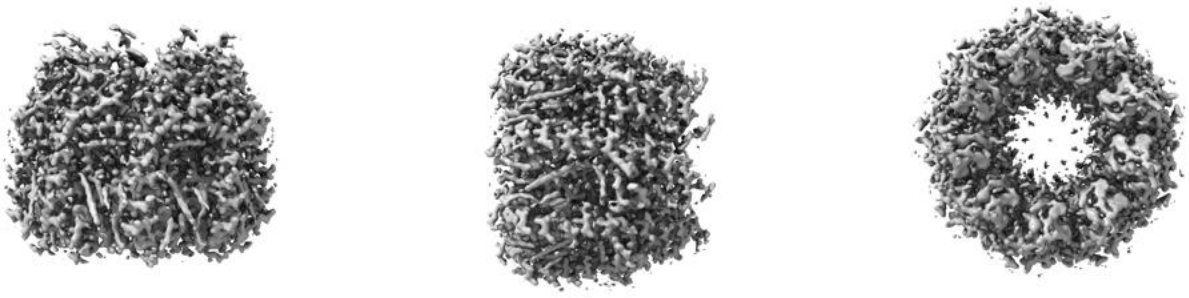


Z

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 0.0305. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

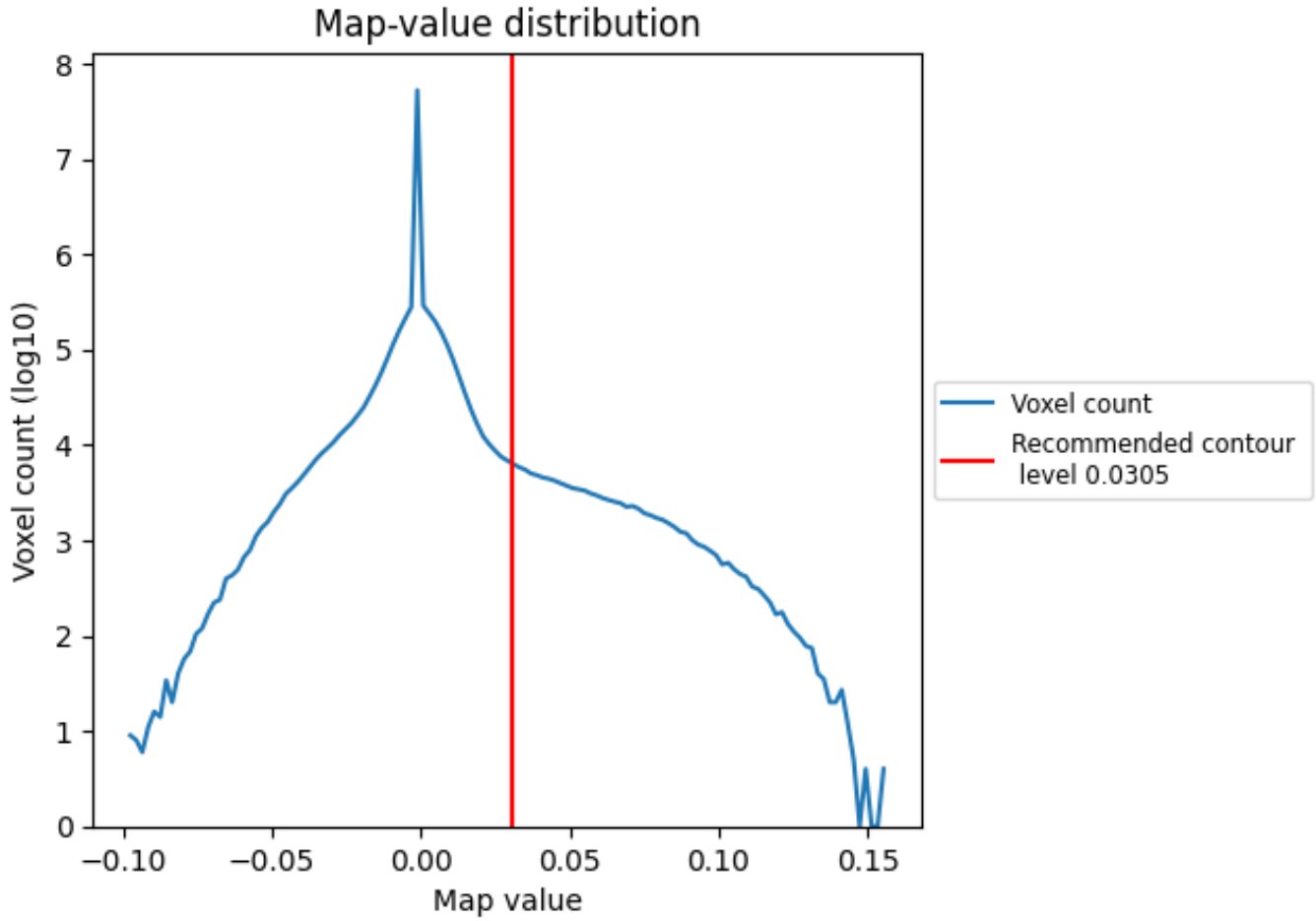
6.6 Mask visualisation (i)

