wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 02:30 AM JST

PDB ID	:	8YIL / pdb_00008yil
EMDB ID	:	EMD-39322
Title	:	Cryo-EM structure of Saccharomyces cerevisiae bc1 complex in YF24228-bound state
Authors	:	Ye, Y.; Li, Z.W.; Yang, G.F.
Deposited on	:	2024-02-29
Resolution	:	2.58 Å(reported)
Based on initial model	:	6YMX

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:

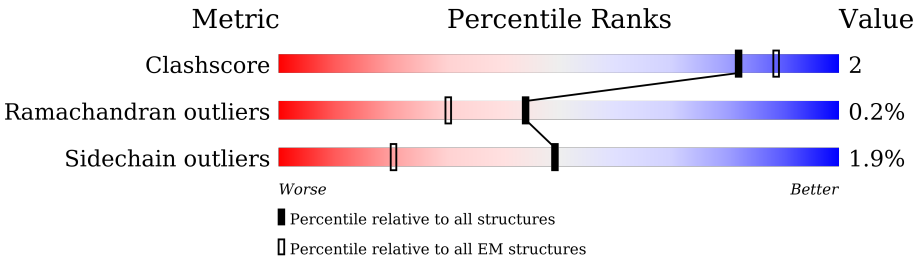
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

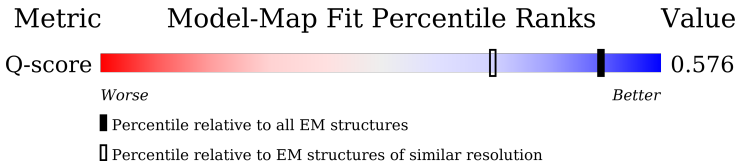
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.58 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	7675 (2.08 - 3.08)

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	431	94% 6%
1	L	431	94% 6%
2	C	385	95% 5%
2	N	385	94% 5% •

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Mol	Chain	Length	Quality of chain
3	B	352	97%
3	M	352	97%
4	D	248	97%
4	O	248	98%
5	E	185	47% 84% 16%
5	P	185	48% 84% 16%
6	F	75	7% 88% 11%
6	Q	75	91% 9%
7	G	126	92% 7%
7	R	126	92% 7%
8	H	93	6% 92% 5%
8	S	93	8% 94%
9	I	55	24% 76% 16% 5%
9	T	55	24% 85% 9%
10	U	52	81% 67% 10% 15%
10	V	52	94% 62% 27% 10%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 32326 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 COR1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3344	2110	576	652	6	0	0
1	L	431	3344	2110	576	652	6	0	0

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	385	3090	2082	484	503	21	0	0
2	N	385	3090	2082	484	503	21	0	0

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	352	2735	1747	453	534	1	0	0
3	M	352	2735	1747	453	534	1	0	0

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	248	1961	1249	340	363	9	0	0
4	O	248	1961	1249	340	363	9	0	0

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	185	1411	893	242	266	10	0	0
5	P	185	1411	893	242	266	10	0	0

- Molecule 6 is a protein called QCR6 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	74	624	391	108	123	2	0	0
6	Q	75	633	396	109	126	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	126	1019	653	173	191	2	0	0
7	R	126	1019	653	173	191	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	93	773	510	131	130	2	0	0
8	S	93	773	510	131	130	2	0	0

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	54	442	295	74	73	0	0
9	T	54	443	295	74	74	0	0

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	U	44	347	230	58	57	2	0	0

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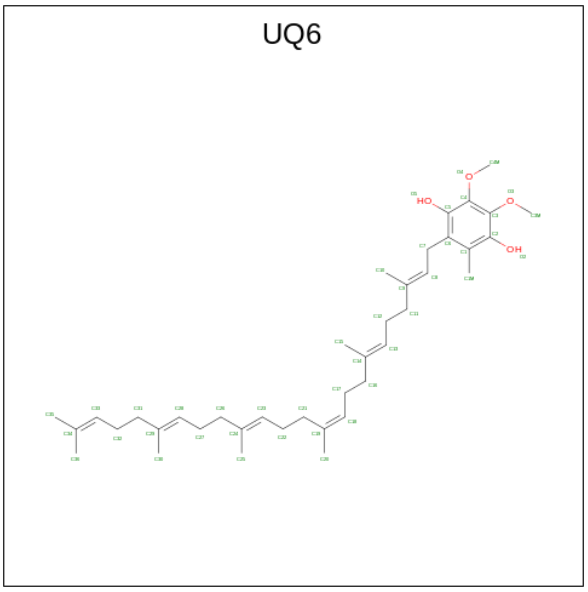
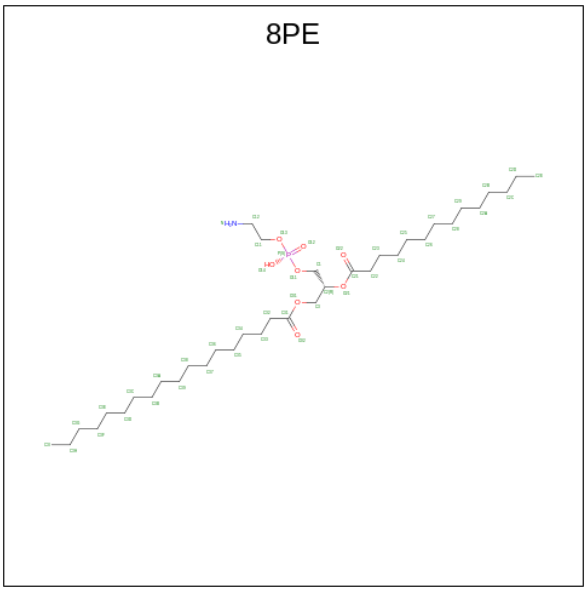
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	V	51	406	272	66	66	2	0	0

- Molecule 11 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$).



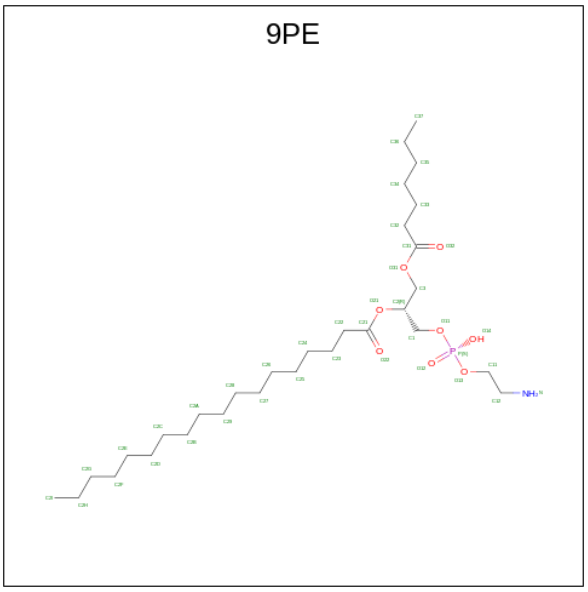
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
11	C	1	43	39	4		0
			Total	C	O		
11	N	1	43	39	4		0

- Molecule 12 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	C	1	47	37	1	8	1	0
			Total	C	N	O	P	
12	S	1	47	37	1	8	1	0

- Molecule 13 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: $C_{30}H_{60}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	C	1	40	30	1	8	1	0

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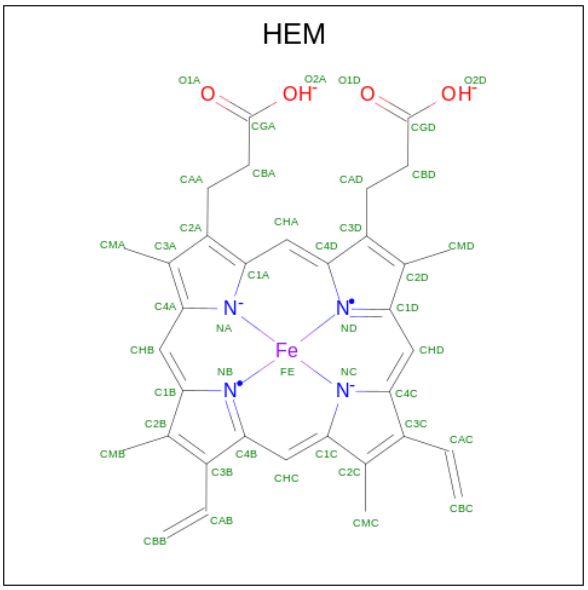
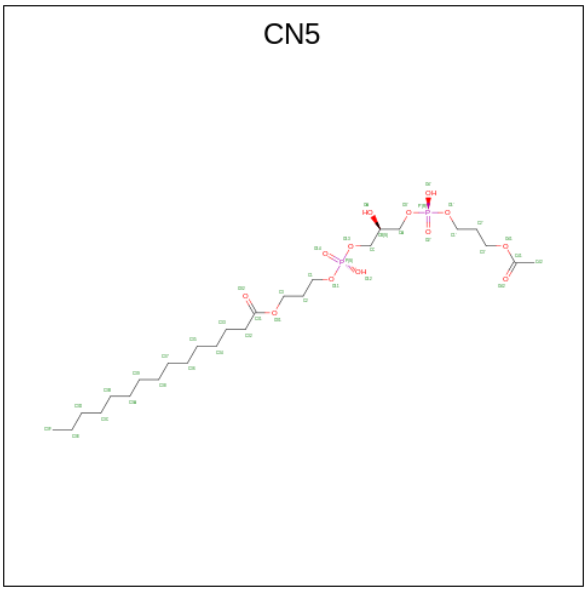
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	N	1	40	30	1	8	1	0

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



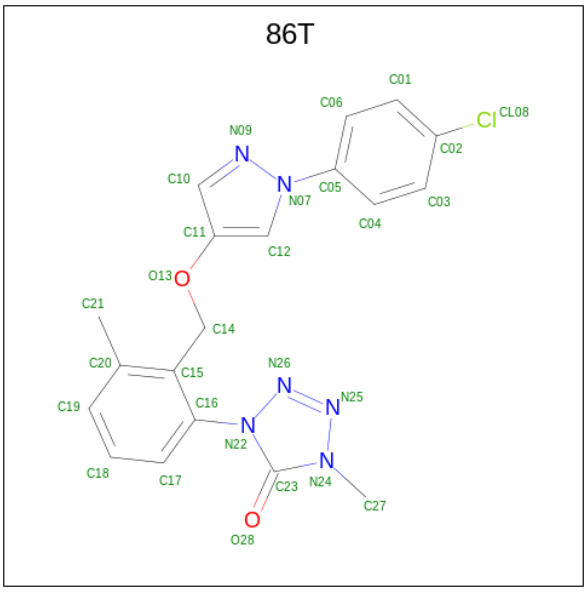
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
14	C	1	43	34	1	4	4	0
14	C	1	43	34	1	4	4	0
14	D	1	43	34	1	4	4	0
14	N	1	43	34	1	4	4	0
14	N	1	43	34	1	4	4	0
14	O	1	43	34	1	4	4	0

- Molecule 15 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-diphosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: $C_{26}H_{52}O_{13}P_2$).



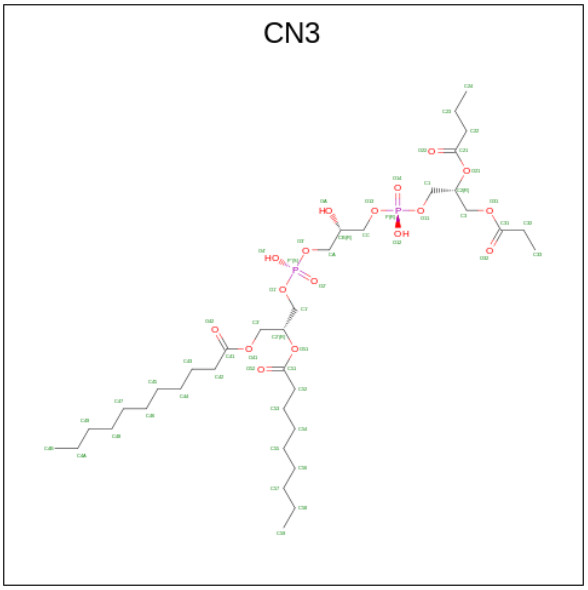
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	C	1	41	26	13	2	0

- Molecule 16 is metyltetraprole (CCD ID: 86T) (formula: $C_{19}H_{17}ClN_6O_2$) (labeled as "Ligand of Interest" by depositor).



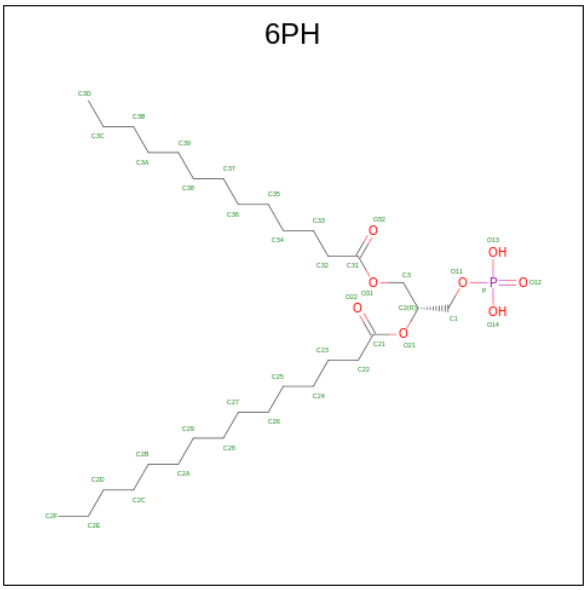
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
16	C	1	28	19	1	6	2	0
16	N	1	28	19	1	6	2	0

- Molecule 17 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanonadec-1-yl undecanoate (CCD ID: CN3) (formula: $C_{36}H_{68}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	C	1	55	36	17	2	0
			Total	C	O	P	
17	N	1	55	36	17	2	0

- Molecule 18 is (1R)-2-(phosphonooxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: $C_{31}H_{61}O_8P$).



