wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 03:36 am BST

PDB ID	:	8ABI / pdb_00008abi
EMDB ID	:	EMD-15322
Title	:	Complex III2 from Yarrowia lipolytica,antimycin A bound, int-position
Authors	:	Wieferig, J.P.; Kuhlbrandt, W.
Deposited on	:	2022-07-04
Resolution	:	3.00 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:

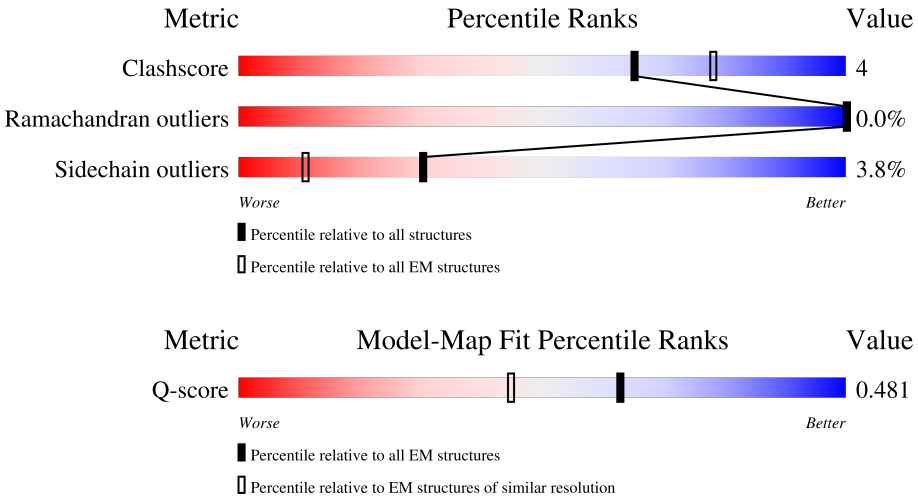
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	C	385	88% 10%
1	N	385	89% 10%
2	E	225	21% 6% 73%
2	P	225	14% 59% 22% 17%

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Mol	Chain	Length	Quality of chain
3	G	128	81% 13%
3	R	128	87% 9%
4	F	137	18% 49% 48%
4	Q	137	15% 47% 48%
5	A	474	5% 83% 8% 8%
5	L	474	84% 7% 8%
6	B	417	5% 84% 12%
6	M	417	5% 82% 14%
7	D	330	66% 8% 26%
7	O	330	66% 8% 26%
8	H	93	81% 10% 9%
8	S	93	81% 10% 9%
9	I	69	71% 7% 22%
9	T	69	68% 10% 22%
10	J	82	83% 9% 9%
10	U	82	77% 15% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	HEC	D	401	X	-	-	-
19	HEC	O	401	X	-	-	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 32548 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	383	Total	C	N	O	S	0	0
			3052	2064	474	496	18		
1	N	383	Total	C	N	O	S	0	0
			3052	2064	474	496	18		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	186	Total	C	N	O	S	0	0
			1445	920	248	268	9		
2	E	61	Total	C	N	O	S	0	0
			465	297	76	89	3		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	124	Total	C	N	O	S	0	0
			994	640	162	190	2		
3	R	124	Total	C	N	O	S	0	0
			994	640	162	190	2		

- Molecule 4 is a protein called YALI0F24673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	71	Total	C	N	O	S	0	0
			579	361	99	115	4		
4	Q	71	Total	C	N	O	S	0	0
			579	361	99	115	4		

- Molecule 5 is a protein called YALI0A14806p.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	438	Total	C	N	O	S	0	0
			3446	2154	603	682	7		
5	L	438	Total	C	N	O	S	0	0
			3446	2154	603	682	7		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	402	Total	C	N	O	S	0	0
			3008	1907	516	583	2		
6	M	402	Total	C	N	O	S	0	0
			3008	1907	516	583	2		

- Molecule 7 is a protein called YALI0A17468p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	244	Total	C	N	O	S	0	0
			1893	1210	323	352	8		
7	O	244	Total	C	N	O	S	0	0
			1893	1210	323	352	8		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	85	Total	C	N	O	S	0	0
			690	459	118	111	2		
8	S	85	Total	C	N	O	S	0	0
			690	459	118	111	2		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	54	Total	C	N	O	S	0	0
			452	297	76	78	1		
9	T	54	Total	C	N	O	S	0	0
			452	297	76	78	1		

- Molecule 10 is a protein called YALI0C12210p.

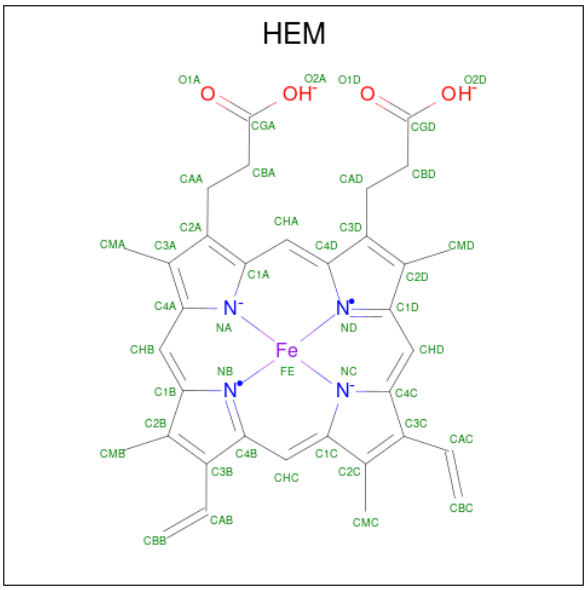
Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	75	Total	C	N	O	0	0
			598	403	99	96		

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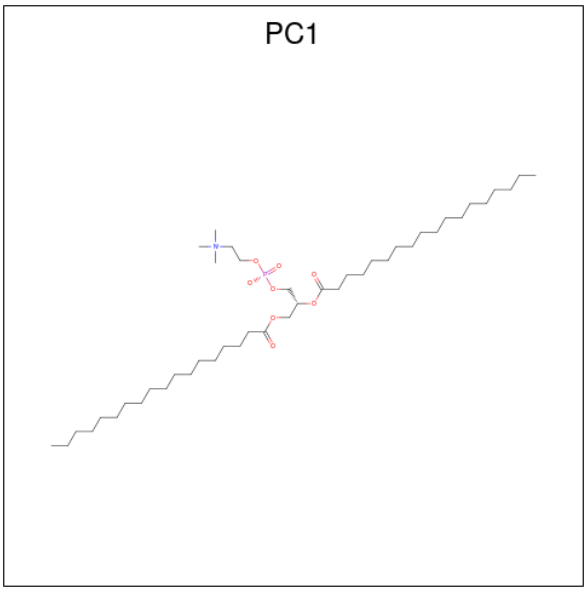
Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	75	Total	C	N	O	0	0
			598	403	99	96		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



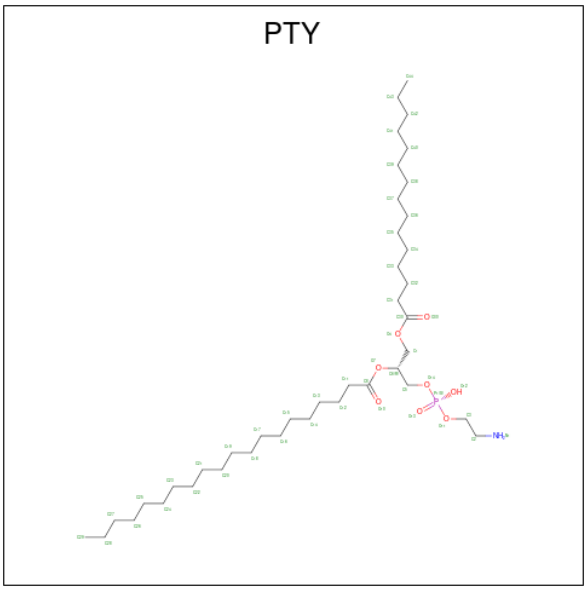
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



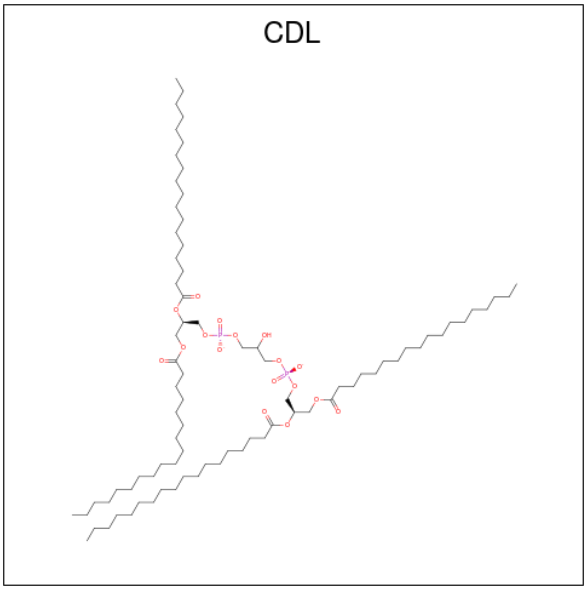
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
12	T	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 13 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	P	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	N	1	Total	C	N	O	P	0
			41	31	1	8	1	
13	E	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



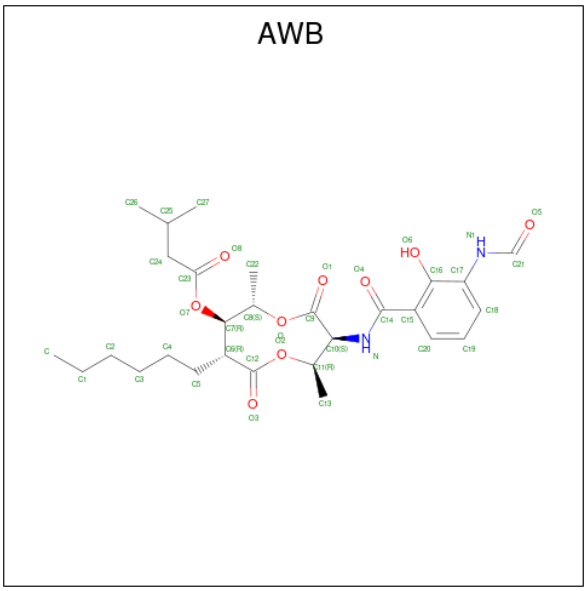
Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	O	P	0
			48	29	17	2	
14	C	1	Total	C	O	P	0
			39	20	17	2	
14	C	1	Total	C	O	P	0
			48	29	17	2	
14	A	1	Total	C	O	P	0
			42	25	15	2	
14	A	1	Total	C	O	P	0
			47	30	15	2	
14	H	1	Total	C	O	P	0
			50	31	17	2	
14	N	1	Total	C	O	P	0
			50	31	17	2	
14	N	1	Total	C	O	P	0
			39	20	17	2	

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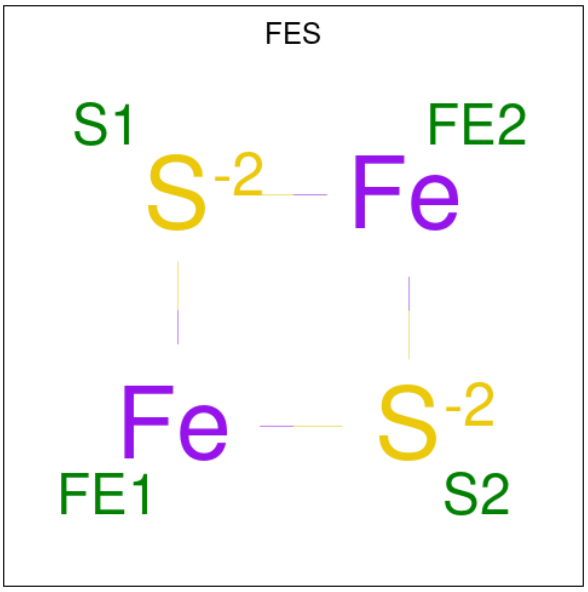
Mol	Chain	Residues	Atoms				AltConf
14	L	1	Total	C	O	P	0
			42	25	15	2	
14	L	1	Total	C	O	P	0
			47	30	15	2	

- Molecule 15 is [(2R,3S,6S,7R,8R)-3-[(3-formamido-2-oxidanyl-phenyl)carbonylamino]-8-hexyl-2,6-dimethyl-4,9-bis(oxidanylidene)-1,5-dioxonan-7-yl] 3-methylbutanoate (CCD ID: AWB) (formula: $C_{28}H_{40}N_2O_9$).



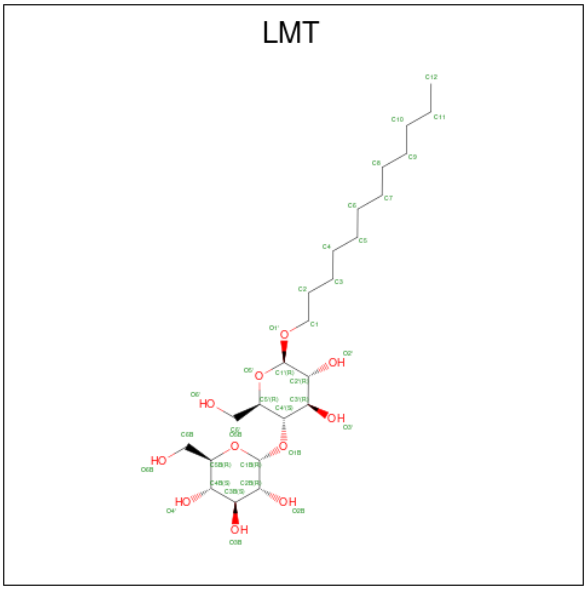
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	N	O	0
			39	28	2	9	
15	N	1	Total	C	N	O	0
			39	28	2	9	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	P	1	Total	Fe	S	0
			4	2	2	

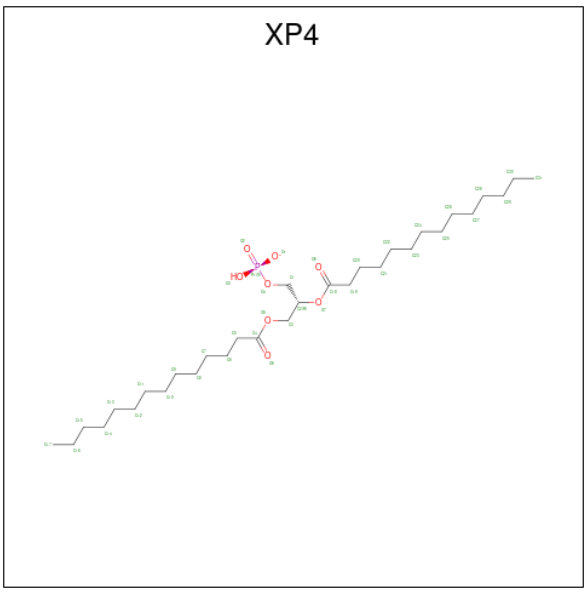
- Molecule 17 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
17	P	1	Total	C	O	0
			35	24	11	
17	J	1	Total	C	O	0
			35	24	11	

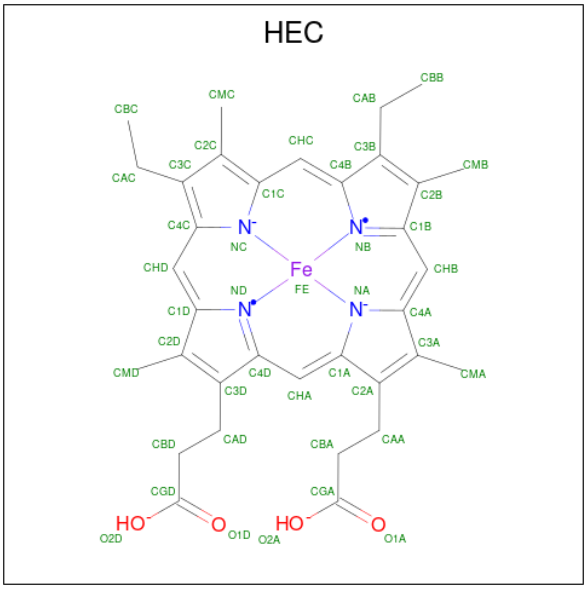
- Molecule 18 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: XP4)

(formula: $C_{31}H_{60}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			24	15	8	1	
18	L	1	Total	C	O	P	0
			24	15	8	1	

- Molecule 19 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



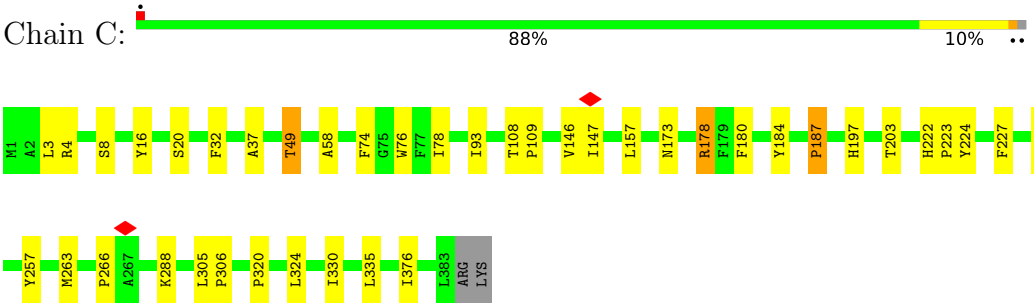
Mol	Chain	Residues	Atoms					AltConf
19	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
19	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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.

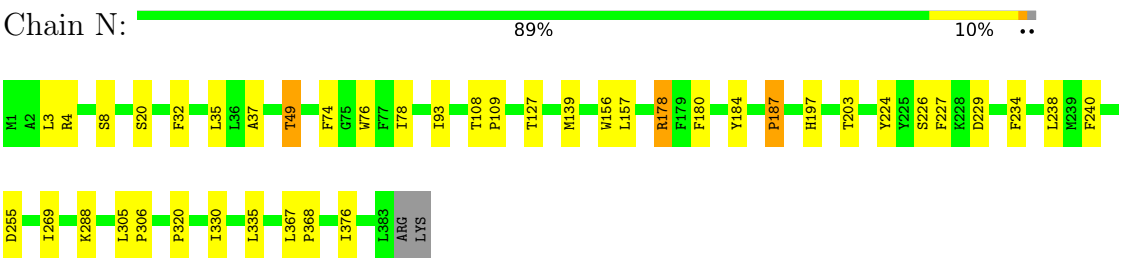
• Molecule 1: Cytochrome b

Chain C:



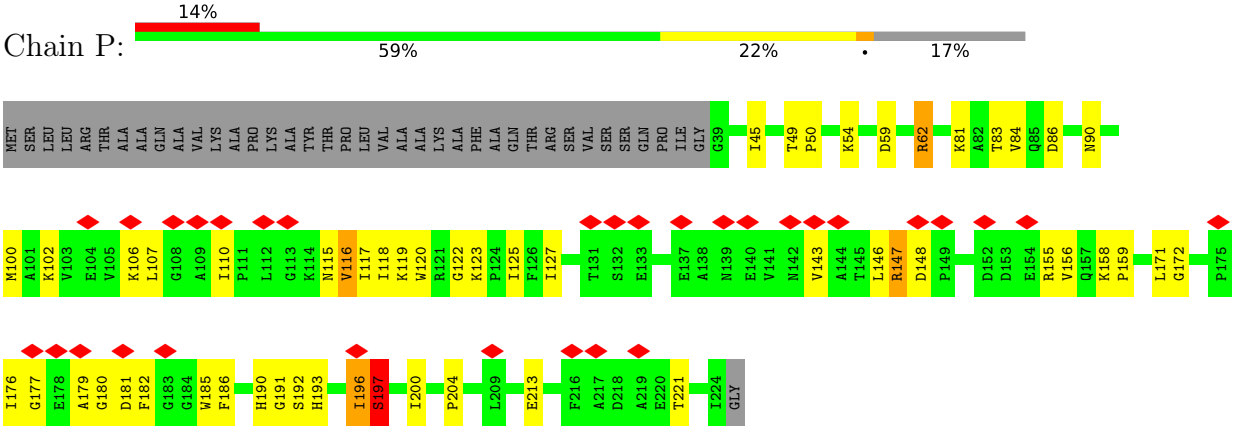
• Molecule 1: Cytochrome b

Chain N:



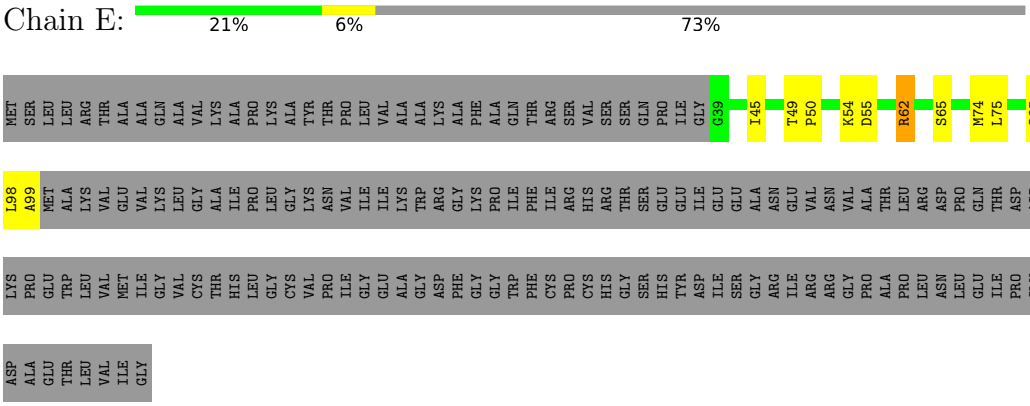
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



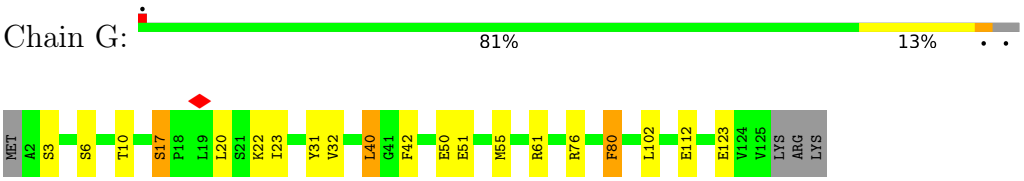
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



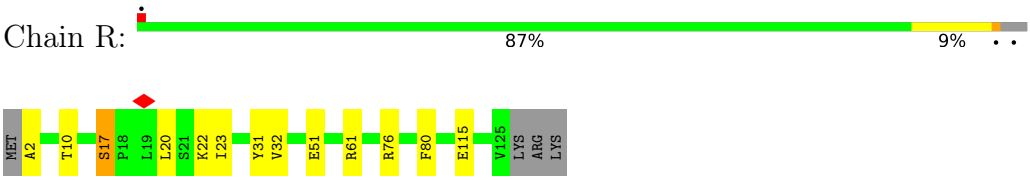
• Molecule 3: Cytochrome b-c1 complex subunit 7

Chain G:



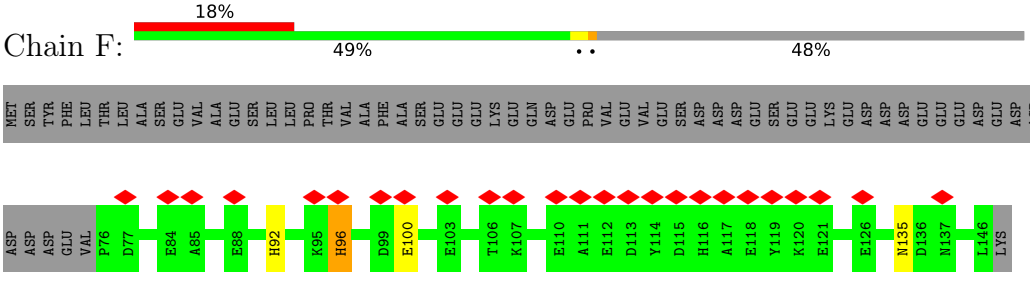
• Molecule 3: Cytochrome b-c1 complex subunit 7

Chain R:



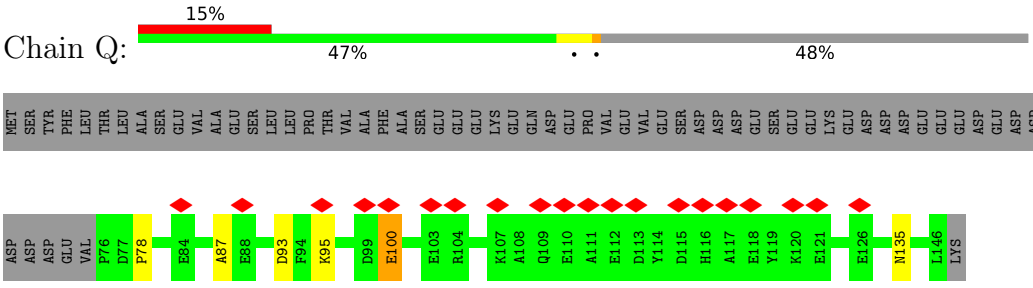
• Molecule 4: YALI0F24673p

Chain F:



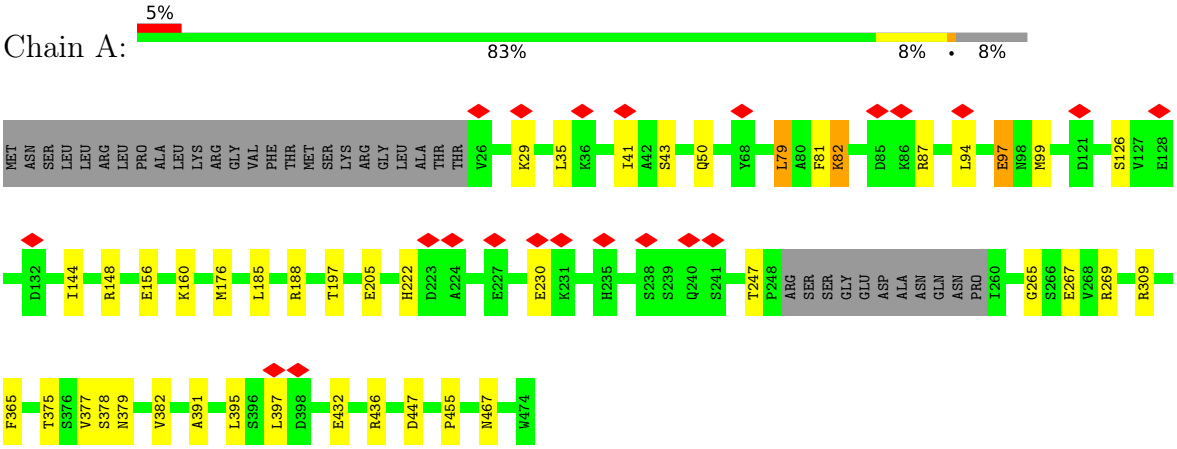
• Molecule 4: YALI0F24673p

Chain Q:



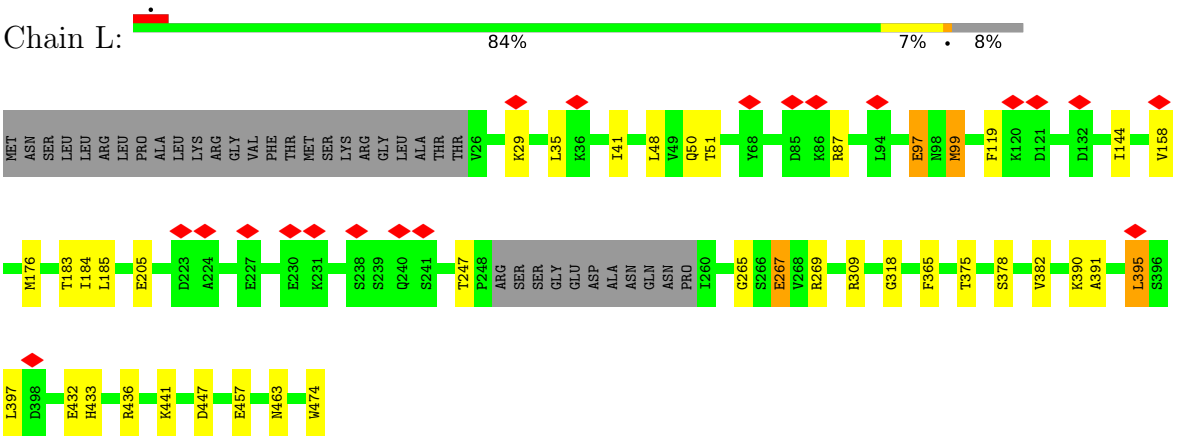
• Molecule 5: YALI0A14806p

Chain A:



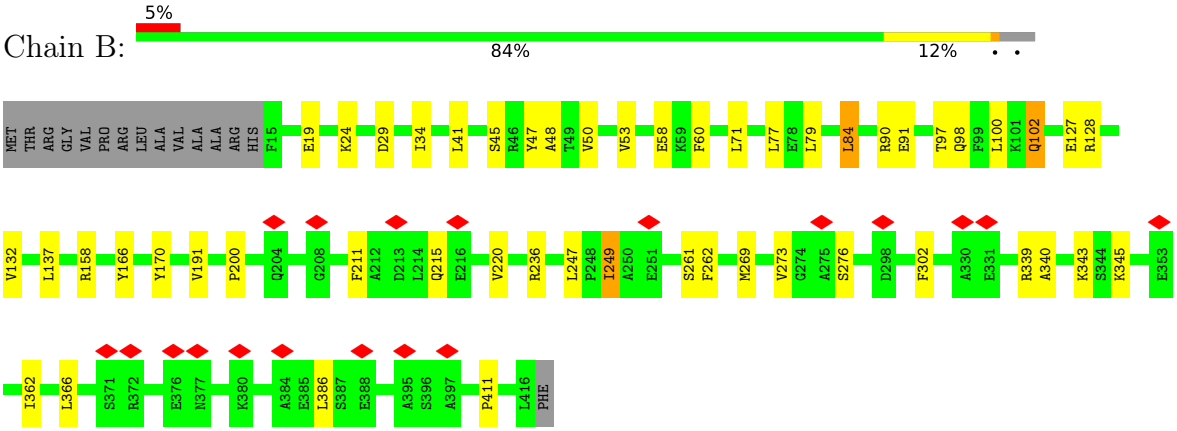
• Molecule 5: YALI0A14806p

Chain L:



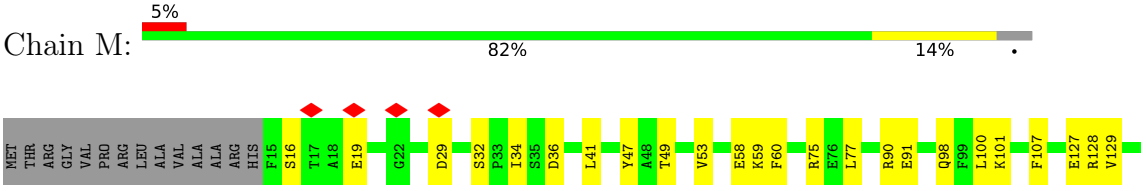
• Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

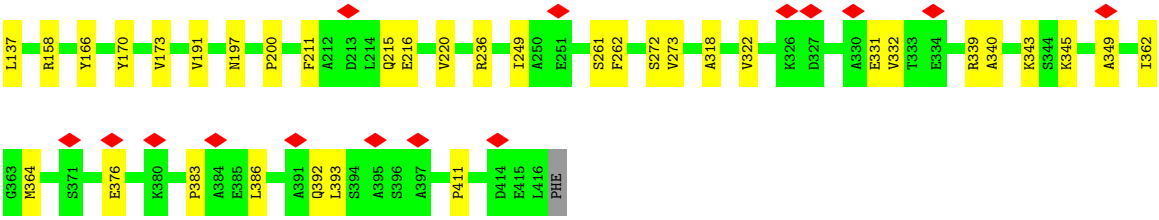
Chain B:



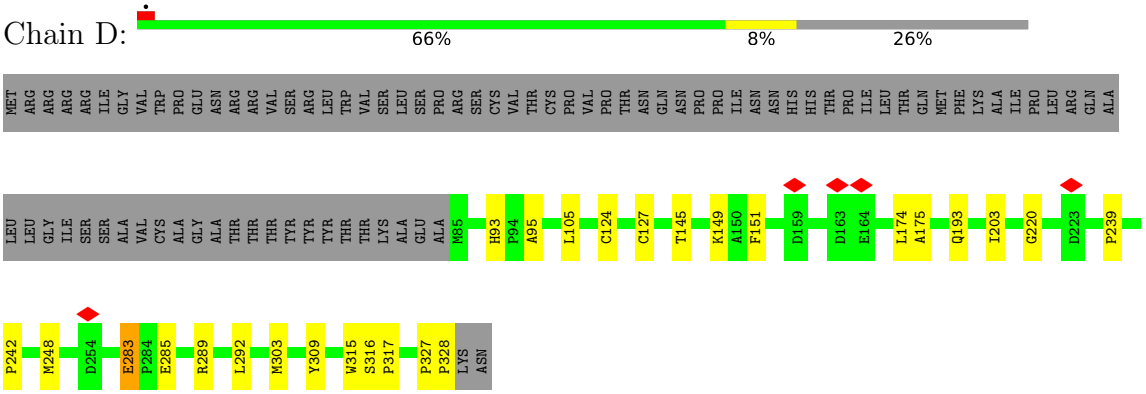
• Molecule 6: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:

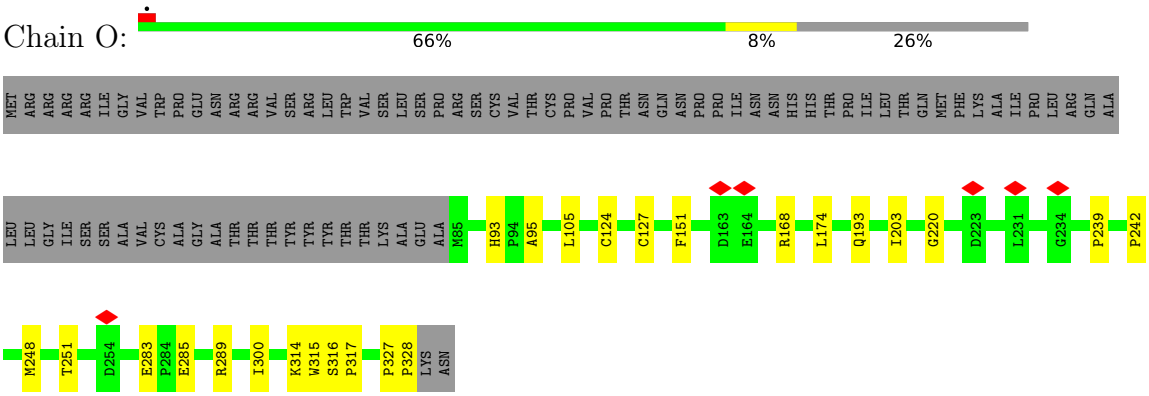




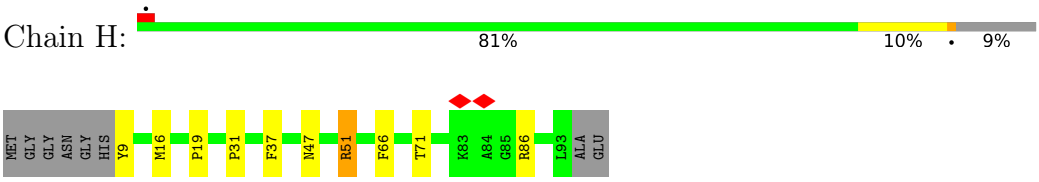
• Molecule 7: YALI0A17468p



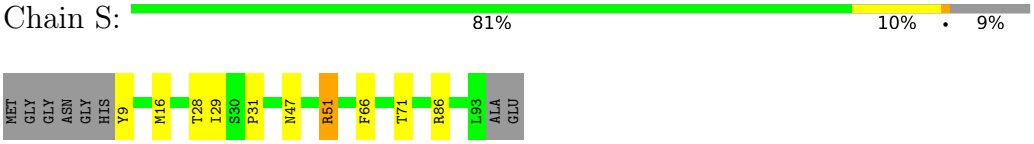
• Molecule 7: YALI0A17468p



• Molecule 8: Cytochrome b-c1 complex subunit 8

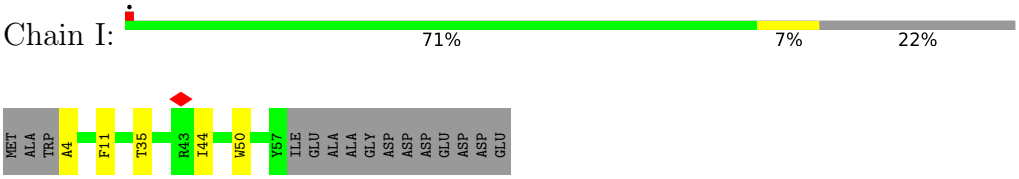


• Molecule 8: Cytochrome b-c1 complex subunit 8



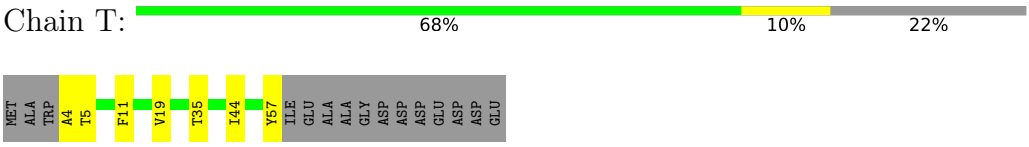
• Molecule 9: Complex III subunit 9

Chain I:



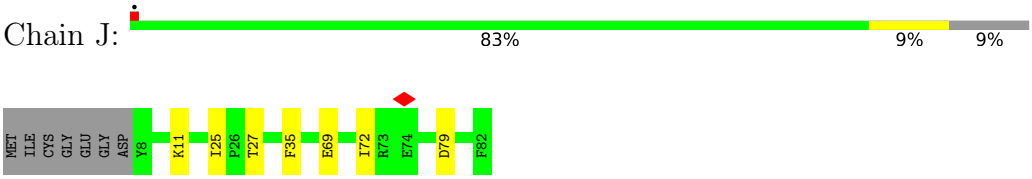
• Molecule 9: Complex III subunit 9

Chain T:



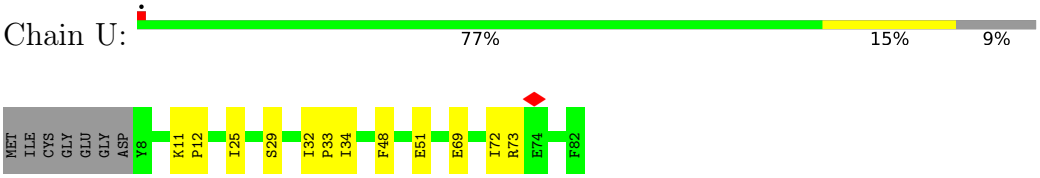
• Molecule 10: YALI0C12210p

Chain J:



• Molecule 10: YALI0C12210p

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	299.16, 299.16, 299.16	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83100003, 0.83100003, 0.83100003	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XP4, HEM, FES, LMT, AWB, CDL, PC1, PTY, HEC

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	C	0.75	0/3153	1.18	13/4305 (0.3%)
1	N	0.75	0/3153	1.17	8/4305 (0.2%)
2	E	0.69	0/474	1.18	2/637 (0.3%)
2	P	0.56	0/1479	1.19	6/2003 (0.3%)
3	G	0.64	0/1012	1.13	2/1373 (0.1%)
3	R	0.63	1/1012 (0.1%)	1.13	0/1373
4	F	0.52	0/595	1.17	1/805 (0.1%)
4	Q	0.52	0/595	1.23	3/805 (0.4%)
5	A	0.63	0/3510	1.17	7/4768 (0.1%)
5	L	0.63	0/3510	1.18	9/4768 (0.2%)
6	B	0.59	0/3069	1.17	8/4178 (0.2%)
6	M	0.59	0/3069	1.17	10/4178 (0.2%)
7	D	0.64	0/1950	1.16	5/2656 (0.2%)
7	O	0.64	0/1950	1.14	5/2656 (0.2%)
8	H	0.64	1/717 (0.1%)	1.14	3/975 (0.3%)
8	S	0.64	1/717 (0.1%)	1.13	2/975 (0.2%)
9	I	0.68	1/465 (0.2%)	1.17	3/629 (0.5%)
9	T	0.70	1/465 (0.2%)	1.19	4/629 (0.6%)
10	J	0.59	0/620	1.14	1/846 (0.1%)
10	U	0.60	0/620	1.12	0/846
All	All	0.65	5/32135 (0.0%)	1.17	92/43710 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	4	ALA	N-CA	7.83	1.61	1.46
9	I	4	ALA	N-CA	7.51	1.60	1.46
8	H	9	TYR	N-CA	5.95	1.57	1.46
8	S	9	TYR	N-CA	5.70	1.57	1.46
3	R	2	ALA	N-CA	5.25	1.56	1.46

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	90	ARG	CG-CD-NE	-8.27	93.81	112.00
7	O	283	GLU	CB-CA-C	-8.18	98.38	111.14
6	B	215	GLN	CB-CA-C	-8.03	95.44	109.64
6	B	90	ARG	CG-CD-NE	-7.93	94.55	112.00
6	M	215	GLN	CB-CA-C	-7.90	95.65	109.64

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	C	3052	0	3113	33	0
1	N	3052	0	3113	31	0
2	E	465	0	459	7	0
2	P	1445	0	1426	33	0
3	G	994	0	1022	8	0
3	R	994	0	1022	7	0
4	F	579	0	511	1	0
4	Q	579	0	511	2	0
5	A	3446	0	3369	24	0
5	L	3446	0	3369	19	0
6	B	3008	0	2991	25	0
6	M	3008	0	2991	26	0
7	D	1893	0	1834	27	0
7	O	1893	0	1834	23	0
8	H	690	0	673	6	0
8	S	690	0	673	8	0
9	I	452	0	435	2	0
9	T	452	0	435	3	0
10	J	598	0	615	3	0
10	U	598	0	615	7	0
11	C	86	0	60	9	0
11	N	86	0	60	8	0
12	C	38	0	50	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	I	32	0	38	0	0
12	N	38	0	50	1	0
12	T	32	0	38	2	0
13	C	41	0	58	3	0
13	E	41	0	58	3	0
13	N	41	0	58	8	0
13	P	41	0	58	10	0
14	A	89	0	85	3	0
14	C	135	0	102	8	0
14	H	50	0	44	2	0
14	L	89	0	85	2	0
14	N	89	0	66	2	0
15	C	39	0	39	1	0
15	N	39	0	39	1	0
16	P	4	0	0	0	0
17	J	35	0	46	1	0
17	P	35	0	46	0	0
18	A	24	0	22	1	0
18	L	24	0	22	0	0
19	D	43	0	32	12	0
19	O	43	0	32	11	0
All	All	32548	0	32199	260	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.

The worst 5 of 260 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)
7:D:124:CYS:SG	19:D:401:HEC:HBB3	1.61	1.40
2:P:84:VAL:CG2	13:P:303:PTY:H441	1.60	1.28
7:O:124:CYS:SG	19:O:401:HEC:HBB3	1.71	1.26
7:D:124:CYS:SG	19:D:401:HEC:CBB	2.34	1.15
7:D:127:CYS:SG	19:D:401:HEC:CAC	2.35	1.15

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	C	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
1	N	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
2	E	59/225 (26%)	58 (98%)	1 (2%)	0	100	100
2	P	184/225 (82%)	171 (93%)	12 (6%)	1 (0%)	24	60
3	G	122/128 (95%)	122 (100%)	0	0	100	100
3	R	122/128 (95%)	122 (100%)	0	0	100	100
4	F	69/137 (50%)	66 (96%)	3 (4%)	0	100	100
4	Q	69/137 (50%)	66 (96%)	3 (4%)	0	100	100
5	A	434/474 (92%)	424 (98%)	10 (2%)	0	100	100
5	L	434/474 (92%)	422 (97%)	12 (3%)	0	100	100
6	B	400/417 (96%)	382 (96%)	18 (4%)	0	100	100
6	M	400/417 (96%)	386 (96%)	14 (4%)	0	100	100
7	D	242/330 (73%)	239 (99%)	3 (1%)	0	100	100
7	O	242/330 (73%)	239 (99%)	3 (1%)	0	100	100
8	H	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
8	S	83/93 (89%)	82 (99%)	1 (1%)	0	100	100
9	I	52/69 (75%)	50 (96%)	2 (4%)	0	100	100
9	T	52/69 (75%)	50 (96%)	2 (4%)	0	100	100
10	J	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
10	U	73/82 (89%)	71 (97%)	2 (3%)	0	100	100
All	All	3955/4680 (84%)	3849 (97%)	105 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	172	GLY

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	C	331/333 (99%)	323 (98%)	8 (2%)	43 73
1	N	331/333 (99%)	325 (98%)	6 (2%)	51 77
2	E	49/182 (27%)	44 (90%)	5 (10%)	7 29
2	P	154/182 (85%)	136 (88%)	18 (12%)	5 23
3	G	113/117 (97%)	103 (91%)	10 (9%)	9 35
3	R	113/117 (97%)	109 (96%)	4 (4%)	32 65
4	F	61/123 (50%)	58 (95%)	3 (5%)	22 56
4	Q	61/123 (50%)	60 (98%)	1 (2%)	55 79
5	A	377/407 (93%)	364 (97%)	13 (3%)	32 66
5	L	377/407 (93%)	362 (96%)	15 (4%)	28 62
6	B	311/322 (97%)	293 (94%)	18 (6%)	18 51
6	M	311/322 (97%)	294 (94%)	17 (6%)	19 53
7	D	192/268 (72%)	190 (99%)	2 (1%)	68 84
7	O	192/268 (72%)	191 (100%)	1 (0%)	81 89
8	H	67/71 (94%)	66 (98%)	1 (2%)	57 80
8	S	67/71 (94%)	66 (98%)	1 (2%)	57 80
9	I	46/57 (81%)	46 (100%)	0	100 100
9	T	46/57 (81%)	46 (100%)	0	100 100
10	J	63/68 (93%)	61 (97%)	2 (3%)	34 67
10	U	63/68 (93%)	61 (97%)	2 (3%)	34 67
All	All	3325/3896 (85%)	3198 (96%)	127 (4%)	30 63

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	77	LEU
6	M	60	PHE
7	D	283	GLU

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Mol	Chain	Res	Type
6	M	58	GLU
6	M	343	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	90	ASN
5	L	159	ASN
3	R	84	HIS
5	L	50	GLN
6	M	63	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

31 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	$\#\|Z\| > 2$
19	HEC	O	401	7	50,50,50	2.57	25 (50%)	68,82,82	2.74	32 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	PTY	E	401	-	40,40,49	0.53	0	43,45,54	0.62	0
14	CDL	H	701	-	49,49,99	0.40	0	55,61,111	0.67	1 (1%)
15	AWB	N	506	-	40,40,40	0.46	0	36,54,54	0.87	0
12	PC1	T	201	-	31,31,53	0.41	0	37,39,61	0.80	1 (2%)
14	CDL	A	3001	-	41,41,99	0.61	0	45,51,111	0.81	1 (2%)
14	CDL	A	3002	-	46,46,99	0.42	0	51,56,111	0.94	3 (5%)
14	CDL	C	508	-	47,47,99	0.58	0	53,59,111	1.01	4 (7%)
15	AWB	C	506	-	40,40,40	0.49	0	36,54,54	0.90	1 (2%)
11	HEM	N	502	1	50,50,50	1.60	11 (22%)	66,82,82	2.49	27 (40%)
13	PTY	P	303	-	40,40,49	0.54	0	43,45,54	0.66	1 (2%)
11	HEM	C	502	1	50,50,50	1.53	8 (16%)	66,82,82	2.58	27 (40%)
12	PC1	I	201	-	31,31,53	0.44	0	37,39,61	0.63	1 (2%)
17	LMT	P	302	-	36,36,36	0.53	0	47,47,47	1.05	5 (10%)
13	PTY	C	504	-	40,40,49	0.39	0	43,45,54	0.64	1 (2%)
18	XP4	A	3003	-	23,23,39	1.51	2 (8%)	27,28,44	2.57	9 (33%)
17	LMT	J	101	-	36,36,36	0.60	0	47,47,47	1.17	4 (8%)
12	PC1	C	503	-	37,37,53	0.82	1 (2%)	43,45,61	1.14	5 (11%)
14	CDL	N	504	-	49,49,99	0.40	0	55,61,111	0.70	0
12	PC1	N	503	-	37,37,53	0.75	1 (2%)	43,45,61	1.02	5 (11%)
14	CDL	N	507	-	38,38,99	0.55	0	44,50,111	1.26	5 (11%)
19	HEC	D	401	7	50,50,50	2.58	24 (48%)	68,82,82	2.77	30 (44%)
13	PTY	N	505	-	40,40,49	0.41	0	43,45,54	0.87	3 (6%)
18	XP4	L	3003	-	23,23,39	1.45	2 (8%)	27,28,44	2.46	8 (29%)
14	CDL	C	505	-	47,47,99	0.56	0	53,59,111	1.10	5 (9%)
14	CDL	L	3001	-	41,41,99	0.51	0	45,51,111	0.84	1 (2%)
11	HEM	N	501	1	50,50,50	1.67	11 (22%)	66,82,82	2.30	28 (42%)
16	FES	P	301	2	0,4,4	-	-	-		
14	CDL	C	507	-	38,38,99	0.48	0	44,50,111	1.21	4 (9%)
14	CDL	L	3002	-	46,46,99	0.40	0	51,56,111	0.81	3 (5%)
11	HEM	C	501	1	50,50,50	1.64	10 (20%)	66,82,82	2.29	30 (45%)

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
19	HEC	O	401	7	1/1/3/7	8/14/54/54	-
13	PTY	E	401	-	-	26/44/44/53	-
14	CDL	H	701	-	-	34/59/59/110	-
15	AWB	N	506	-	-	12/38/53/53	0/1/2/2
12	PC1	T	201	-	-	12/35/35/57	-
14	CDL	A	3002	-	-	30/54/54/110	-
14	CDL	A	3001	-	-	17/48/48/110	-
14	CDL	C	508	-	-	28/57/57/110	-
15	AWB	C	506	-	-	9/38/53/53	0/1/2/2
11	HEM	N	502	1	-	4/14/54/54	-
13	PTY	P	303	-	-	24/44/44/53	-
11	HEM	C	502	1	-	4/14/54/54	-
12	PC1	I	201	-	-	12/35/35/57	-
17	LMT	P	302	-	-	5/21/61/61	0/2/2/2
13	PTY	C	504	-	-	29/44/44/53	-
18	XP4	A	3003	-	-	3/24/24/41	-
17	LMT	J	101	-	-	12/21/61/61	0/2/2/2
12	PC1	C	503	-	-	10/41/41/57	-
14	CDL	N	504	-	-	36/59/59/110	-
12	PC1	N	503	-	-	15/41/41/57	-
19	HEC	D	401	7	1/1/3/7	8/14/54/54	-
14	CDL	N	507	-	-	28/48/48/110	-
13	PTY	N	505	-	-	30/44/44/53	-
18	XP4	L	3003	-	-	3/24/24/41	-
14	CDL	C	505	-	-	31/57/57/110	-
14	CDL	L	3001	-	-	24/48/48/110	-
11	HEM	N	501	1	-	4/14/54/54	-
16	FES	P	301	2	-	-	0/1/1/1
14	CDL	C	507	-	-	29/48/48/110	-
14	CDL	L	3002	-	-	26/54/54/110	-
11	HEM	C	501	1	-	5/14/54/54	-

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	O	401	HEC	C4B-NB	-6.25	1.29	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	401	HEC	C4B-NB	-6.06	1.29	1.40
18	A	3003	XP4	O7-C18	5.08	1.46	1.35
18	L	3003	XP4	O7-C18	5.00	1.46	1.35
19	D	401	HEC	C1D-ND	-4.84	1.32	1.40

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	502	HEM	CHD-C4C-NC	9.07	134.25	124.44
19	O	401	HEC	C1B-C2B-C3B	-8.07	98.47	106.96
11	N	502	HEM	CHD-C4C-NC	8.00	133.09	124.44
18	L	3003	XP4	O7-C18-C19	7.98	125.77	111.09
18	A	3003	XP4	O7-C18-C19	7.95	125.71	111.09

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	D	401	HEC	NA
19	O	401	HEC	NA

5 of 518 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	201	PC1	C11-O13-P-O12
12	T	201	PC1	C11-O13-P-O12
12	T	201	PC1	O21-C2-C3-O31
13	C	504	PTY	C11-C8-O7-C6
13	C	504	PTY	C3-O11-P1-O13

There are no ring outliers.