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

7 Map analysis

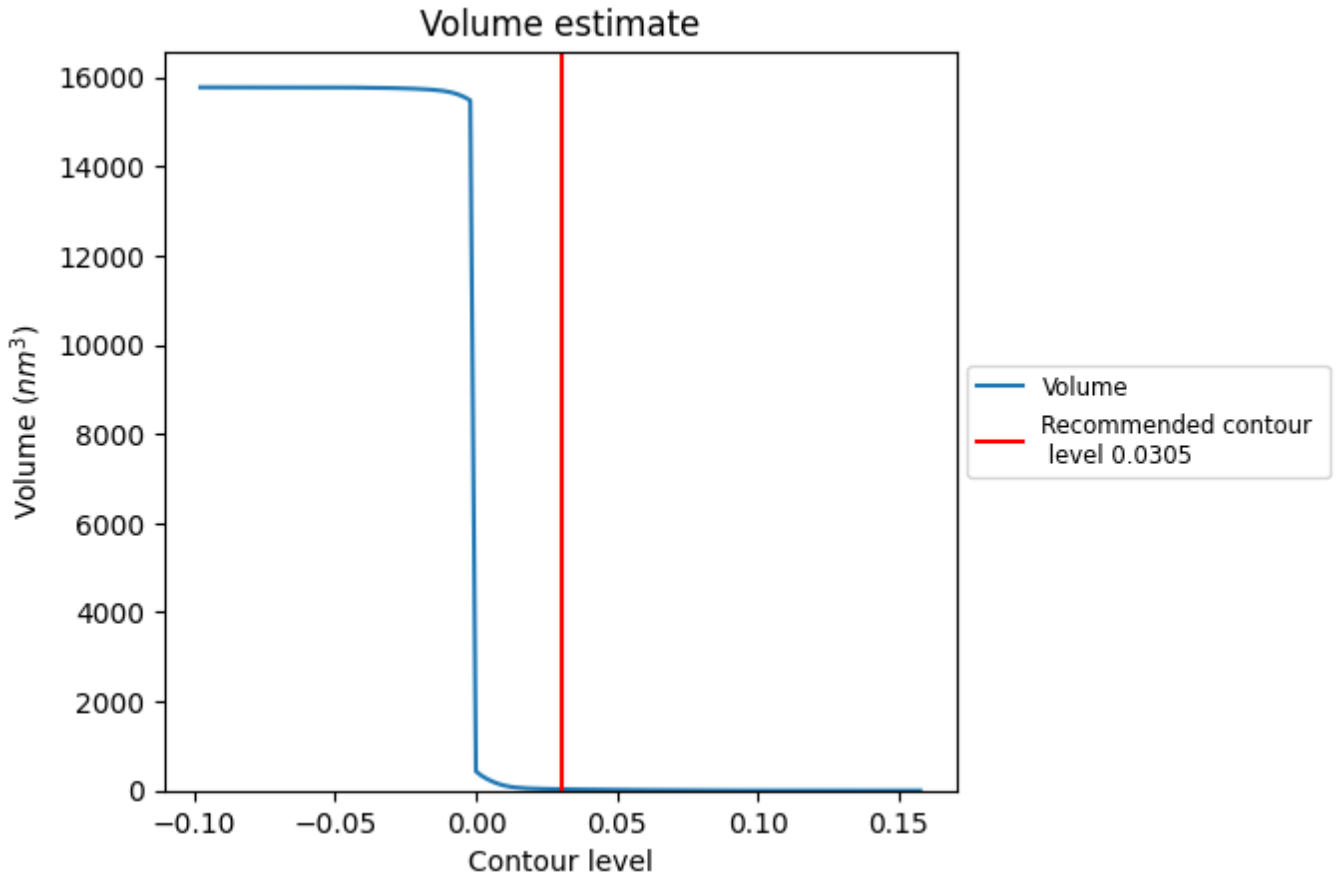
This section contains the results of statistical analysis of the map.

