wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 05:04 pm BST

PDB ID	:	9SFJ / pdb_00009sfj
EMDB ID	:	EMD-54826
Title	:	E.coli cytochrome bd-I dimer in the MK bound open and closed state
Authors	:	van der Velden, T.T.; Kaystha, K.; Bruenle, S.; Jeuken, L.J.C.
Deposited on	:	2025-08-19
Resolution	:	2.52 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:

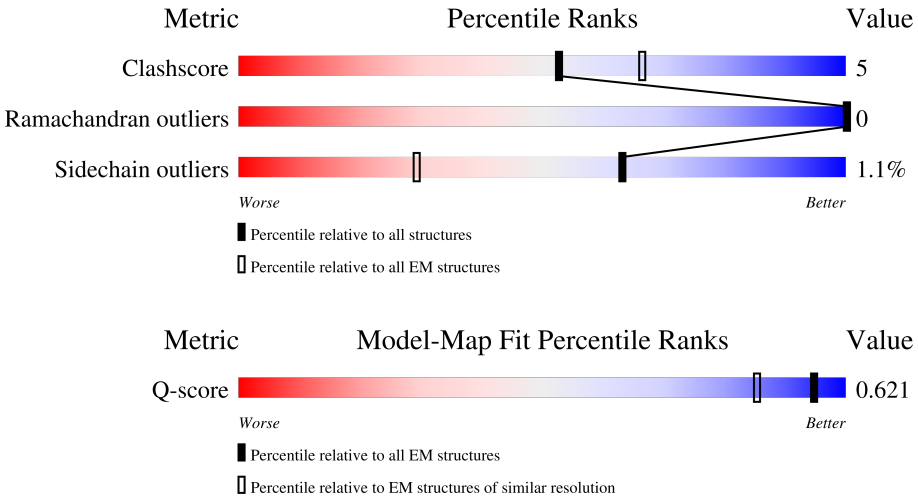
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.52 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.



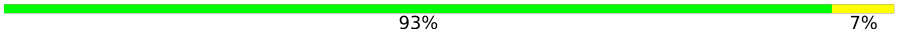
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7226 (2.02 - 3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	522	82% 7% 10%
1	a	522	88% 11%
2	B	379	92% 8%
2	b	379	91% 9%

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Mol	Chain	Length	Quality of chain
3	H	29	
3	h	29	
4	X	37	
4	x	37	

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
6	A1JN4	A	602	X	-	-	-
6	A1JN4	a	607	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 31200 atoms, of which 15734 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 bd-I ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	468	Total	C	H	N	O	S	0	0
			7407	2434	3717	594	637	25		
1	a	514	Total	C	H	N	O	S	0	0
			8116	2668	4068	649	706	25		

- Molecule 2 is a protein called Cytochrome bd-I ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	379	Total	C	H	N	O	S	0	0
			6021	1986	3025	483	505	22		
2	b	379	Total	C	H	N	O	S	0	0
			6021	1986	3025	483	505	22		

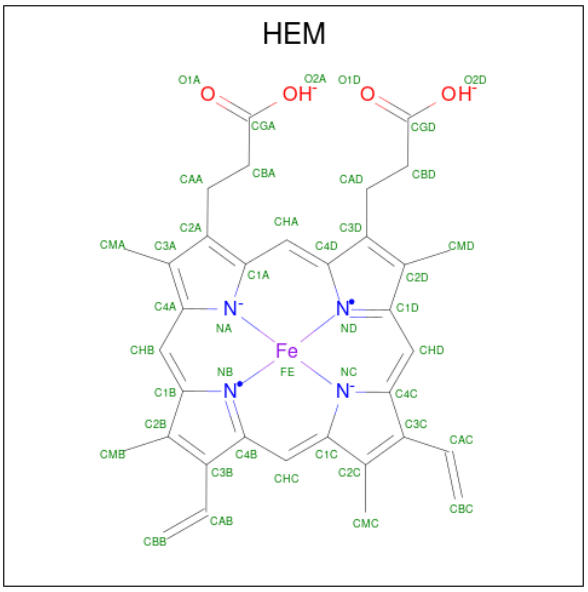
- Molecule 3 is a protein called Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF).

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	29	Total	C	H	N	O	S	0	0
			424	139	215	32	37	1		
3	h	29	Total	C	H	N	O	S	0	0
			432	139	222	32	38	1		

- Molecule 4 is a protein called Cytochrome bd-I ubiquinol oxidase subunit X.

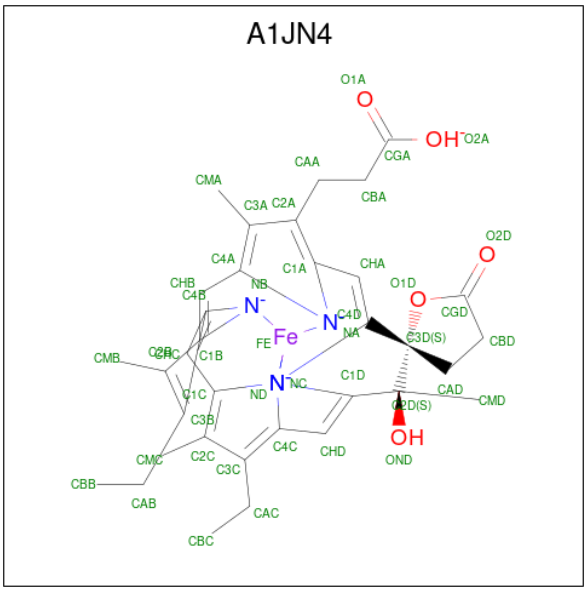
Mol	Chain	Residues	Atoms						AltConf	Trace
4	X	30	Total	C	H	N	O	S	0	0
			451	157	219	34	39	2		
4	x	30	Total	C	H	N	O	S	0	0
			451	157	219	34	39	2		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



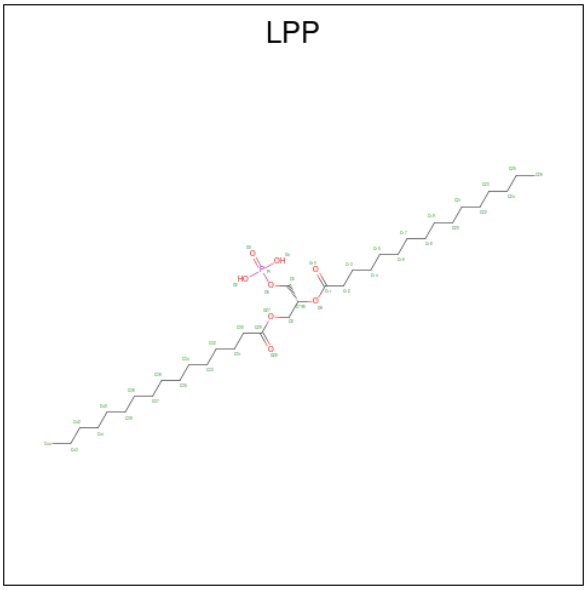
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	a	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 6 is TRANS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: A1JN4) (formula: $C_{34}H_{36}FeN_4O_5$).



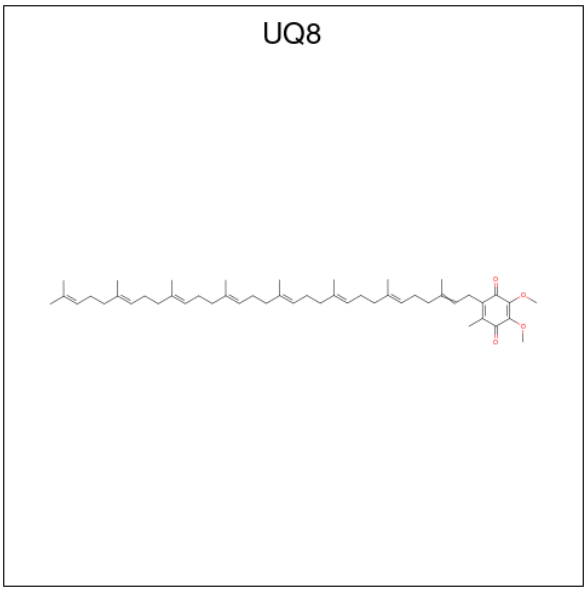
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	Fe	H	N	O	0
			75	34	1	31	4	5	
6	a	1	Total	C	Fe	H	N	O	0
			75	34	1	31	4	5	

- Molecule 7 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$).



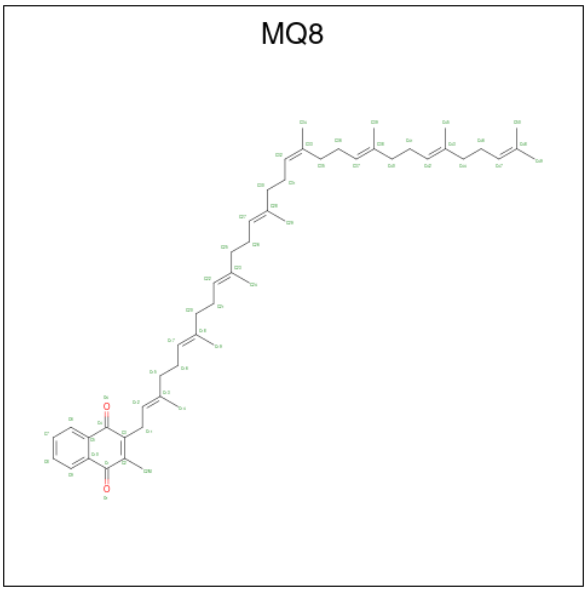
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	O	P	0
			111	35	67	8	1	
7	B	1	Total	C	H	O	P	0
			111	35	67	8	1	
7	a	1	Total	C	H	O	P	0
			111	35	67	8	1	
7	a	1	Total	C	H	O	P	0
			111	35	67	8	1	
7	b	1	Total	C	H	O	P	0
			111	35	67	8	1	
7	x	1	Total	C	H	O	P	0
			111	35	67	8	1	

- Molecule 8 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



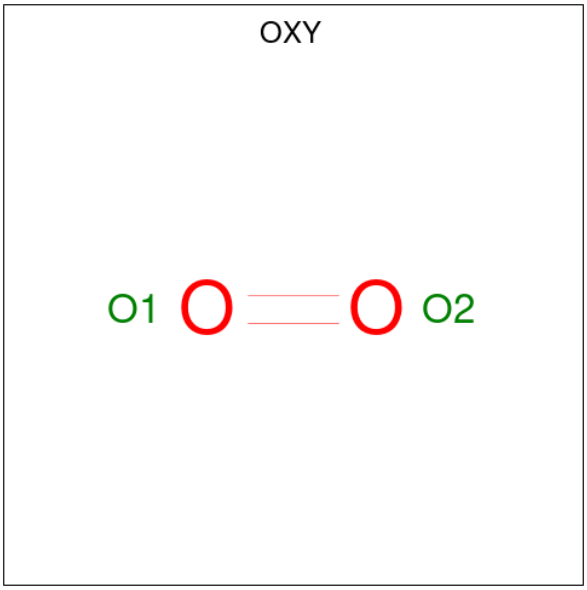
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	H	O	0
			127	49	74	4	
8	B	1	Total	C	H	O	0
			127	49	74	4	
8	a	1	Total	C	H	O	0
			127	49	74	4	
8	b	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 9 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	H	O	0
			125	51	72	2	
9	a	1	Total	C	H	O	0
			125	51	72	2	

- Molecule 10 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		AltConf
10	a	1	Total	O	0
			2	2	

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	O	0
			1	1	
11	B	1	Total	O	0
			1	1	
11	a	3	Total	O	0
			3	3	
11	b	4	Total	O	0
			4	4	

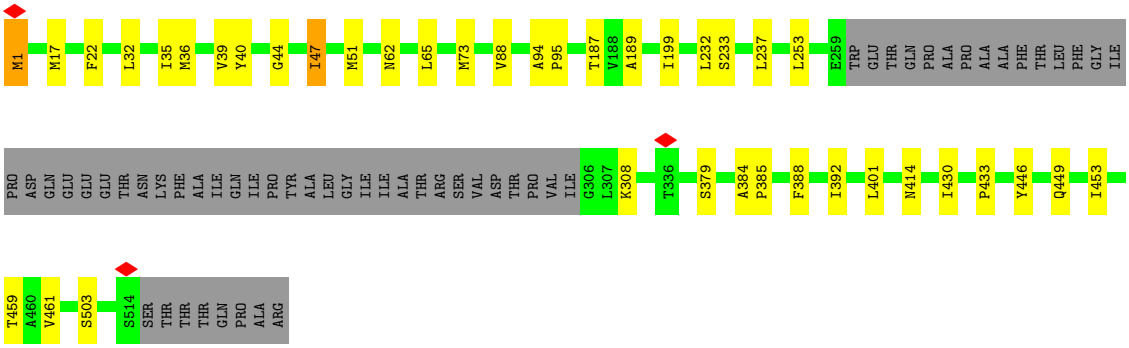
3 Residue-property plots (i)

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 bd-I ubiquinol oxidase subunit 1

Chain A:

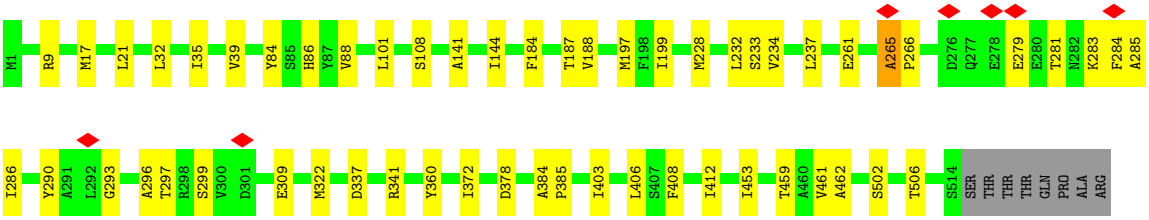




• Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 1

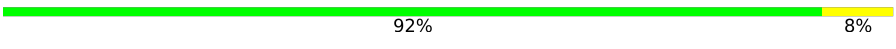
Chain a:





• Molecule 2: Cytochrome bd-I ubiquinol oxidase subunit 2

Chain B:

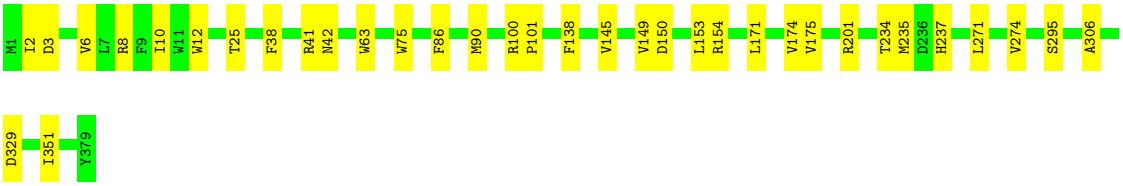




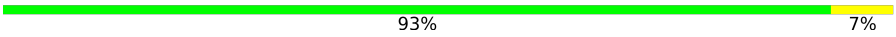
• Molecule 2: Cytochrome bd-I ubiquinol oxidase subunit 2