27 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	O	401	HEC	11	0
13	E	401	PTY	3	0
14	H	701	CDL	2	0
15	N	506	AWB	1	0
12	T	201	PC1	2	0
14	A	3001	CDL	2	0
14	A	3002	CDL	2	0
14	C	508	CDL	2	0

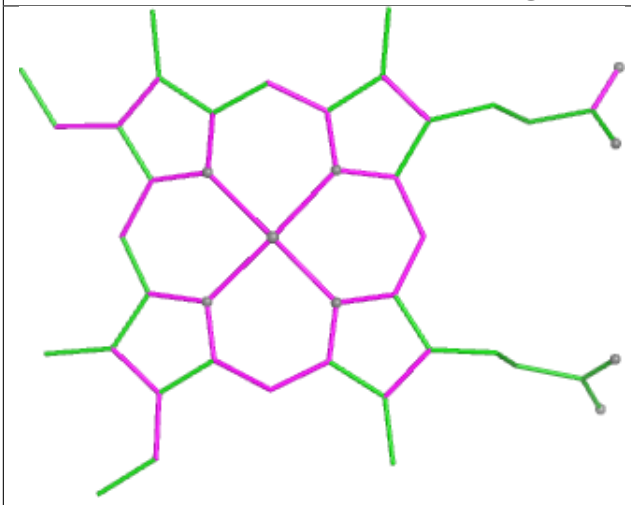
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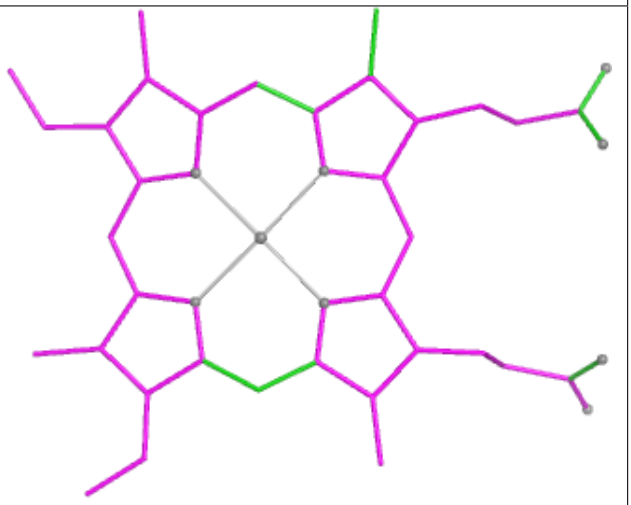
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	506	AWB	1	0
11	N	502	HEM	3	0
13	P	303	PTY	10	0
11	C	502	HEM	3	0
13	C	504	PTY	3	0
18	A	3003	XP4	1	0
17	J	101	LMT	1	0
12	C	503	PC1	2	0
14	N	504	CDL	2	0
12	N	503	PC1	1	0
14	N	507	CDL	1	0
19	D	401	HEC	12	0
13	N	505	PTY	8	0
14	C	505	CDL	2	0
14	L	3001	CDL	1	0
11	N	501	HEM	5	0
14	C	507	CDL	4	0
14	L	3002	CDL	2	0
11	C	501	HEM	6	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.

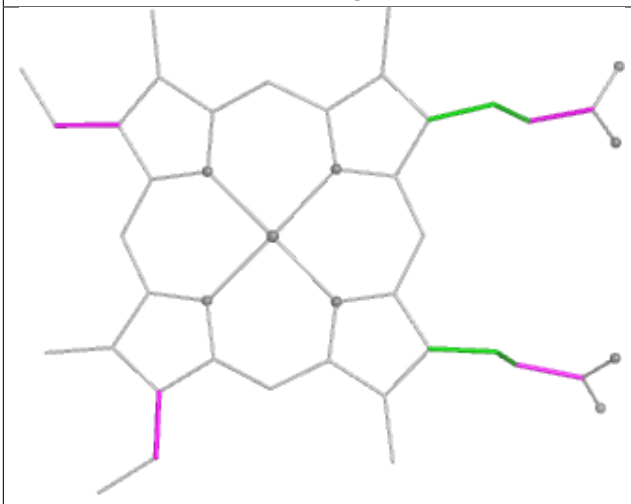
Ligand HEC O 401



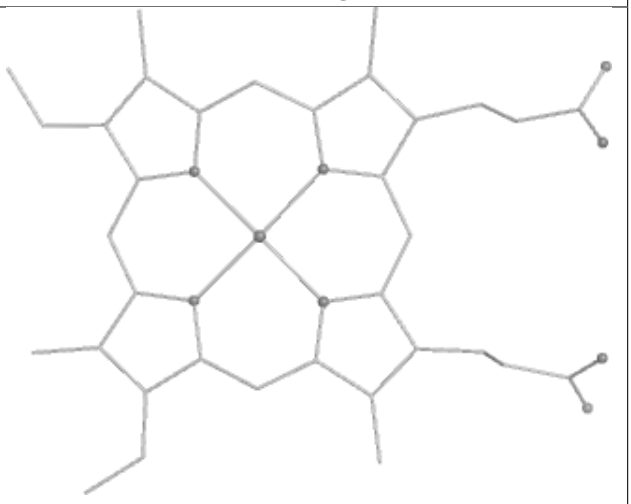
Bond lengths



Bond angles

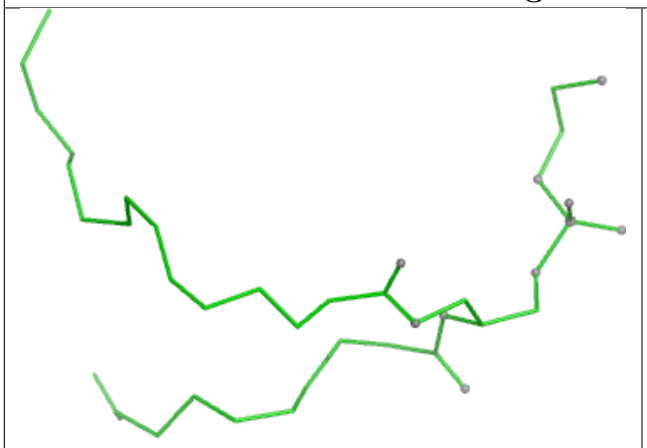


Torsions

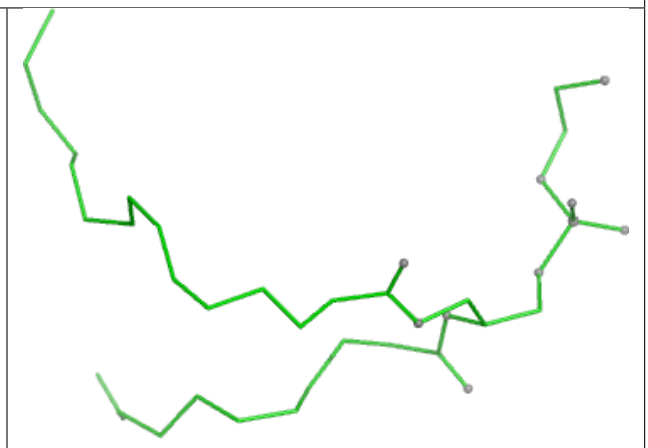


Rings

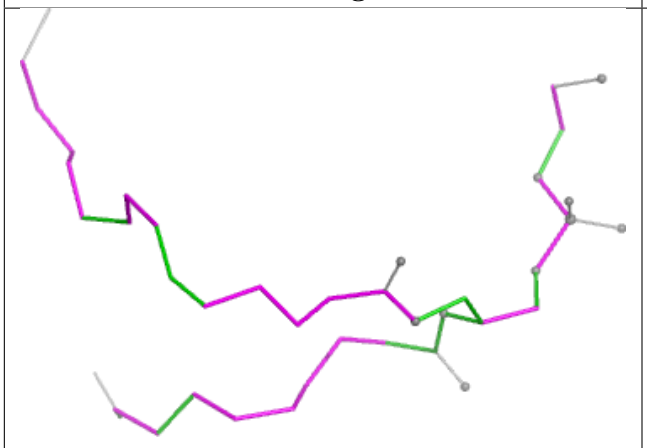
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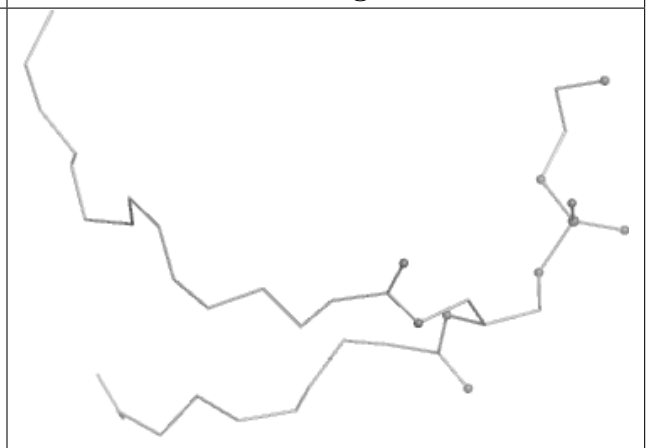
Bond lengths



Bond angles

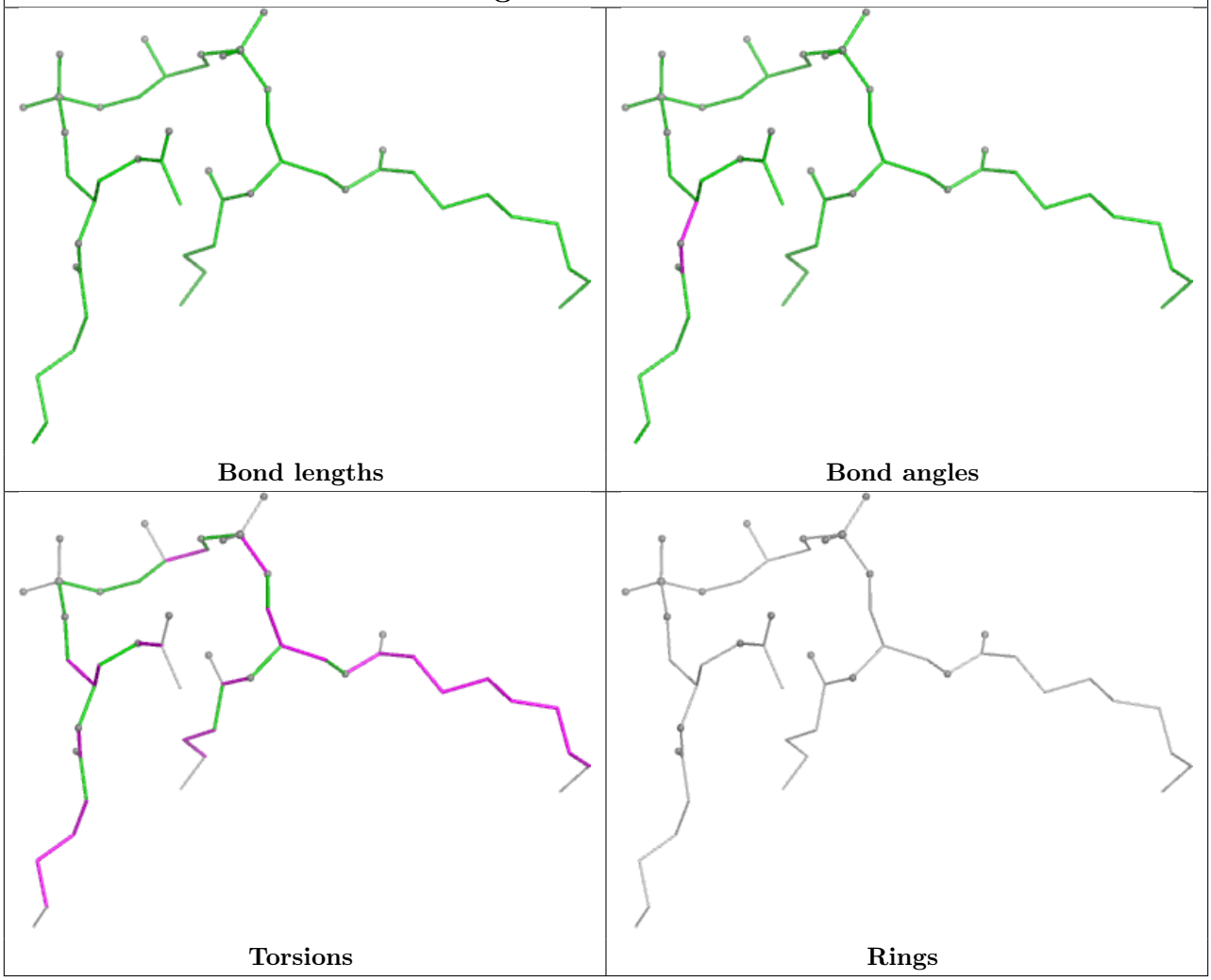


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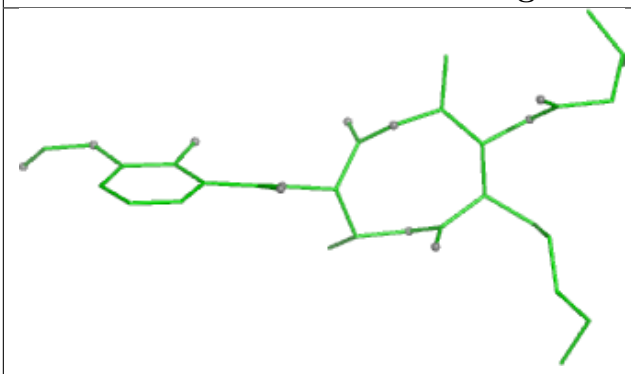


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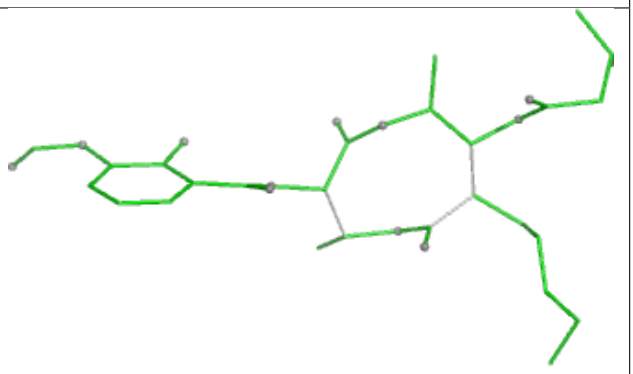
Ligand CDL H 701



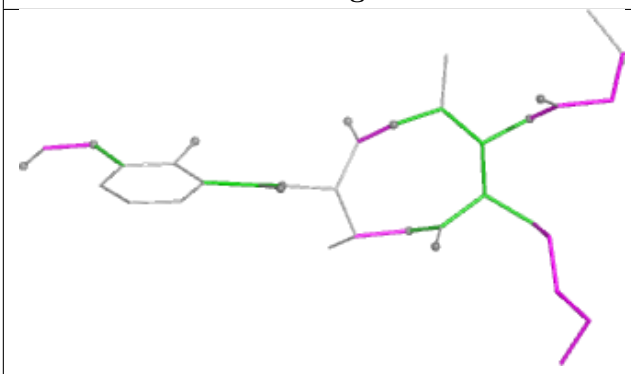
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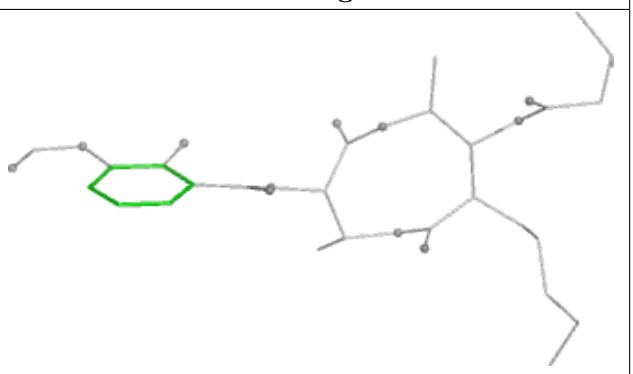
Bond lengths



Bond angles

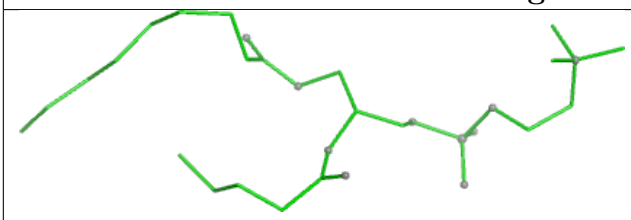


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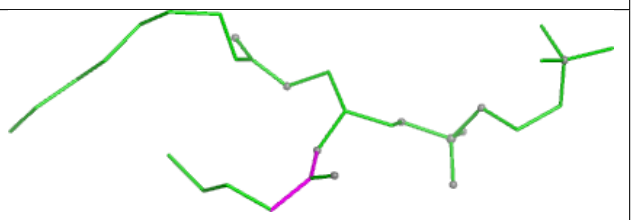


Rings

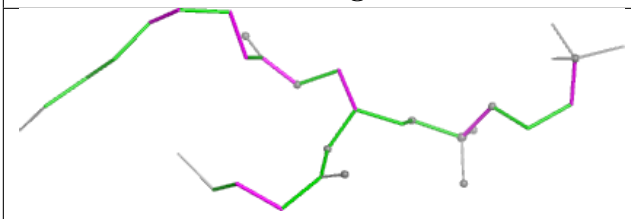
Ligand PC1 T 201



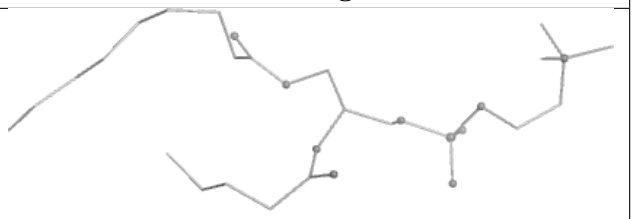
Bond lengths



Bond angles

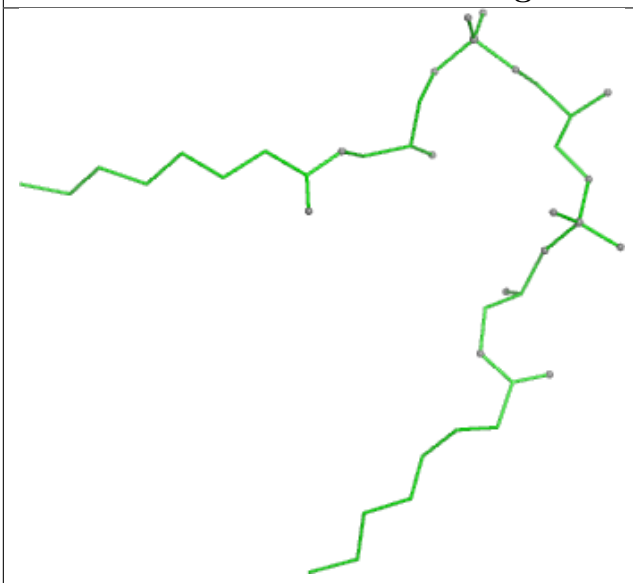


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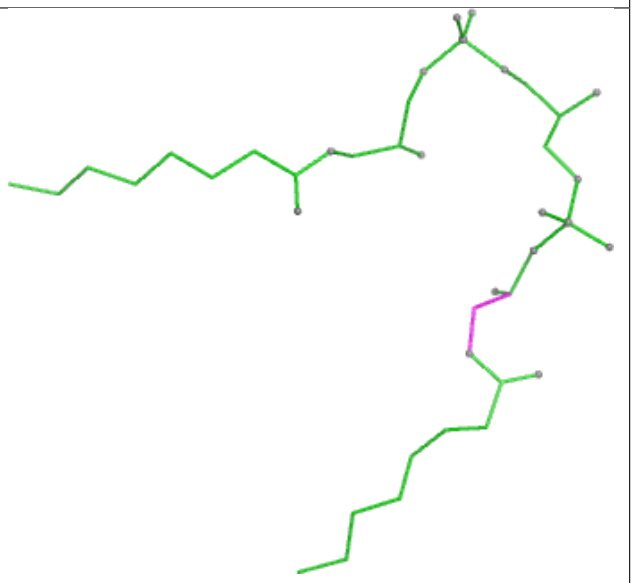


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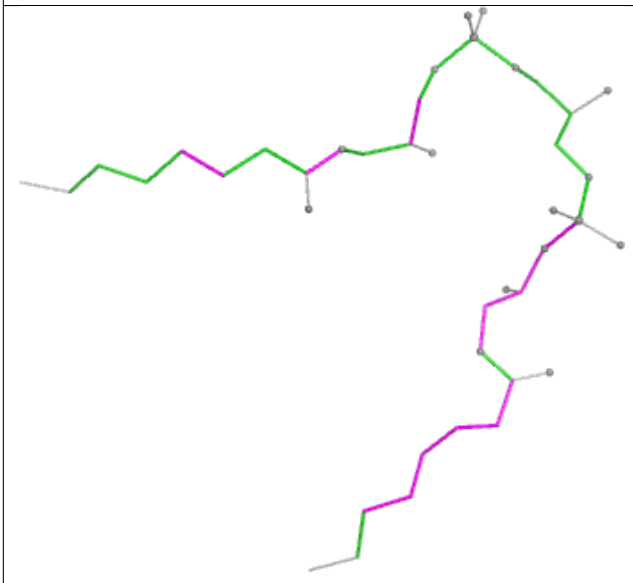
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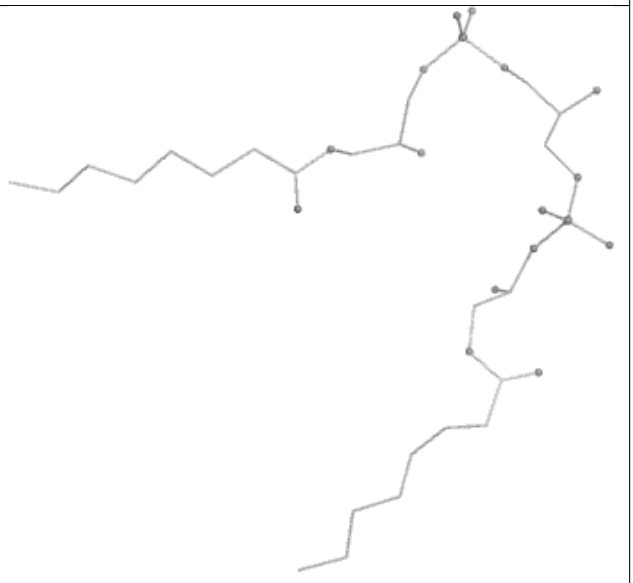
Bond lengths