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.

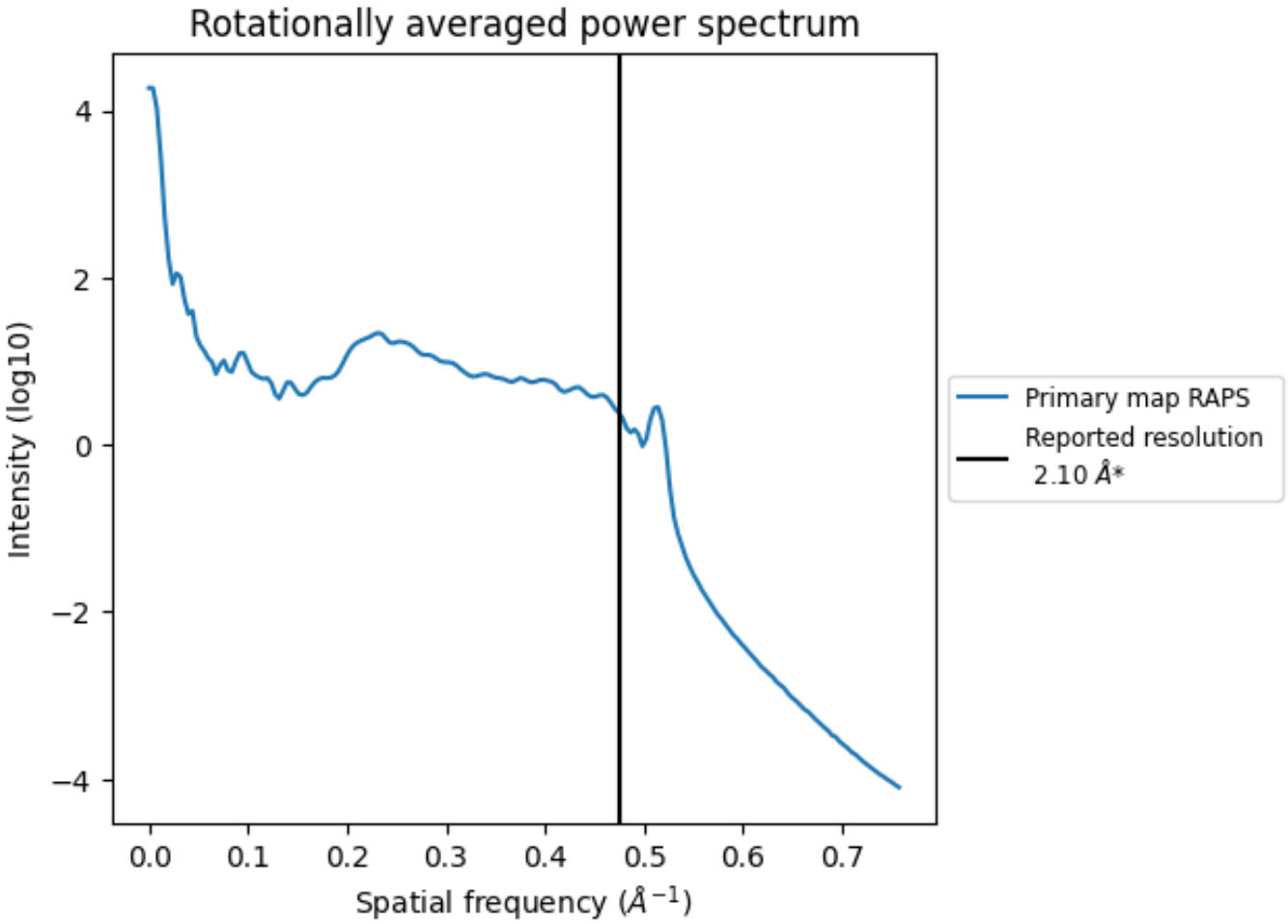
7.2 Volume estimate (i)



The volume at the recommended contour level is 30 nm^3; this corresponds to an approximate mass of 27 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)