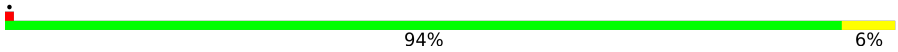
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	O	1	40	31	8	1	0

3 Residue-property plots (i)

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

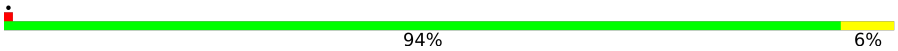
• Molecule 1: COR1 isoform 1

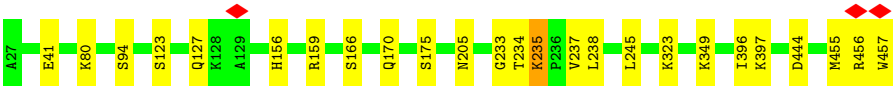
Chain A:



• Molecule 1: COR1 isoform 1

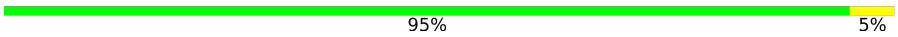
Chain L:





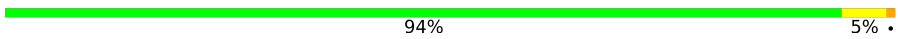
• Molecule 2: Cytochrome b

Chain C:



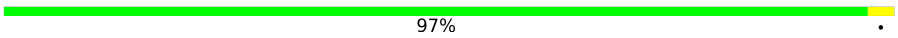
• Molecule 2: Cytochrome b

Chain N:



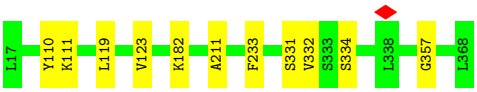
• Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



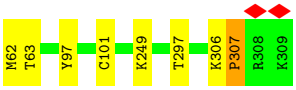
• Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 97%



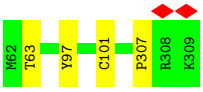
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 97%



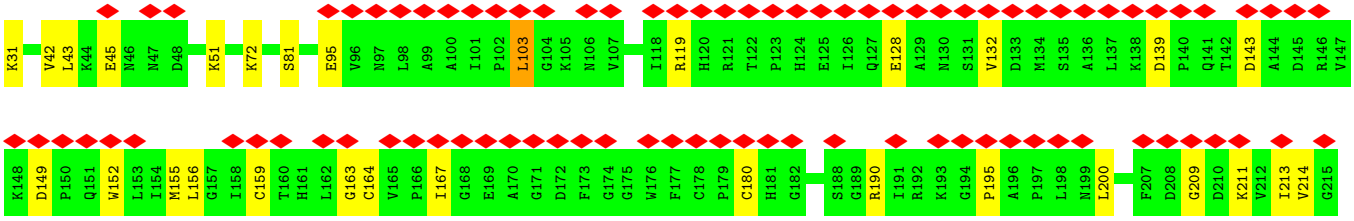
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O: 98%



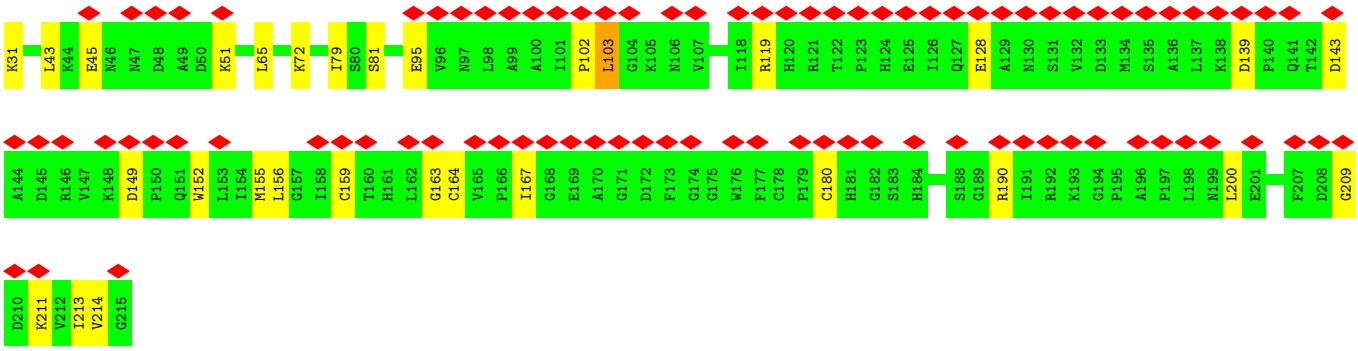
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 47% 84% 16%



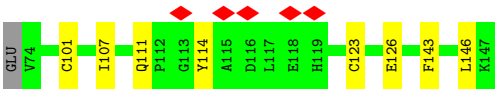
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P: 48% 84% 16%



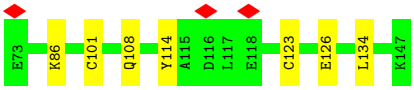
• Molecule 6: QCR6 isoform 1

Chain F: 7% 88% 11%



• Molecule 6: QCR6 isoform 1

Chain Q:



• Molecule 7: Cytochrome b-c1 complex subunit 7

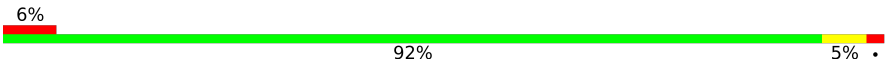
Chain G:

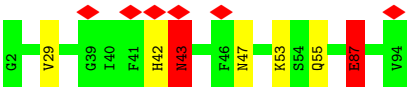
• Molecule 7: Cytochrome b-c1 complex subunit 7

Chain R:

• Molecule 8: Cytochrome b-c1 complex subunit 8

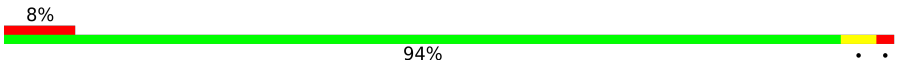
Chain H:

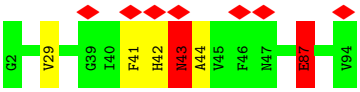




• Molecule 8: Cytochrome b-c1 complex subunit 8

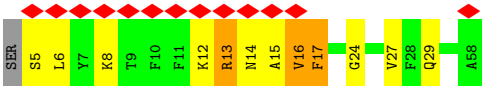
Chain S:





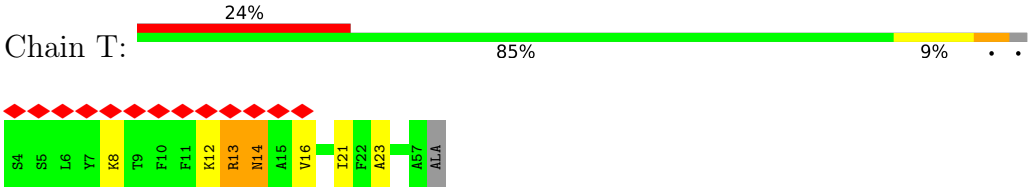
• Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain I:



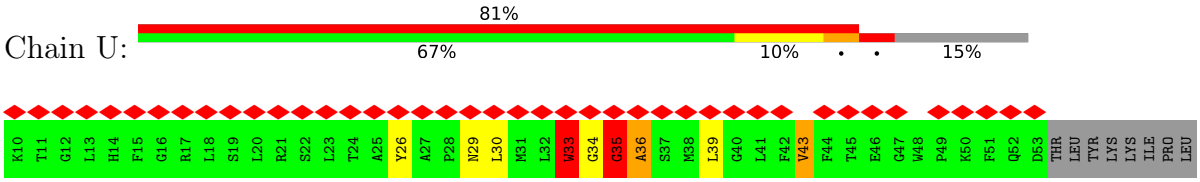
• Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain T:



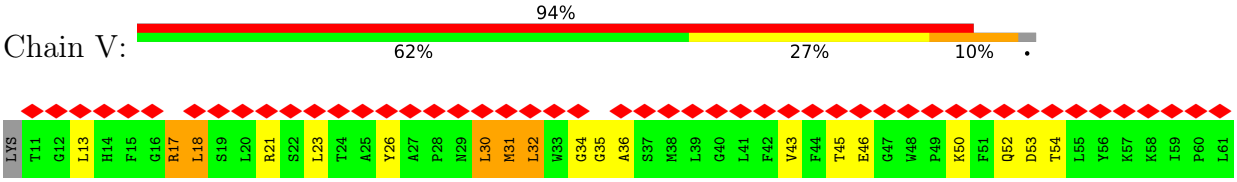
• Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain U:



• Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105757	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.48	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.808	Depositor
Minimum map value	-3.244	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	307.19998, 307.19998, 307.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9599999, 0.9599999, 0.9599999	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 8PE, UQ6, 86T, HEM, CN5, 6PH, 9PE, CN3

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	0.45	3/3405 (0.1%)	0.53	0/4615
1	L	0.49	3/3405 (0.1%)	0.52	0/4615
2	C	0.35	1/3192 (0.0%)	0.49	0/4354
2	N	0.35	1/3192 (0.0%)	0.48	1/4354 (0.0%)
3	B	0.30	1/2781 (0.0%)	0.42	0/3764
3	M	0.30	1/2781 (0.0%)	0.43	0/3764
4	D	0.26	0/2022	0.43	1/2751 (0.0%)
4	O	0.26	0/2022	0.43	1/2751 (0.0%)
5	E	0.41	1/1444 (0.1%)	0.77	4/1957 (0.2%)
5	P	0.63	1/1444 (0.1%)	0.76	3/1957 (0.2%)
6	F	0.27	0/638	0.52	0/858
6	Q	0.25	0/647	0.65	1/870 (0.1%)
7	G	0.51	1/1040 (0.1%)	0.73	6/1408 (0.4%)
7	R	0.42	1/1040 (0.1%)	0.60	2/1408 (0.1%)
8	H	0.58	1/804 (0.1%)	0.92	6/1088 (0.6%)
8	S	0.47	2/804 (0.2%)	0.92	5/1088 (0.5%)
9	I	0.63	1/455 (0.2%)	0.76	3/614 (0.5%)
9	T	0.28	0/456	0.65	1/615 (0.2%)
10	U	0.57	1/358 (0.3%)	1.11	4/483 (0.8%)
10	V	0.72	1/419 (0.2%)	0.94	1/567 (0.2%)
All	All	0.41	20/32349 (0.1%)	0.58	39/43881 (0.1%)

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
1	L	0	1
2	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	2
6	Q	0	1
8	H	0	1
8	S	0	1
9	I	0	1
9	T	0	1
10	V	0	1
All	All	0	11

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	233	GLY	C-N	21.12	1.59	1.33
5	P	102	PRO	C-N	19.26	1.58	1.33
1	A	233	GLY	C-N	16.53	1.53	1.33
7	G	2	PRO	C-N	13.58	1.50	1.33
8	H	43	ASN	C-N	13.03	1.51	1.34

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	43	ASN	O-C-N	-18.98	97.34	122.59
8	S	43	ASN	CA-C-N	12.45	139.24	120.31
8	S	43	ASN	C-N-CA	12.45	139.24	120.31
8	S	43	ASN	O-C-N	-11.66	107.09	122.59
7	G	2	PRO	CA-C-N	-9.86	106.10	120.89

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	ARG	Peptide
2	C	346	VAL	Peptide
8	H	43	ASN	Mainchain
2	N	107	ARG	Sidechain
2	N	346	VAL	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	3344	0	3323	12	0
1	L	3344	0	3323	11	0
2	C	3090	0	3129	12	0
2	N	3090	0	3129	16	0
3	B	2735	0	2774	6	0
3	M	2735	0	2774	5	0
4	D	1961	0	1890	8	0
4	O	1961	0	1890	1	0
5	E	1411	0	1390	13	0
5	P	1411	0	1390	12	0
6	F	624	0	583	10	0
6	Q	633	0	589	5	0
7	G	1019	0	1034	5	0
7	R	1019	0	1034	6	0
8	H	773	0	736	5	0
8	S	773	0	736	3	0
9	I	442	0	440	8	0
9	T	443	0	440	6	0
10	U	347	0	345	12	0
10	V	406	0	414	15	0
11	C	43	0	60	4	0
11	N	43	0	60	4	0
12	C	47	0	73	3	0
12	S	47	0	73	1	0
13	C	40	0	59	1	0
13	N	40	0	59	1	0
14	C	86	0	60	0	0
14	D	43	0	30	0	0
14	N	86	0	60	2	0
14	O	43	0	30	1	0
15	C	41	0	50	4	0
16	C	28	0	0	0	0
16	N	28	0	0	0	0
17	C	55	0	66	0	0
17	N	55	0	66	0	0
18	O	40	0	59	2	0
All	All	32326	0	32168	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 161 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)
5:E:164:CYS:HB3	5:E:180:CYS:SG	1.89	1.13
5:P:164:CYS:HB3	5:P:180:CYS:SG	1.89	1.13
6:F:101:CYS:HB3	6:F:123:CYS:SG	2.29	0.72
10:V:46:GLU:HA	10:V:52:GLN:HE21	1.54	0.72
1:A:75:ASN:HD22	1:A:144:VAL:CG2	2.04	0.70

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	429/431 (100%)	396 (92%)	33 (8%)	0	100	100
1	L	429/431 (100%)	396 (92%)	33 (8%)	0	100	100
2	C	383/385 (100%)	368 (96%)	14 (4%)	1 (0%)	36	56
2	N	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	36	56
3	B	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
3	M	350/352 (99%)	336 (96%)	14 (4%)	0	100	100
4	D	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
4	O	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
5	E	183/185 (99%)	152 (83%)	30 (16%)	1 (0%)	24	44
5	P	183/185 (99%)	154 (84%)	29 (16%)	0	100	100
6	F	72/75 (96%)	68 (94%)	4 (6%)	0	100	100
6	Q	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
7	G	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
7	R	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
8	H	91/93 (98%)	79 (87%)	12 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
9	I	52/55 (94%)	48 (92%)	4 (8%)	0	100	100
9	T	52/55 (94%)	49 (94%)	3 (6%)	0	100	100
10	U	42/52 (81%)	32 (76%)	9 (21%)	1 (2%)	4	8
10	V	49/52 (94%)	36 (74%)	11 (22%)	2 (4%)	2	2
All	All	3952/4004 (99%)	3677 (93%)	269 (7%)	6 (0%)	44	63

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	V	17	ARG
10	V	54	THR
2	N	347	PRO
10	U	35	GLY
2	C	347	PRO

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	370/370 (100%)	363 (98%)	7 (2%)	50	73
1	L	370/370 (100%)	363 (98%)	7 (2%)	50	73
2	C	338/338 (100%)	336 (99%)	2 (1%)	78	89
2	N	338/338 (100%)	335 (99%)	3 (1%)	70	85
3	B	301/301 (100%)	301 (100%)	0	100	100
3	M	301/301 (100%)	301 (100%)	0	100	100
4	D	206/206 (100%)	205 (100%)	1 (0%)	81	91
4	O	206/206 (100%)	205 (100%)	1 (0%)	81	91
5	E	151/151 (100%)	137 (91%)	14 (9%)	8	18
5	P	151/151 (100%)	137 (91%)	14 (9%)	8	18
6	F	67/68 (98%)	66 (98%)	1 (2%)	57	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Q	68/68 (100%)	68 (100%)	0	100	100
7	G	110/110 (100%)	108 (98%)	2 (2%)	51	74
7	R	110/110 (100%)	108 (98%)	2 (2%)	51	74
8	H	77/77 (100%)	76 (99%)	1 (1%)	61	81
8	S	77/77 (100%)	75 (97%)	2 (3%)	40	66
9	I	44/45 (98%)	42 (96%)	2 (4%)	24	47
9	T	45/45 (100%)	43 (96%)	2 (4%)	25	48
10	U	35/43 (81%)	34 (97%)	1 (3%)	37	63
10	V	42/43 (98%)	39 (93%)	3 (7%)	13	29
All	All	3407/3418 (100%)	3342 (98%)	65 (2%)	49	73

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	R	17	LYS
9	T	13	ARG
2	N	160	ASP
5	E	214	VAL
9	T	16	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	57	GLN
6	Q	87	ASN
1	L	149	GLN
8	S	21	GLN
10	U	14	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)

