wwPDB EM Validation Summary Report

Dec 16, 2024 – 05:00 PM EST

PDB ID	:	7RJE
EMDB ID	:	EMD-24486
Title	:	Complex III2 from Candida albicans, Inz-5 bound
Authors	:	Di Trani, J.M.; Rubinstein, J.L.
Deposited on	:	2021-07-20
Resolution	:	3.30 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 ⓘ symbol.

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

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

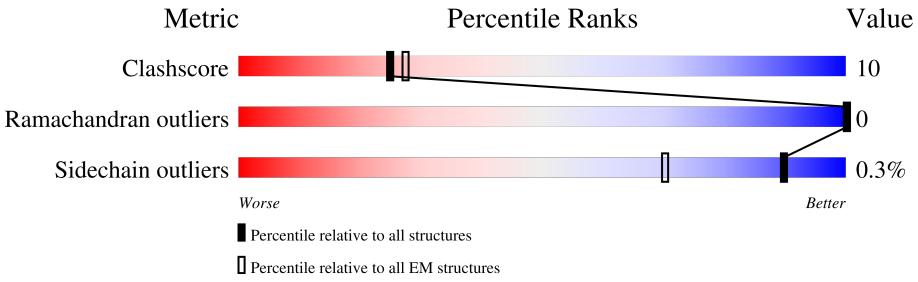
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	K	387	77% 21%
1	T	387	80% 19%
2	A	439	79% 16% 5%
2	E	439	78% 17% 5%
3	B	374	76% 22%
3	L	374	78% 19%
4	D	288	61% 23% 16%
4	N	288	63% 21% 16%

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Mol	Chain	Length	Quality of chain
5	G	127	82% 14%
5	P	127	83% 13%
6	F	95	72% 21% 7%
6	O	95	73% 20% 7%
7	H	135	47% 6% 47%
7	Q	135	45% 8% 47%
8	I	65	42% 17% 42%
8	R	65	43% 15% 42%
9	C	213	60% 74% 11% 15%
9	M	213	61% 74% 11% 15%

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
13	FES	M	301	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 57440 atoms, of which 28132 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	K	384	Total	C	H	N	O	S	0	0
			6146	2060	3088	478	503	17		
1	T	384	Total	C	H	N	O	S	0	0
			6146	2060	3088	478	503	17		

- Molecule 2 is a protein called Ubiquinol--cytochrome-c reductase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	417	Total	C	H	N	O	S	0	0
			6359	2012	3162	547	635	3		
2	E	417	Total	C	H	N	O	S	0	0
			6359	2012	3162	547	635	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	364	Total	C	H	N	O	S	0	0
			5392	1708	2692	443	548	1		
3	L	364	Total	C	H	N	O	S	0	0
			5392	1708	2692	443	548	1		

- Molecule 4 is a protein called Ubiquinol--cytochrome-c reductase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	243	Total	C	H	N	O	S	0	0
			3713	1215	1812	332	348	6		
4	N	243	Total	C	H	N	O	S	0	0
			3713	1215	1812	332	348	6		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	122	Total	C	H	N	O	S	0	0
			1978	629	1002	161	183	3		
5	P	122	Total	C	H	N	O	S	0	0
			1978	629	1002	161	183	3		

- Molecule 6 is a protein called Ubiquinol--cytochrome-c reductase subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	88	Total	C	H	N	O	S	0	0
			1410	472	687	124	126	1		
6	O	88	Total	C	H	N	O	S	0	0
			1410	472	687	124	126	1		

- Molecule 7 is a protein called Ubiquinol--cytochrome-c reductase subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	72	Total	C	H	N	O	S	0	0
			1104	363	522	105	108	6		
7	Q	72	Total	C	H	N	O	S	0	0
			1104	363	522	105	108	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	47	GLU	ASP	conflict	UNP A0A1D8PJT8
Q	47	GLU	ASP	conflict	UNP A0A1D8PJT8