Chain b:





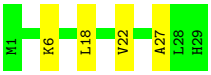
• Molecule 3: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)





• Molecule 3: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)





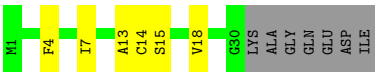
• Molecule 4: Cytochrome bd-I ubiquinol oxidase subunit X





• Molecule 4: Cytochrome bd-I ubiquinol oxidase subunit X





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.005	Depositor
Minimum map value	-1.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, OXY, MQ8, A1JN4, LPP, UQ8

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.16	0/3784	0.42	6/5122 (0.1%)
1	a	0.16	0/4154	0.27	0/5634
2	B	0.14	0/3083	0.32	2/4212 (0.0%)
2	b	0.15	0/3083	0.31	2/4212 (0.0%)
3	H	0.12	0/210	0.19	0/286
3	h	0.15	0/211	0.32	0/286
4	X	0.15	0/239	0.25	0/326
4	x	0.14	0/239	0.20	0/326
All	All	0.15	0/15003	0.33	10/20404 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	MET	CA-C-N	10.32	141.25	121.54
1	A	1	MET	C-N-CA	10.32	141.25	121.54
1	A	47	ILE	CA-C-N	9.27	134.39	120.31
1	A	47	ILE	C-N-CA	9.27	134.39	120.31
1	A	503	SER	CA-C-N	8.19	132.08	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	265	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3690	3717	3726	30	0
1	a	4048	4068	4078	36	0
2	B	2996	3025	3025	21	0
2	b	2996	3025	3025	22	0
3	H	209	215	238	2	0
3	h	210	222	238	3	0
4	X	232	219	230	3	0
4	x	232	219	230	3	0
5	A	86	60	60	13	0
5	a	86	60	60	14	0
6	A	44	31	0	0	0
6	a	44	31	0	1	0
7	A	44	67	67	4	0
7	B	44	67	67	0	0
7	a	88	134	134	3	0
7	b	44	67	67	0	0
7	x	44	67	67	0	0
8	A	53	74	74	10	0
8	B	53	74	74	5	0
8	a	53	74	74	12	0
8	b	53	74	74	8	0
9	A	53	72	72	7	0
9	a	53	72	72	6	0
10	a	2	0	0	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	a	3	0	0	1	0
11	b	4	0	0	0	0
All	All	15466	15734	15752	165	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 5.

The worst 5 of 165 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:a:309:GLU:N	1:a:309:GLU:OE1	2.09	0.85
7:A:603:LPP:H442	7:A:603:LPP:H261	1.58	0.84
1:A:187:THR:OG1	5:A:601:HEM:O1A	1.96	0.82
5:A:604:HEM:HBC2	5:A:604:HEM:HHD	1.62	0.82
8:a:604:UQ8:H10A	8:a:604:UQ8:C15	2.10	0.81

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/522 (89%)	457 (98%)	7 (2%)	0	100	100
1	a	512/522 (98%)	502 (98%)	10 (2%)	0	100	100
2	B	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
2	b	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
3	H	27/29 (93%)	27 (100%)	0	0	100	100
3	h	27/29 (93%)	27 (100%)	0	0	100	100
4	X	28/37 (76%)	28 (100%)	0	0	100	100
4	x	28/37 (76%)	28 (100%)	0	0	100	100
All	All	1840/1934 (95%)	1813 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	381/426 (89%)	379 (100%)	2 (0%)	81 91
1	a	419/426 (98%)	412 (98%)	7 (2%)	53 77
2	B	313/313 (100%)	309 (99%)	4 (1%)	61 81
2	b	313/313 (100%)	310 (99%)	3 (1%)	68 85
3	H	24/24 (100%)	24 (100%)	0	100 100
3	h	24/24 (100%)	24 (100%)	0	100 100
4	X	23/28 (82%)	23 (100%)	0	100 100
4	x	23/28 (82%)	22 (96%)	1 (4%)	26 49
All	All	1520/1582 (96%)	1503 (99%)	17 (1%)	63 83

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	145	VAL
4	x	15	SER
1	a	234	VAL
1	a	261	GLU
1	a	290	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	X	26	HIS
1	a	152	GLN
2	b	374	ASN
1	a	263	GLN
2	B	56	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

19 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	$\#\|Z\| > 2$
8	UQ8	A	605	-	53,53,53	1.21	2 (3%)	64,67,67	1.51	14 (21%)
10	OXY	a	608	6	1,1,1	0.15	0	-		
6	A1JN4	A	602	1	46,52,52	2.91	14 (30%)	62,89,89	4.63	38 (61%)
7	LPP	B	401	-	43,43,43	1.09	2 (4%)	47,48,48	1.16	2 (4%)
6	A1JN4	a	607	10,1	46,52,52	2.90	16 (34%)	62,89,89	4.61	39 (62%)
9	MQ8	a	605	-	54,54,54	2.74	24 (44%)	66,69,69	7.78	27 (40%)
5	HEM	A	604	1	50,50,50	1.44	7 (14%)	66,82,82	1.31	8 (12%)
7	LPP	a	606	-	43,43,43	1.11	2 (4%)	47,48,48	1.18	3 (6%)
7	LPP	x	101	-	43,43,43	1.10	2 (4%)	47,48,48	1.11	2 (4%)
8	UQ8	b	402	-	53,53,53	2.31	15 (28%)	64,67,67	4.01	26 (40%)
5	HEM	A	601	1	50,50,50	1.43	6 (12%)	66,82,82	1.32	7 (10%)
9	MQ8	A	606	-	54,54,54	2.76	24 (44%)	66,69,69	7.87	28 (42%)
7	LPP	A	603	-	43,43,43	1.07	2 (4%)	47,48,48	1.08	2 (4%)
7	LPP	b	401	-	43,43,43	1.10	2 (4%)	47,48,48	1.14	2 (4%)
8	UQ8	B	402	-	53,53,53	2.27	15 (28%)	64,67,67	4.11	26 (40%)
5	HEM	a	601	1	50,50,50	1.38	6 (12%)	66,82,82	1.30	6 (9%)
7	LPP	a	602	-	43,43,43	1.08	2 (4%)	47,48,48	1.16	2 (4%)
5	HEM	a	603	1	50,50,50	1.44	7 (14%)	66,82,82	1.32	9 (13%)
8	UQ8	a	604	-	53,53,53	1.18	2 (3%)	64,67,67	1.49	13 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	a	603	1	-	6/14/54/54	-
5	HEM	A	604	1	-	6/14/54/54	-
7	LPP	a	606	-	-	24/45/45/45	-
8	UQ8	A	605	-	-	8/51/75/75	0/1/1/1
8	UQ8	a	604	-	-	12/51/75/75	0/1/1/1
7	LPP	A	603	-	-	14/45/45/45	-
7	LPP	b	401	-	-	23/45/45/45	-
6	A1JN4	A	602	1	1/1/12/12	6/9/89/89	0/1/9/9
7	LPP	B	401	-	-	21/45/45/45	-
7	LPP	x	101	-	-	21/45/45/45	-
5	HEM	a	601	1	-	5/14/54/54	-
8	UQ8	B	402	-	-	7/51/75/75	0/1/1/1
8	UQ8	b	402	-	-	9/51/75/75	0/1/1/1
5	HEM	A	601	1	-	3/14/54/54	-
9	MQ8	a	605	-	-	11/47/67/67	0/2/2/2
6	A1JN4	a	607	10,1	1/1/12/12	5/9/89/89	0/1/9/9
9	MQ8	A	606	-	-	11/47/67/67	0/2/2/2
7	LPP	a	602	-	-	20/45/45/45	-

The worst 5 of 150 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	A1JN4	C3D-C2D	-11.70	1.26	1.55
6	a	607	A1JN4	C3D-C2D	-11.64	1.26	1.55
8	b	402	UQ8	C6-C1	10.23	1.53	1.35
8	B	402	UQ8	C6-C1	10.05	1.53	1.35
9	a	605	MQ8	C3-C2	8.00	1.49	1.35

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	606	MQ8	C30-C28-C27	21.03	163.67	121.12
9	A	606	MQ8	C44-C43-C42	20.90	163.41	121.12
9	a	605	MQ8	C30-C28-C27	20.57	162.73	121.12
9	a	605	MQ8	C44-C43-C42	20.24	162.07	121.12
9	A	606	MQ8	C19-C18-C17	17.02	167.33	123.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	602	A1JN4	NB
6	a	607	A1JN4	NB

5 of 212 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	HEM	C1A-C2A-CAA-CBA
5	A	601	HEM	C3A-C2A-CAA-CBA
5	a	601	HEM	C1A-C2A-CAA-CBA
7	A	603	LPP	C12-C11-O9-C7
7	B	401	LPP	C6-O5-P1-O2

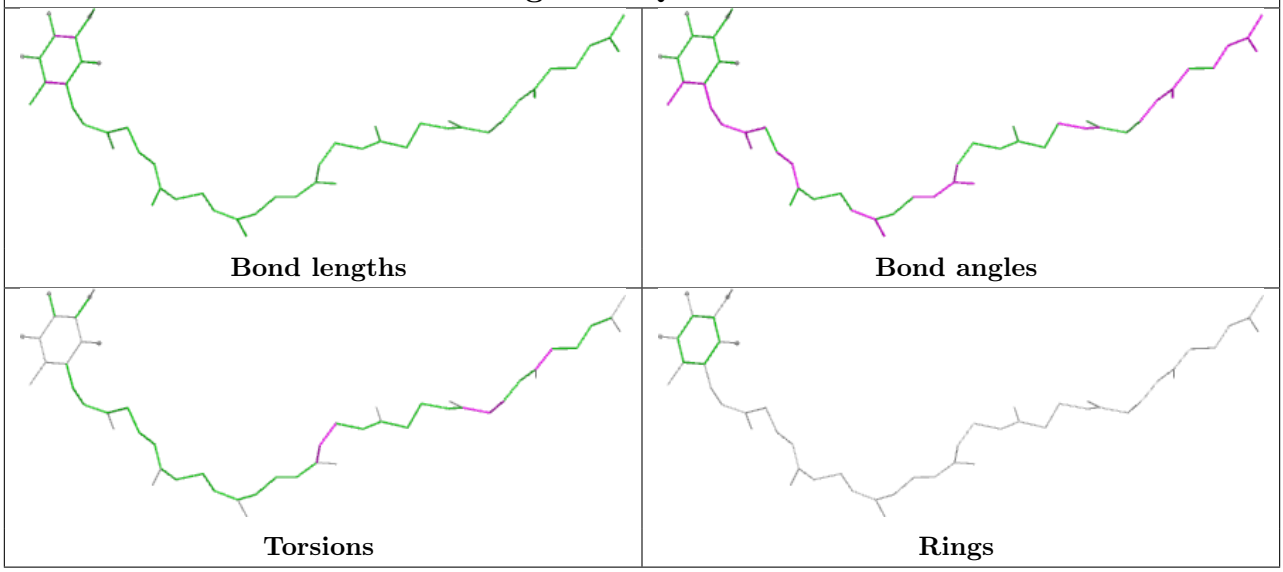
There are no ring outliers.

13 monomers are involved in 82 short contacts:

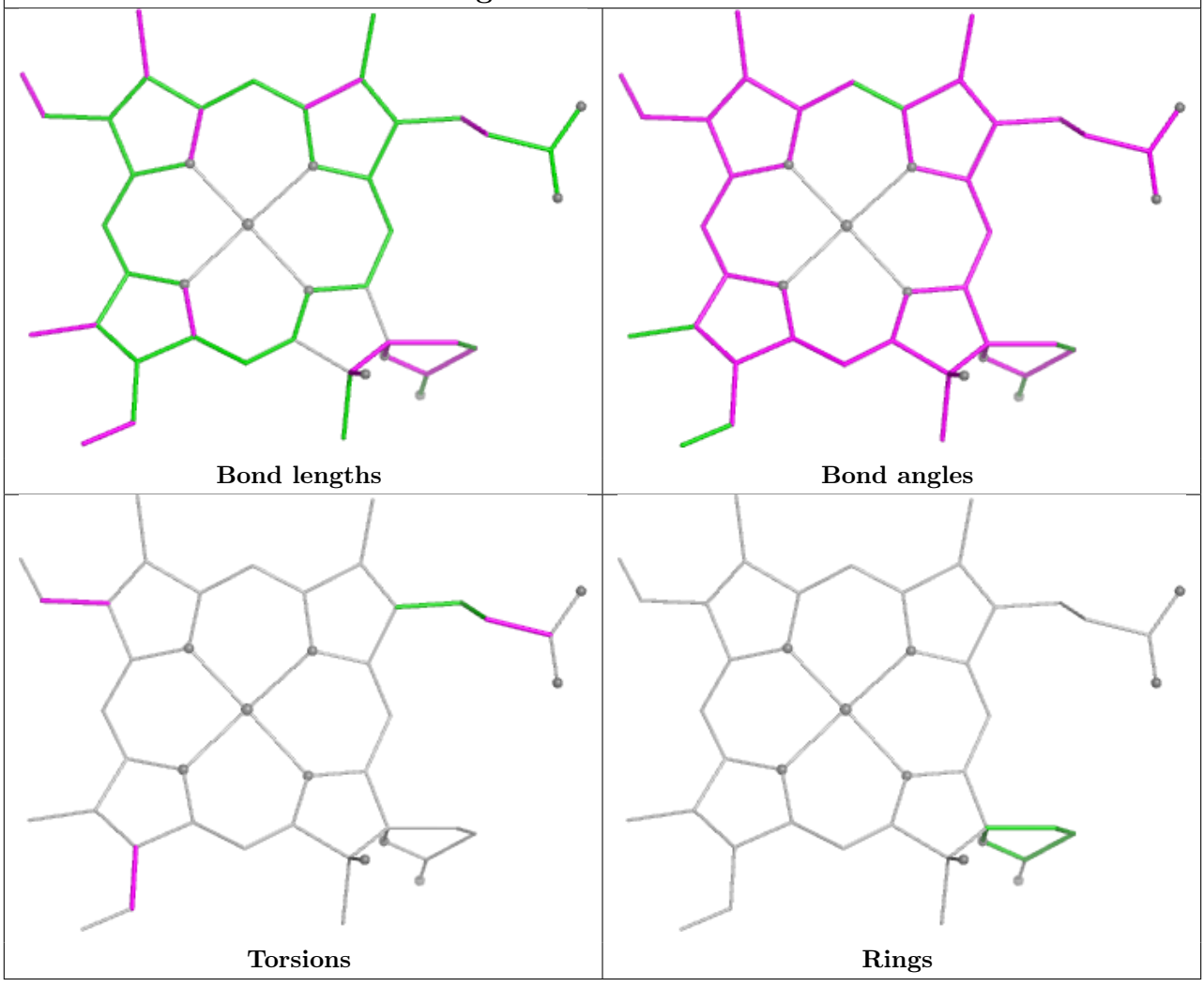
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	605	UQ8	10	0
6	a	607	A1JN4	1	0
9	a	605	MQ8	6	0
5	A	604	HEM	6	0
8	b	402	UQ8	8	0
5	A	601	HEM	7	0
9	A	606	MQ8	7	0
7	A	603	LPP	4	0
8	B	402	UQ8	5	0
5	a	601	HEM	7	0
7	a	602	LPP	3	0
5	a	603	HEM	7	0
8	a	604	UQ8	12	0

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.