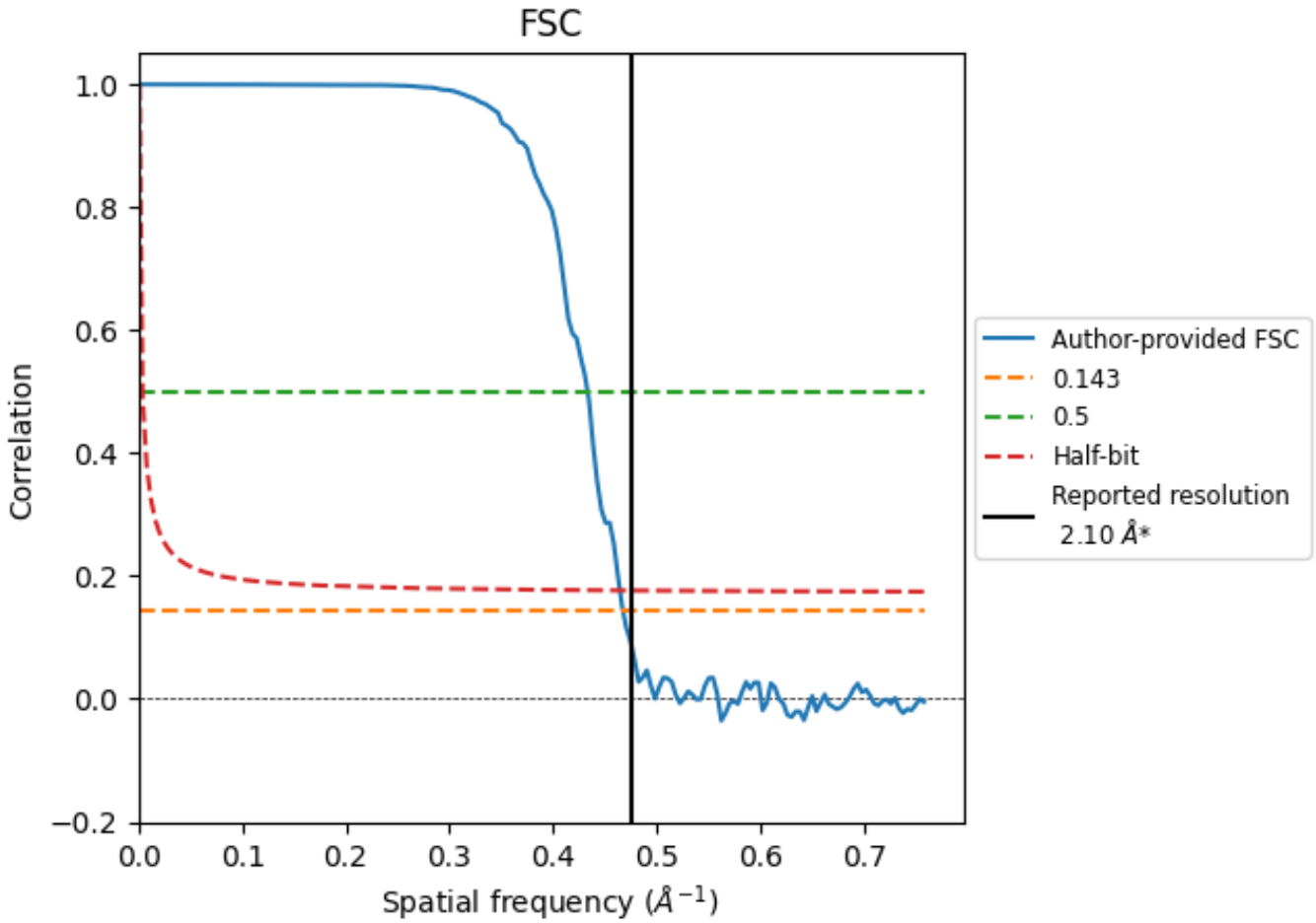


*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

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 0.476 Å^{-1}

8.2 Resolution estimates (i)

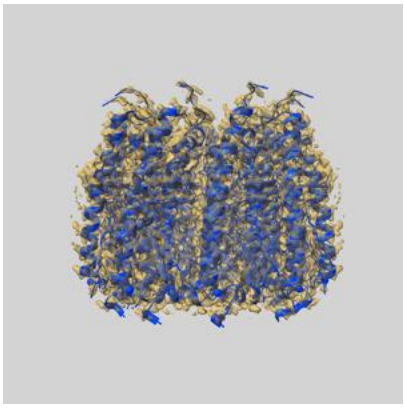
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.14	2.31	2.15
Unmasked-calculated*	-	-	-

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

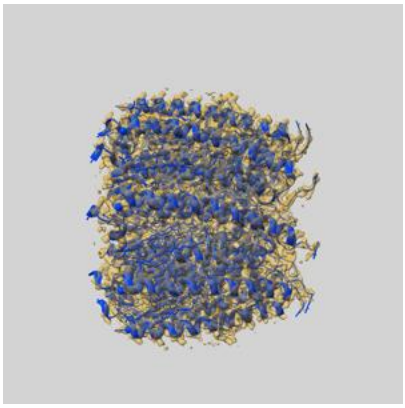
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13307 and PDB model 7PBW. Per-residue inclusion information can be found in section 3 on page 12.