Bond angles

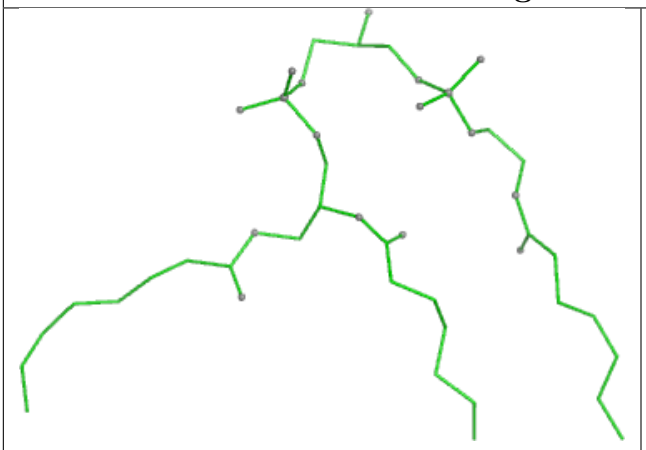


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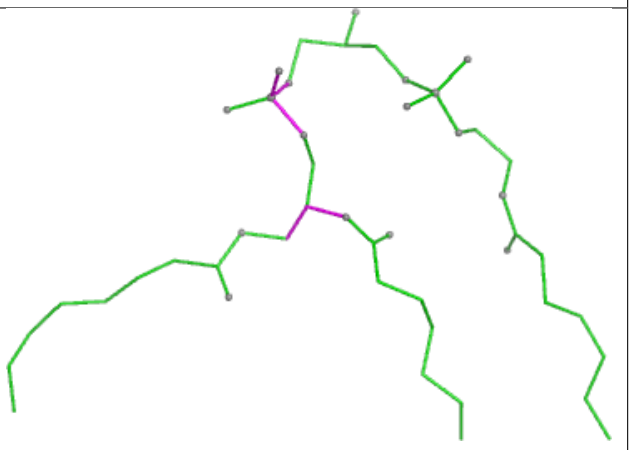


Rings

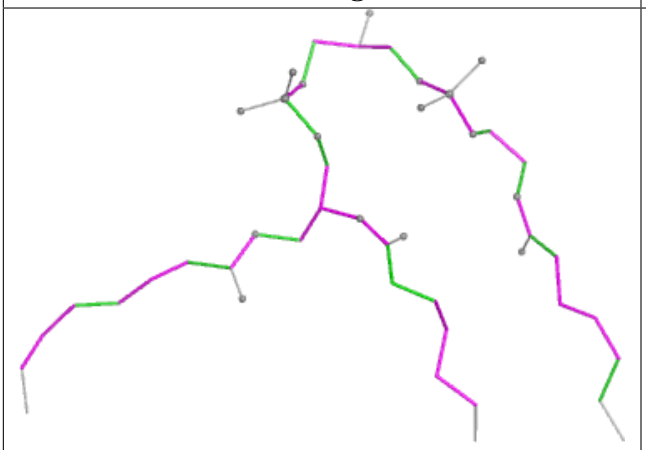
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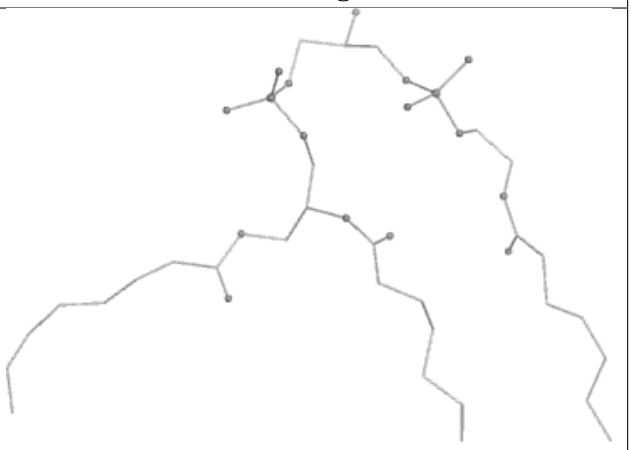
Bond lengths



Bond angles

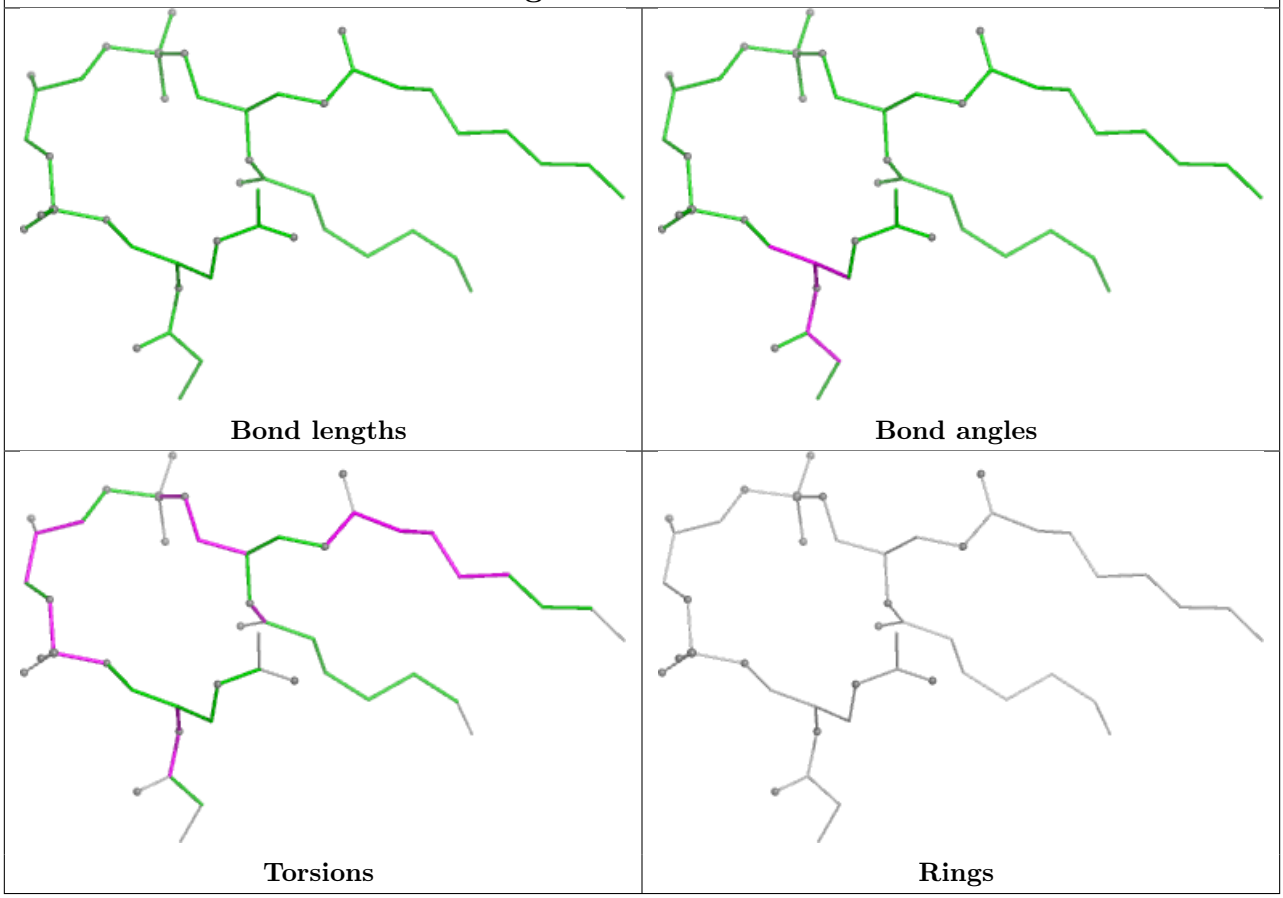


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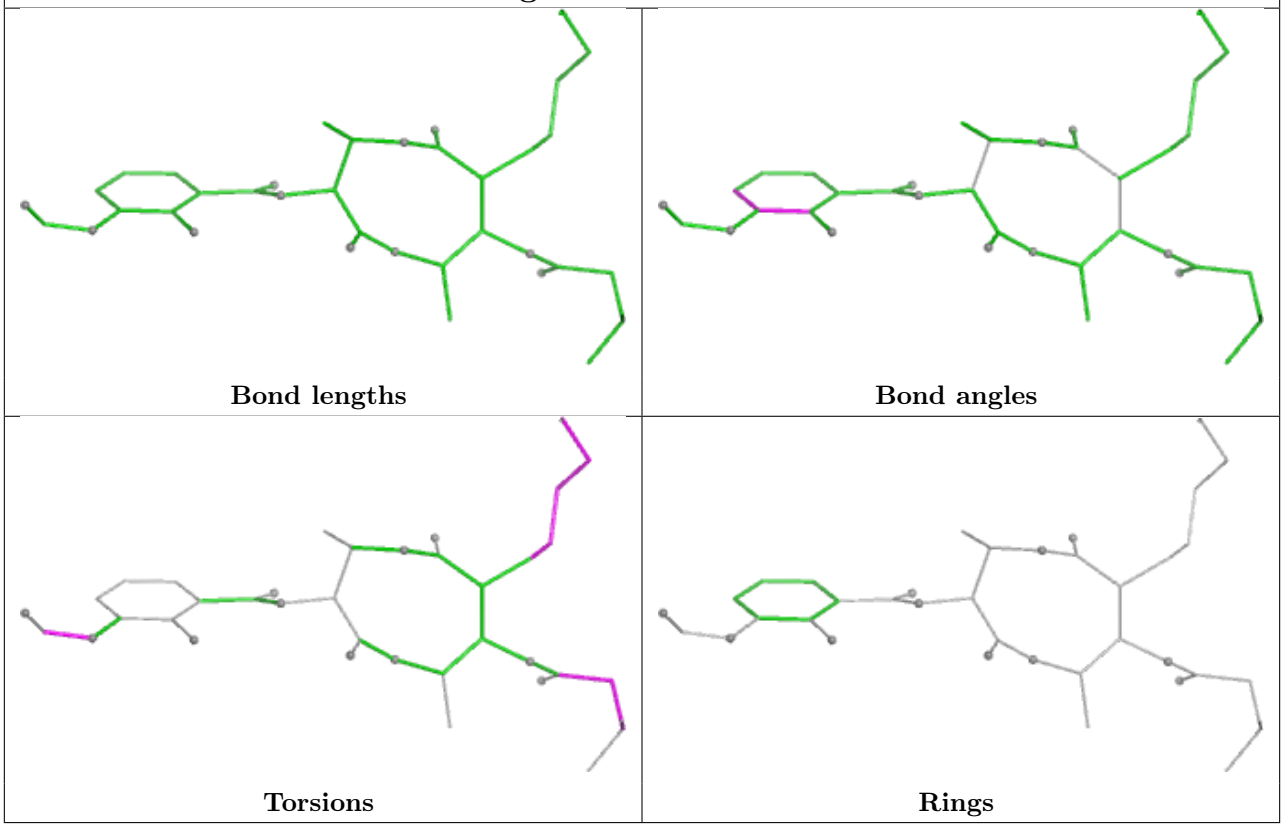


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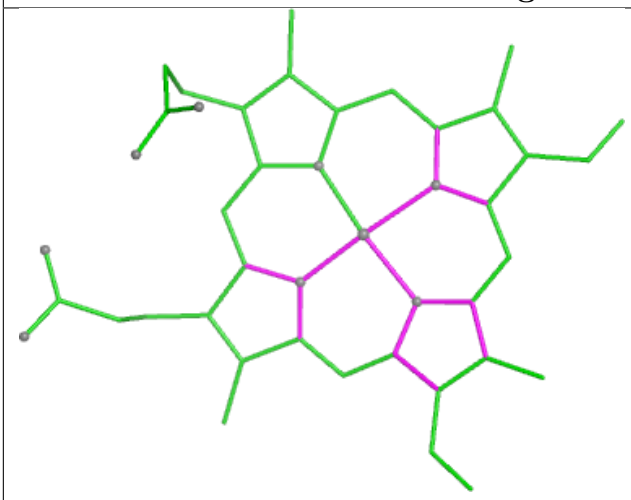
Ligand CDL C 508



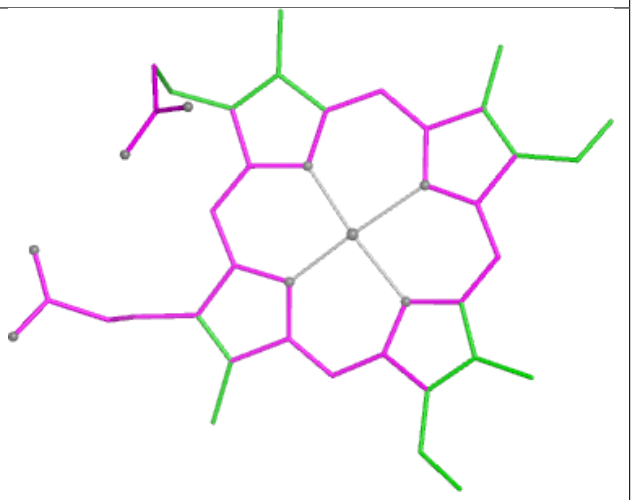
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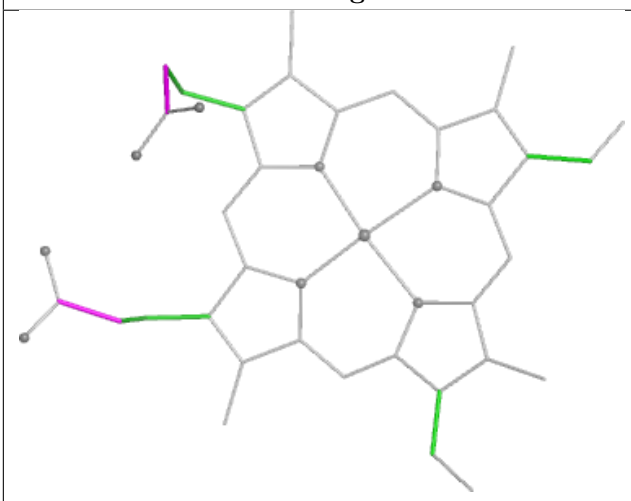
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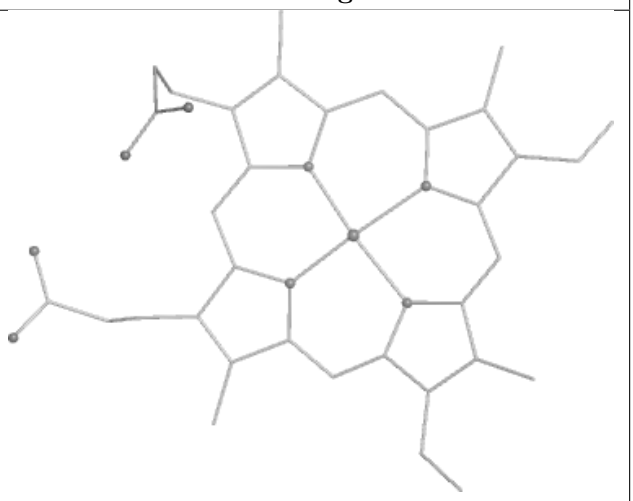
Bond lengths



Bond angles

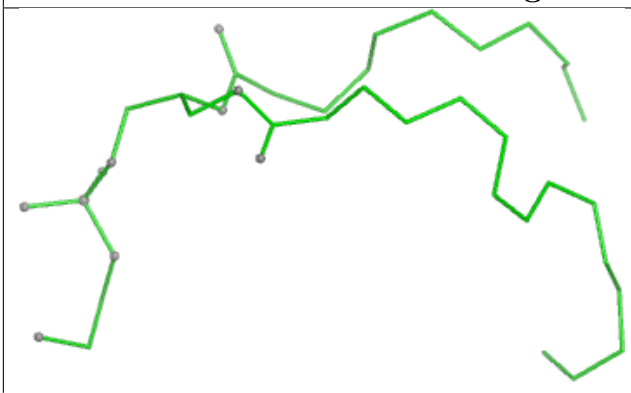


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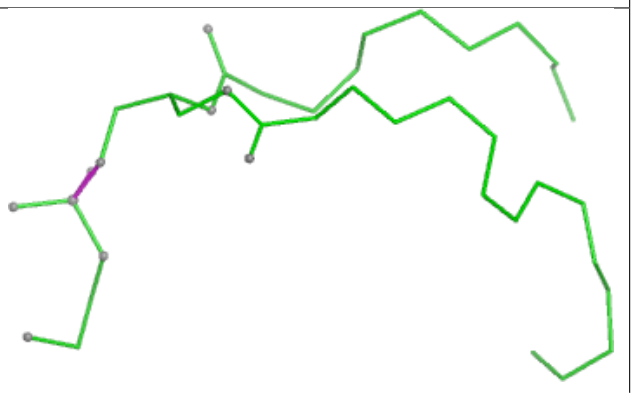


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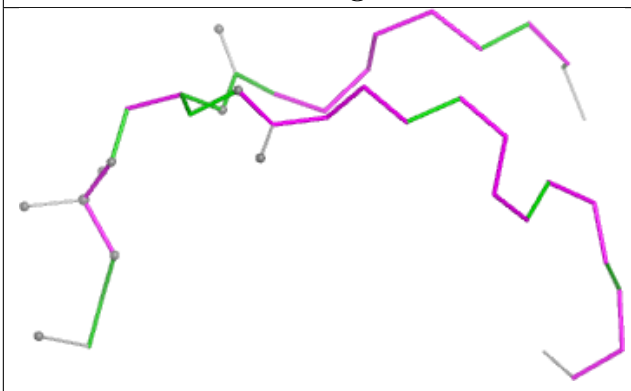
Ligand PTY P 303



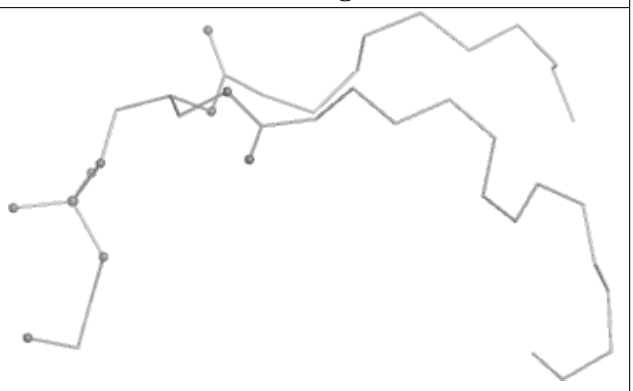
Bond lengths



Bond angles

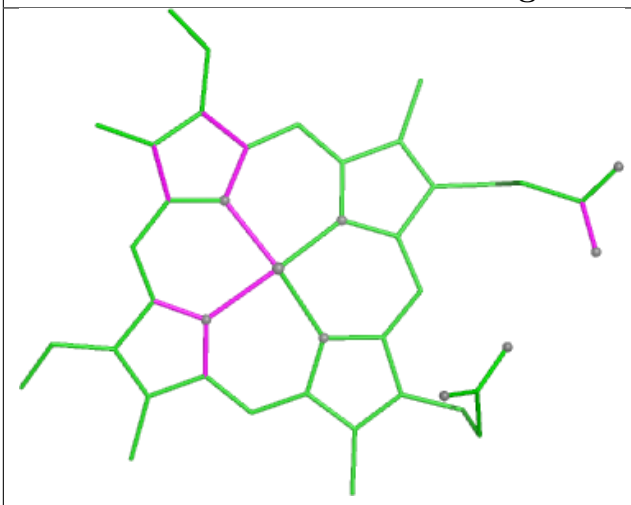


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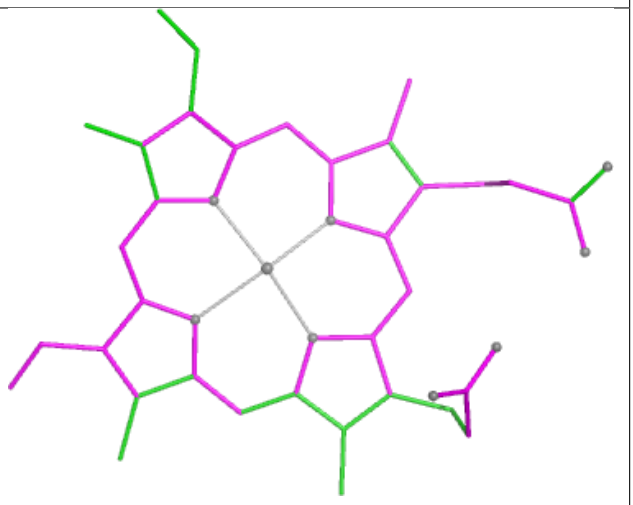


Rings

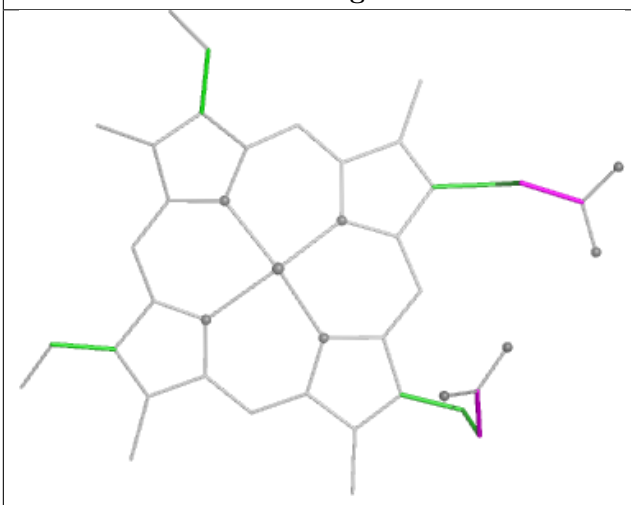
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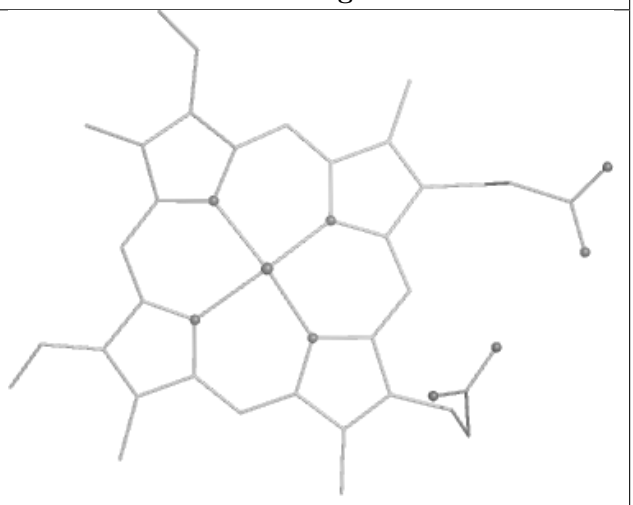
Bond lengths



Bond angles

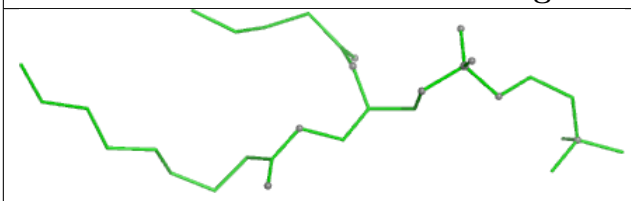


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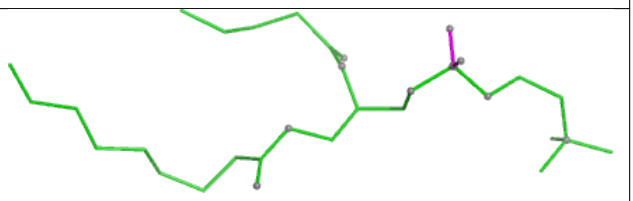


Rings

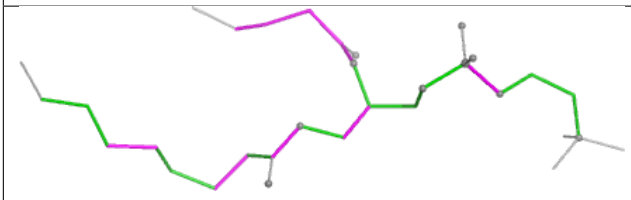
Ligand PC1 I 201



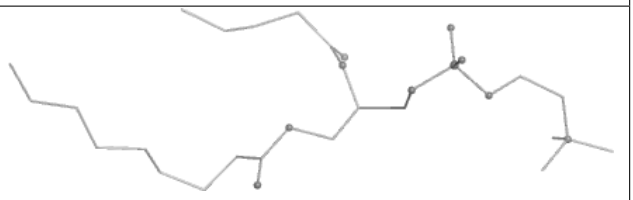
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Bond angles