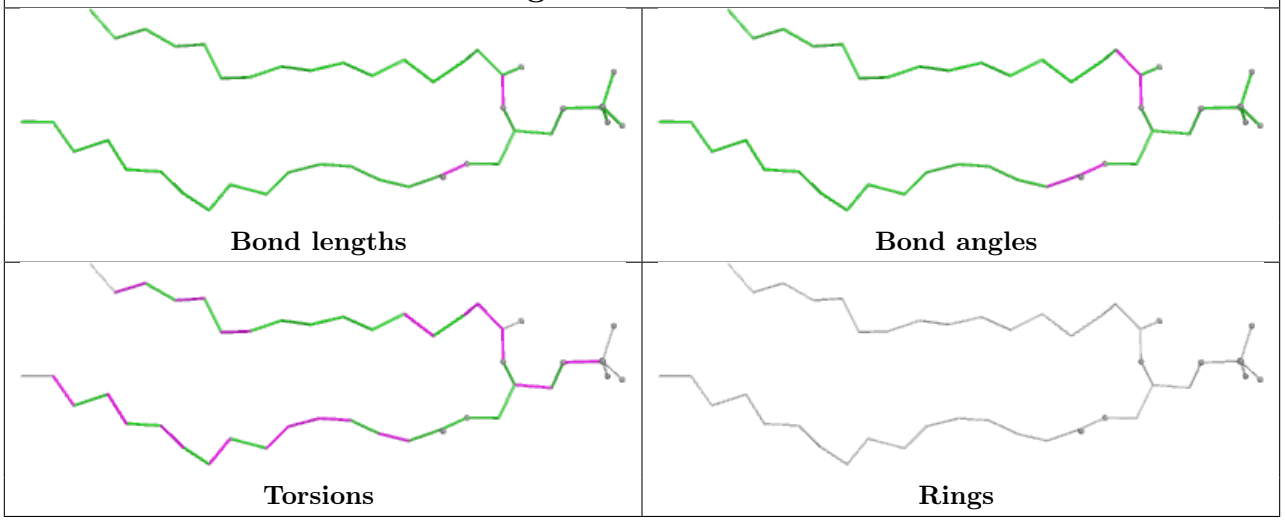
Ligand UQ8 A 605



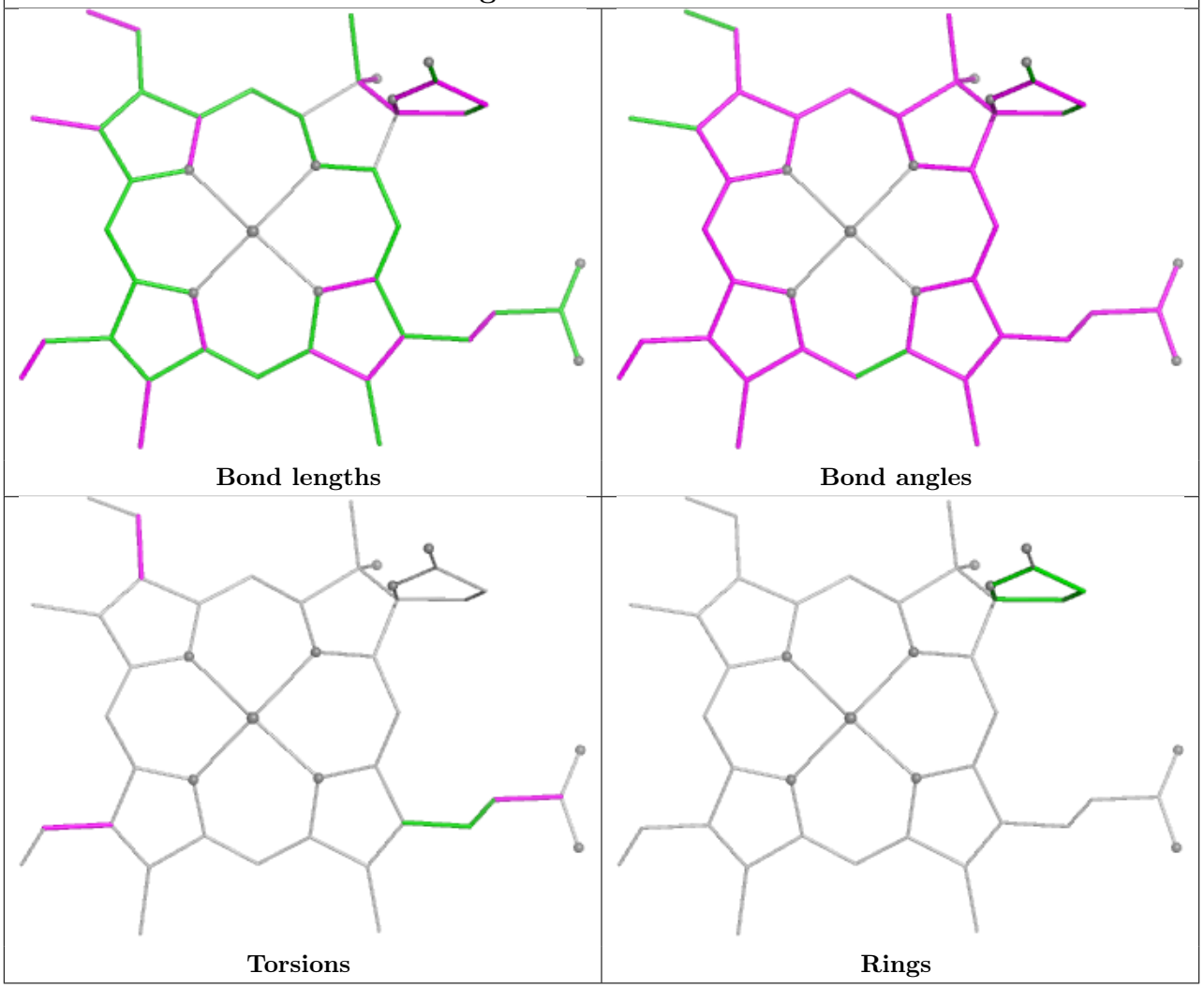
Ligand A1JN4 A 602



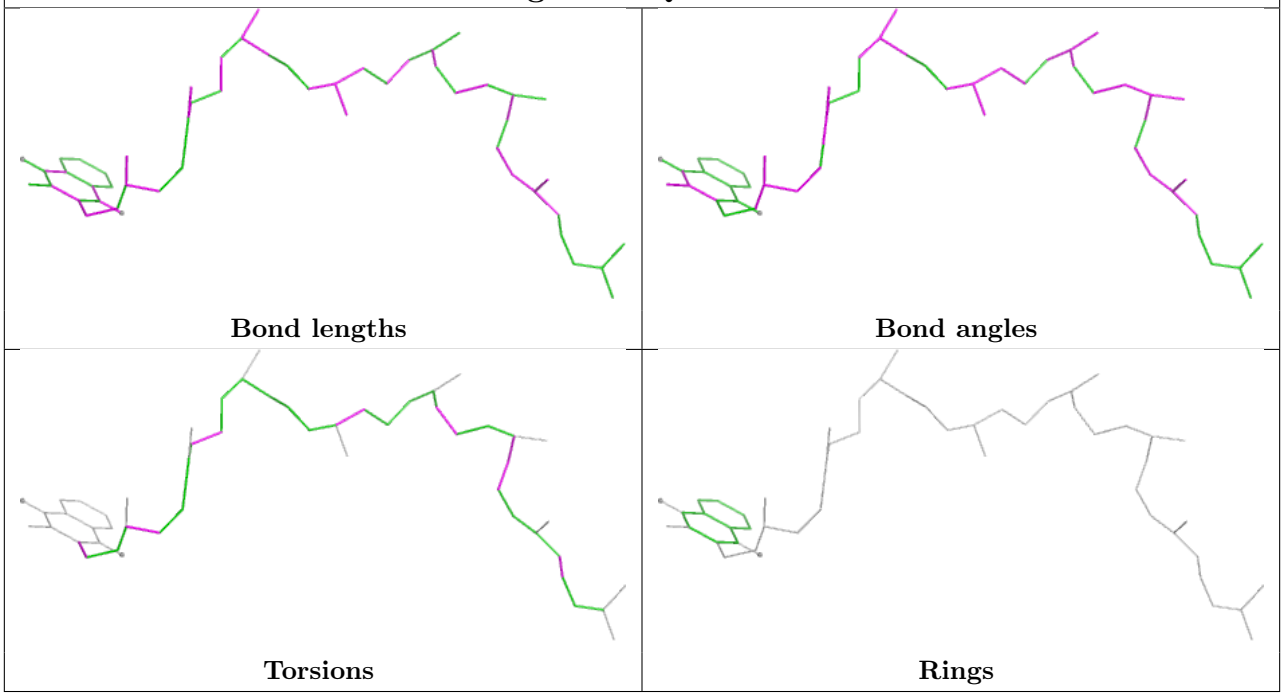
Ligand LPP B 401



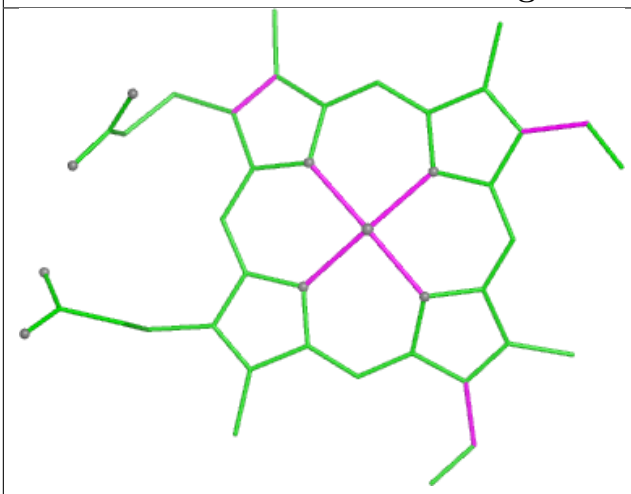
Ligand A1JN4 a 607



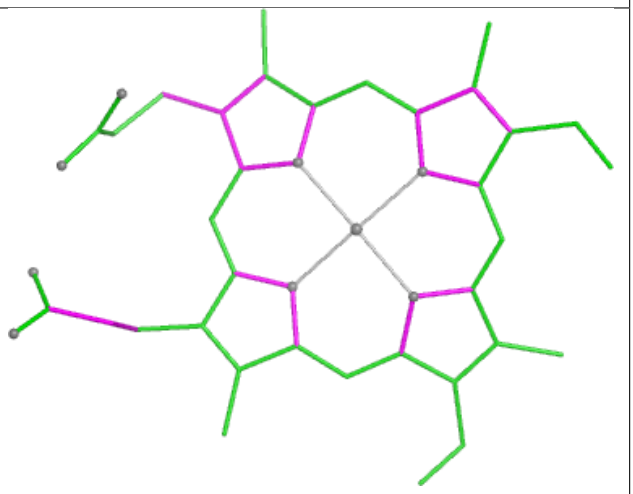
Ligand MQ8 a 605



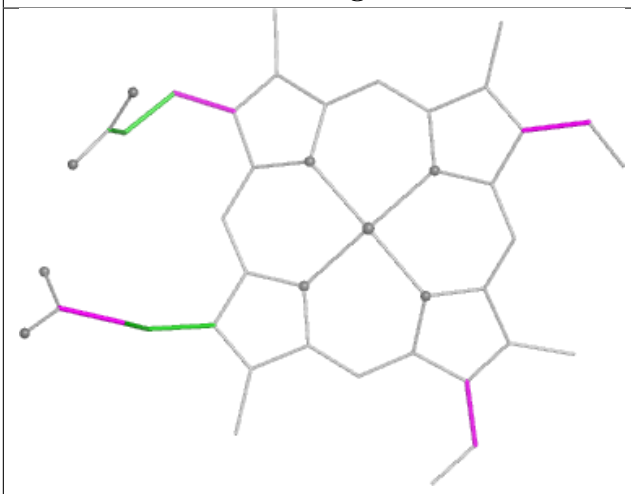
Ligand HEM A 604



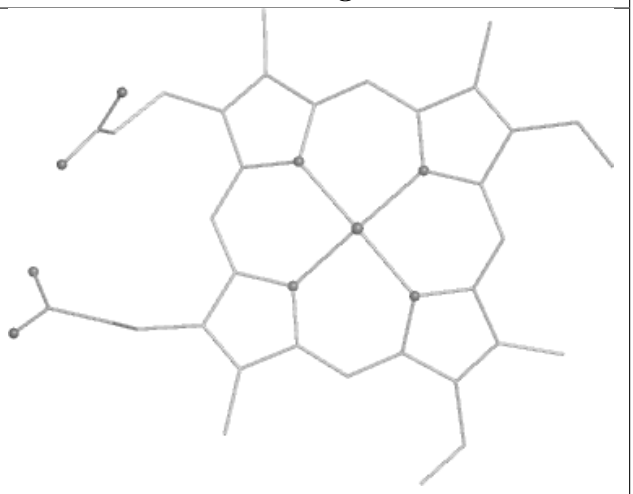
Bond lengths



Bond angles

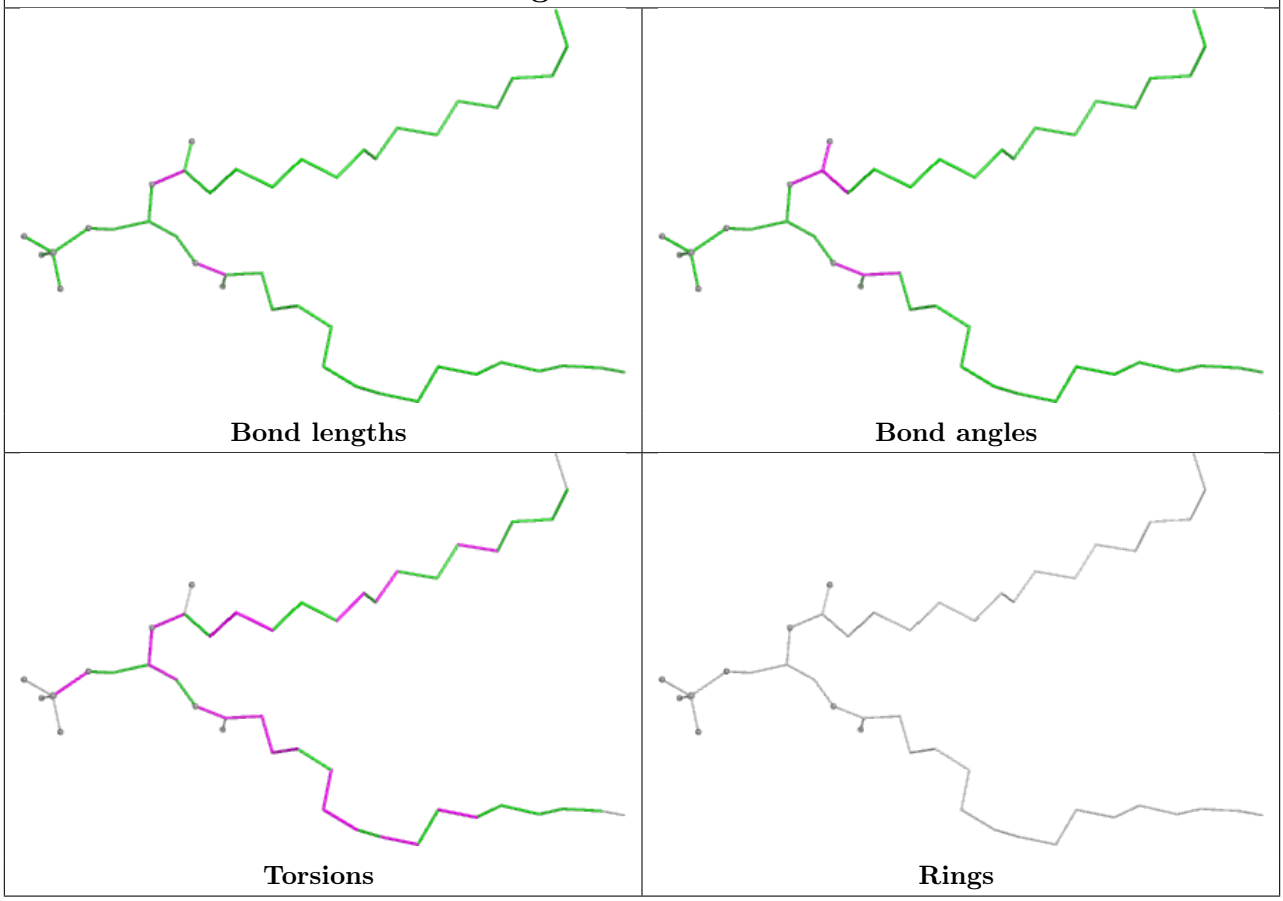


Torsions

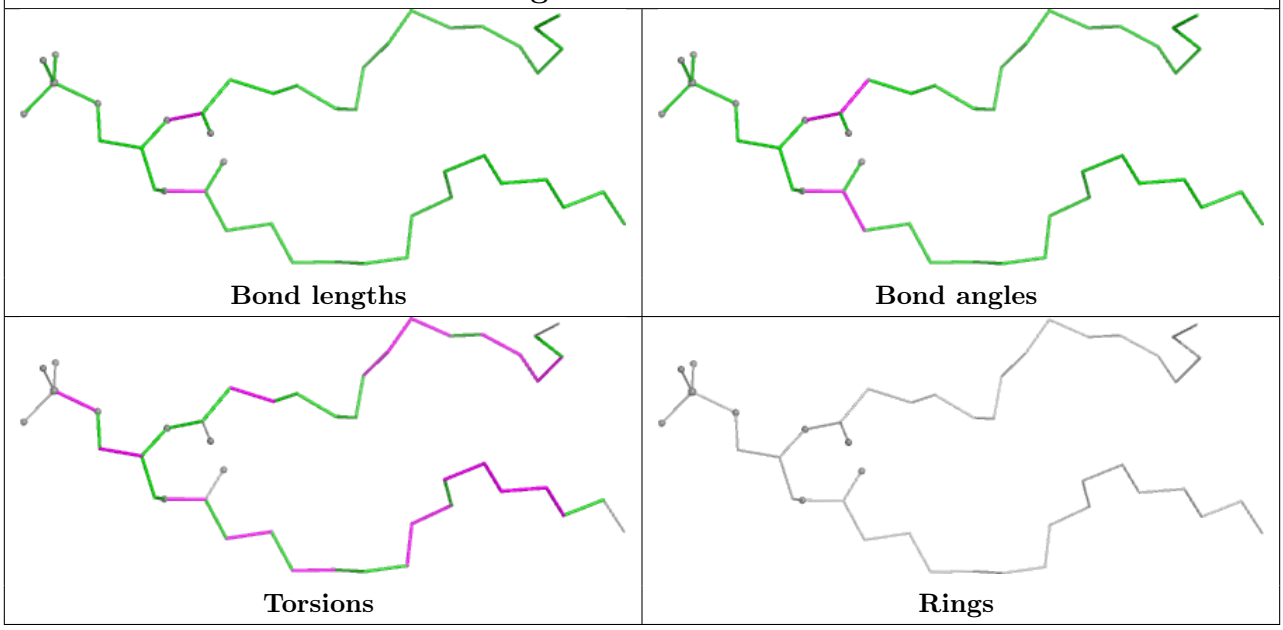


Rings

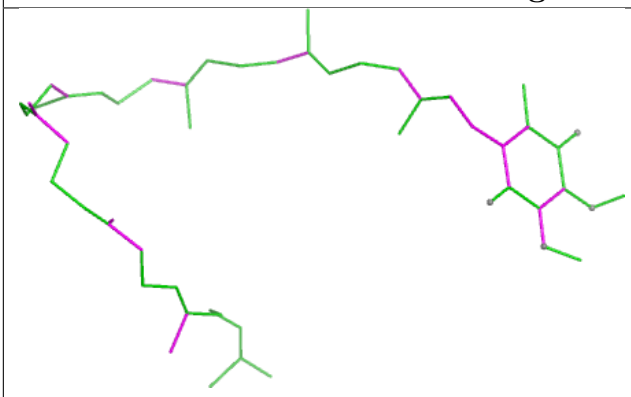
Ligand LPP a 606