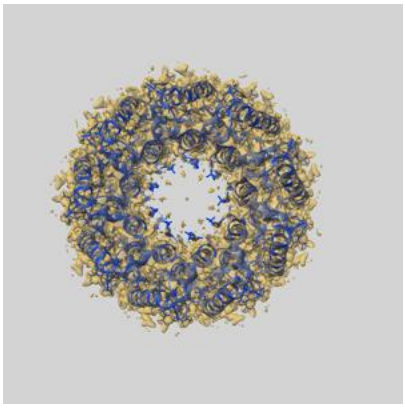
9.1 Map-model overlay



X



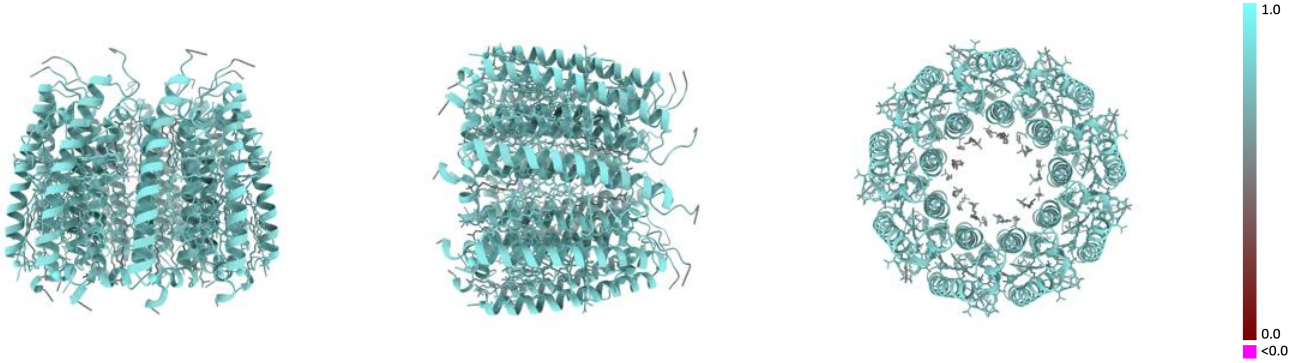
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0305 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.

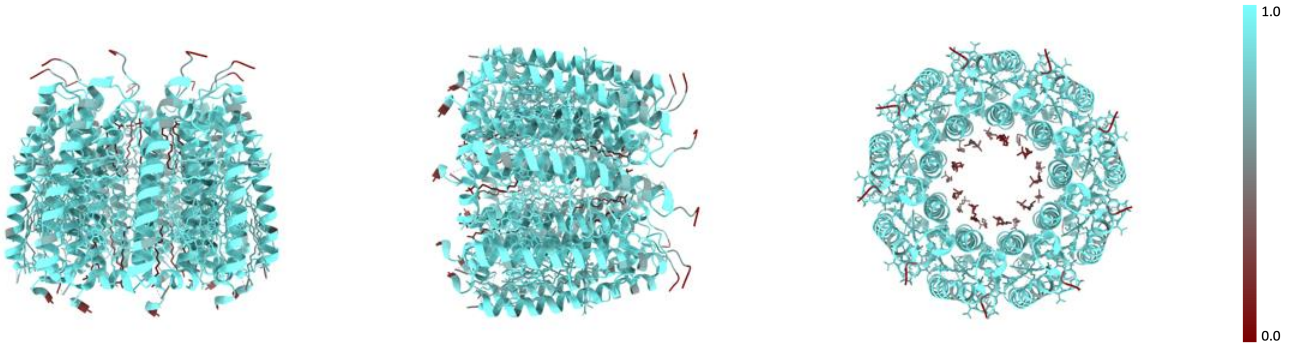
9.2 Q-score mapped to coordinate model



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.