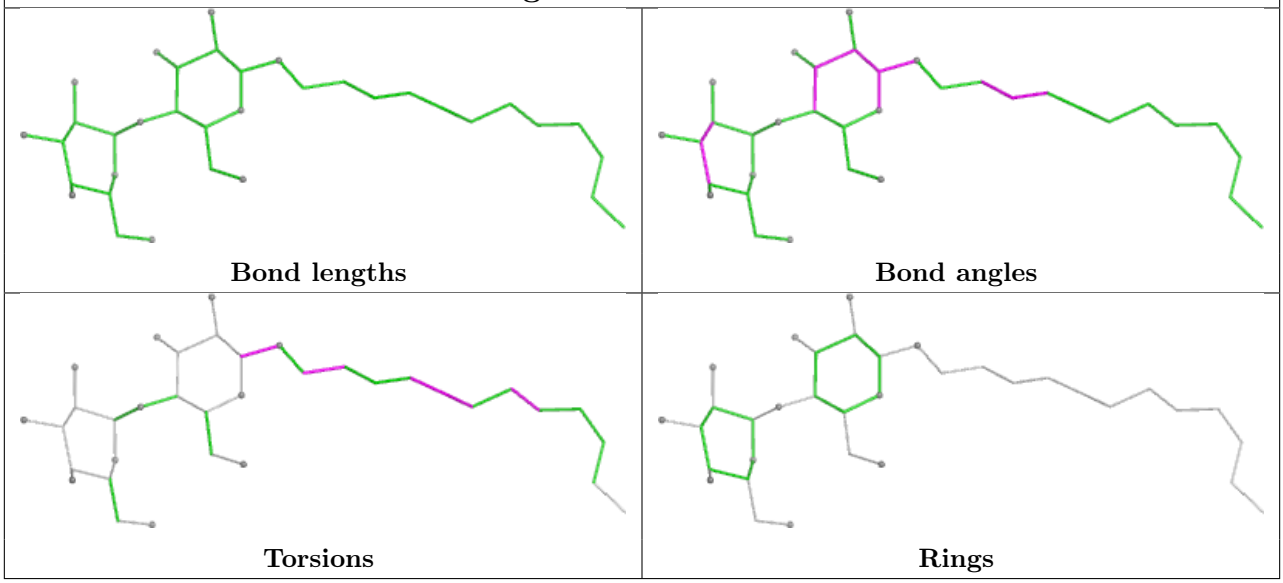


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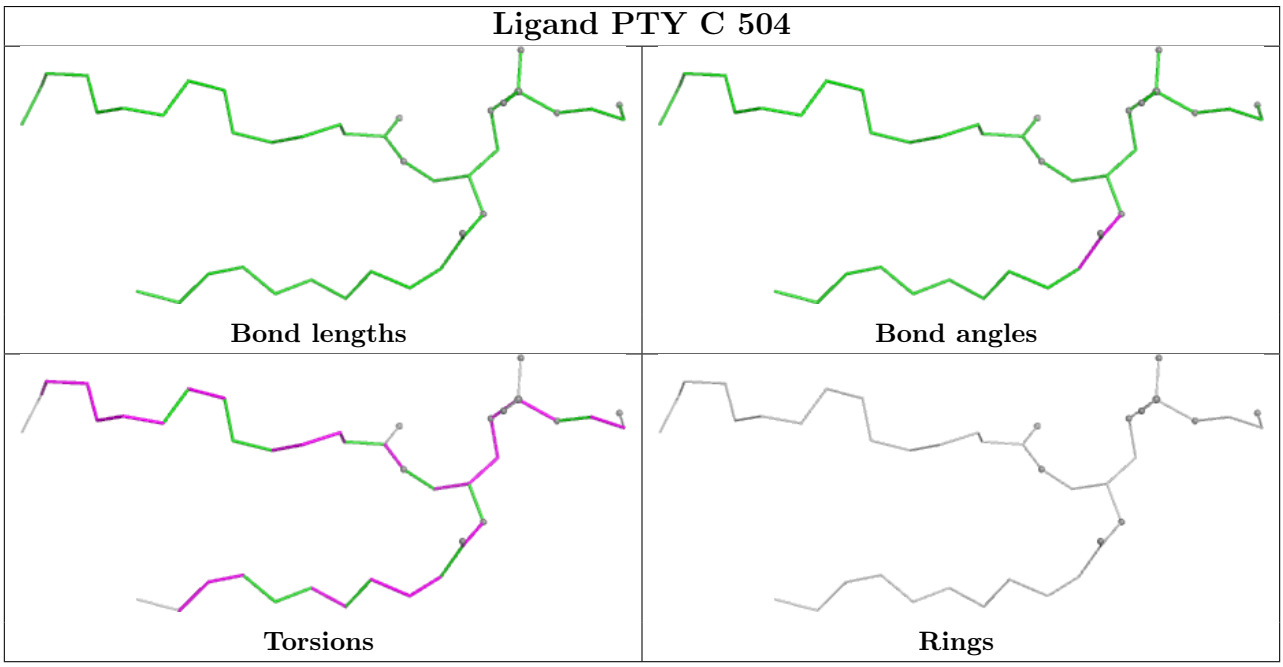


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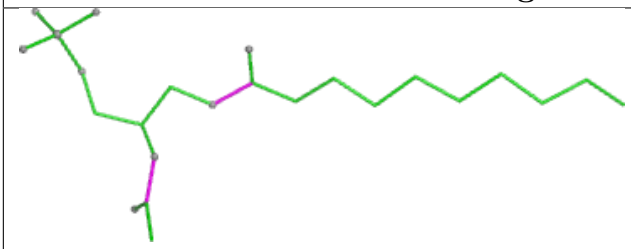
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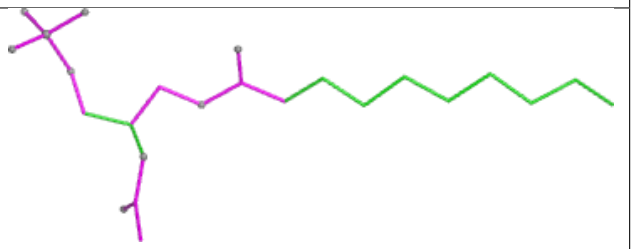
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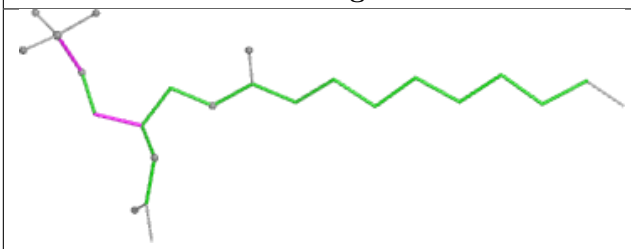
Ligand XP4 A 3003



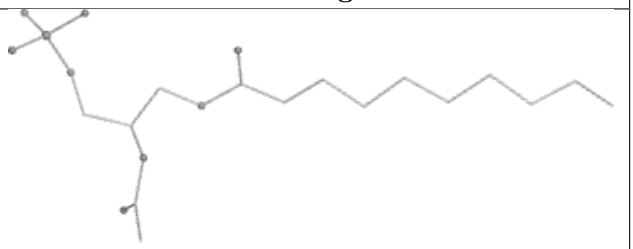
Bond lengths



Bond angles

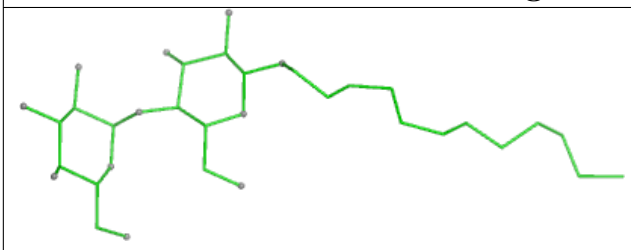


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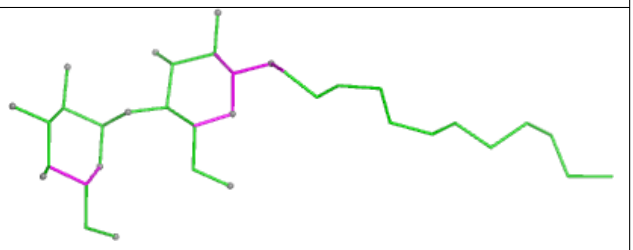


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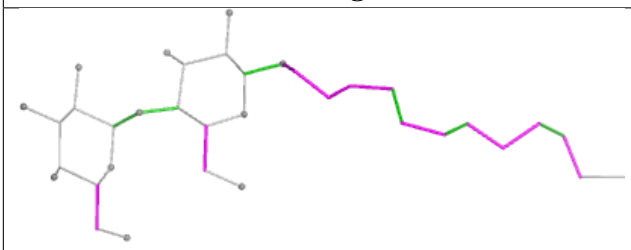
Ligand LMT J 101



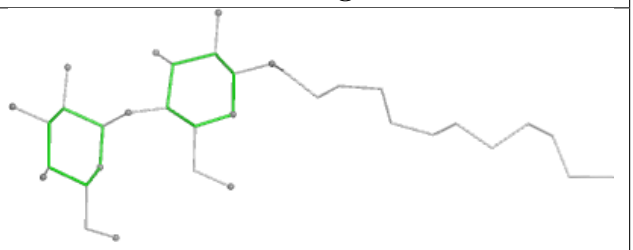
Bond lengths



Bond angles

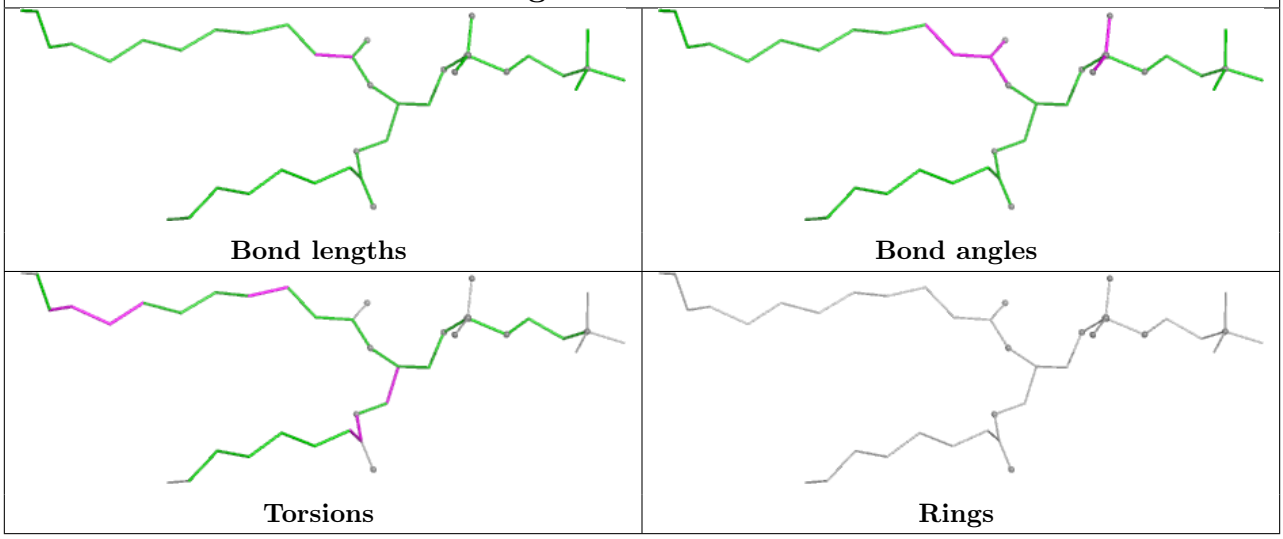


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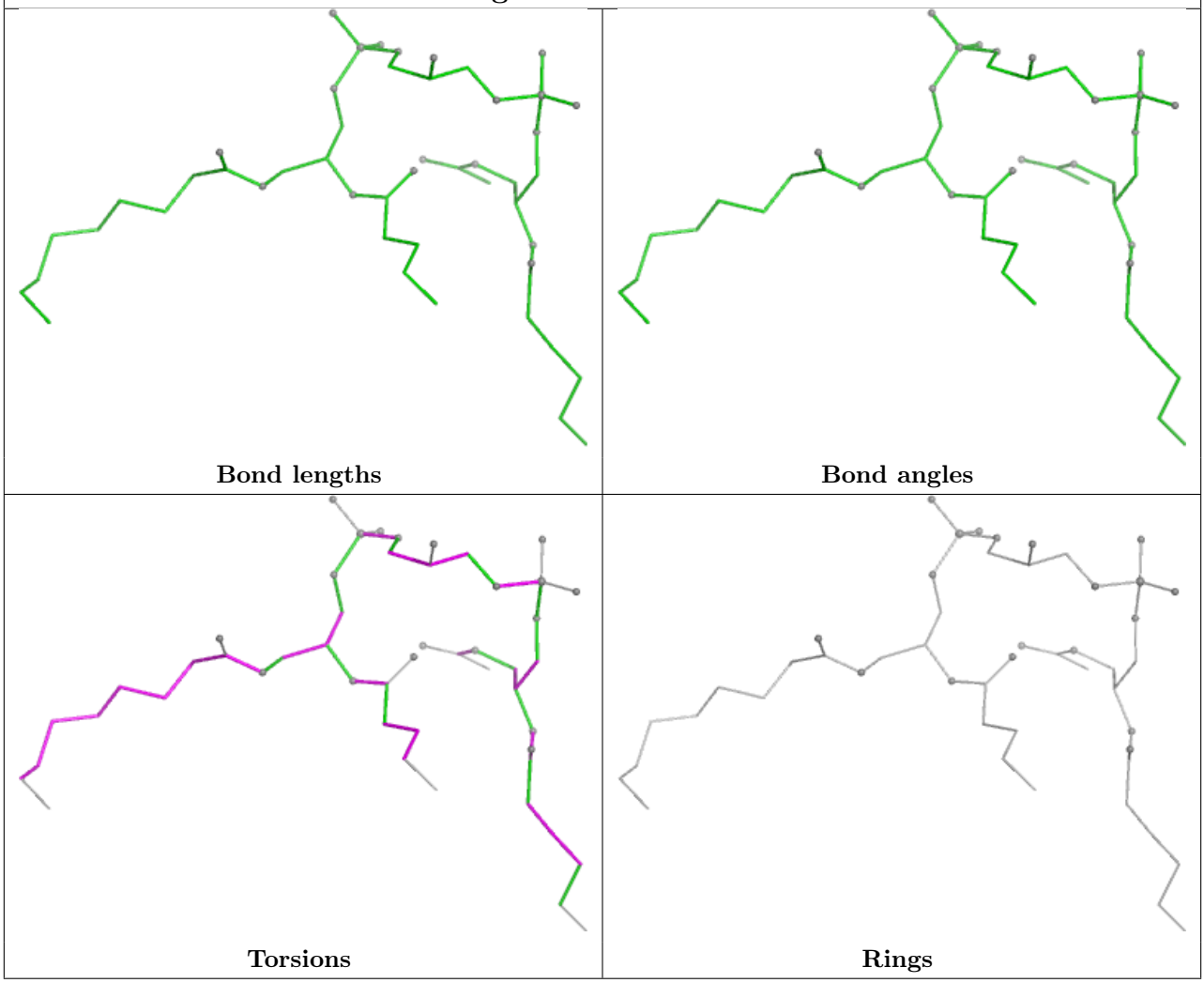