18 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	$\#\|Z\| > 2$
14	HEM	O	401	4	50,50,50	1.35	7 (14%)	66,82,82	1.43	11 (16%)
11	UQ6	N	406	-	43,43,43	1.68	11 (25%)	51,55,55	1.48	8 (15%)
14	HEM	N	405	2	50,50,50	1.38	6 (12%)	66,82,82	1.26	7 (10%)
13	9PE	N	403	-	39,39,39	0.94	4 (10%)	42,44,44	1.11	2 (4%)
13	9PE	C	403	-	39,39,39	0.93	4 (10%)	42,44,44	1.02	2 (4%)
16	86T	N	401	-	30,31,31	0.52	0	37,44,44	1.19	3 (8%)
18	6PH	O	402	-	39,39,39	0.93	3 (7%)	43,44,44	1.16	2 (4%)
15	CN5	C	405	-	40,40,40	0.35	0	44,48,48	0.42	0
17	CN3	N	402	-	54,54,54	1.16	7 (12%)	60,66,66	1.27	4 (6%)
14	HEM	N	404	2	50,50,50	1.48	8 (16%)	66,82,82	1.71	15 (22%)
14	HEM	D	401	4	50,50,50	1.27	5 (10%)	66,82,82	1.26	7 (10%)
16	86T	C	406	-	30,31,31	0.51	0	37,44,44	1.19	2 (5%)
14	HEM	C	408	2	50,50,50	1.34	6 (12%)	66,82,82	1.19	6 (9%)
12	8PE	S	101	-	46,46,46	0.90	4 (8%)	49,51,51	1.07	2 (4%)
14	HEM	C	404	2	50,50,50	1.46	8 (16%)	66,82,82	1.68	13 (19%)
11	UQ6	C	401	-	43,43,43	1.57	8 (18%)	51,55,55	1.52	10 (19%)
17	CN3	C	407	-	54,54,54	1.16	8 (14%)	60,66,66	1.19	4 (6%)
12	8PE	C	402	-	46,46,46	0.48	0	49,51,51	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEM	O	401	4	-	3/14/54/54	-
11	UQ6	N	406	-	-	13/39/39/39	0/1/1/1
14	HEM	N	405	2	-	4/14/54/54	-
13	9PE	N	403	-	-	23/43/43/43	-
13	9PE	C	403	-	-	17/43/43/43	-
16	86T	N	401	-	-	0/13/13/13	0/4/4/4
18	6PH	O	402	-	-	26/41/41/41	-
15	CN5	C	405	-	-	27/44/44/44	-
17	CN3	N	402	-	-	36/65/65/65	-
14	HEM	N	404	2	-	5/14/54/54	-
14	HEM	D	401	4	-	0/14/54/54	-
16	86T	C	406	-	-	0/13/13/13	0/4/4/4
14	HEM	C	408	2	-	3/14/54/54	-
12	8PE	S	101	-	-	18/50/50/50	-
14	HEM	C	404	2	-	4/14/54/54	-
11	UQ6	C	401	-	-	6/39/39/39	0/1/1/1
17	CN3	C	407	-	-	25/65/65/65	-
12	8PE	C	402	-	-	30/50/50/50	-

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	406	UQ6	C7-C6	5.24	1.57	1.51
11	C	401	UQ6	C7-C6	4.76	1.56	1.51
14	C	404	HEM	FE-ND	4.03	2.07	1.94
14	N	404	HEM	FE-ND	3.76	2.06	1.94
11	N	406	UQ6	C16-C14	3.70	1.59	1.51

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	C	404	HEM	CAD-C3D-C4D	5.76	134.73	124.66
14	N	404	HEM	CAD-C3D-C4D	5.36	134.03	124.66
14	C	404	HEM	CAD-C3D-C2D	-5.10	118.37	127.88
14	N	404	HEM	CAD-C3D-C2D	-4.75	119.03	127.88
16	N	401	86T	C05-N07-C12	-4.49	122.78	129.04

There are no chirality outliers.

5 of 240 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	401	UQ6	C9-C11-C12-C13
11	C	401	UQ6	C19-C21-C22-C23
11	N	406	UQ6	C1-C6-C7-C8
11	N	406	UQ6	C23-C24-C26-C27
11	N	406	UQ6	C25-C24-C26-C27

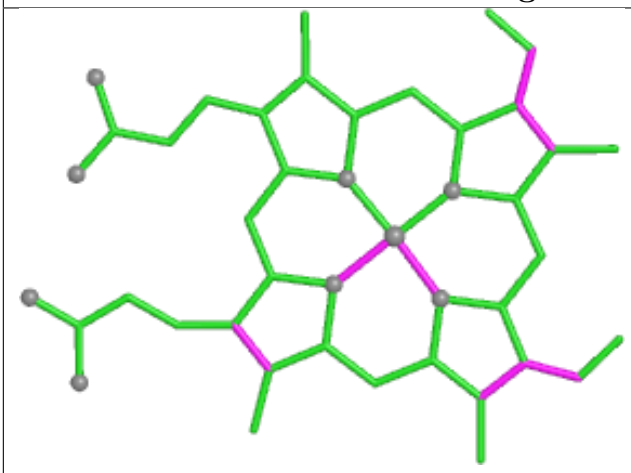
There are no ring outliers.

10 monomers are involved in 20 short contacts:

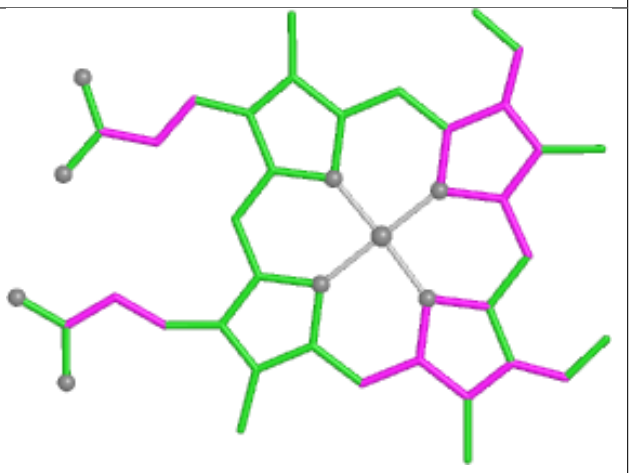
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	O	401	HEM	1	0
11	N	406	UQ6	4	0
13	N	403	9PE	1	0
13	C	403	9PE	1	0
18	O	402	6PH	2	0
15	C	405	CN5	4	0
14	N	404	HEM	2	0
12	S	101	8PE	1	0
11	C	401	UQ6	4	0
12	C	402	8PE	3	0

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.