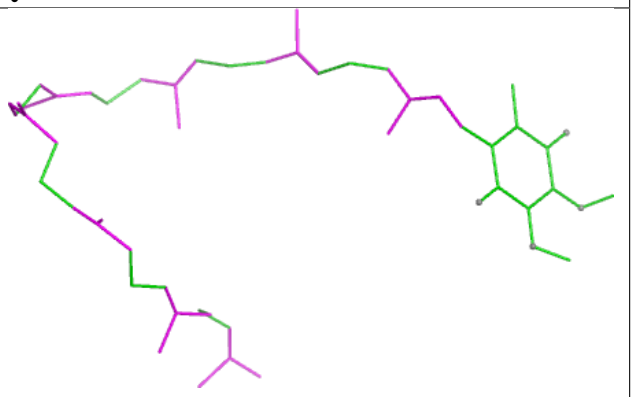
Ligand LPP x 101



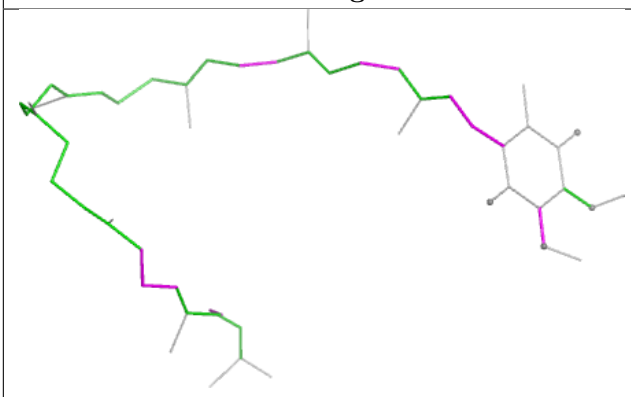
Ligand UQ8 b 402



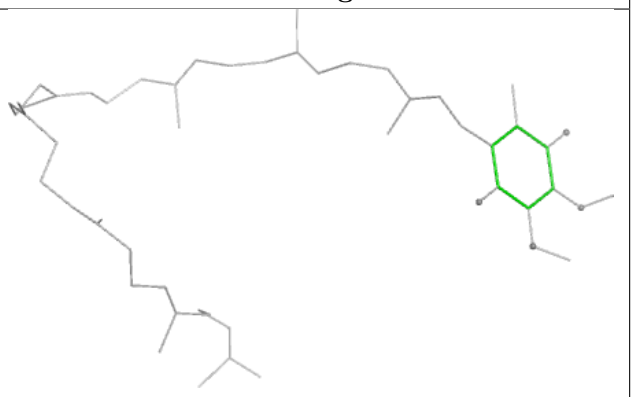
Bond lengths



Bond angles

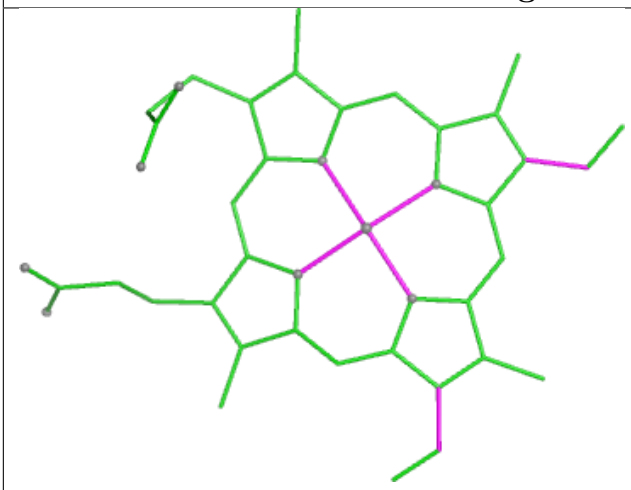


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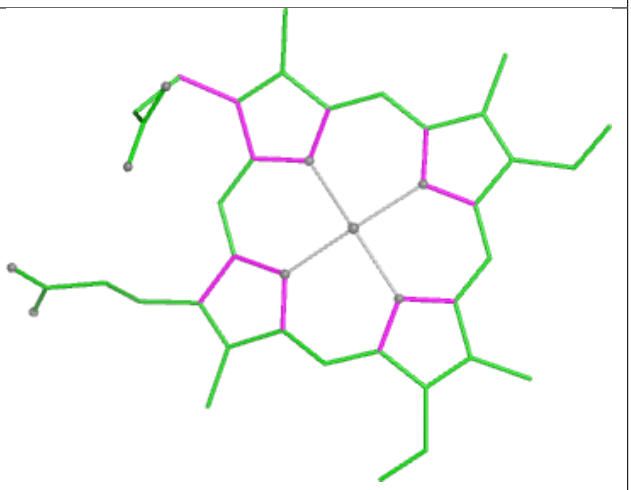


Rings

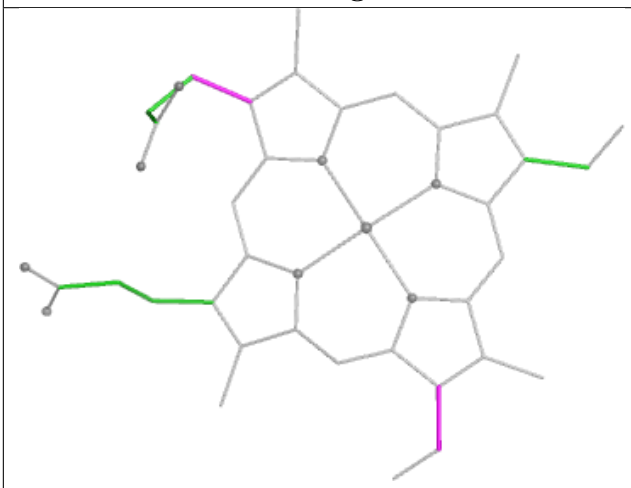
Ligand HEM A 601



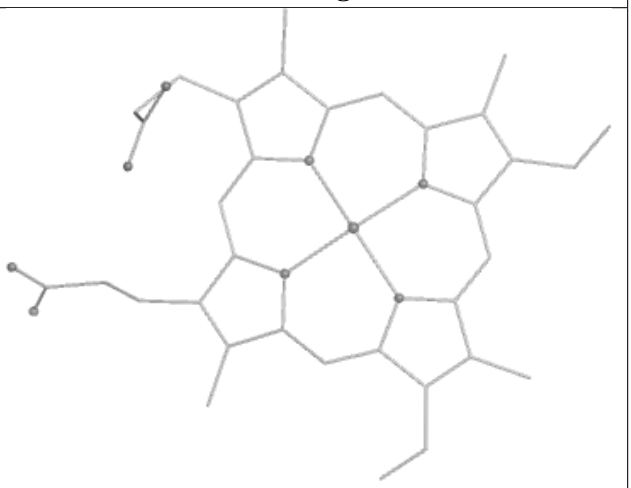
Bond lengths



Bond angles

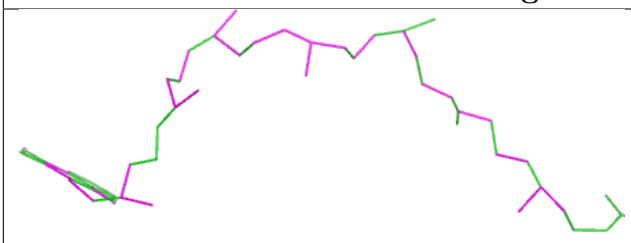


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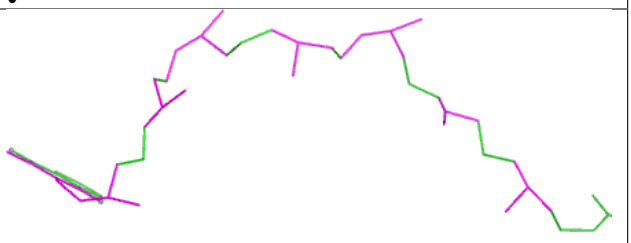