Rings

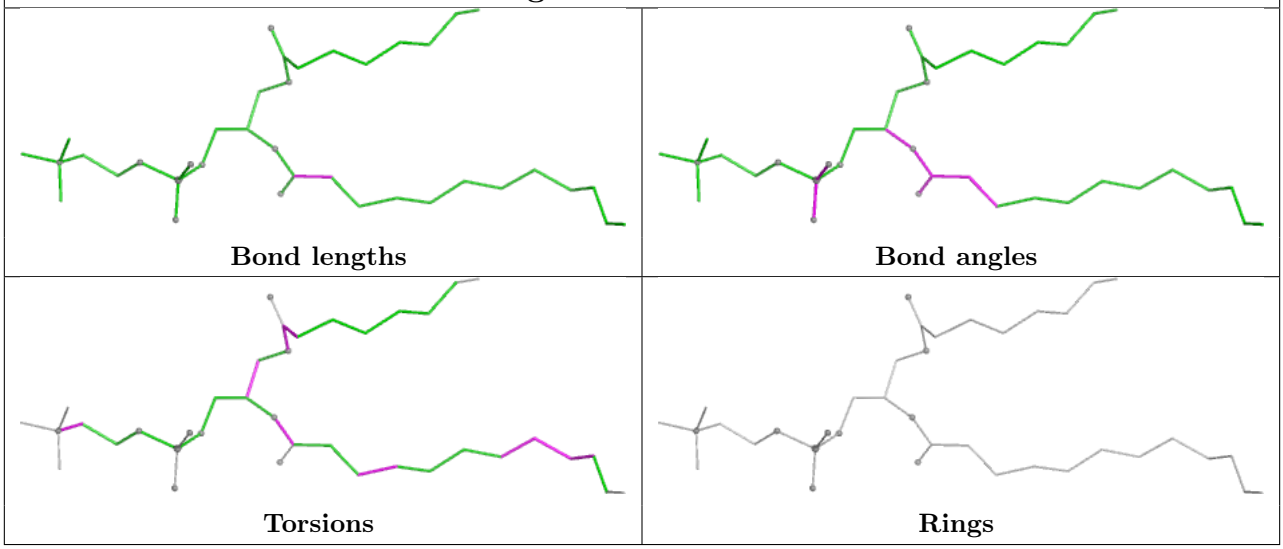
Ligand PC1 C 503



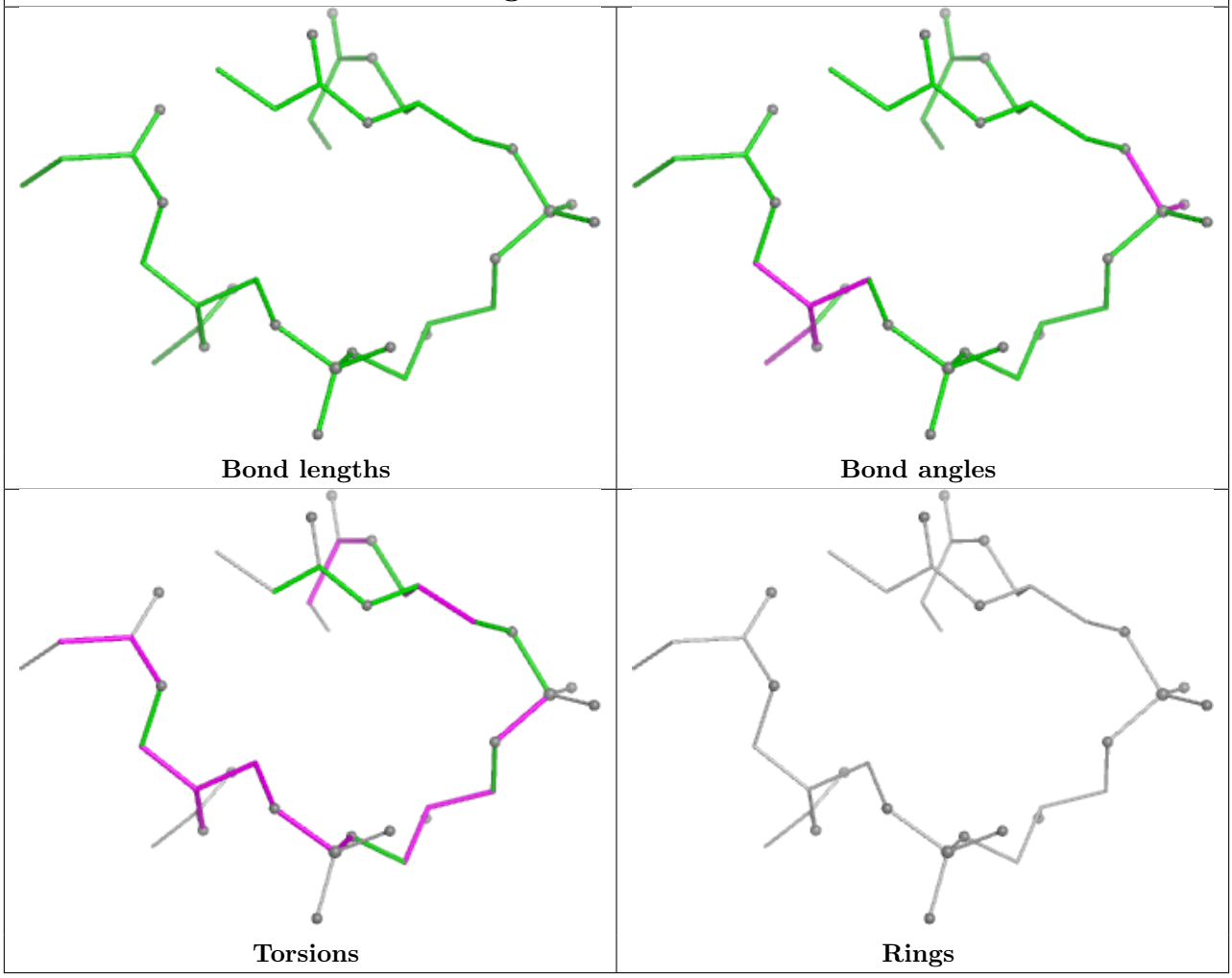
Ligand CDL N 504



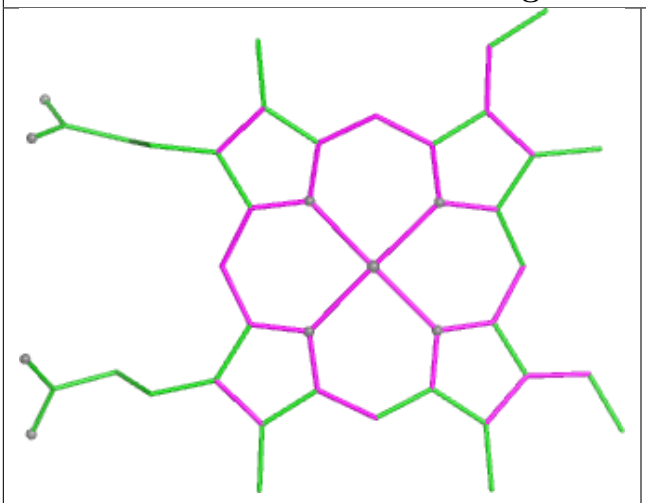
Ligand PC1 N 503



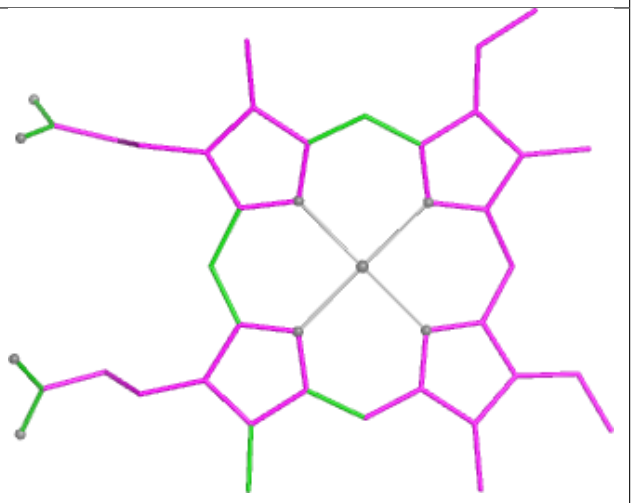
Ligand CDL N 507



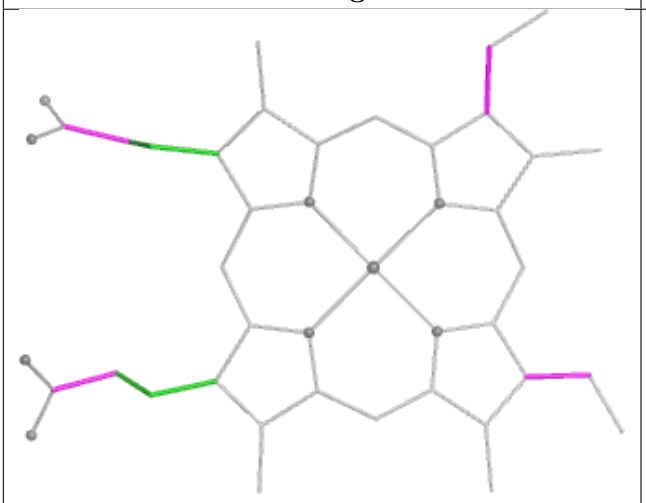
Ligand HEC D 401



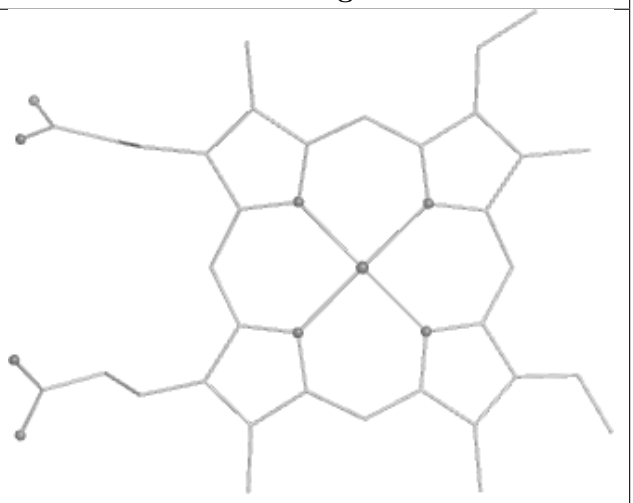
Bond lengths



Bond angles

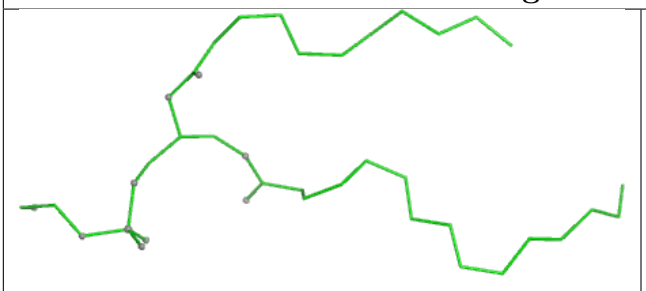


Torsions

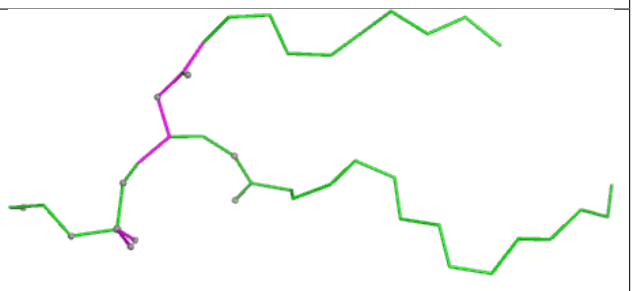


Rings

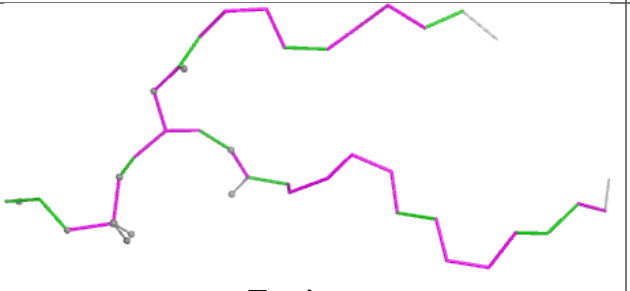
Ligand PTY N 505



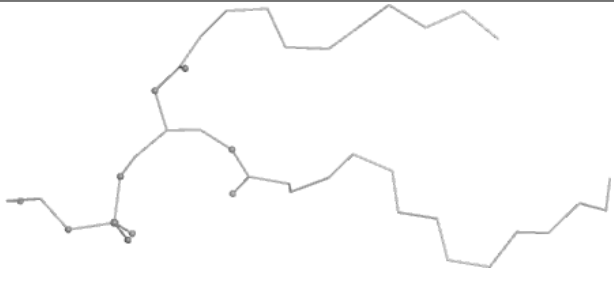
Bond lengths



Bond angles

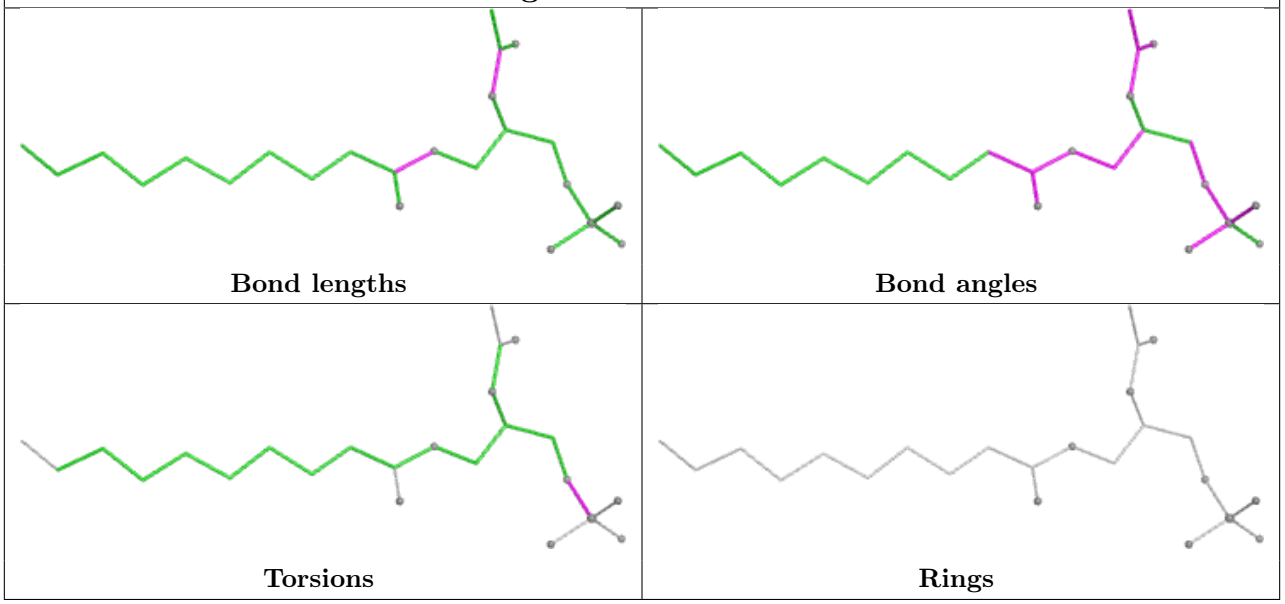


Torsions

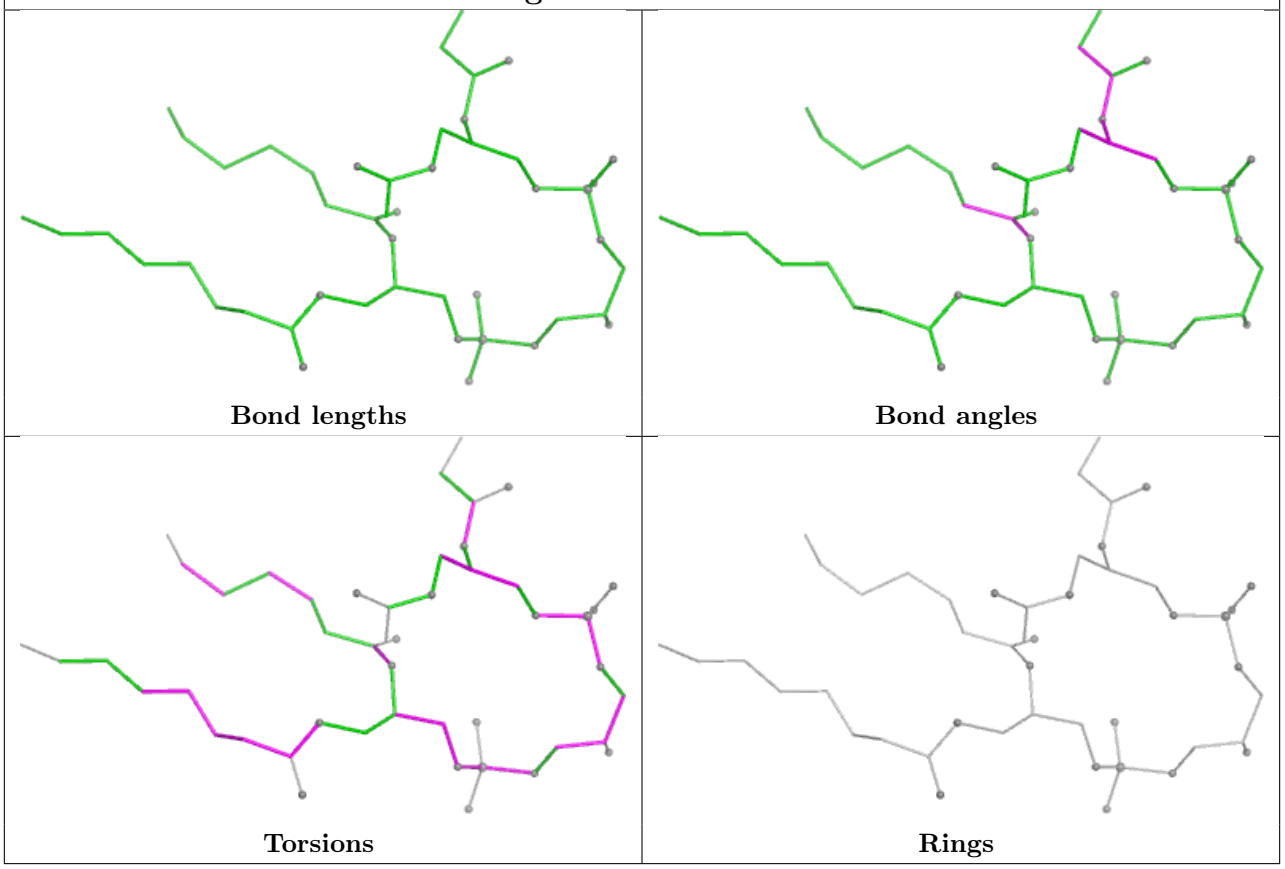


Rings

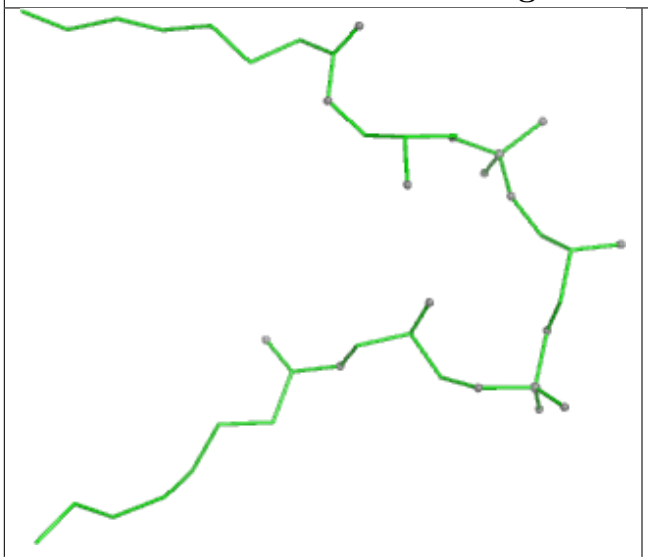
Ligand XP4 L 3003



Ligand CDL C 505



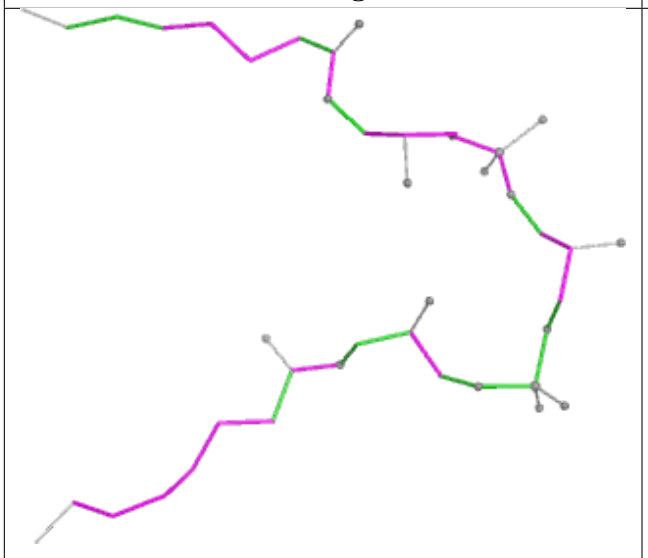
Ligand CDL L 3001



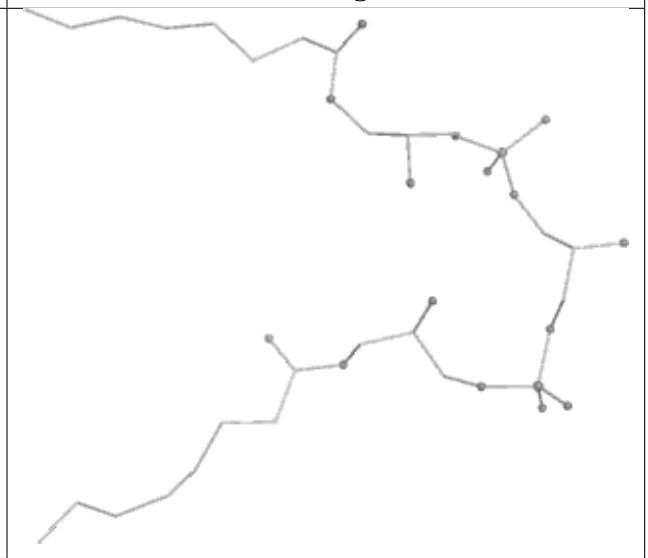
Bond lengths



Bond angles

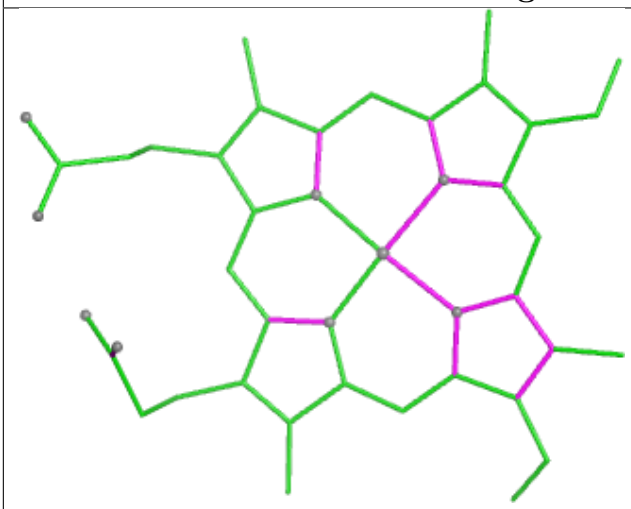


Torsions

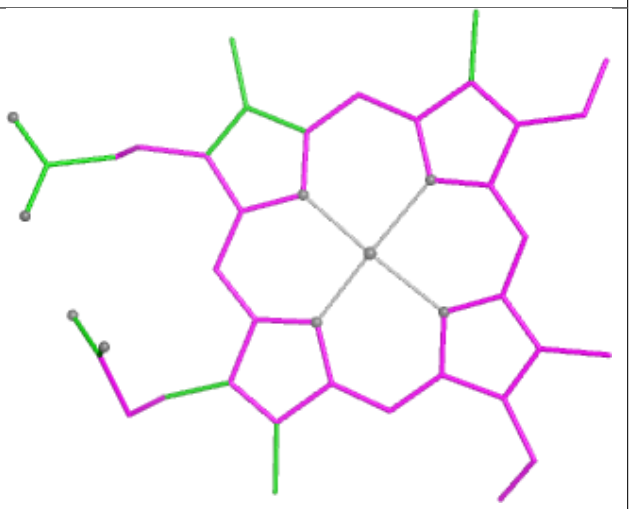


Rings

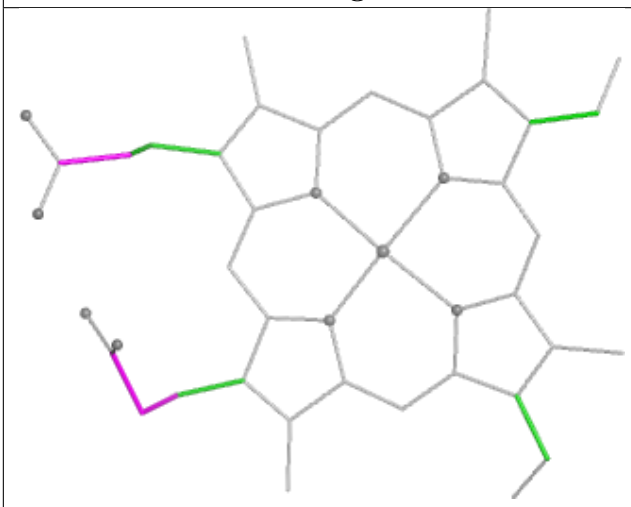
Ligand HEM N 501



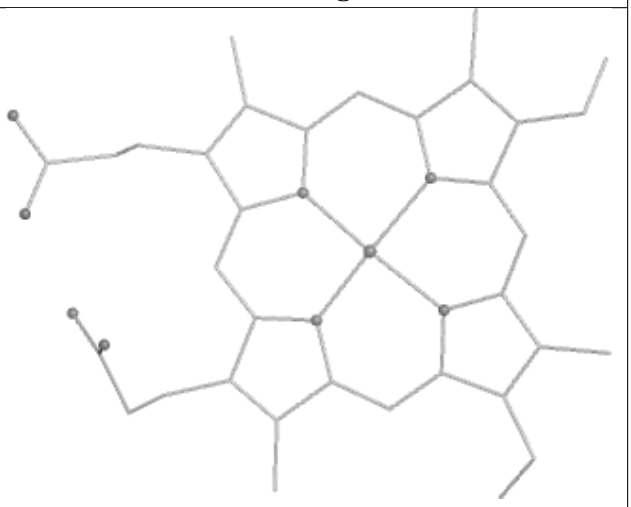
Bond lengths



Bond angles

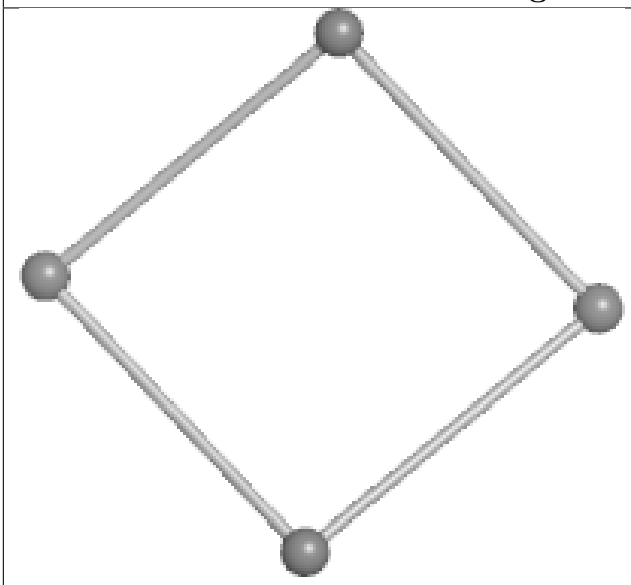


Torsions

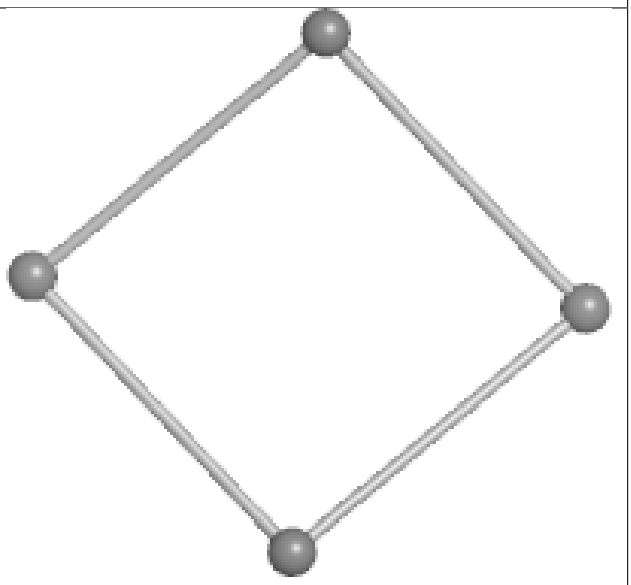


Rings

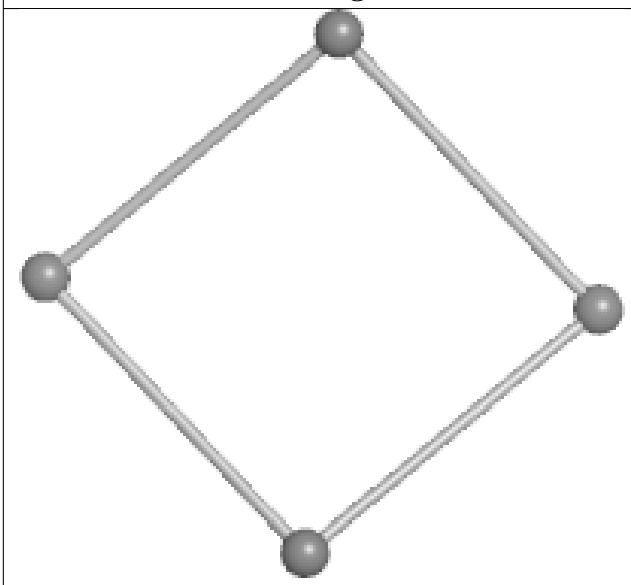
Ligand FES P 301



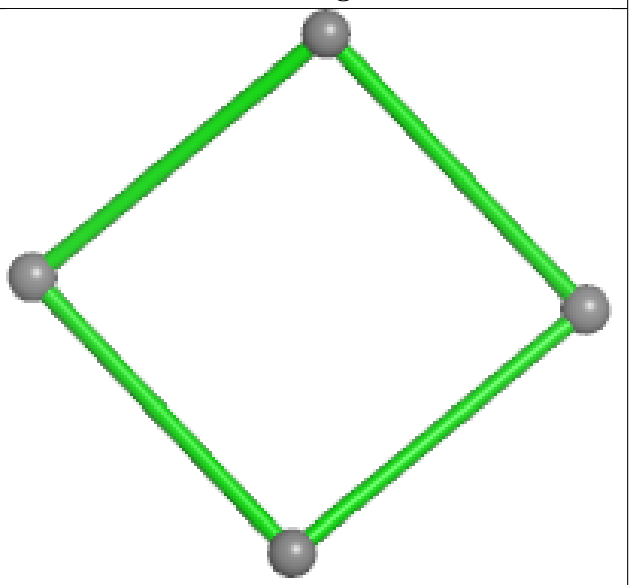
Bond lengths



Bond angles

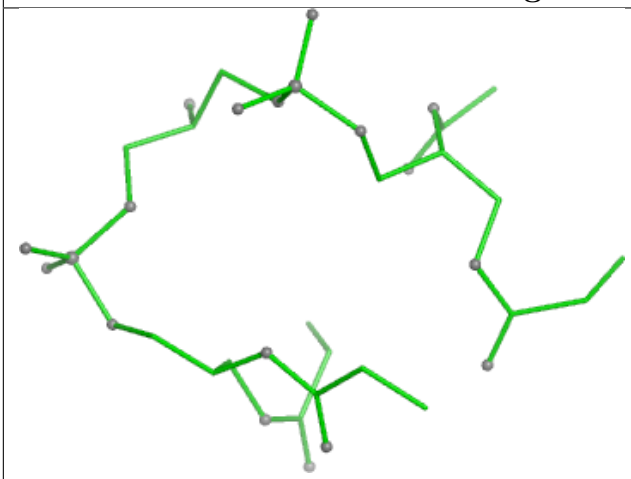


Torsions

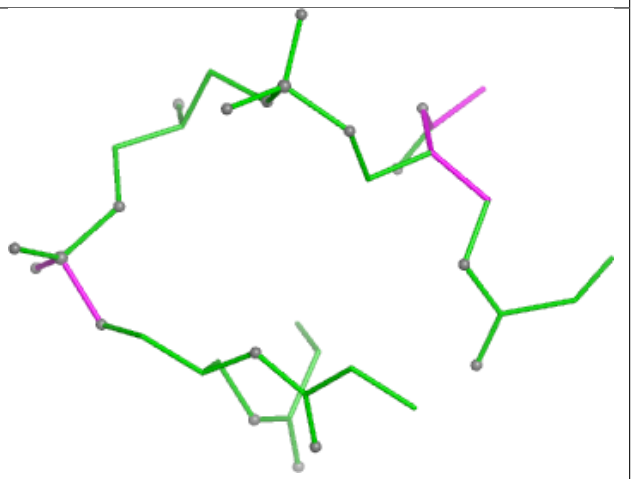


Rings

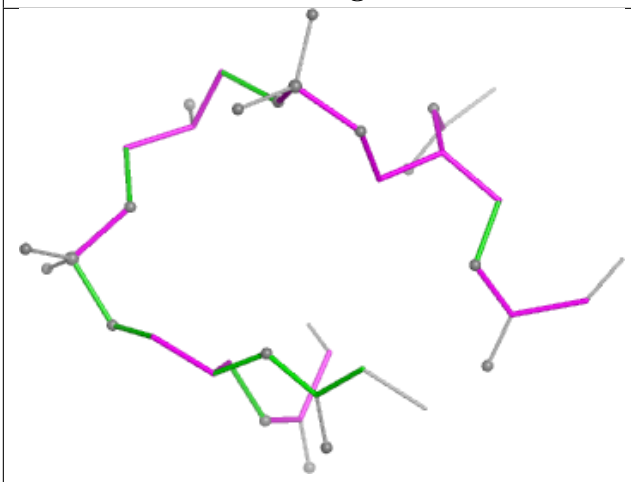
Ligand CDL C 507



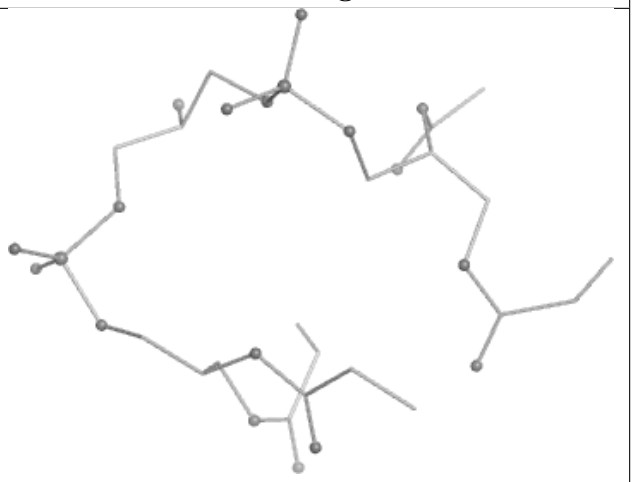
Bond lengths



Bond angles

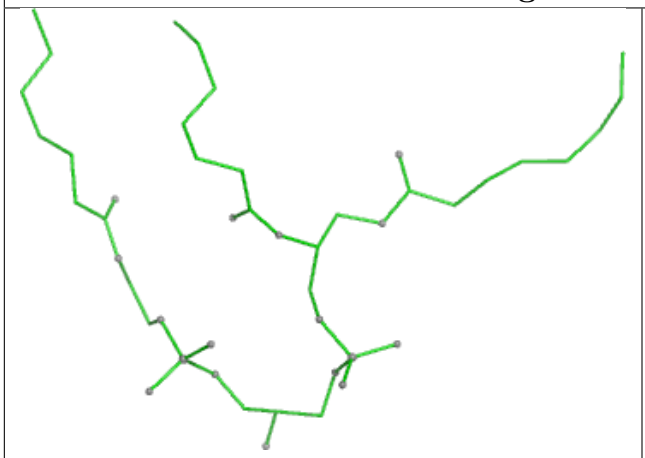


Torsions

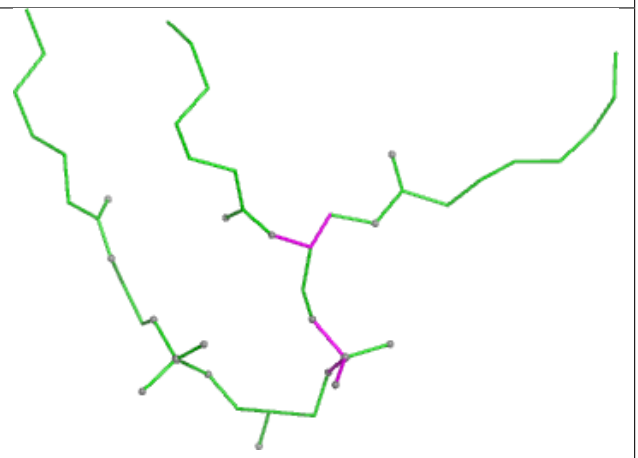


Rings

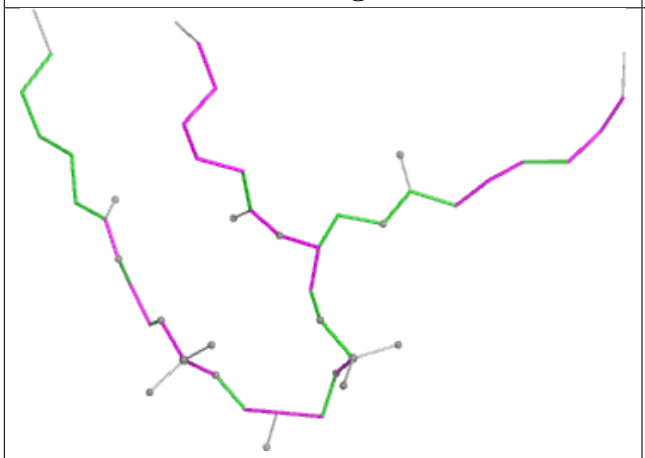
Ligand CDL L 3002



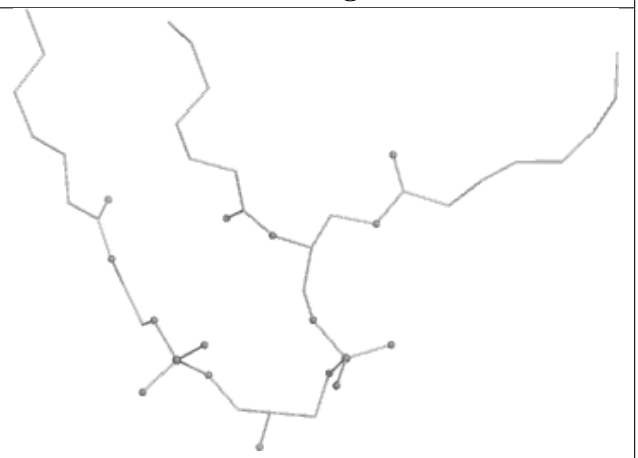
Bond lengths



Bond angles

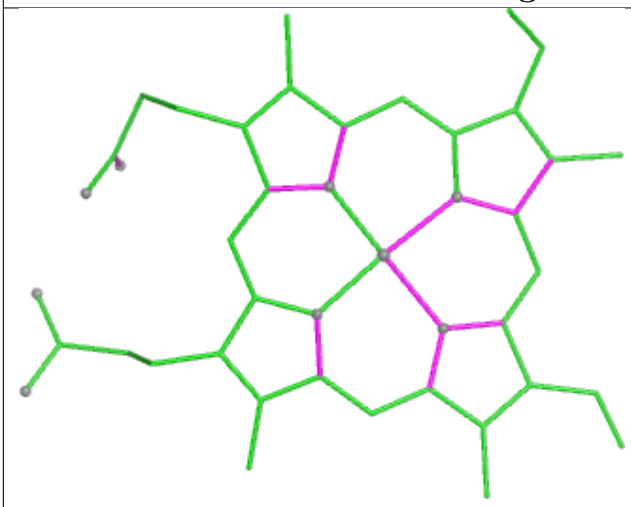


Torsions

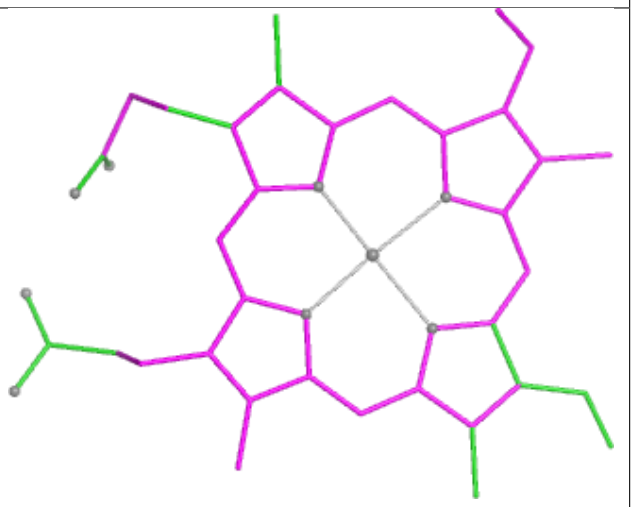