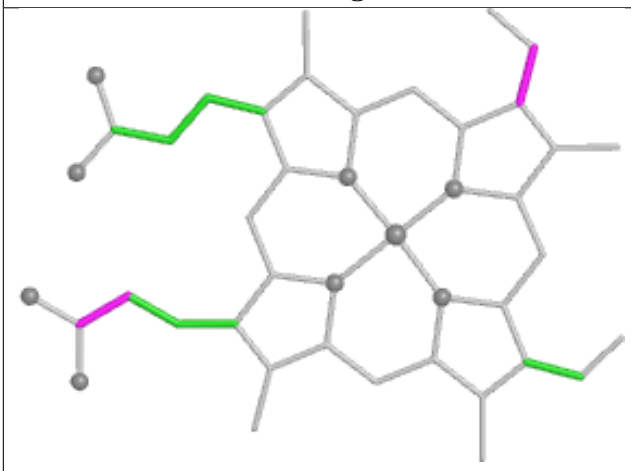
Ligand HEM O 401



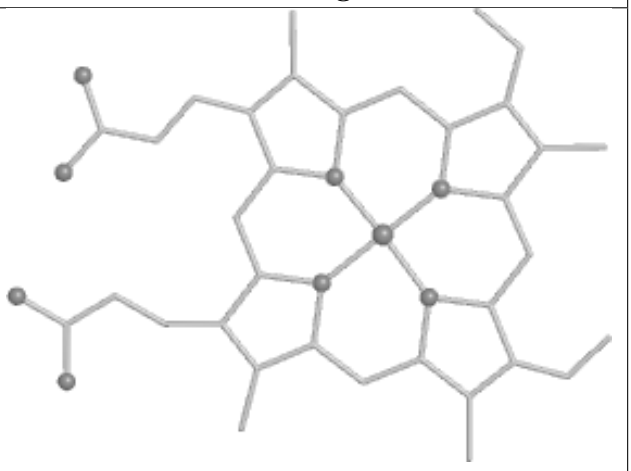
Bond lengths



Bond angles

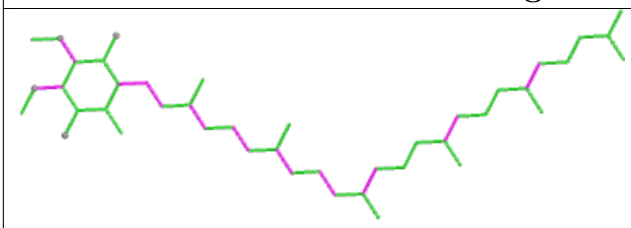


Torsions

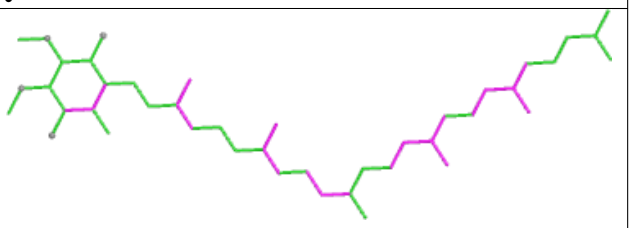


Rings

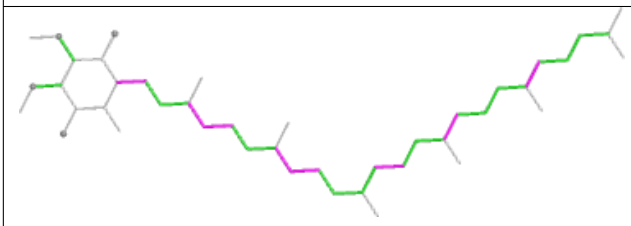
Ligand UQ6 N 406



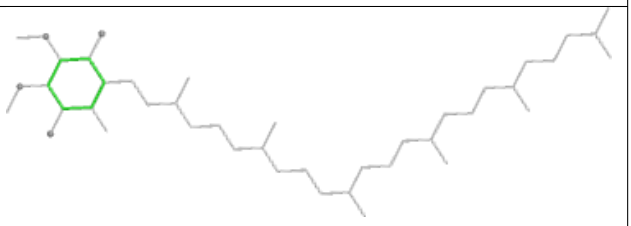
Bond lengths



Bond angles

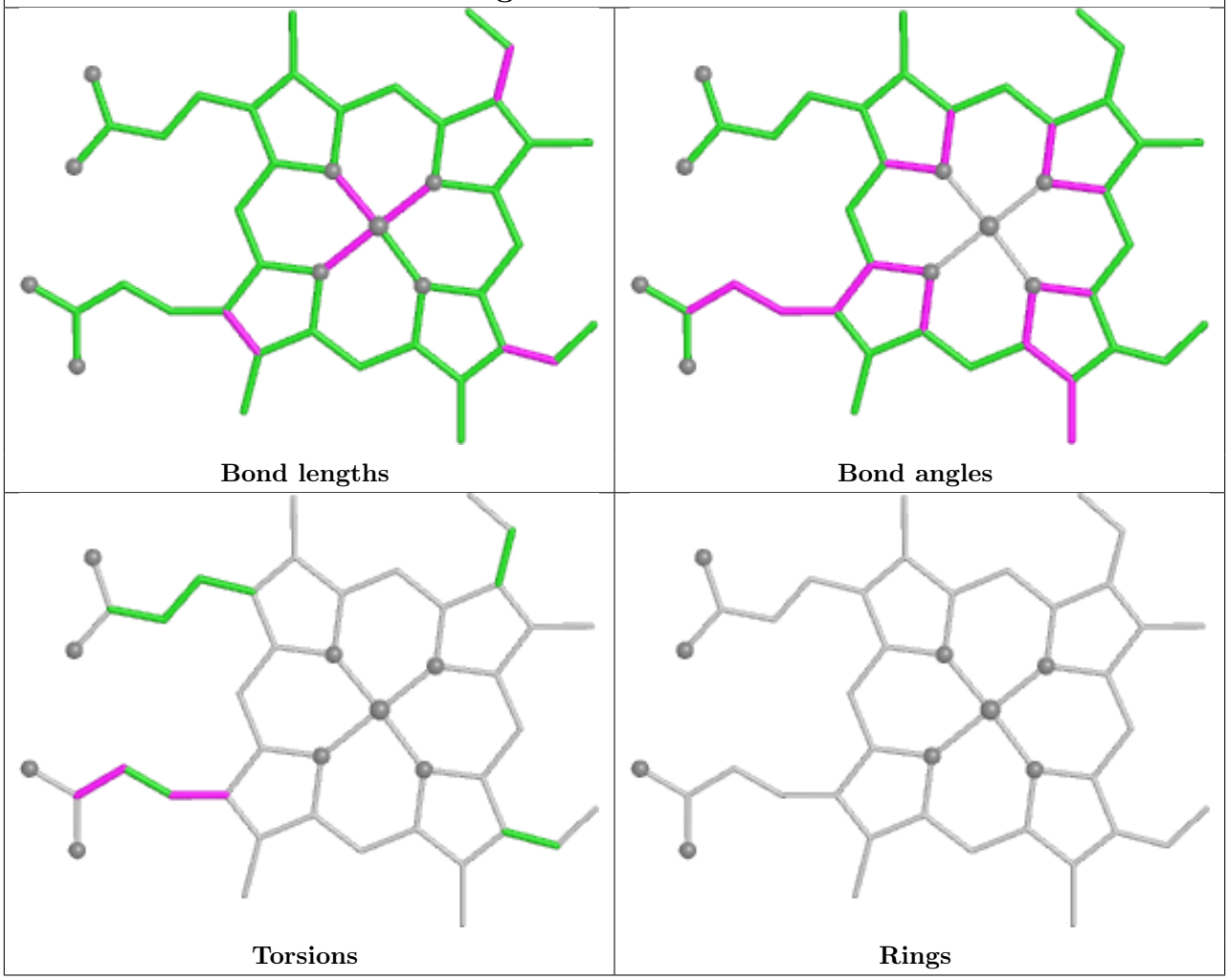


Torsions

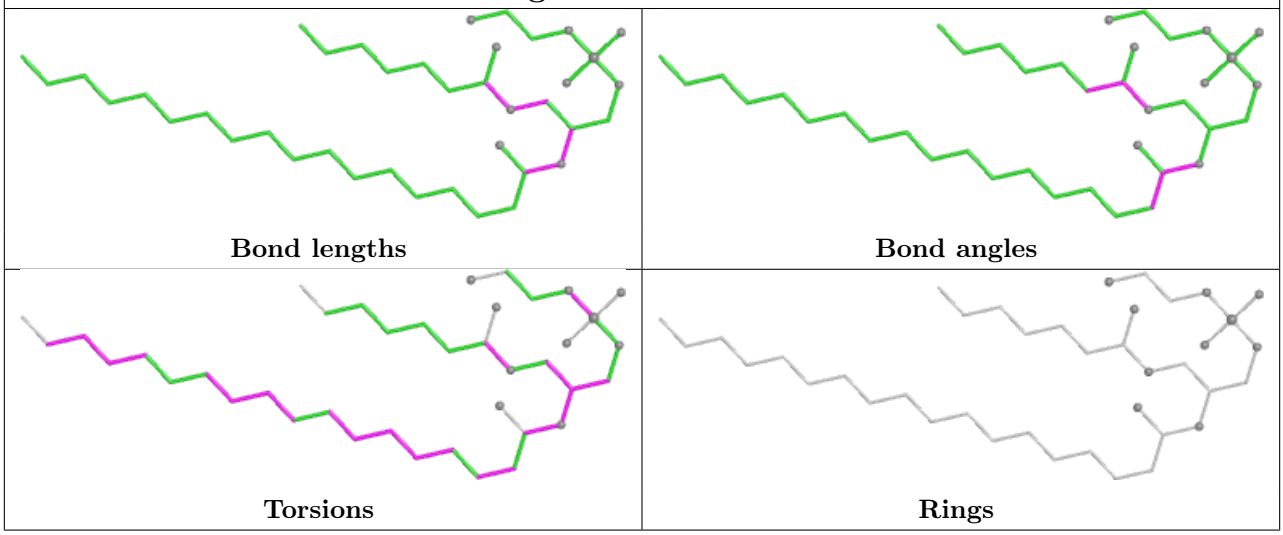


Rings

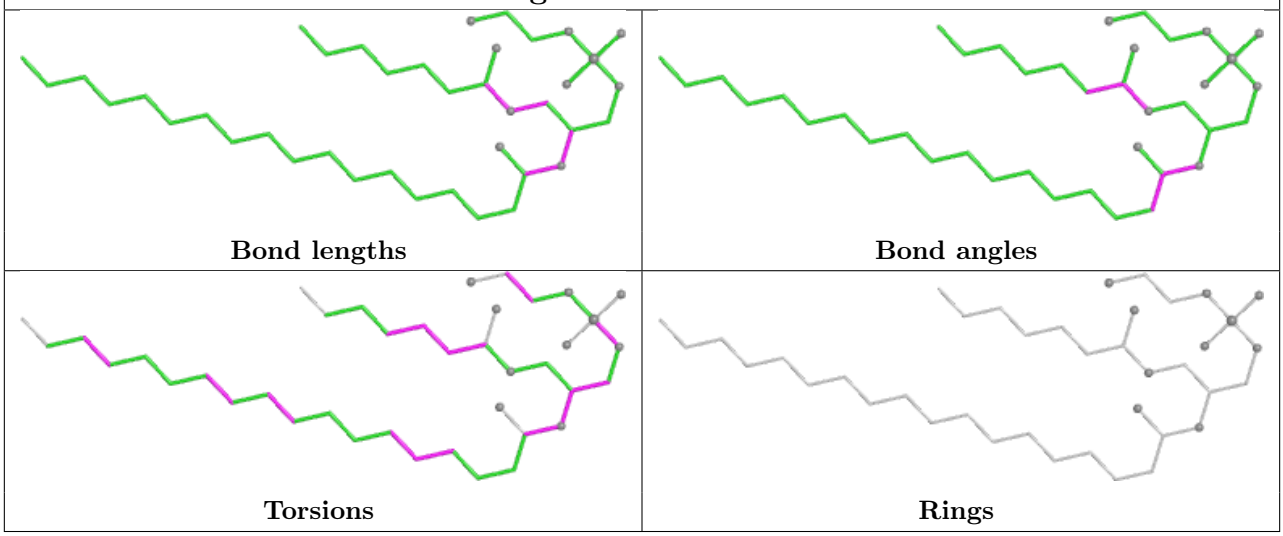
Ligand HEM N 405



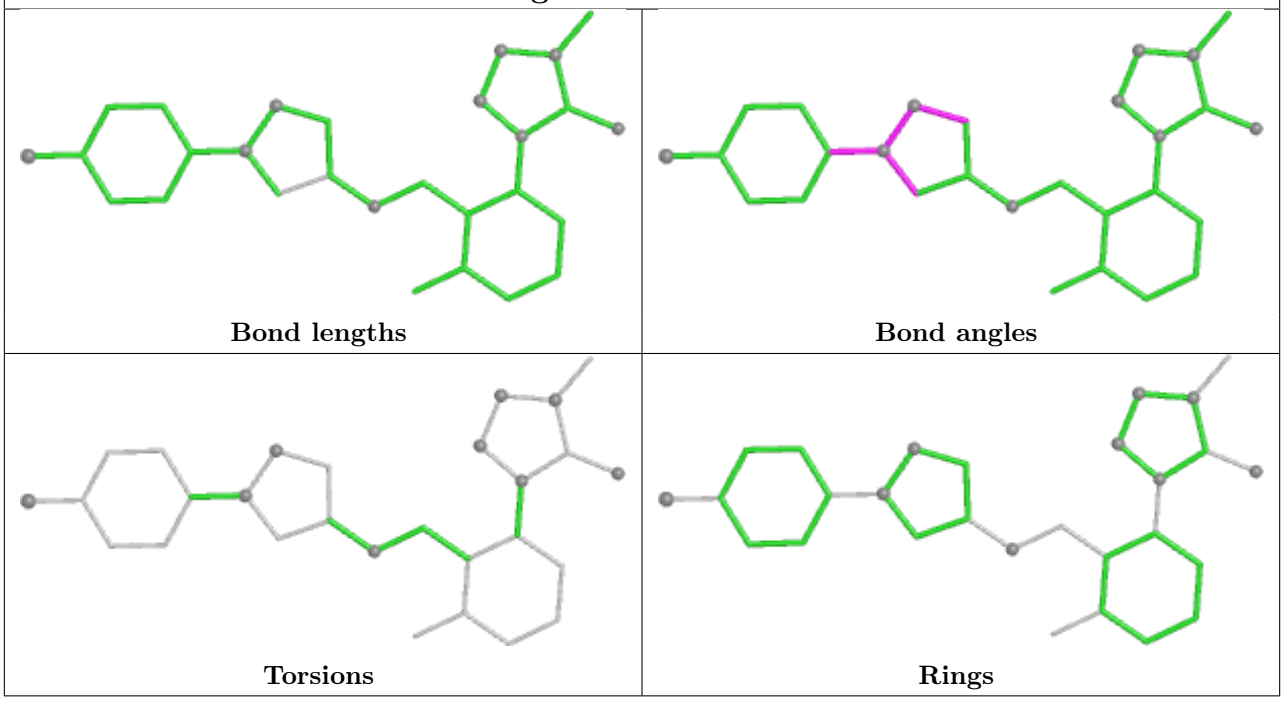
Ligand 9PE N 403

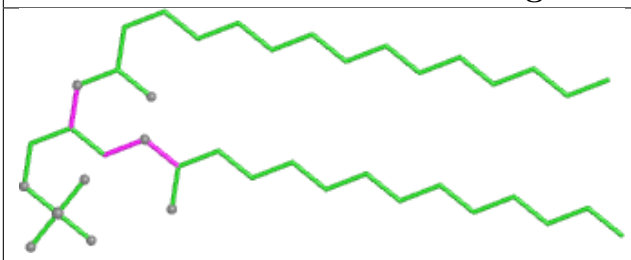
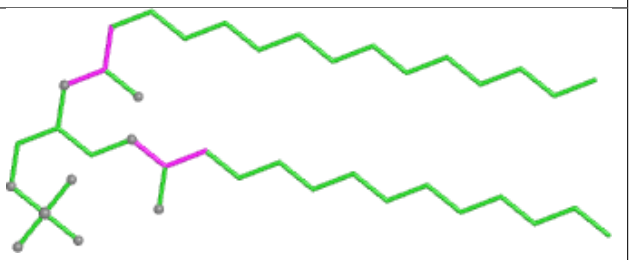
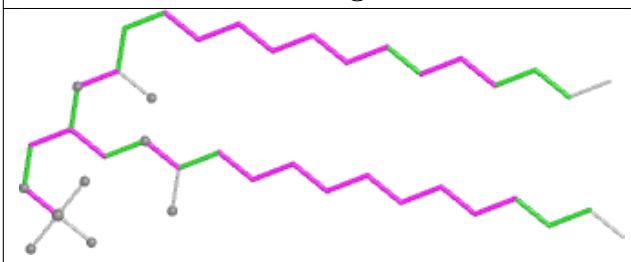
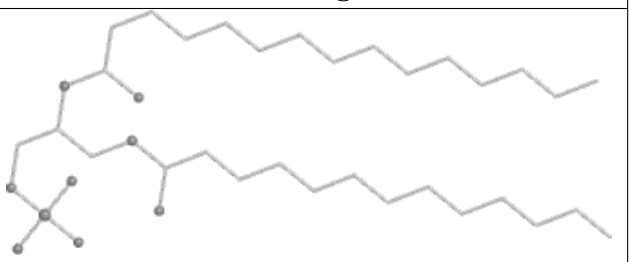


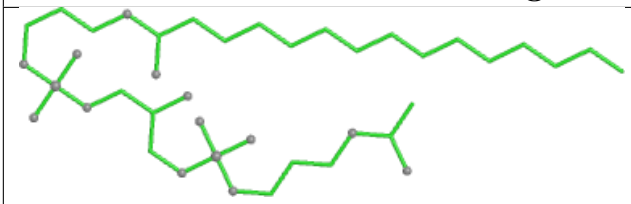
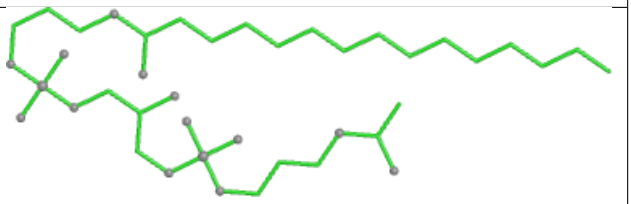
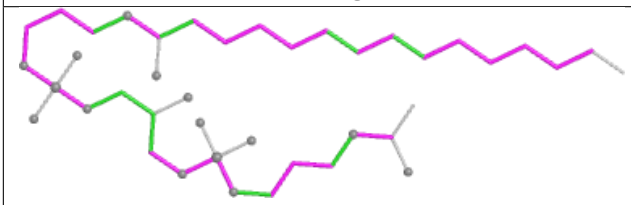
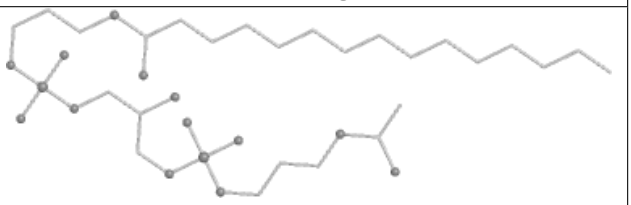
Ligand 9PE C 403



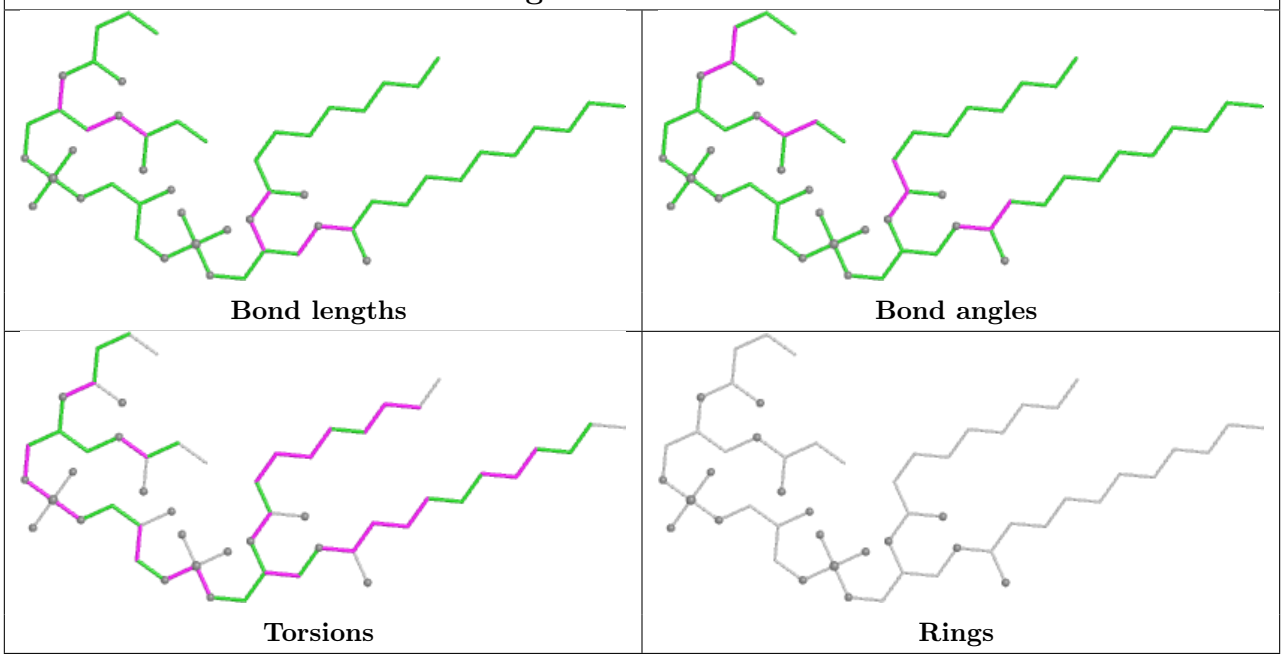
Ligand 86T N 401



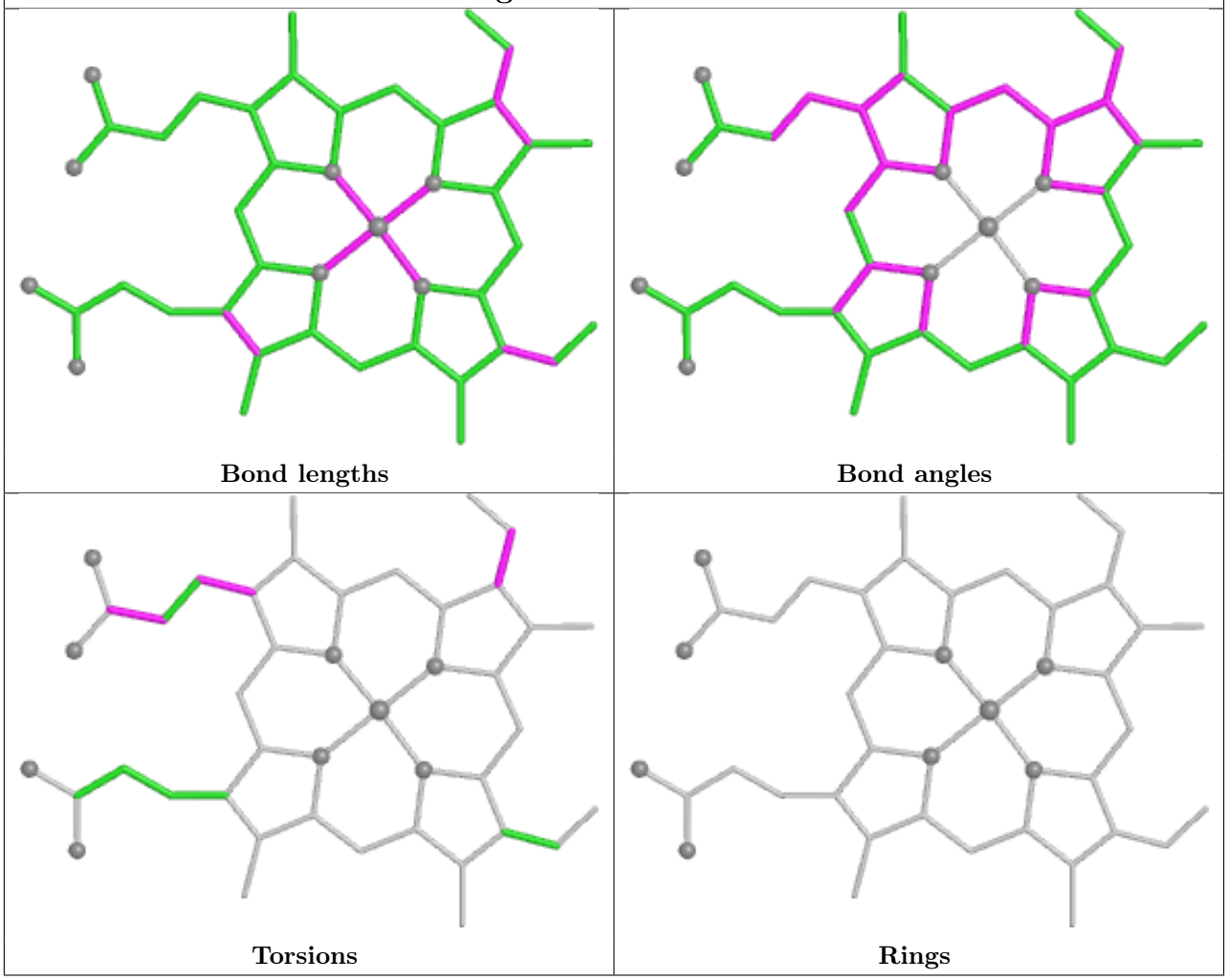
Ligand 6PH O 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CN5 C 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