Rings

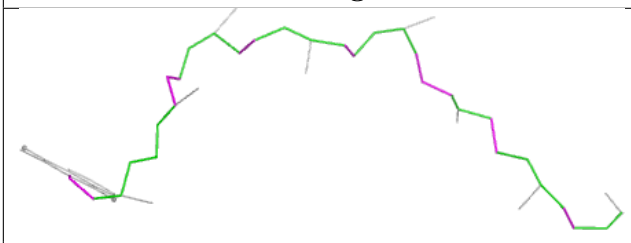
Ligand MQ8 A 606



Bond lengths



Bond angles

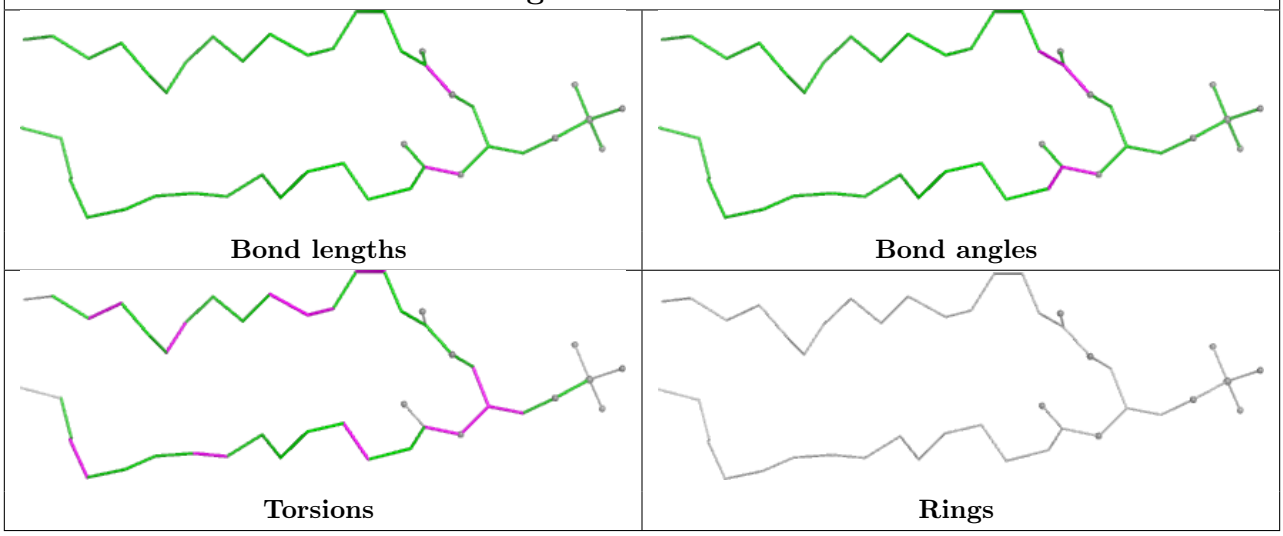


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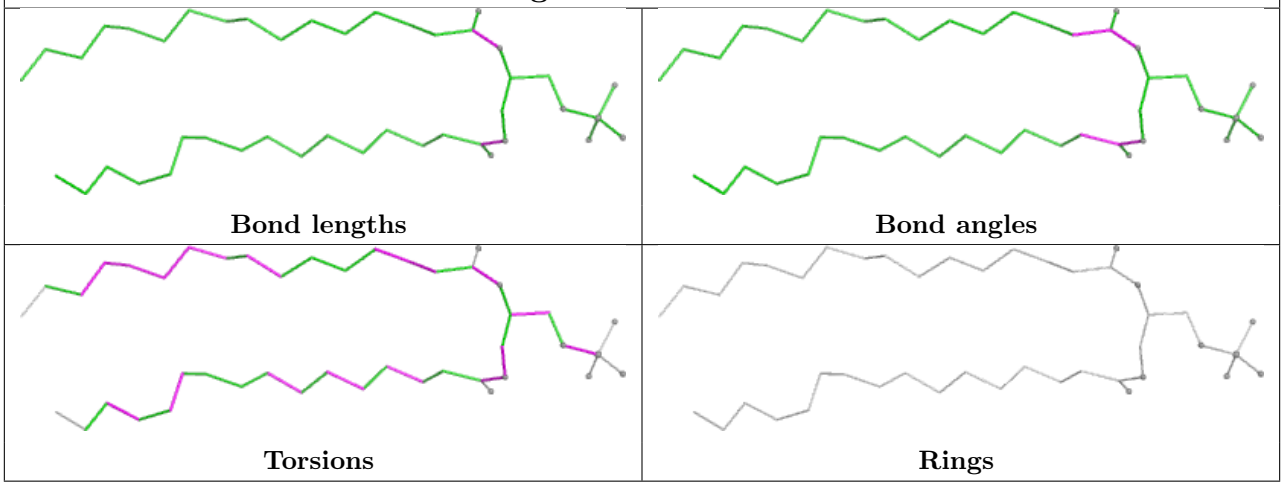


Rings

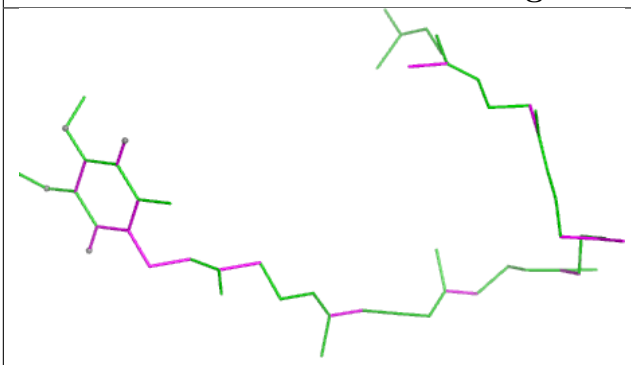
Ligand LPP A 603



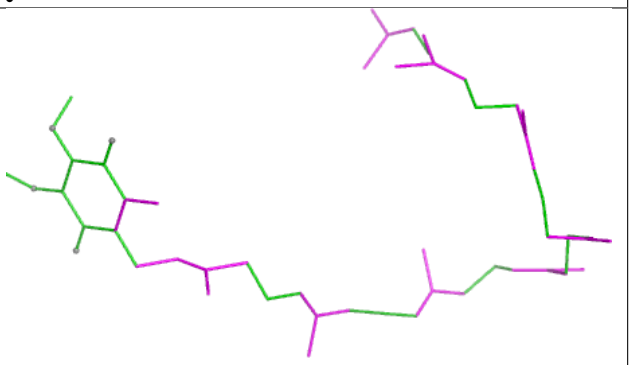
Ligand LPP b 401



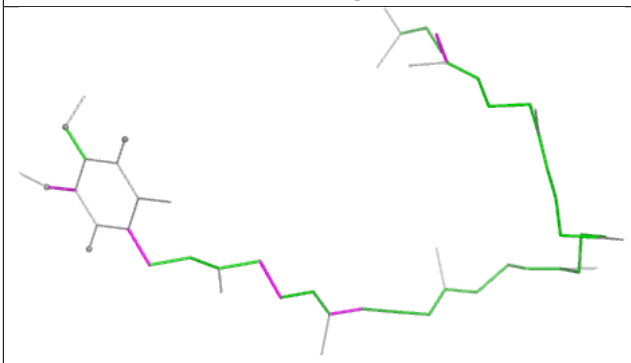
Ligand UQ8 B 402



Bond lengths



Bond angles

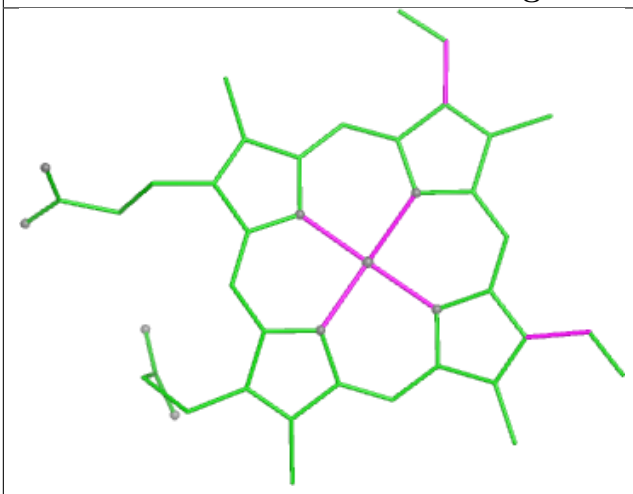


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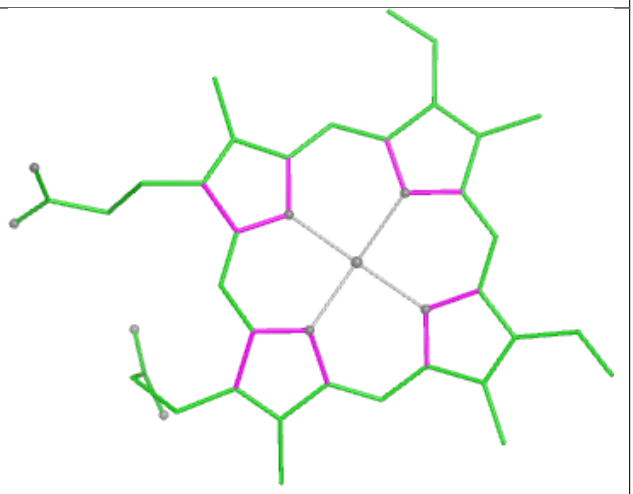


Rings

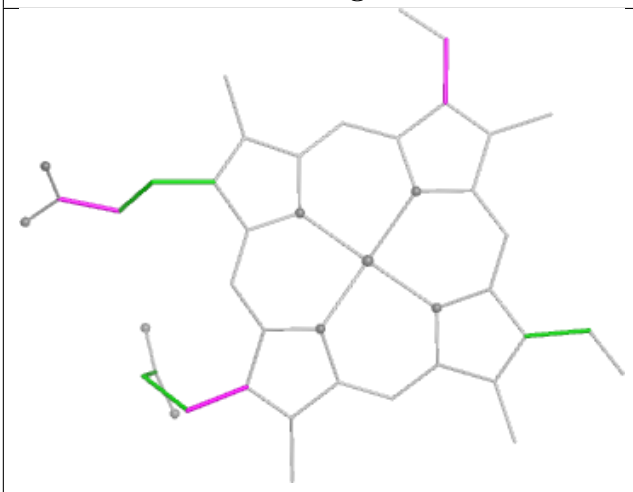
Ligand HEM a 601



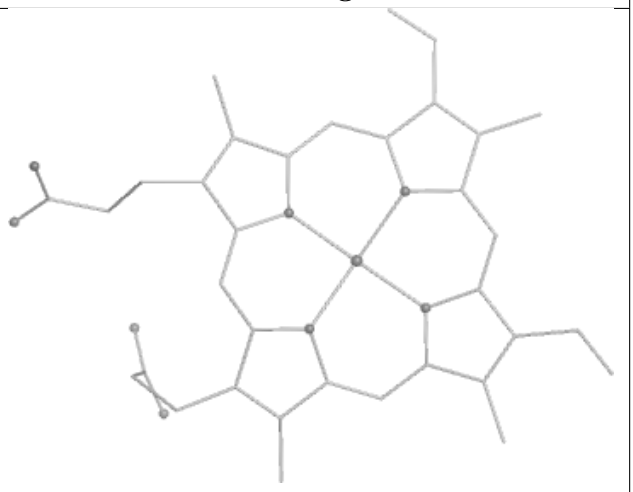
Bond lengths



Bond angles

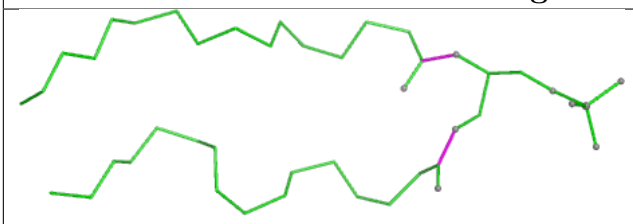


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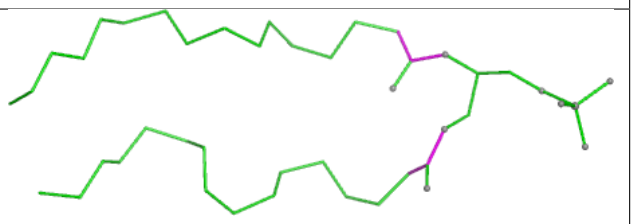