Rings

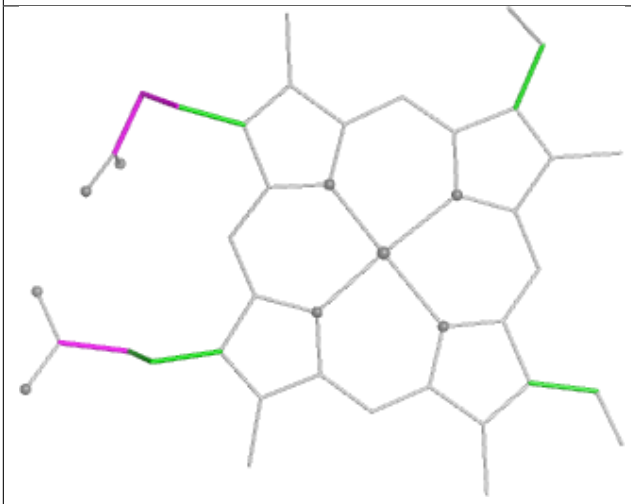
Ligand HEM C 501



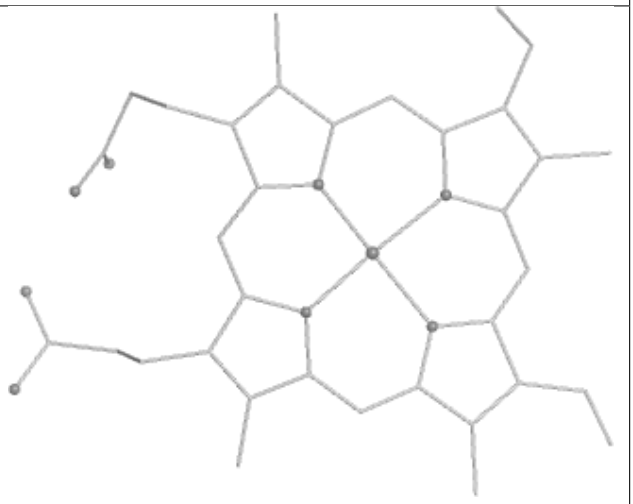
Bond lengths



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.

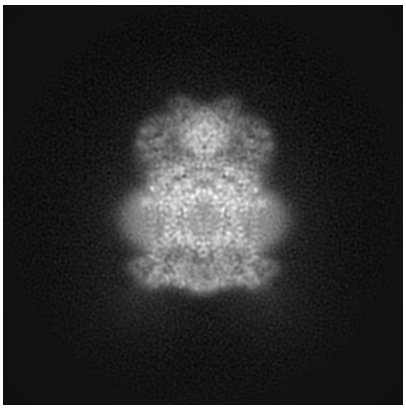
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15322. These allow visual inspection of the internal detail of the map and identification of artifacts.

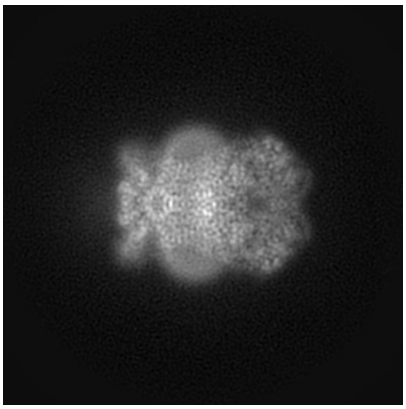
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

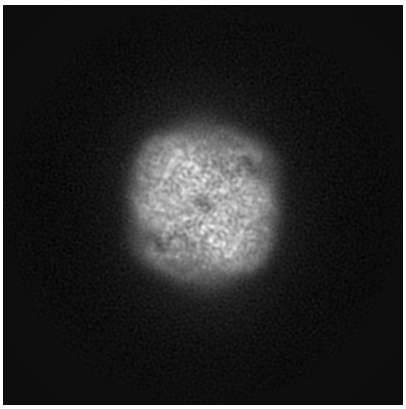
6.1.1 Primary map



X

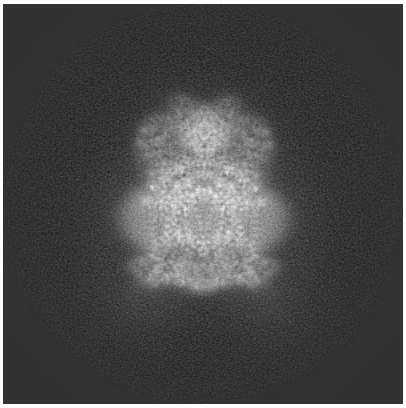


Y

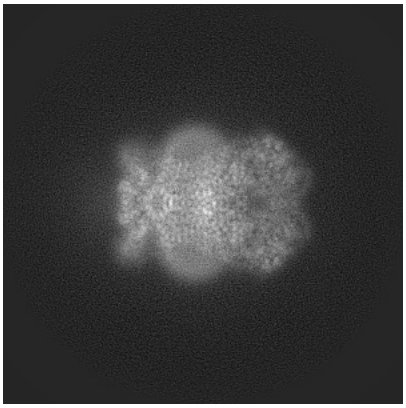


Z

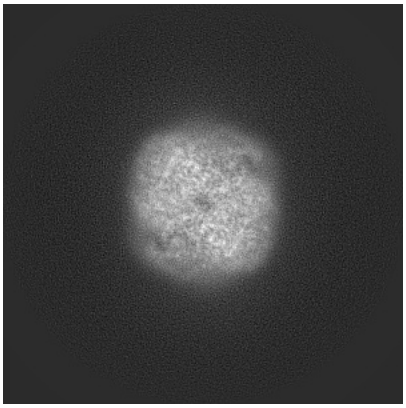
6.1.2 Raw map



X



Y

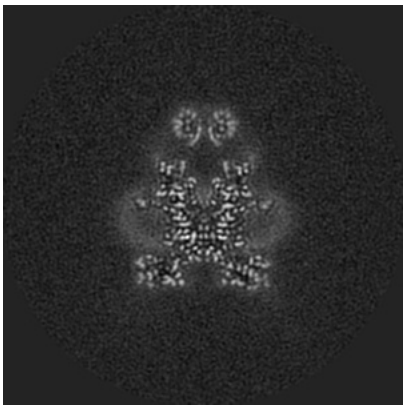


Z

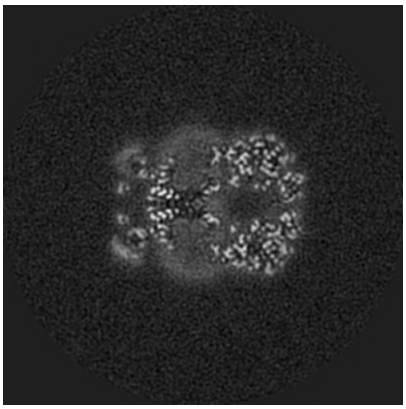
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

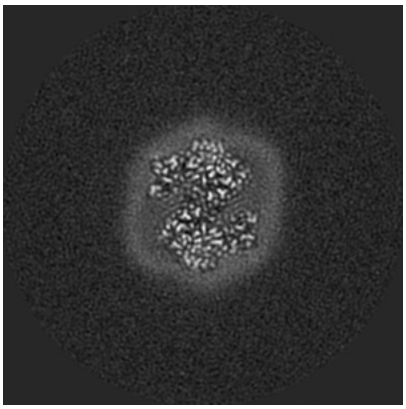
6.2.1 Primary map



X Index: 180

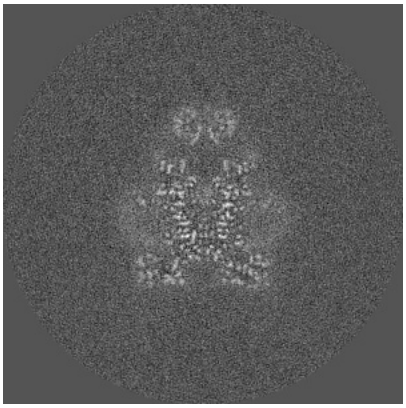


Y Index: 180

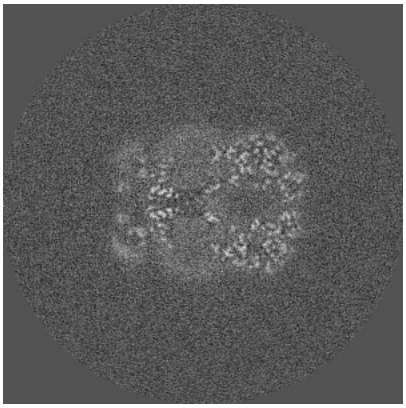


Z Index: 180

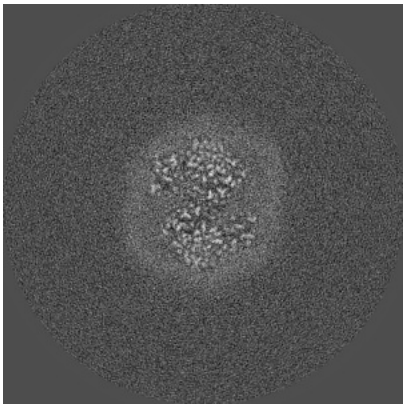
6.2.2 Raw map



X Index: 180



Y Index: 180

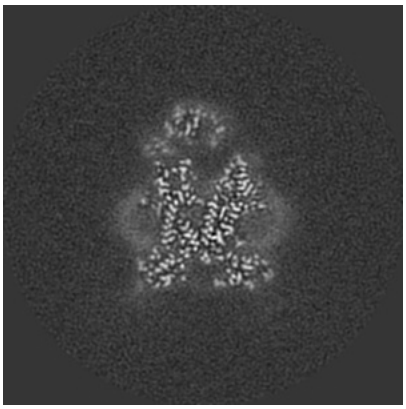


Z Index: 180

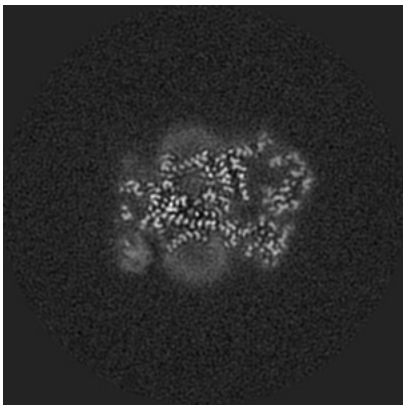
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

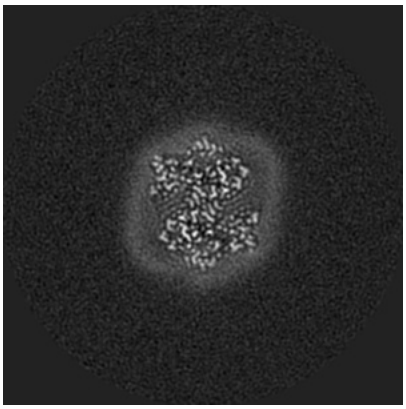
6.3.1 Primary map



X Index: 186

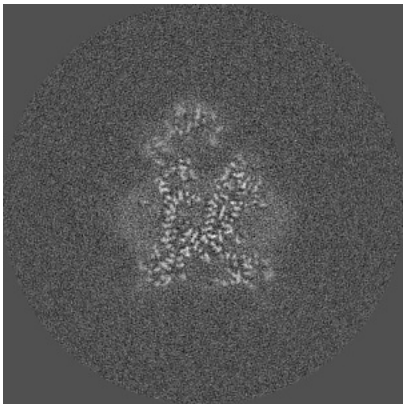


Y Index: 166

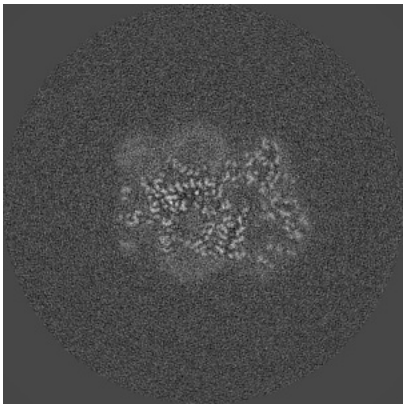


Z Index: 182

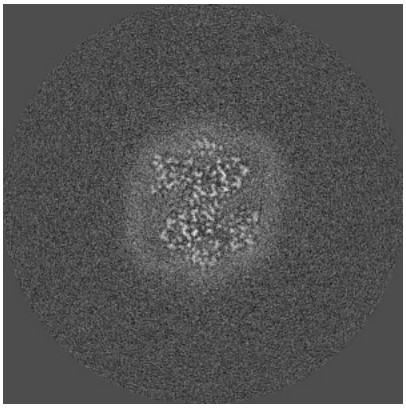
6.3.2 Raw map



X Index: 187



Y Index: 194

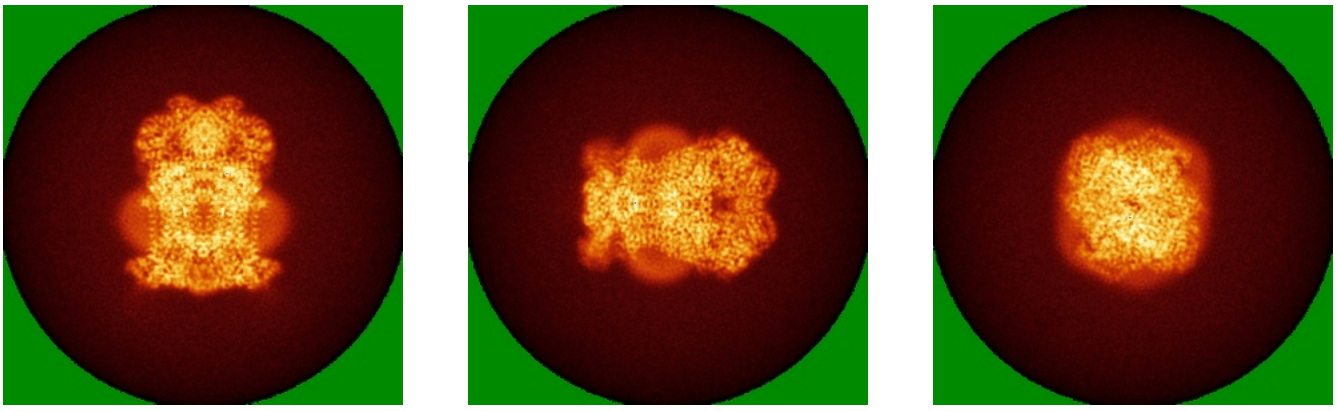


Z Index: 182

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

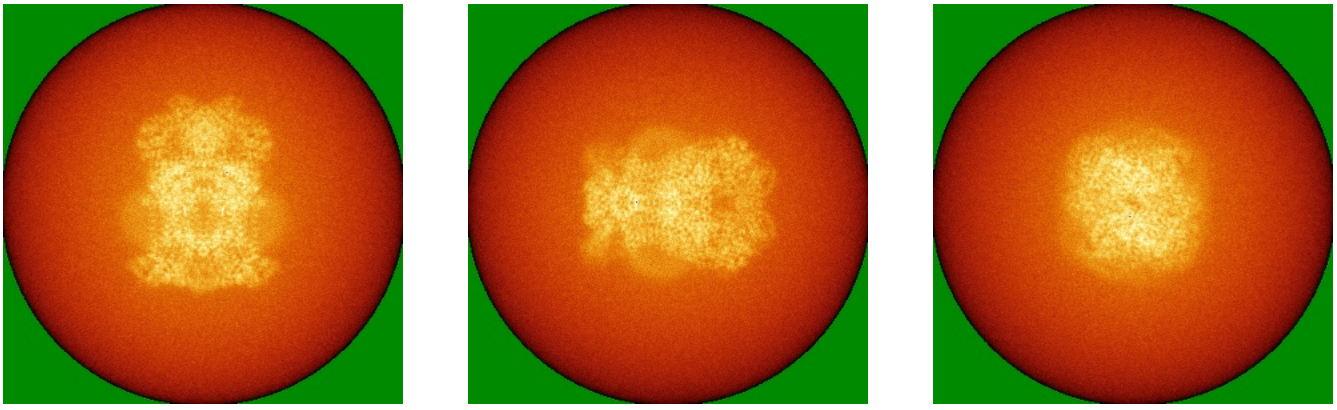
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

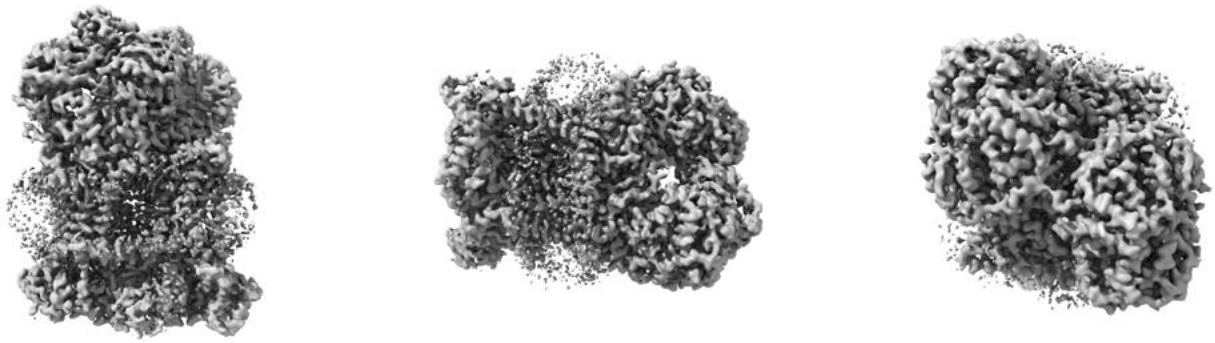


X Y Z

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)

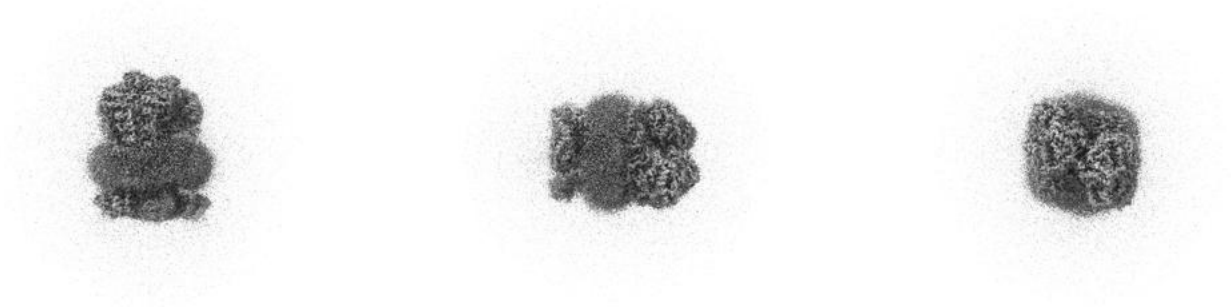
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