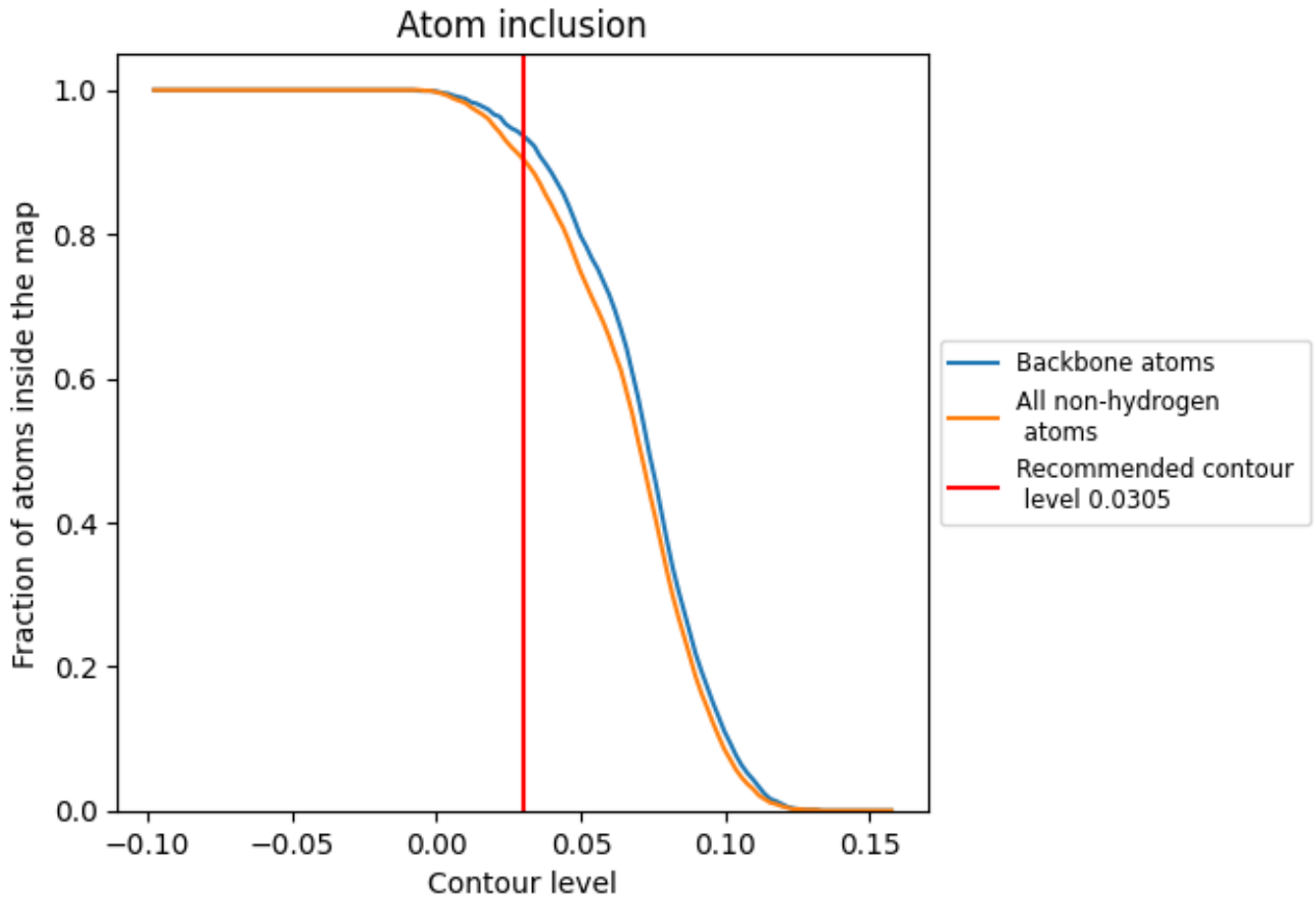
9.3 Atom inclusion mapped to coordinate model



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 (0.0305).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.0305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.7600
AA	0.8970	0.7600
AB	0.9120	0.7630
AC	0.9150	0.7650
AD	0.9120	0.7640
AE	0.9170	0.7690
AF	0.9130	0.7700
AG	0.9080	0.7660
AH	0.9170	0.7690
AI	0.9380	0.7750
BA	0.8760	0.7480
BB	0.8760	0.7500
BC	0.8810	0.7490
BD	0.8850	0.7560
BE	0.8870	0.7490
BF	0.8850	0.7520
BG	0.8870	0.7510
BH	0.8920	0.7480
BI	0.8780	0.7510