Rings

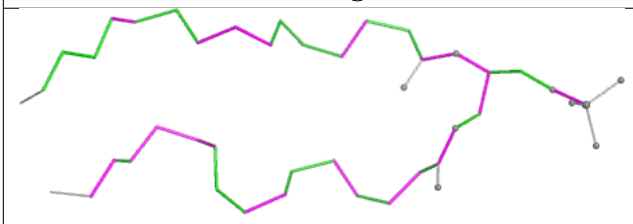
Ligand LPP a 602



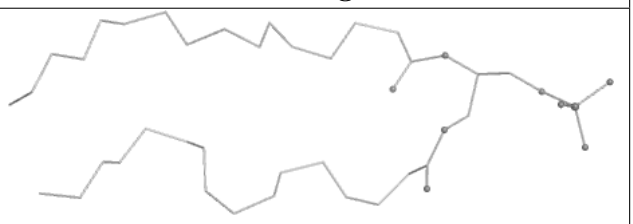
Bond lengths



Bond angles

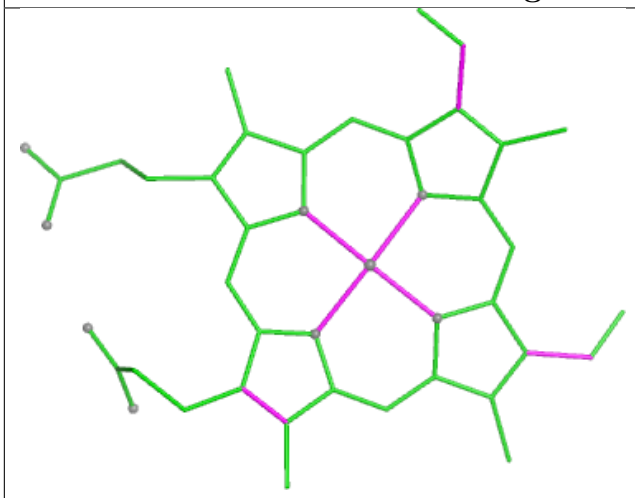


Torsions

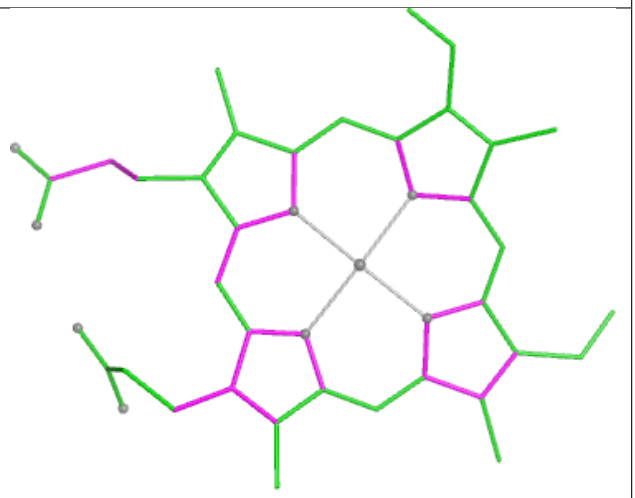


Rings

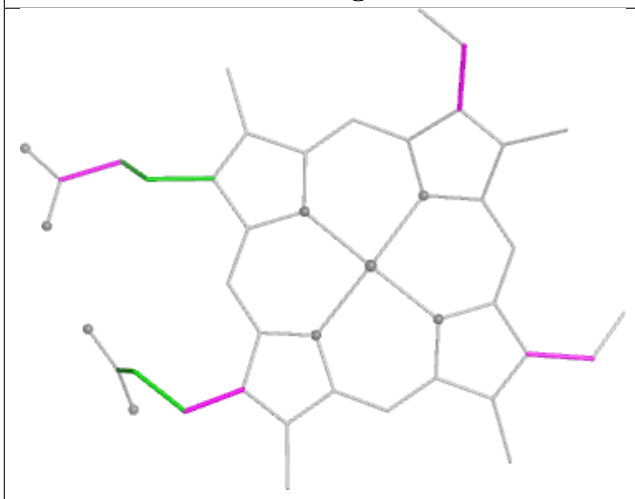
Ligand HEM a 603



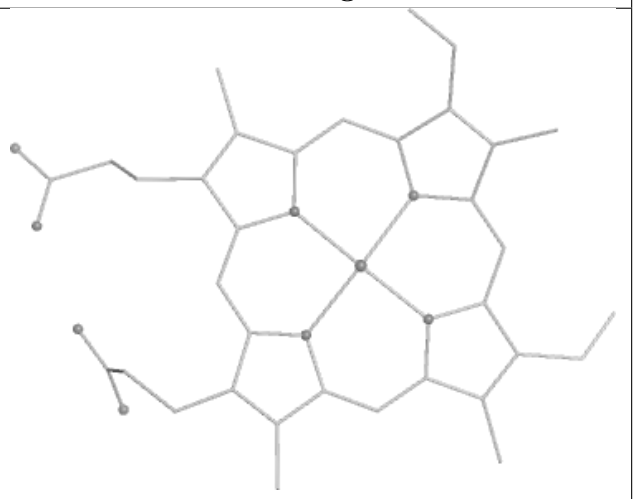
Bond lengths



Bond angles

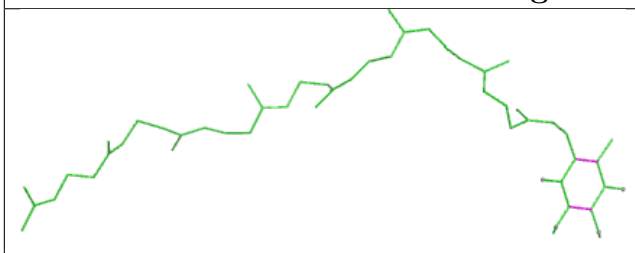


Torsions

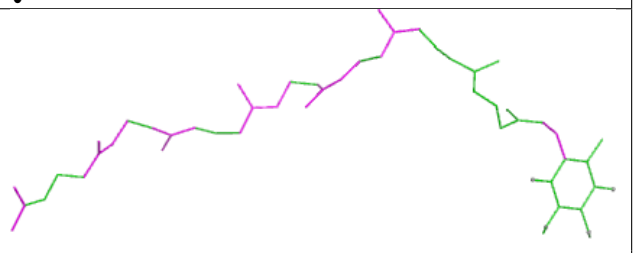


Rings

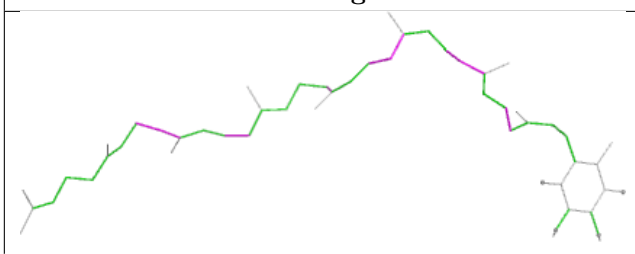
Ligand UQ8 a 604



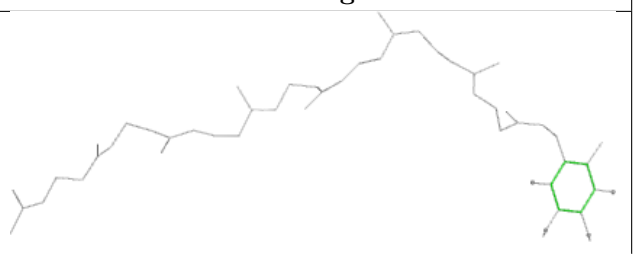
Bond lengths



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.

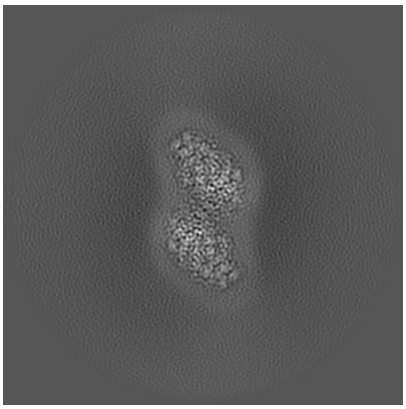
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54826. These allow visual inspection of the internal detail of the map and identification of artifacts.

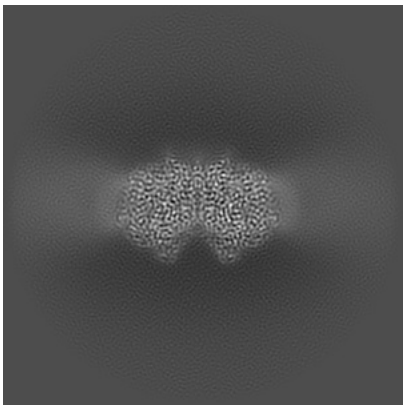
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

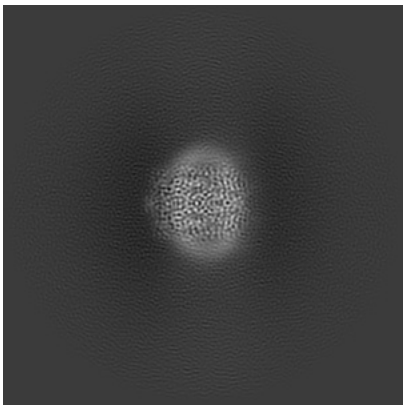
6.1.1 Primary map



X

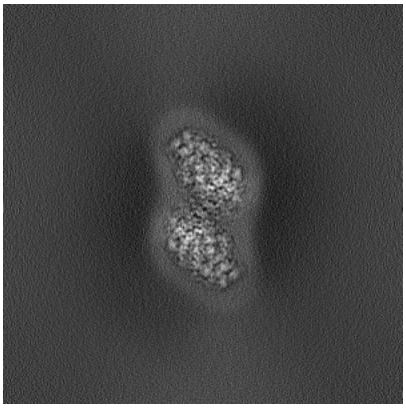


Y

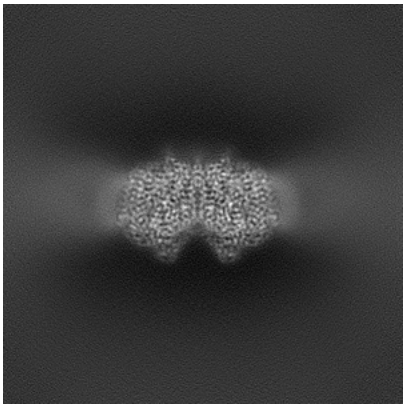


Z

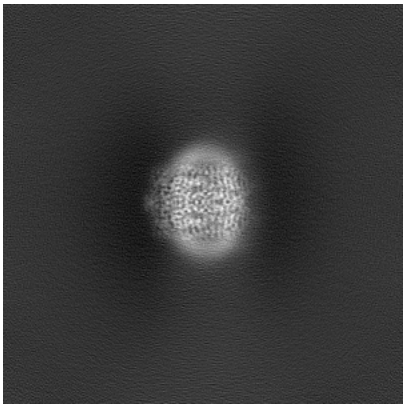
6.1.2 Raw map



X



Y

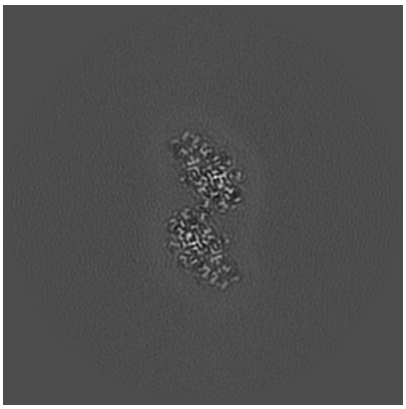


Z

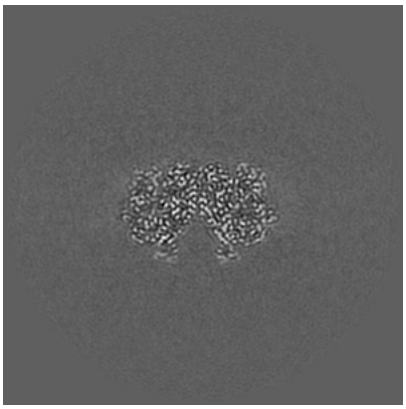
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

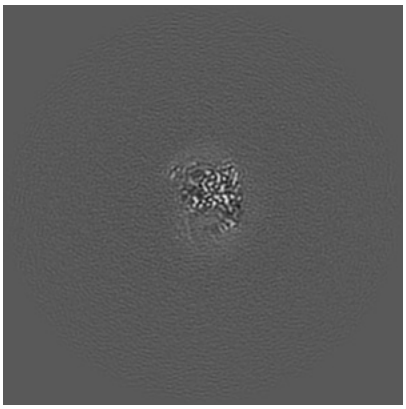
6.2.1 Primary map



X Index: 180

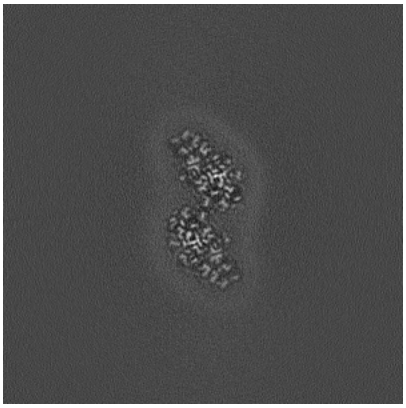


Y Index: 180

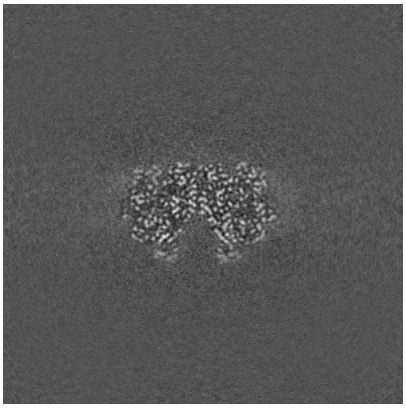


Z Index: 180

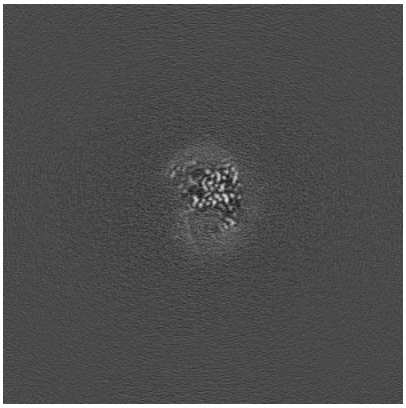
6.2.2 Raw map



X Index: 180



Y Index: 180

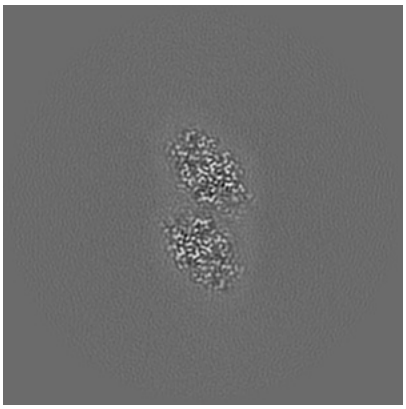


Z Index: 180

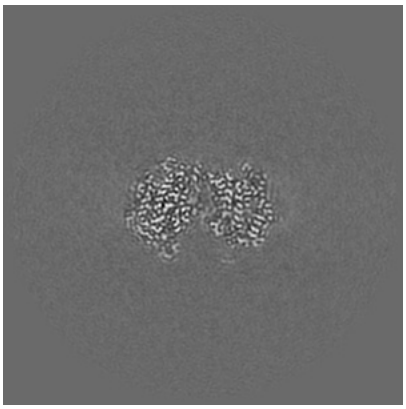
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

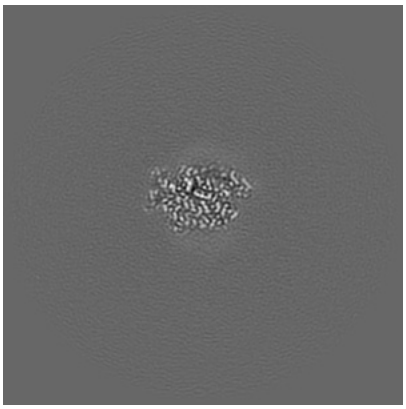
6.3.1 Primary map



X Index: 165

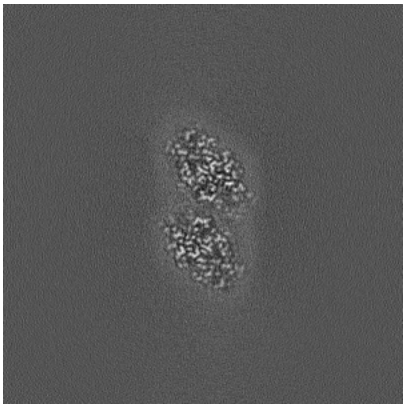


Y Index: 174

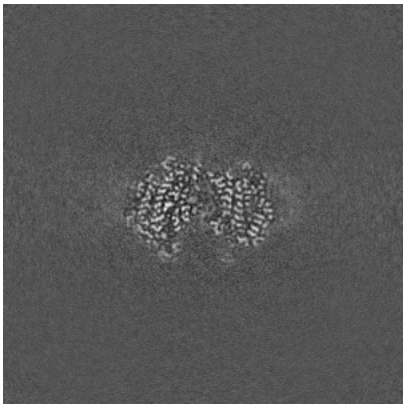


Z Index: 203

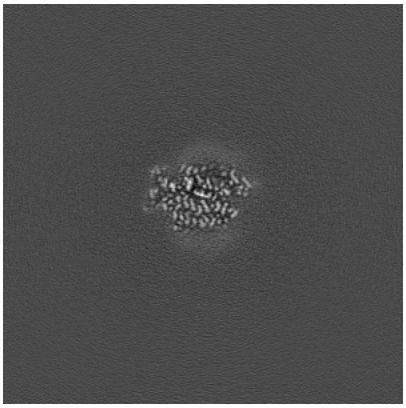
6.3.2 Raw map



X Index: 165



Y Index: 174

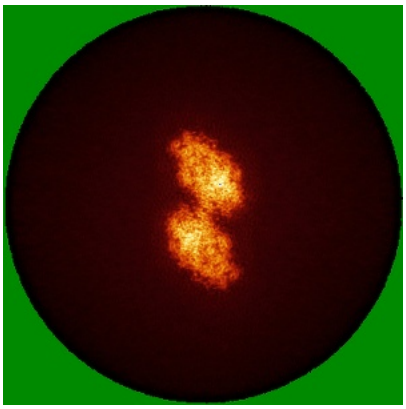


Z Index: 203

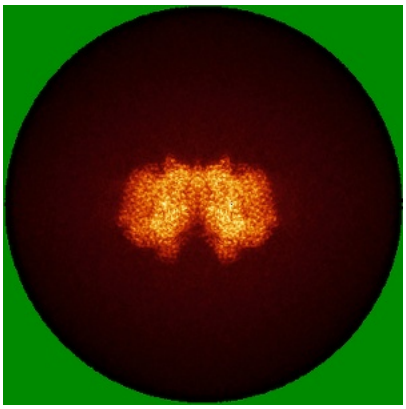
The images above show the largest variance slices of the map in three orthogonal directions.