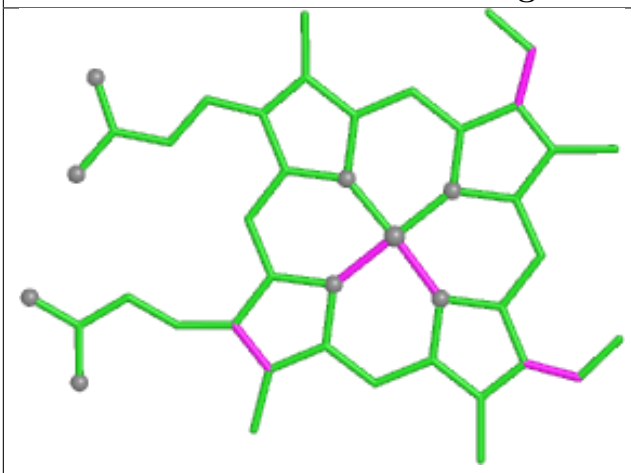
Ligand CN3 N 402



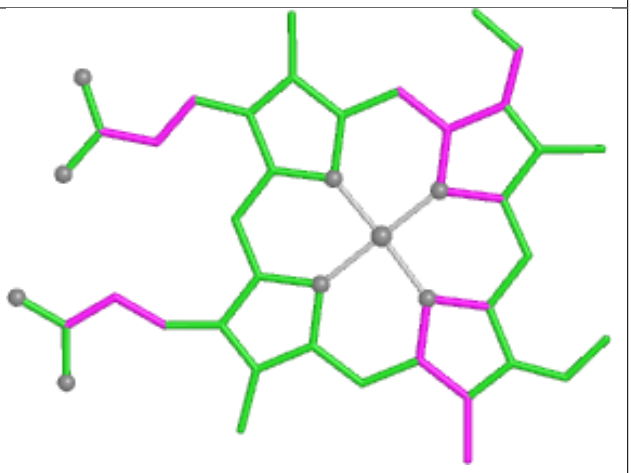
Ligand HEM N 404



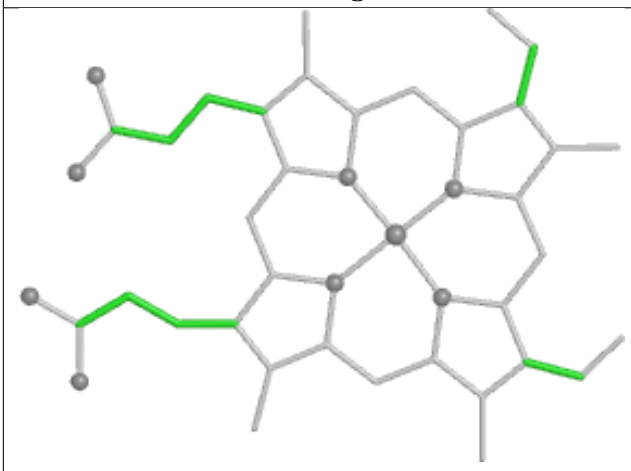
Ligand HEM D 401



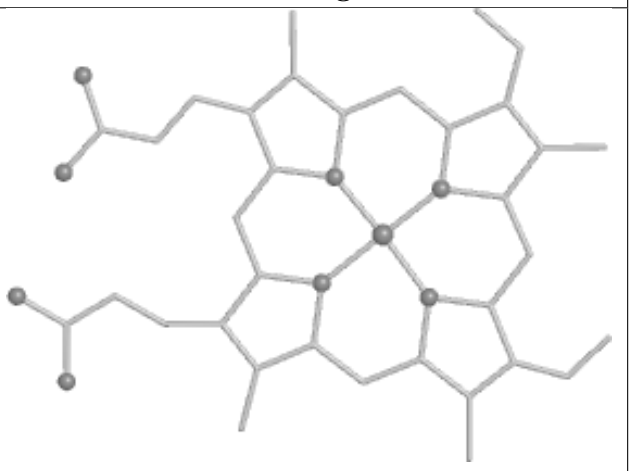
Bond lengths



Bond angles

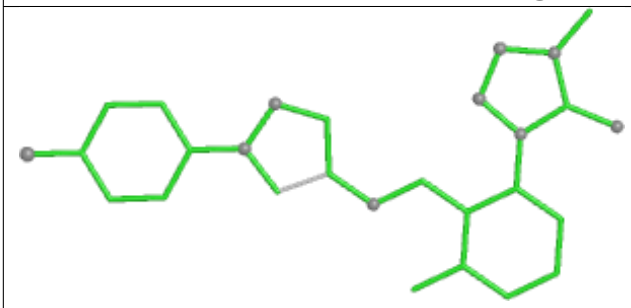


Torsions



Rings

Ligand 86T C 406



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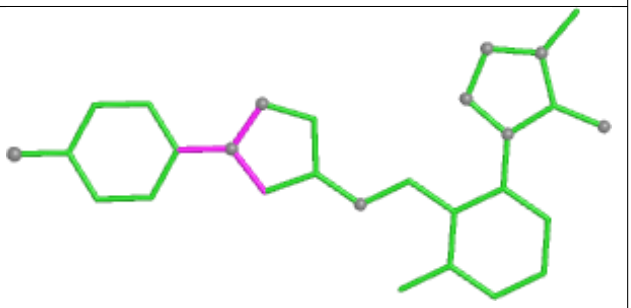
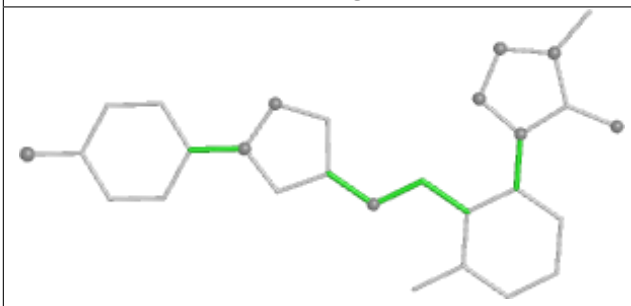


Bond angles



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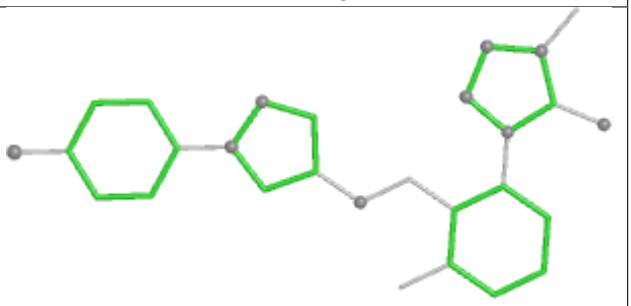

Rings

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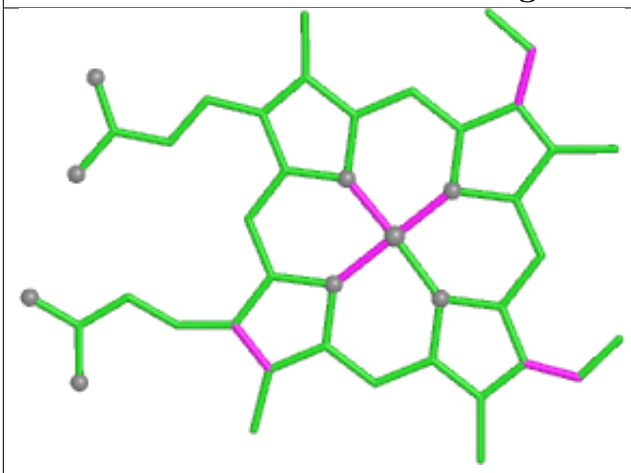
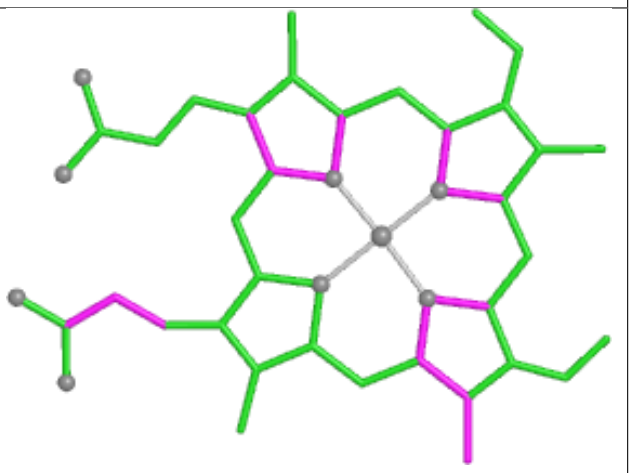
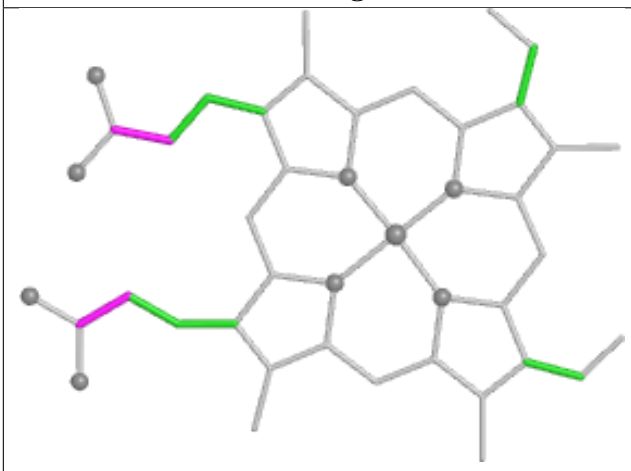


Bond lengths



Bond angles



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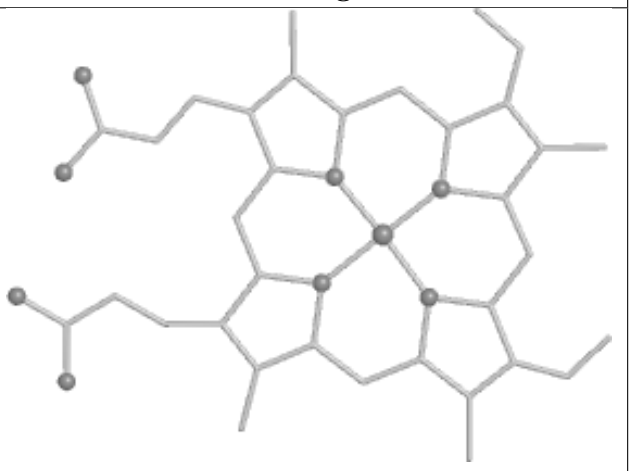
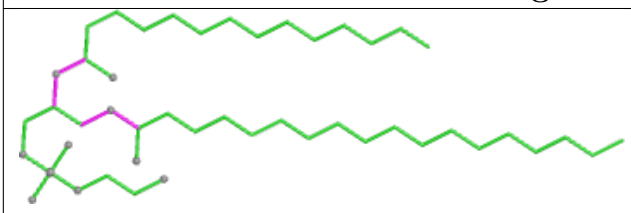
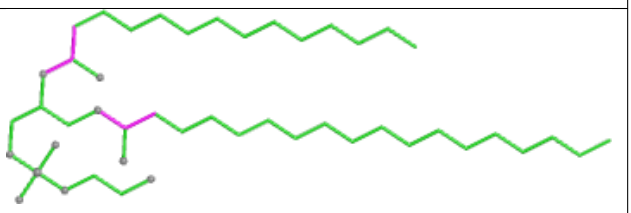