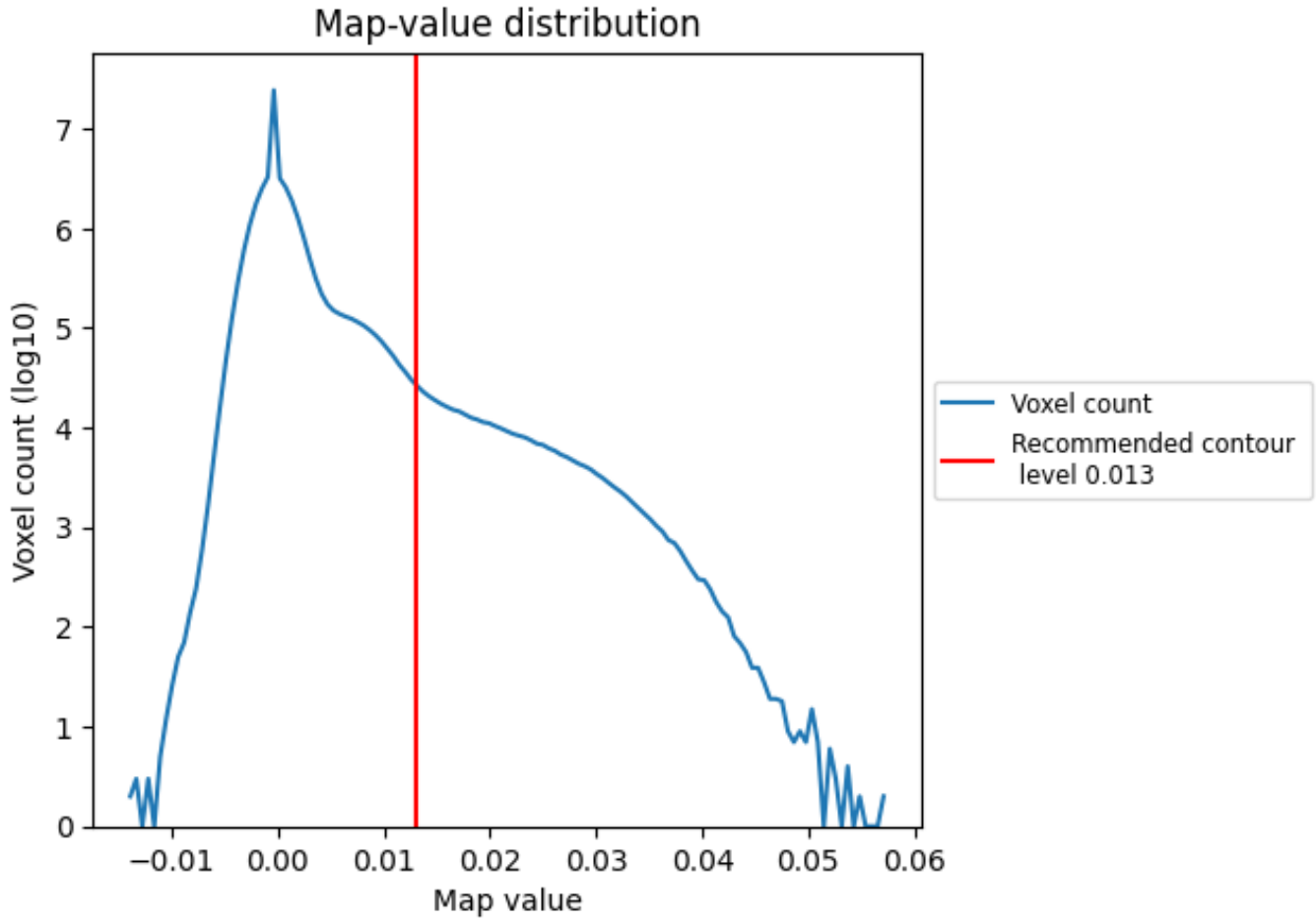
6.6 Mask visualisation (i)

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

7 Map analysis

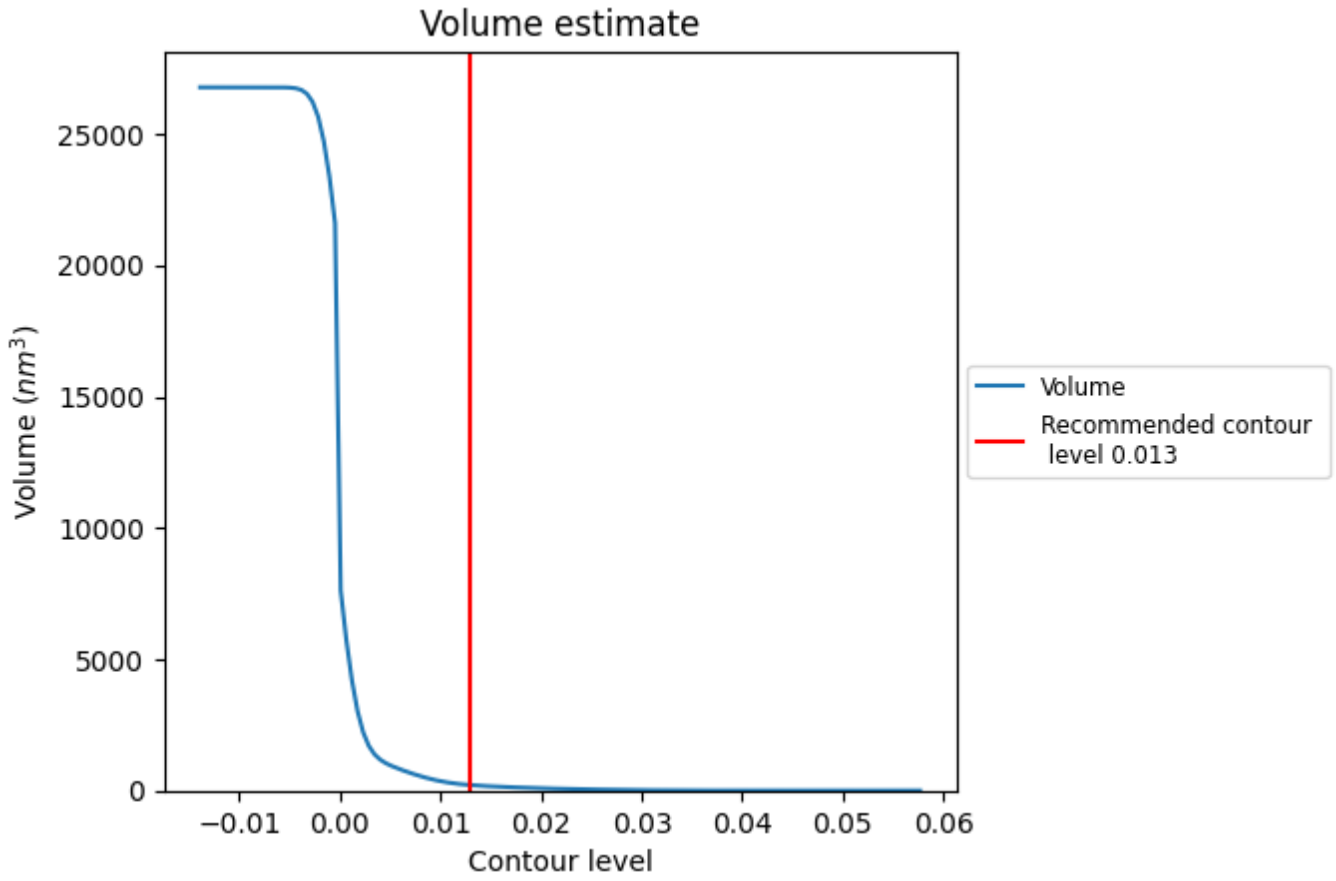
This section contains the results of statistical analysis of the map.

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.

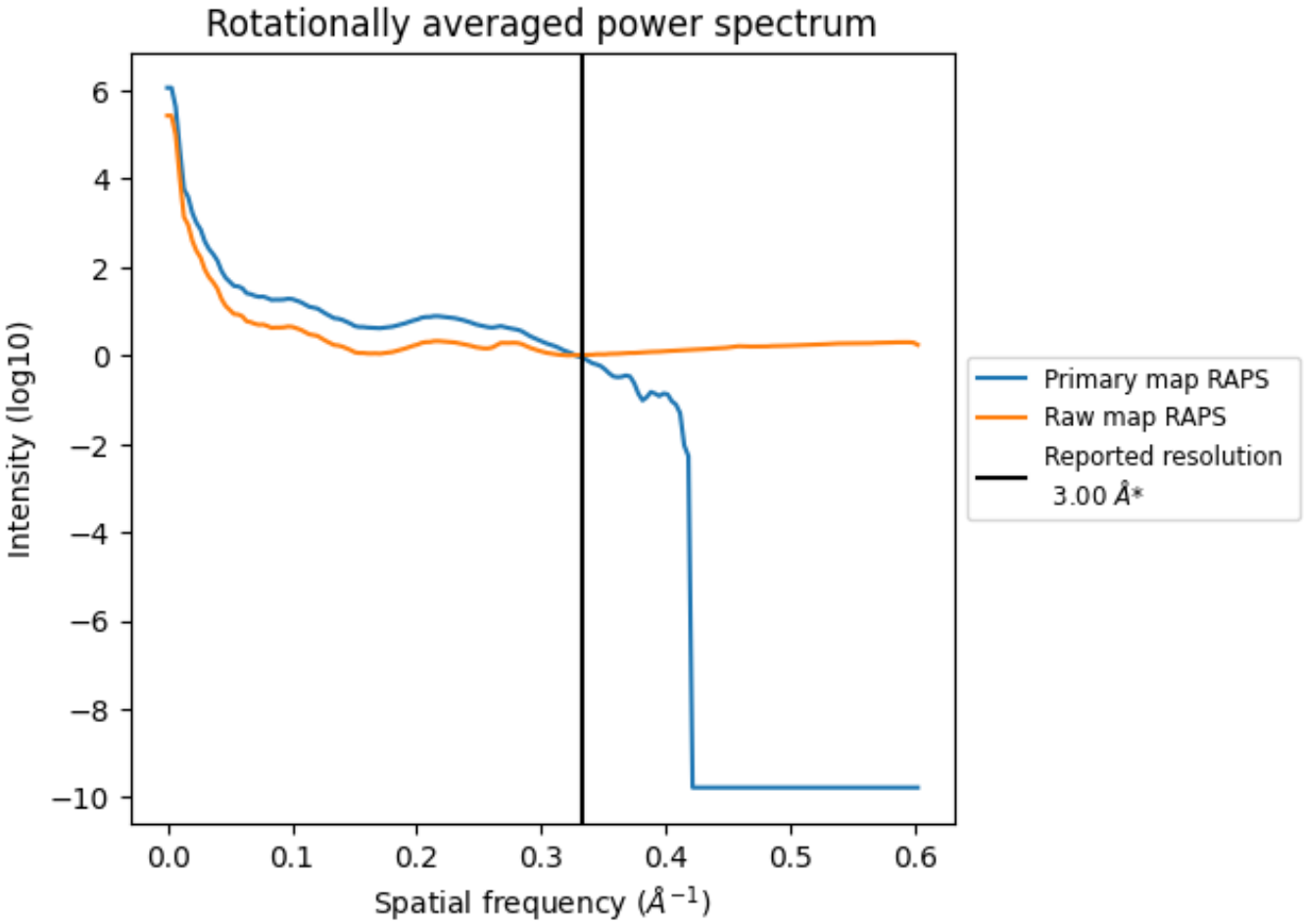
7.2 Volume estimate (i)



The volume at the recommended contour level is 209 nm^3; this corresponds to an approximate mass of 189 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)

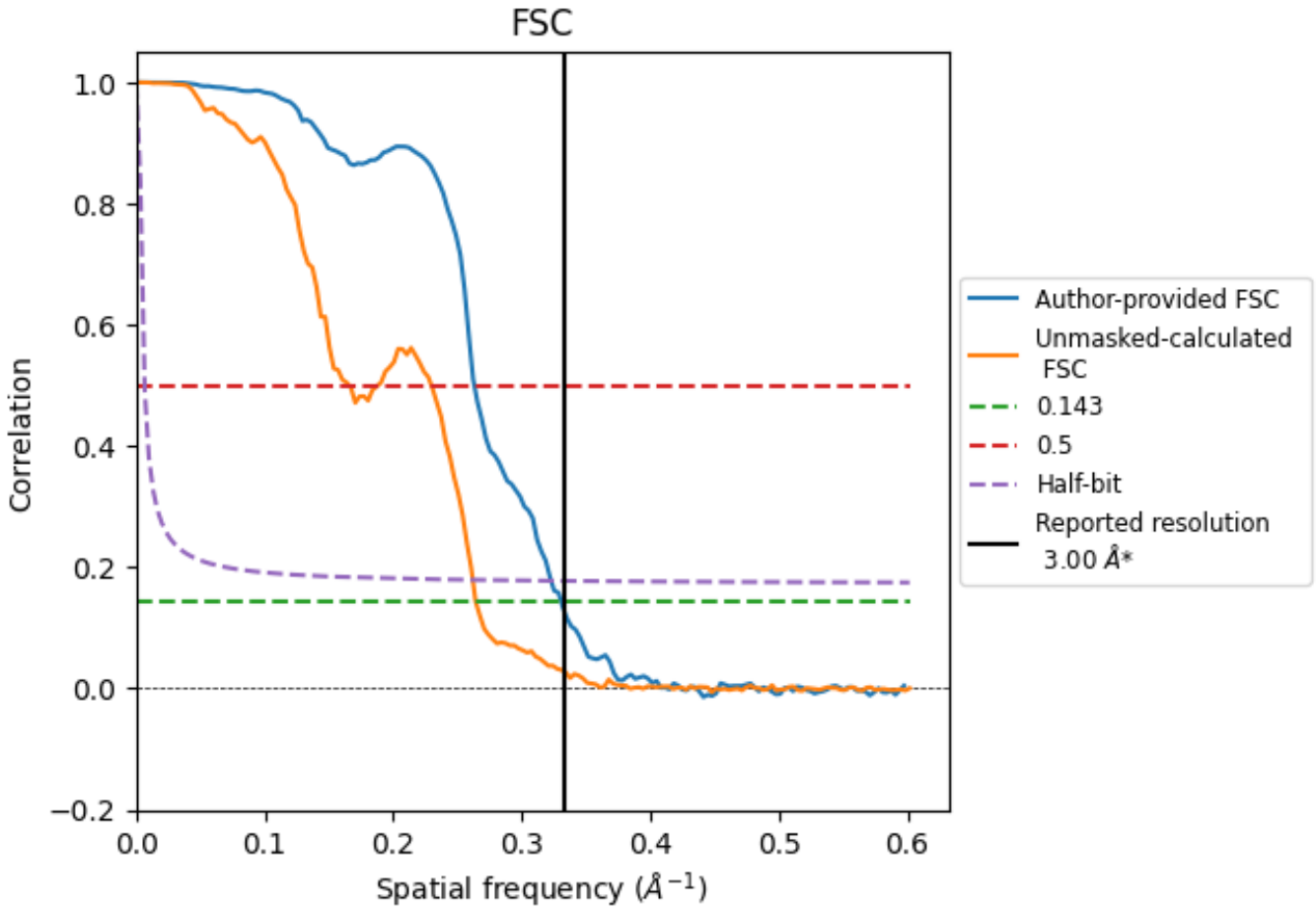


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

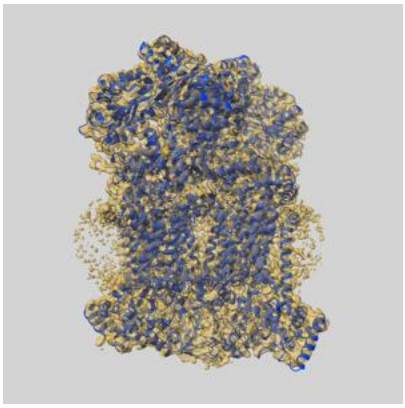
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.80	3.10
Unmasked-calculated*	3.79	6.04	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 3.0 by more than 10 %

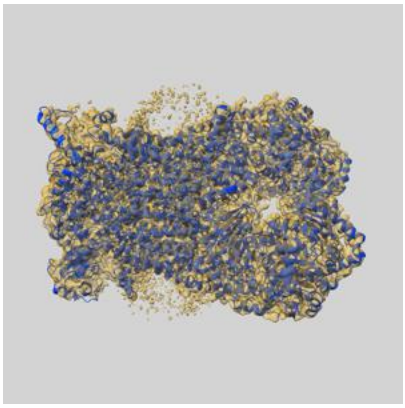
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15322 and PDB model 8ABI. Per-residue inclusion information can be found in section 3 on page 13.

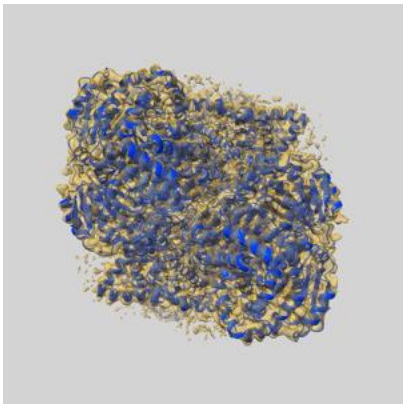
9.1 Map-model overlay



X



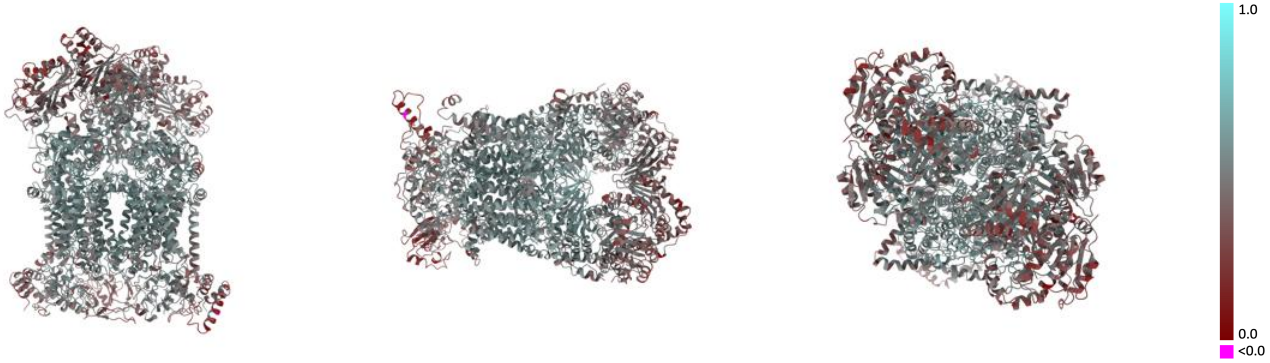
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

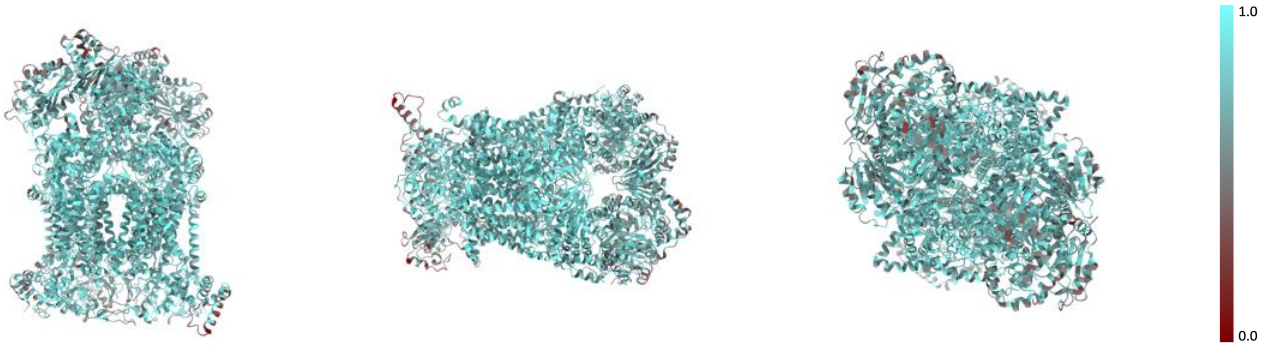
9.2 Q-score mapped to coordinate model (i)



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.

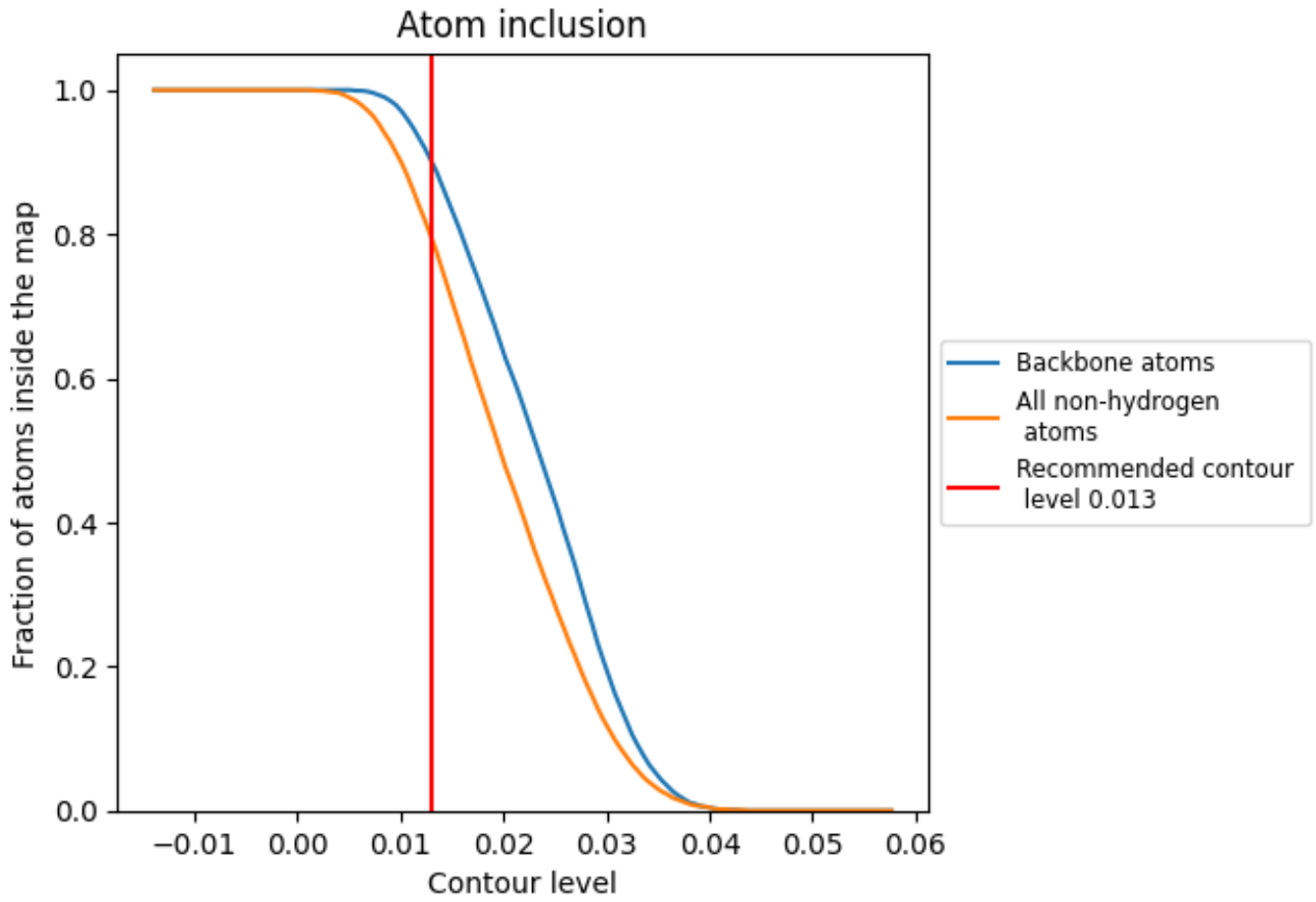
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.4810
A	0.7800	0.4690
B	0.7430	0.4310
C	0.8870	0.5590
D	0.8320	0.4910
E	0.8440	0.5410
F	0.5550	0.2900
G	0.8350	0.5330
H	0.8370	0.5170
I	0.7970	0.5110
J	0.7620	0.4830
L	0.7820	0.4700
M	0.7480	0.4380
N	0.8800	0.5590
O	0.8360	0.4930
P	0.6610	0.3480
Q	0.5740	0.3030
R	0.8320	0.5250
S	0.8540	0.5110
T	0.8290	0.5170
U	0.7960	0.4980