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

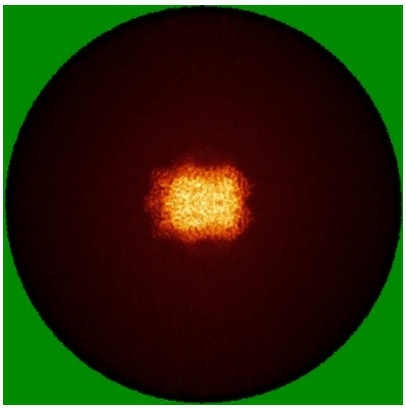
6.4.1 Primary map



X

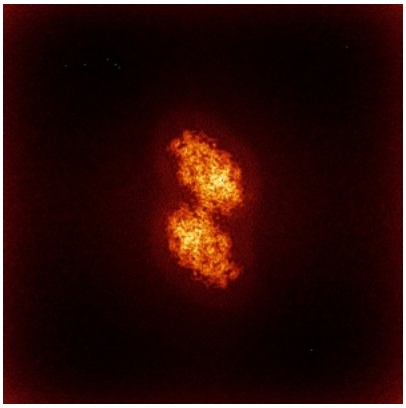


Y

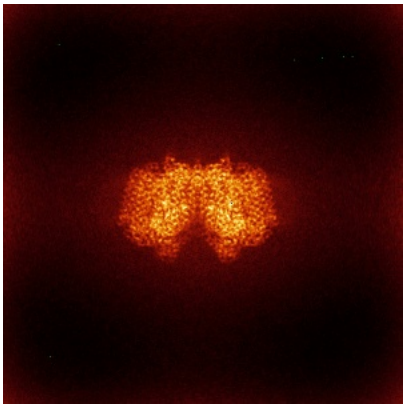


Z

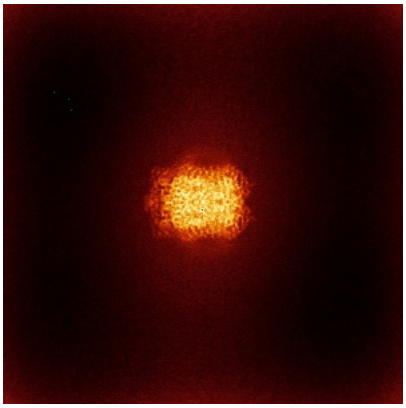
6.4.2 Raw map



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)

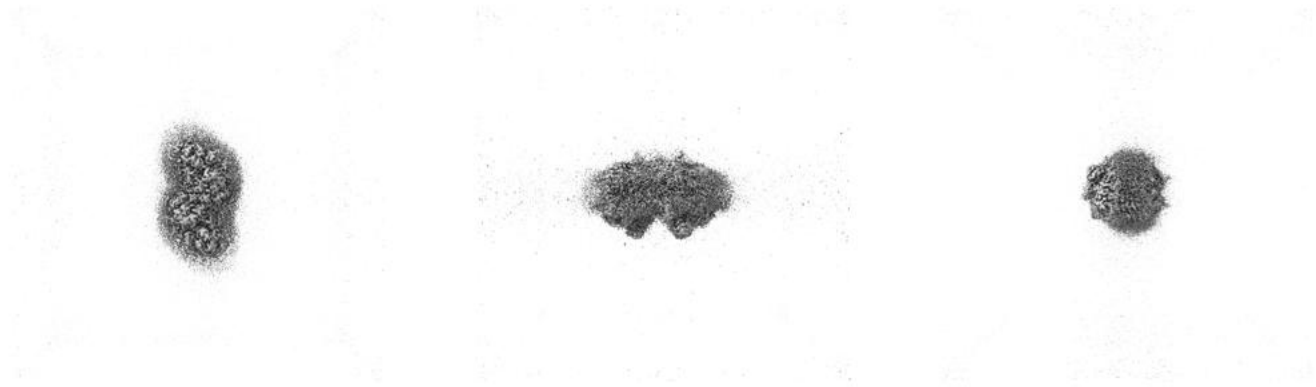
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.125. 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.

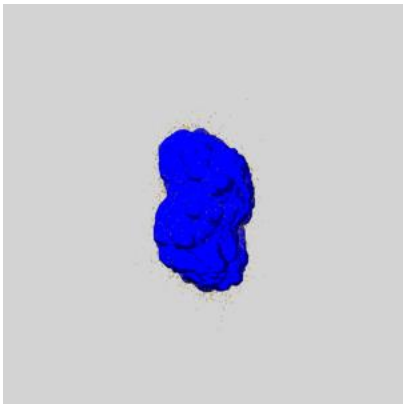
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

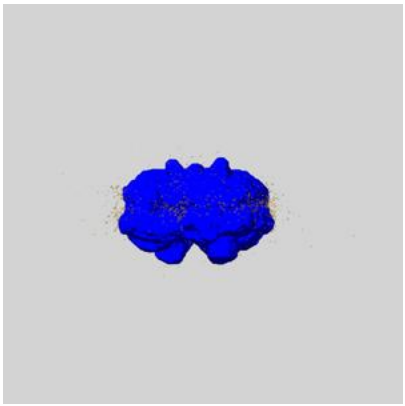
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

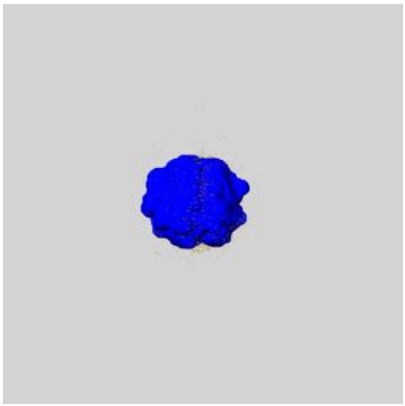
6.6.1 emd_54826_msk_1.map (i)



X



Y

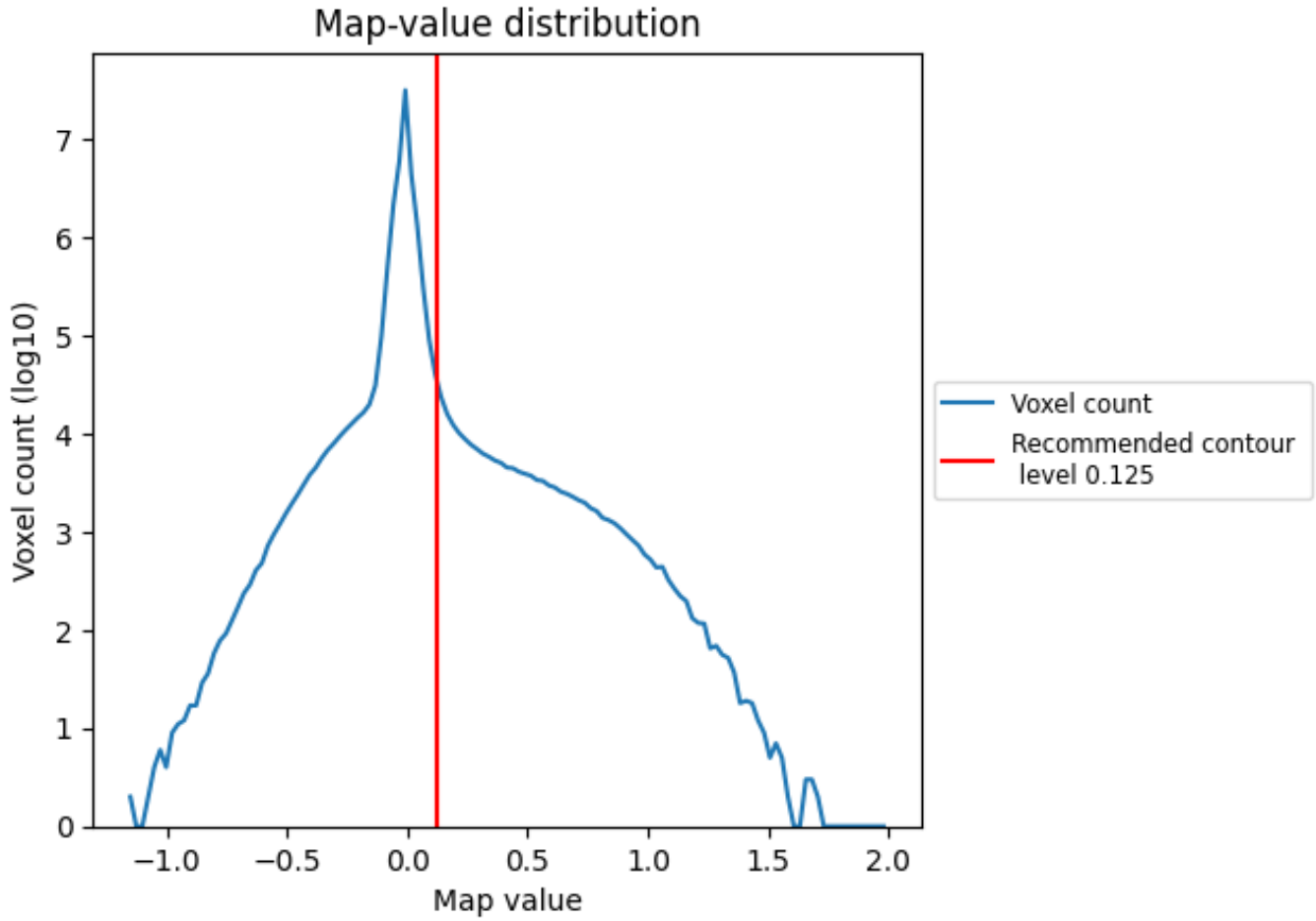


Z

7 Map analysis

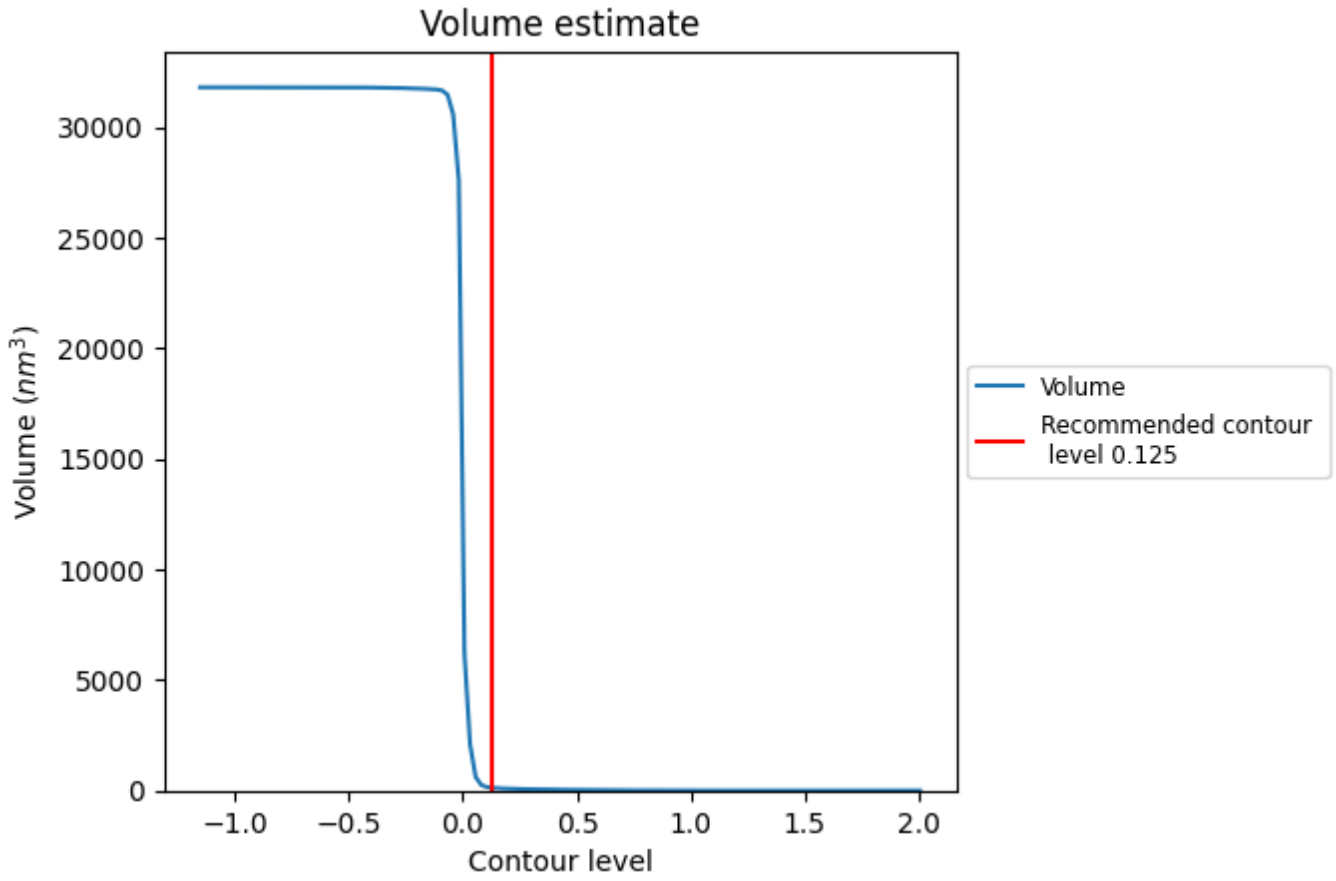
This section contains the results of statistical analysis of the map.

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.