Rings

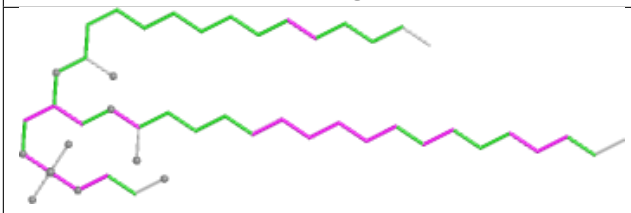
Ligand 8PE S 101



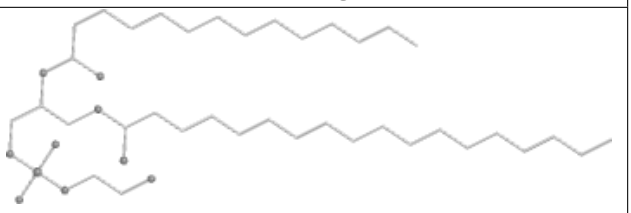
Bond lengths



Bond angles

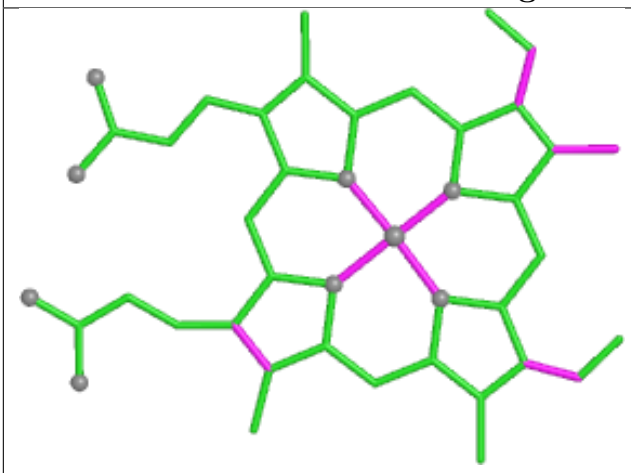


Torsions

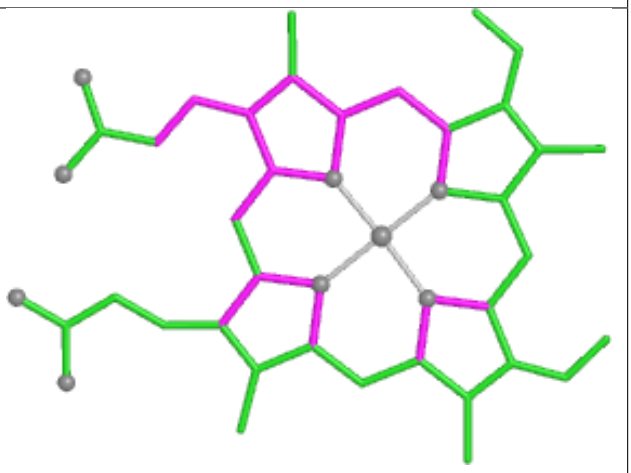


Rings

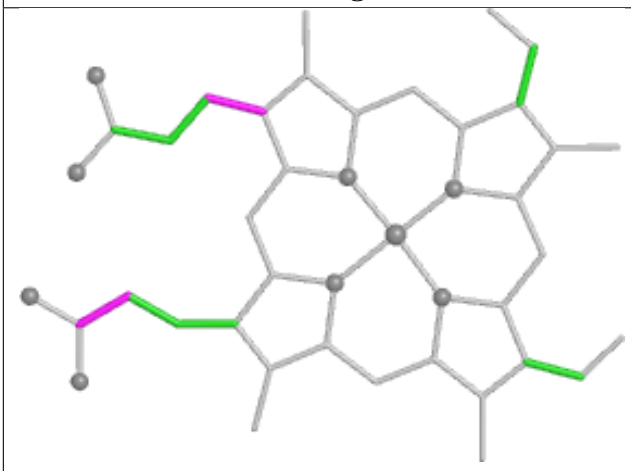
Ligand HEM C 404



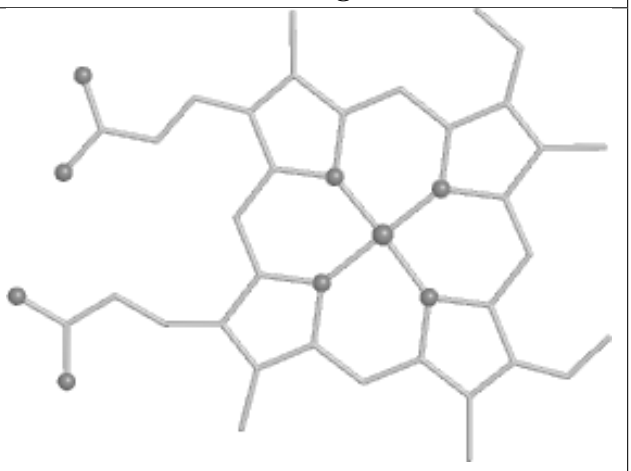
Bond lengths



Bond angles

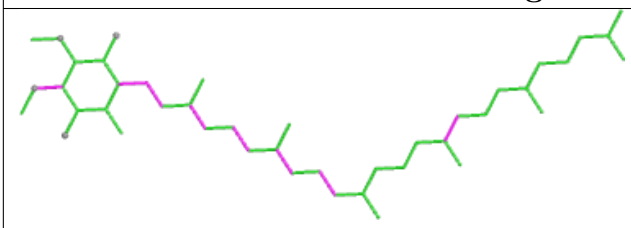


Torsions

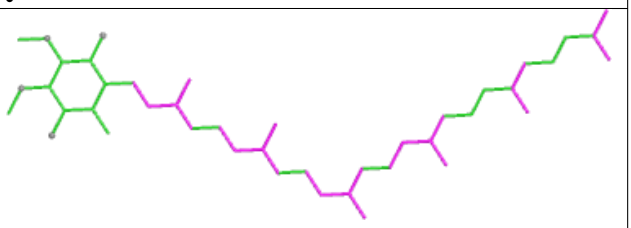


Rings

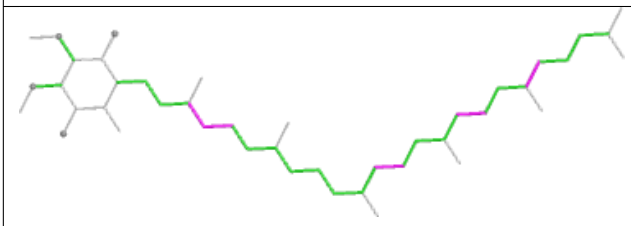
Ligand UQ6 C 401



Bond lengths



Bond angles



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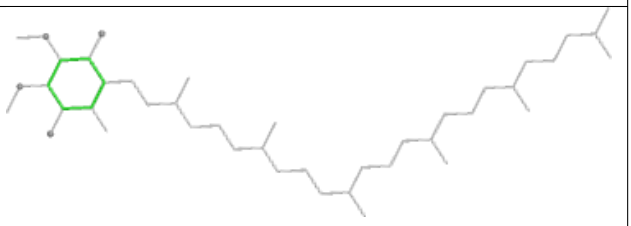
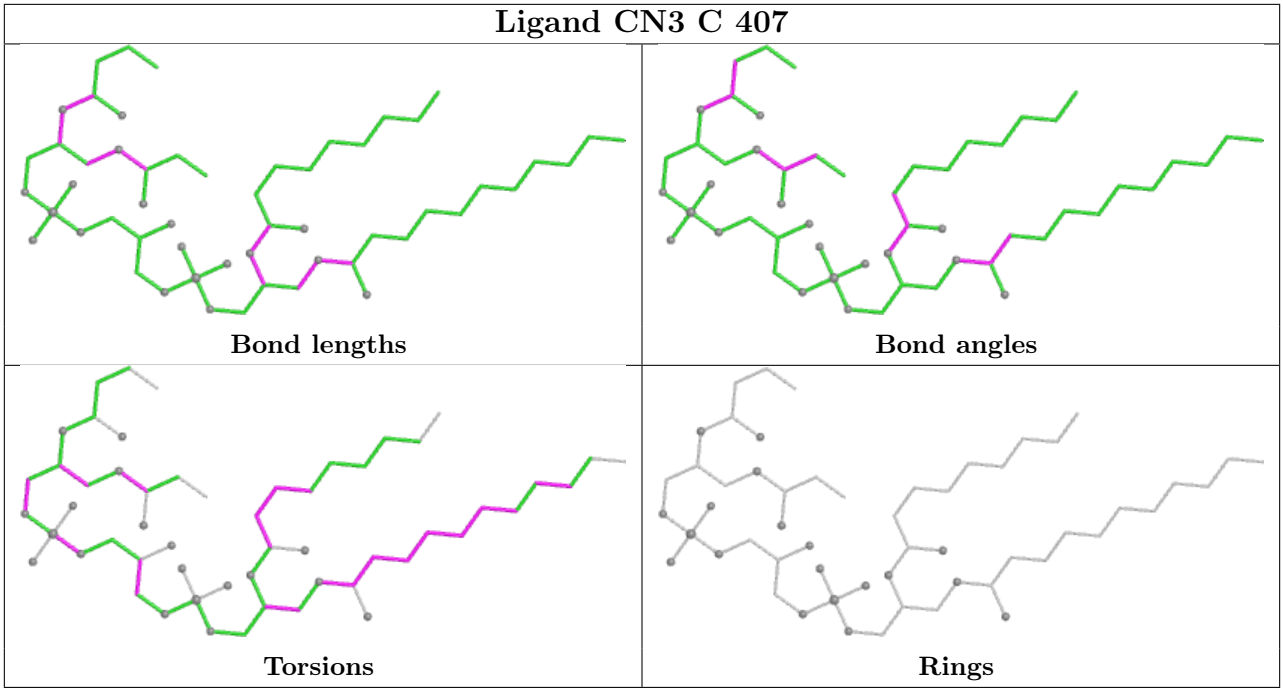
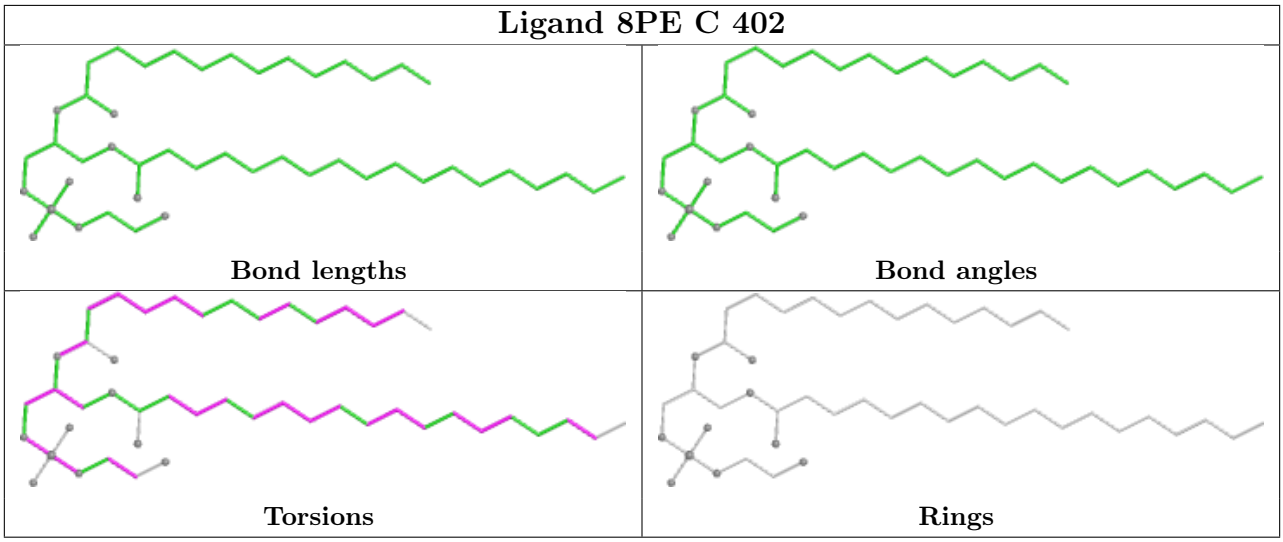


Rings





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.

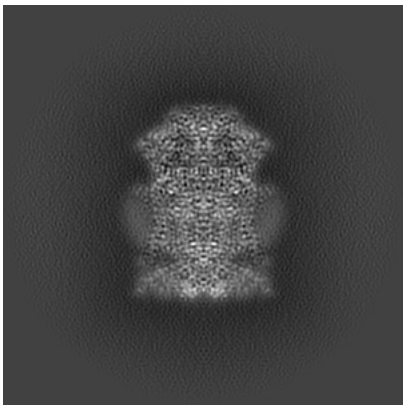
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-39322. These allow visual inspection of the internal detail of the map and identification of artifacts.

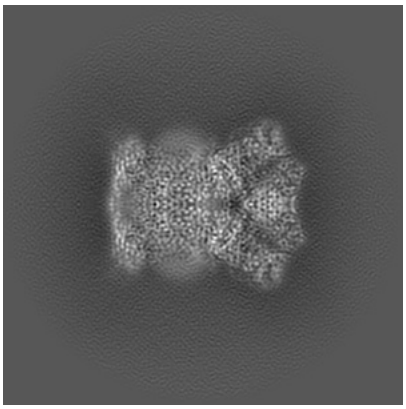
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

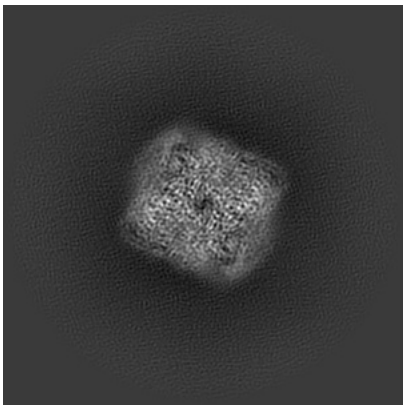
6.1.1 Primary map



X

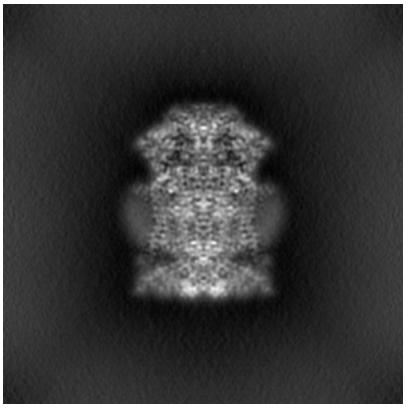


Y

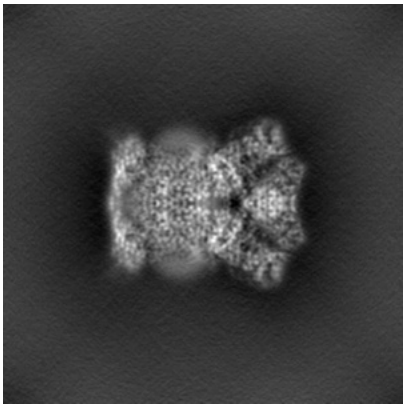


Z

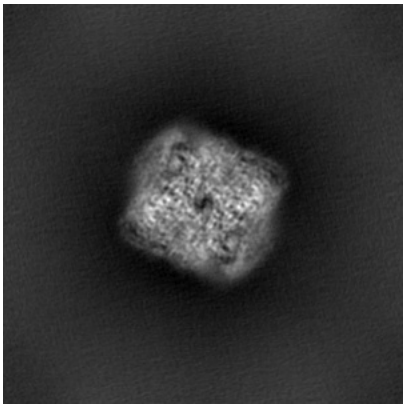
6.1.2 Raw map



X



Y

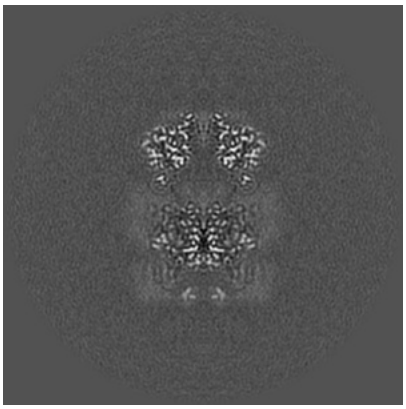


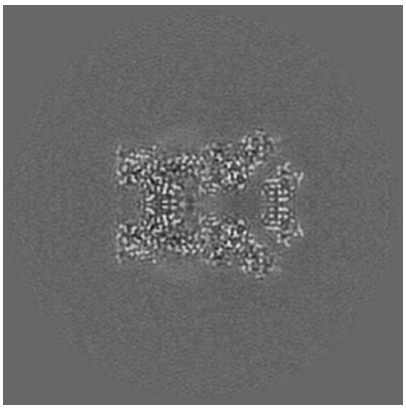
Z

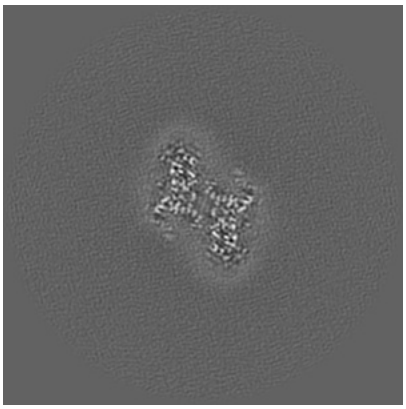
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

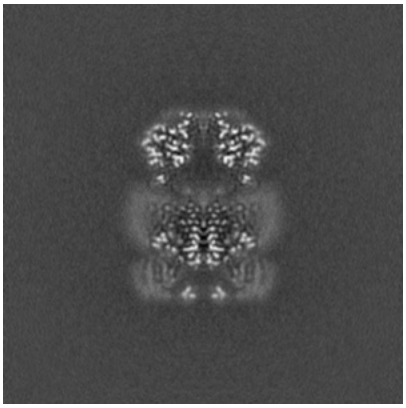
6.2.1 Primary map

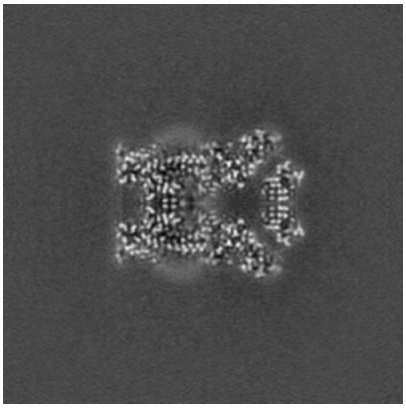

X Index: 160

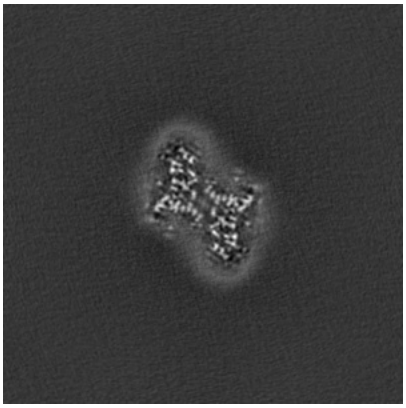

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

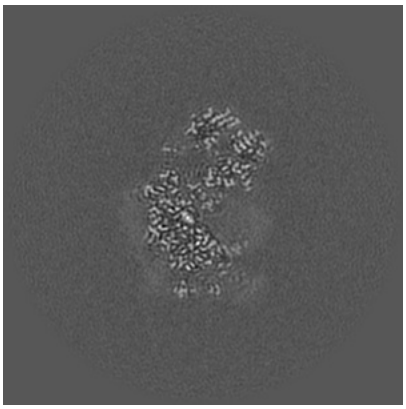

Y Index: 160


Z Index: 160

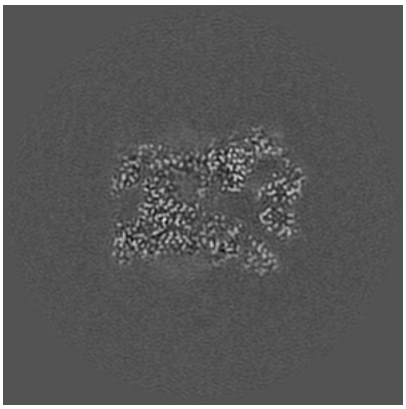
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

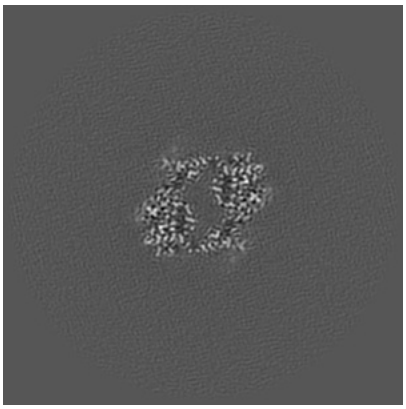
6.3.1 Primary map



X Index: 172

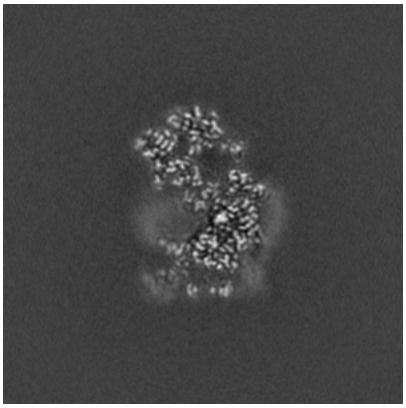


Y Index: 165

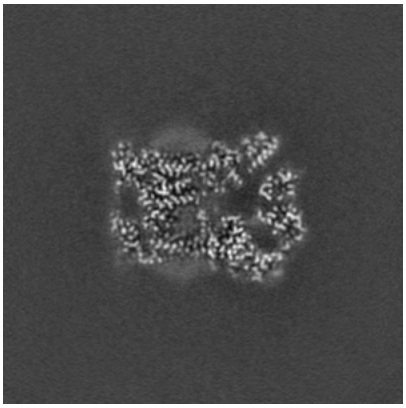


Z Index: 181

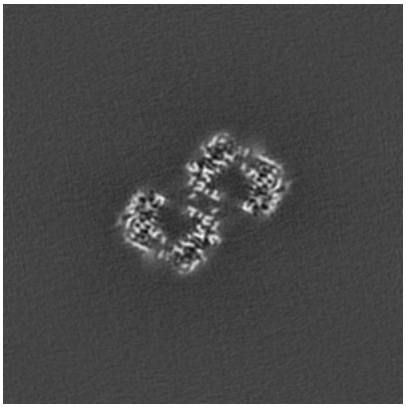
6.3.2 Raw map



X Index: 149



Y Index: 155

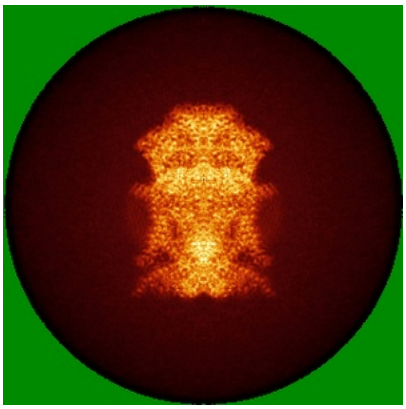


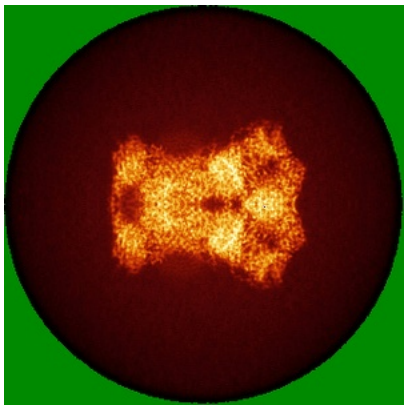
Z Index: 205

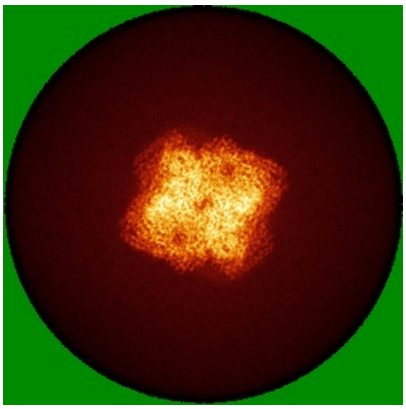
The images above show the largest variance slices of the map in three orthogonal directions.

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

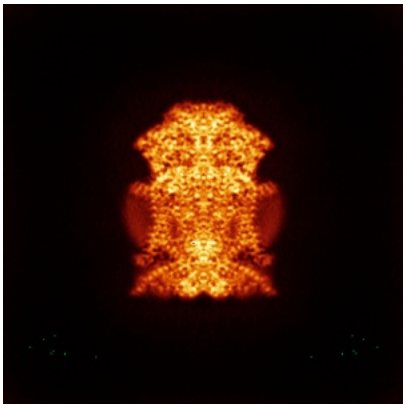
6.4.1 Primary map

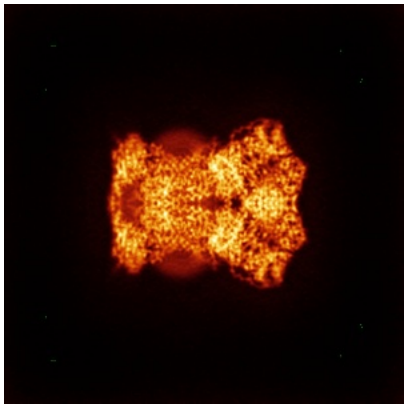

X

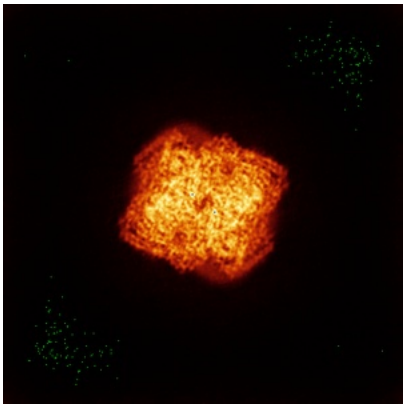

Y


Z

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

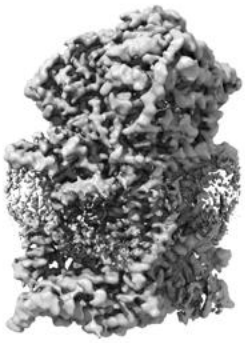
X

Y

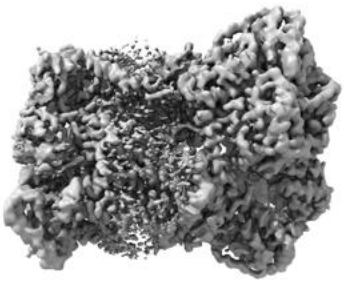
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

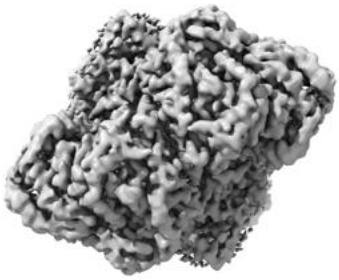
6.5.2 Raw map



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.

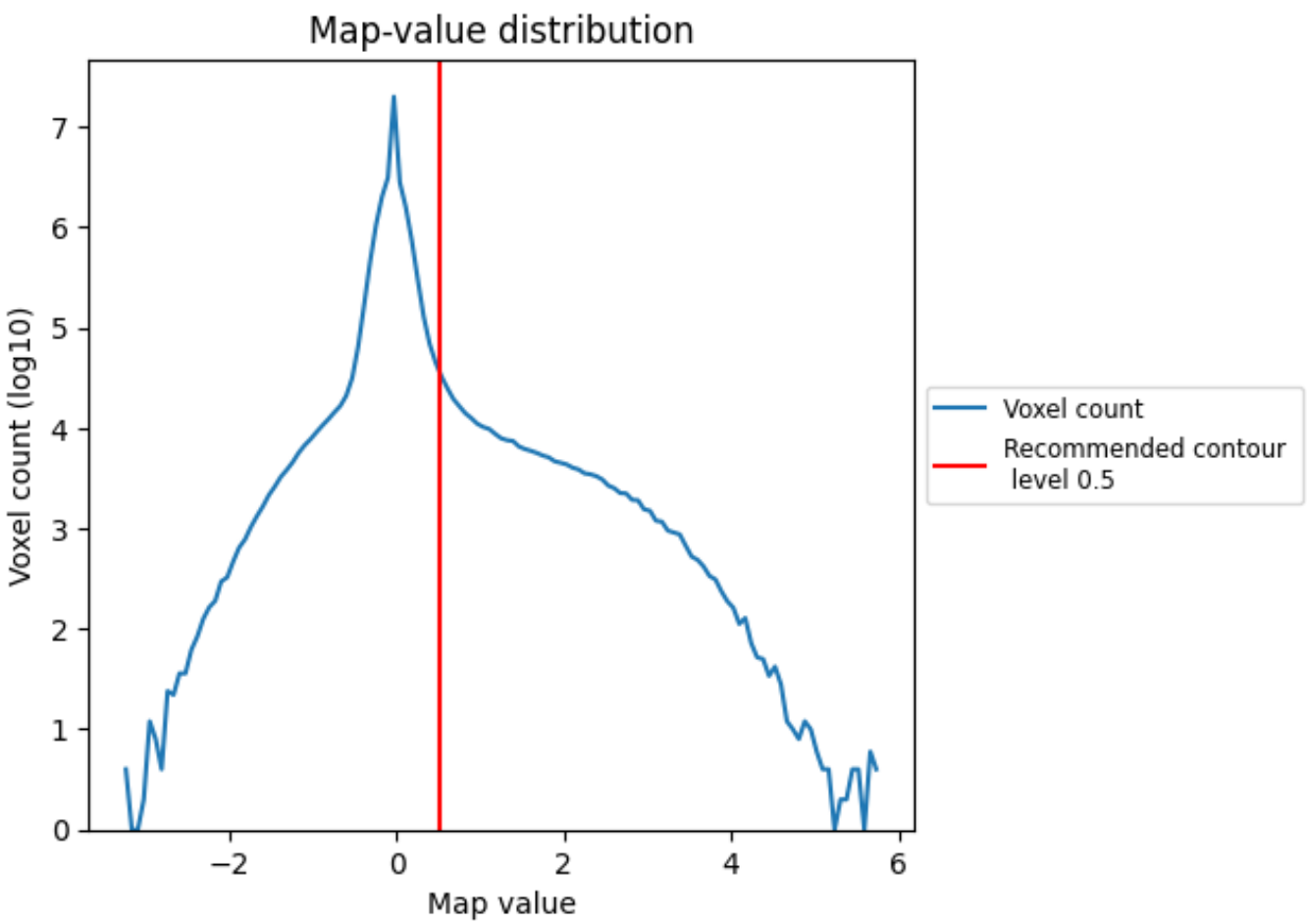
6.6 Mask visualisation (i)

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

7 Map analysis (i)

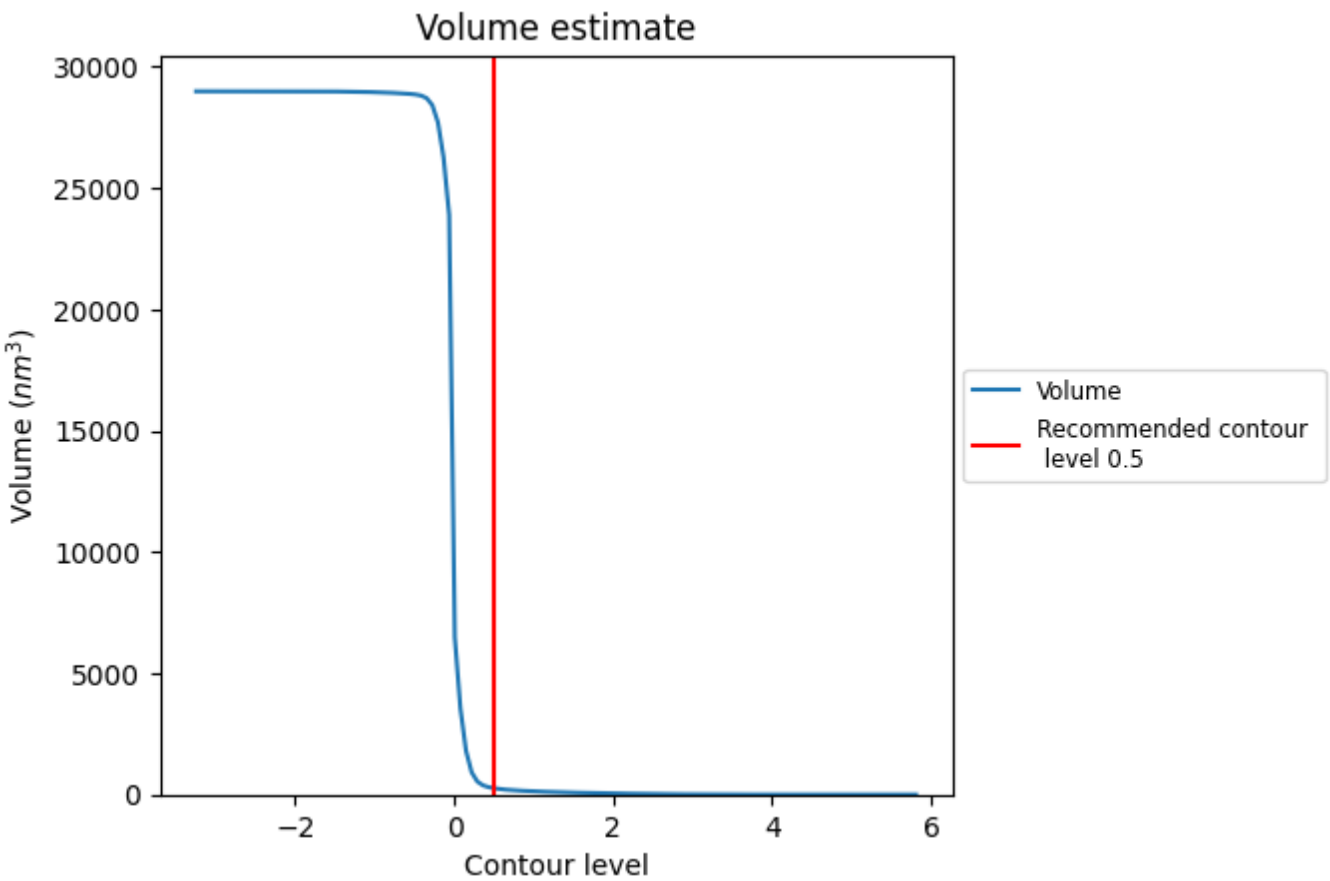
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