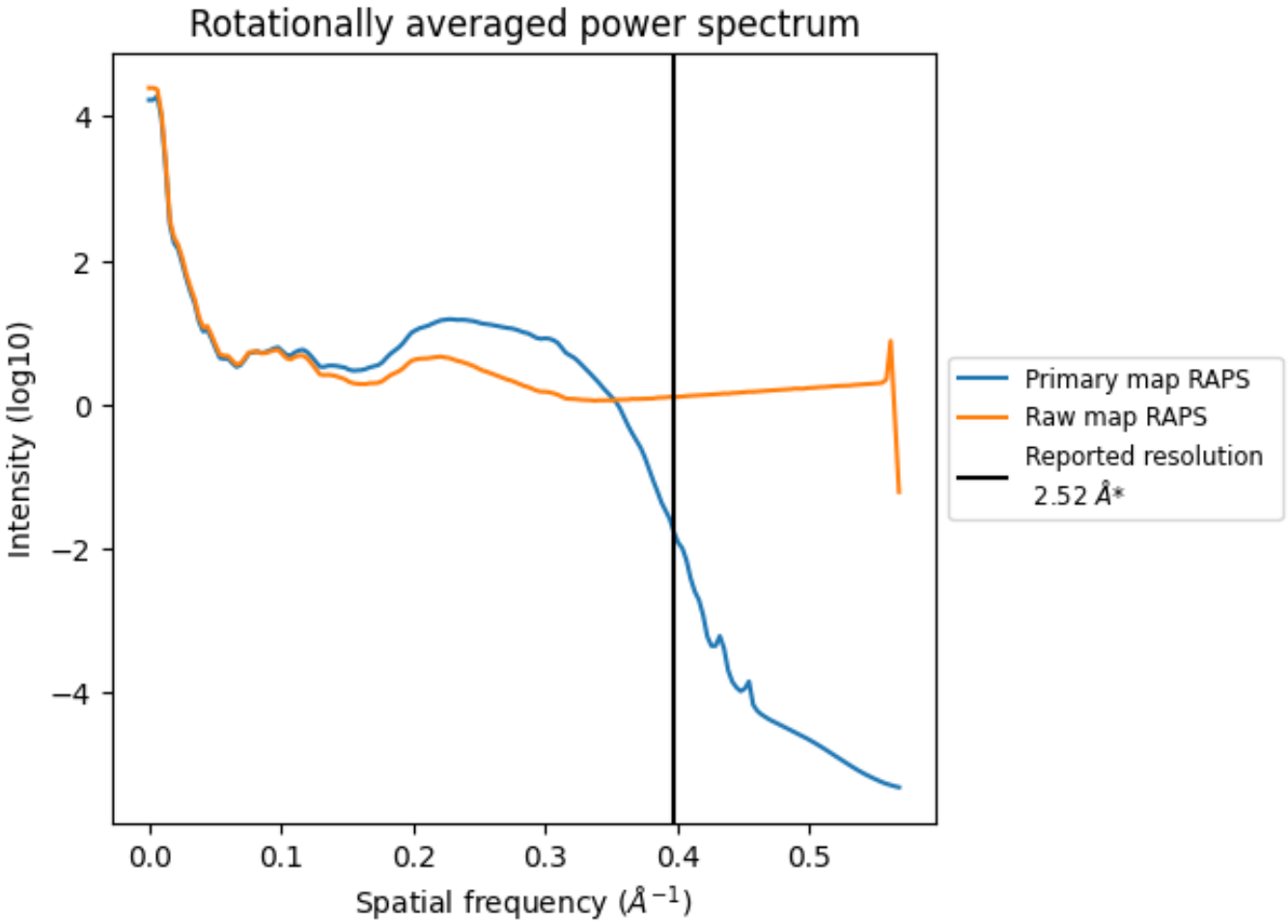
7.2 Volume estimate (i)



The volume at the recommended contour level is 130 nm^3; this corresponds to an approximate mass of 117 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)

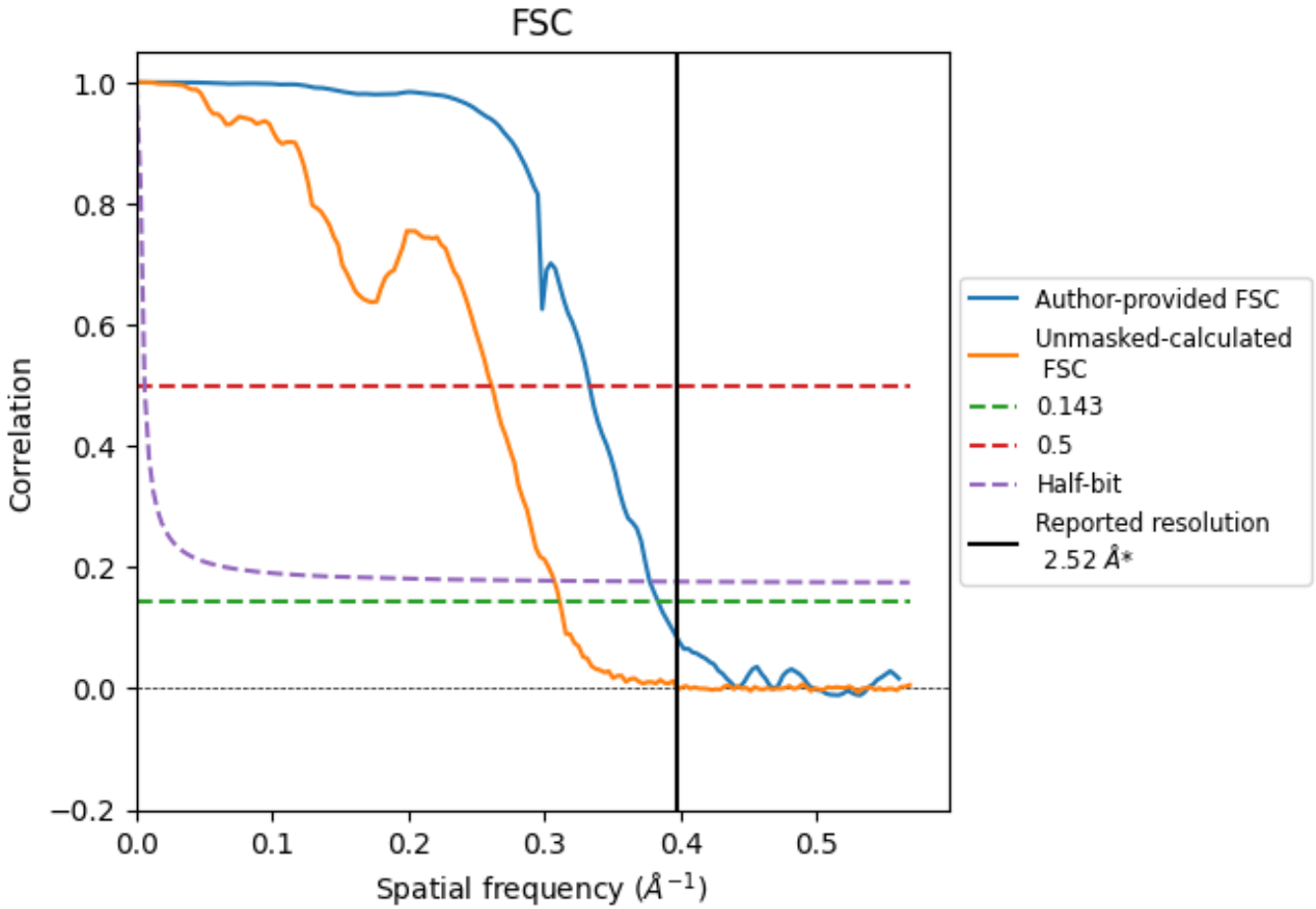


*Reported resolution corresponds to spatial frequency of 0.397 Å^{-1}

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 0.397 Å^{-1}

8.2 Resolution estimates (i)

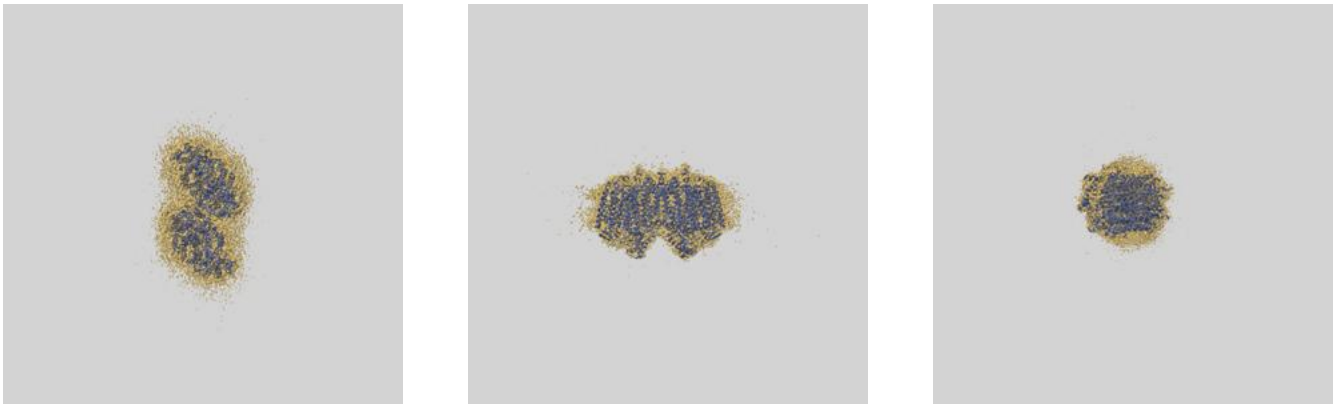
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.61	3.00	2.65
Unmasked-calculated*	3.21	3.83	3.26

*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 3.21 differs from the reported value 2.52 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54826 and PDB model 9SFJ. Per-residue inclusion information can be found in section 3 on page 9.

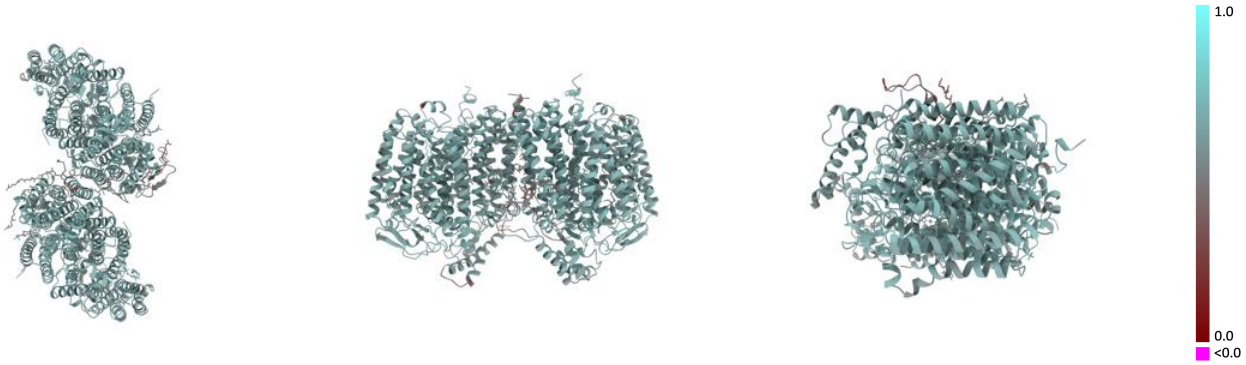
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.125 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.

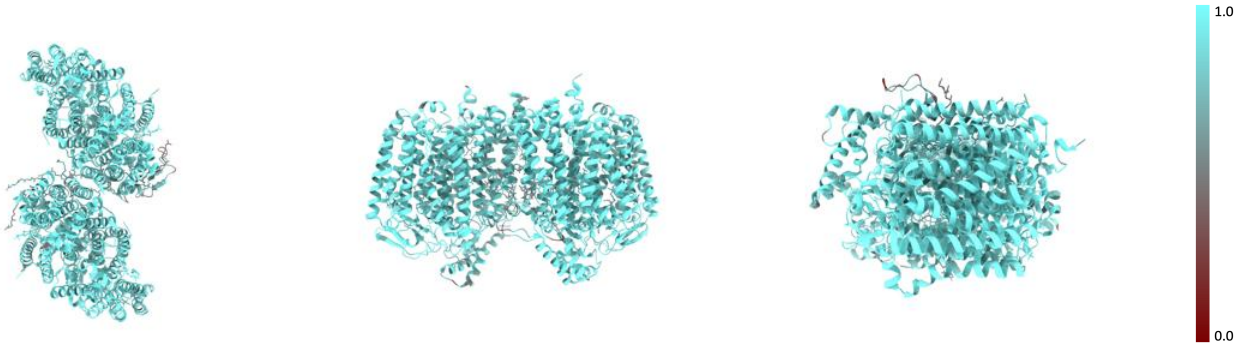
9.2 Q-score mapped to coordinate model (i)



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.

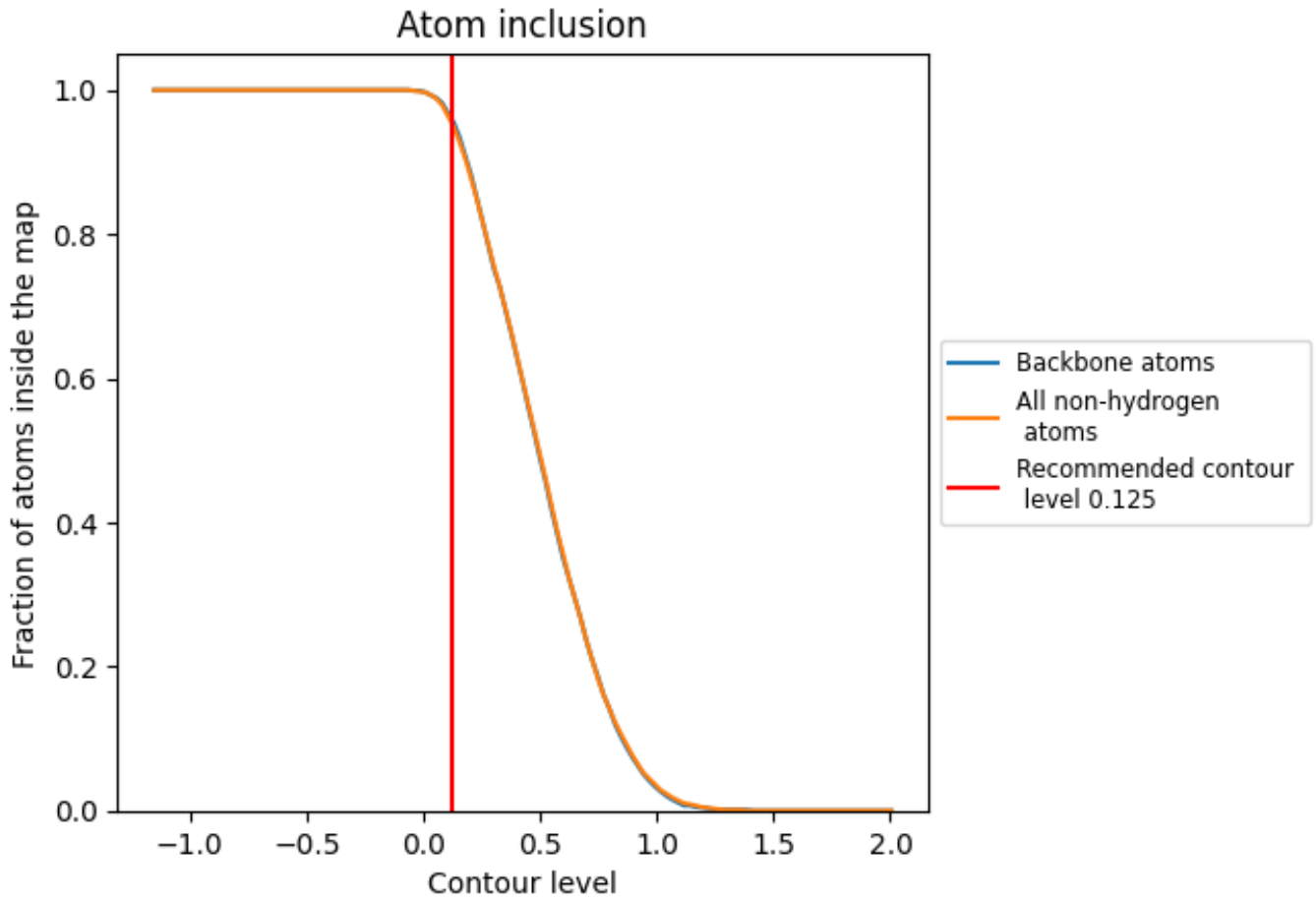
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.125).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.6210
A	0.9470	0.6220
B	0.9580	0.6220
H	0.8760	0.6010
X	0.9430	0.6060
a	0.9370	0.6170
b	0.9670	0.6280
h	0.9330	0.6140
x	0.9450	0.6150