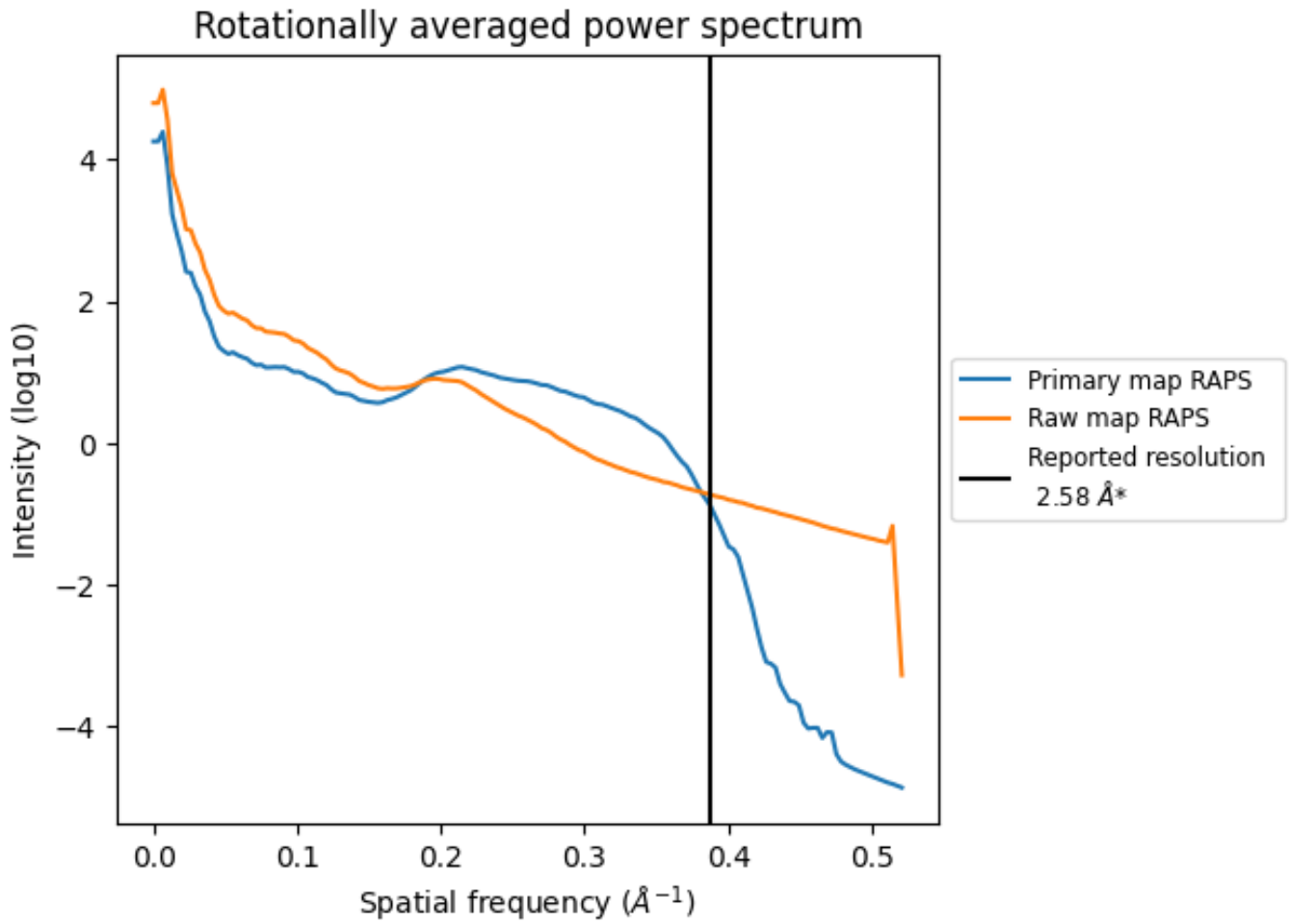
7.2 Volume estimate (i)



The volume at the recommended contour level is 262 nm^3; this corresponds to an approximate mass of 237 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)

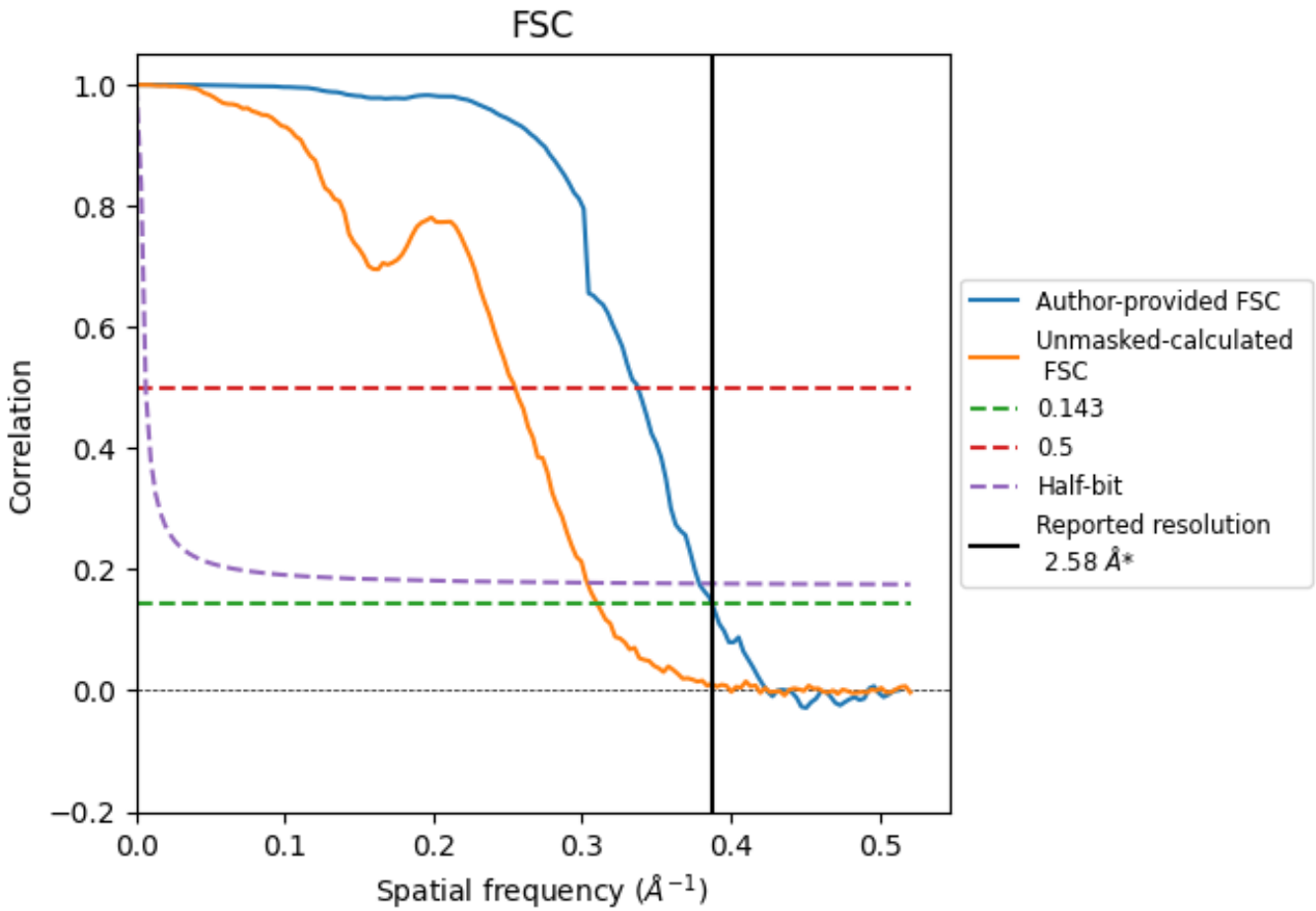


*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

8.2 Resolution estimates (i)

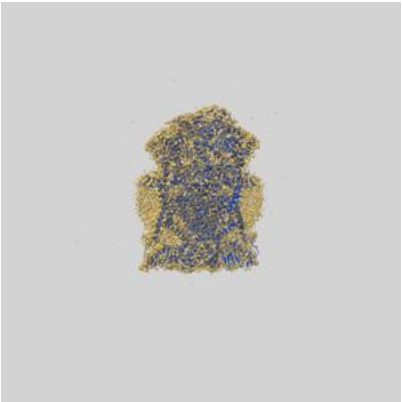
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.58	2.96	2.64
Unmasked-calculated*	3.22	3.92	3.29

*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 3.22 differs from the reported value 2.58 by more than 10 %

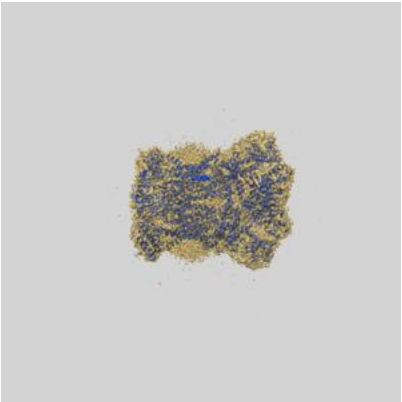
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-39322 and PDB model 8YIL. Per-residue inclusion information can be found in section 3 on page 12.

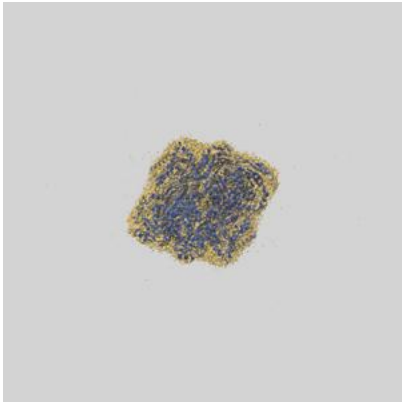
9.1 Map-model overlay (i)



X



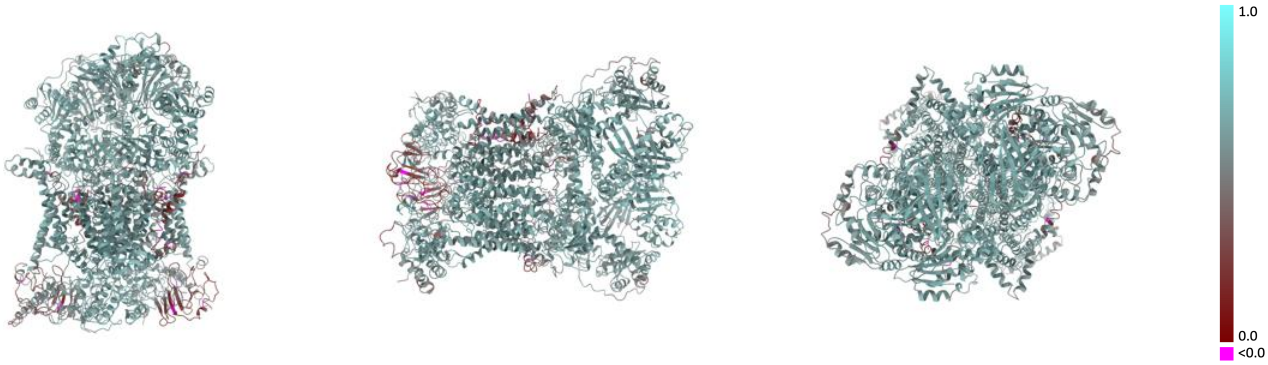
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

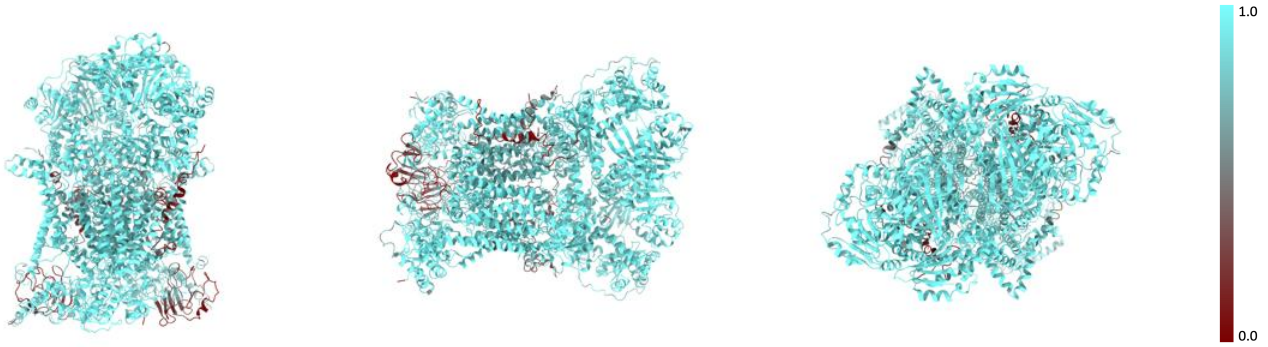
9.2 Q-score mapped to coordinate model (i)



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.

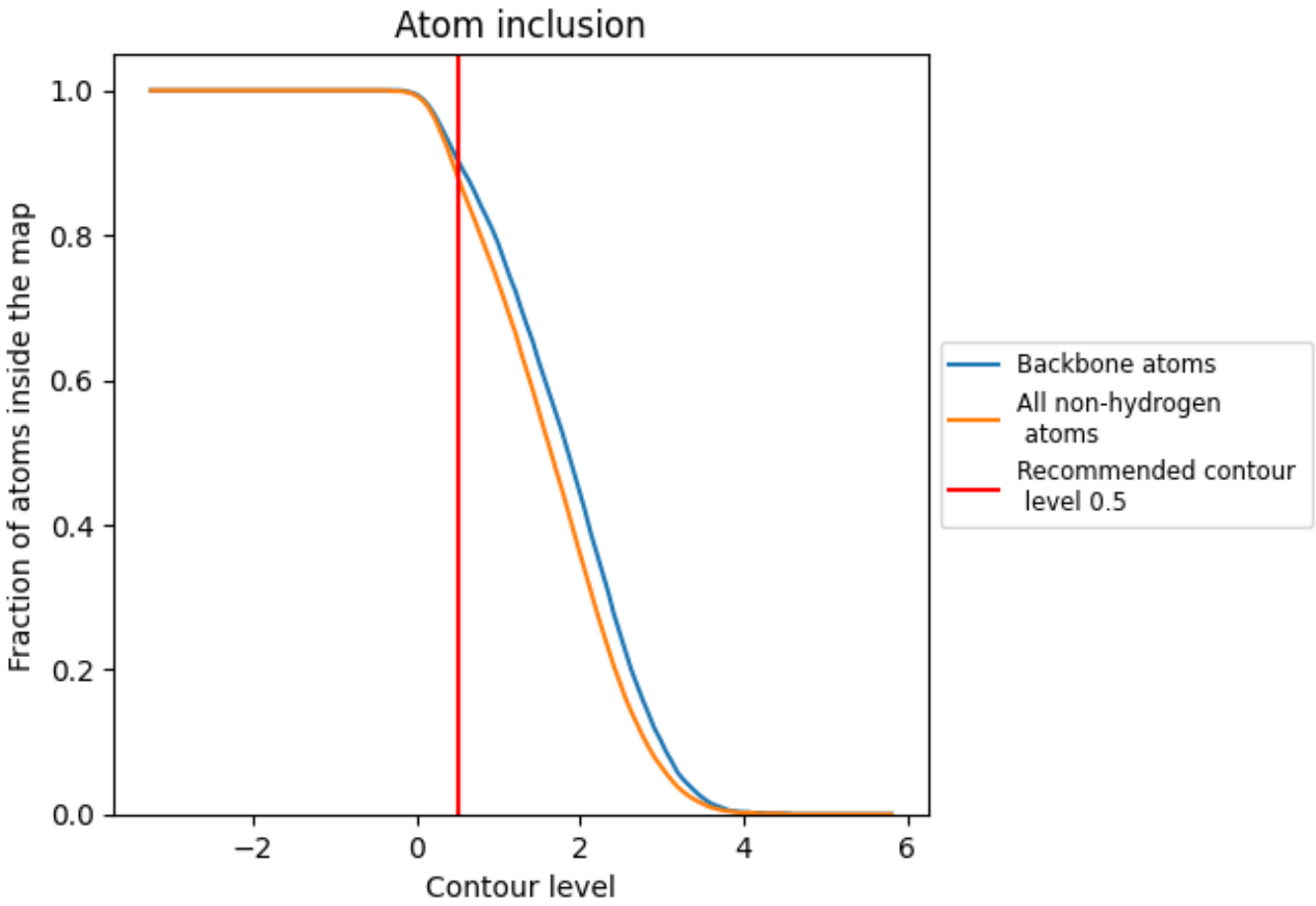
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8820	0.5760
A	0.9560	0.6000
B	0.9720	0.6290
C	0.9720	0.6370
D	0.9650	0.6160
E	0.4880	0.3830
F	0.8210	0.5030
G	0.9370	0.6040
H	0.8440	0.5370
I	0.6700	0.4430
L	0.9560	0.6010
M	0.9710	0.6290
N	0.9740	0.6390
O	0.9660	0.6190
P	0.4760	0.3770
Q	0.8290	0.4980
R	0.9380	0.6030
S	0.8400	0.5340
T	0.6690	0.4720
U	0.1030	0.2300
V	0.0850	0.1980