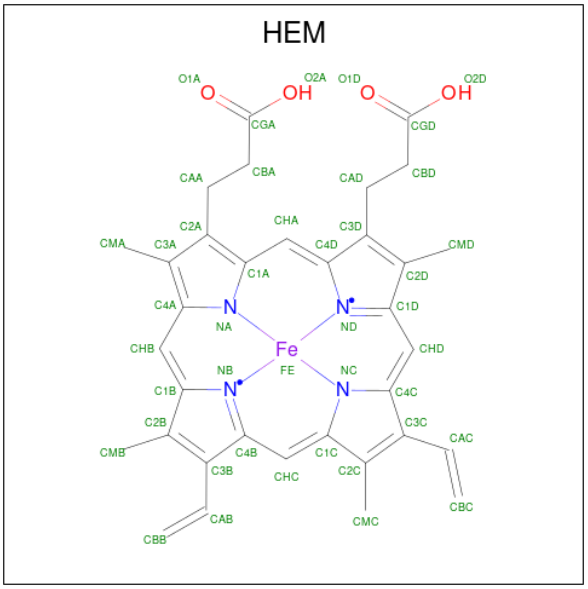
- Molecule 8 is a protein called Ubiquinol--cytochrome-c reductase subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	38	Total	C	H	N	O	0	0
			613	211	300	53	49		
8	R	38	Total	C	H	N	O	0	0
			613	211	300	53	49		

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

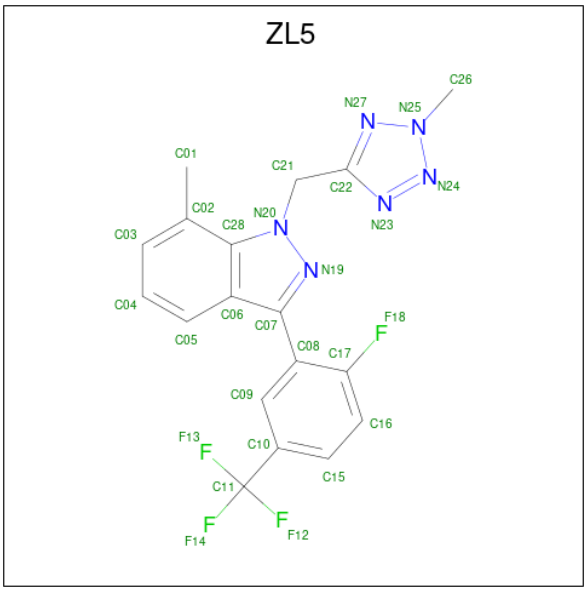
Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	181	Total	C	H	N	O	S	0	0
			1740	638	697	193	210	2		
9	M	181	Total	C	H	N	O	S	0	0
			1740	638	697	193	210	2		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



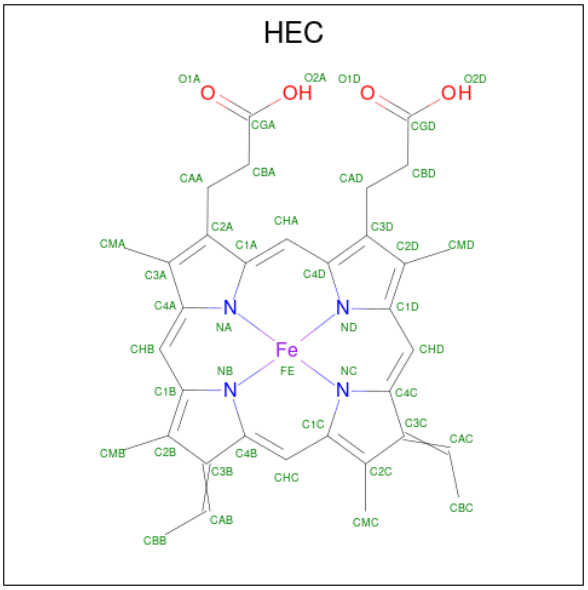
Mol	Chain	Residues	Atoms						AltConf
10	K	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
10	K	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
10	T	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
10	T	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 11 is 3-[2-fluoro-5-(trifluoromethyl)phenyl]-7-methyl-1-[(2-methyl-2H-tetrazol-5-yl)methyl]-1H-indazole (three-letter code: ZL5) (formula: $C_{18}H_{14}F_4N_6$) (labeled as "Ligand of Interest" by depositor).



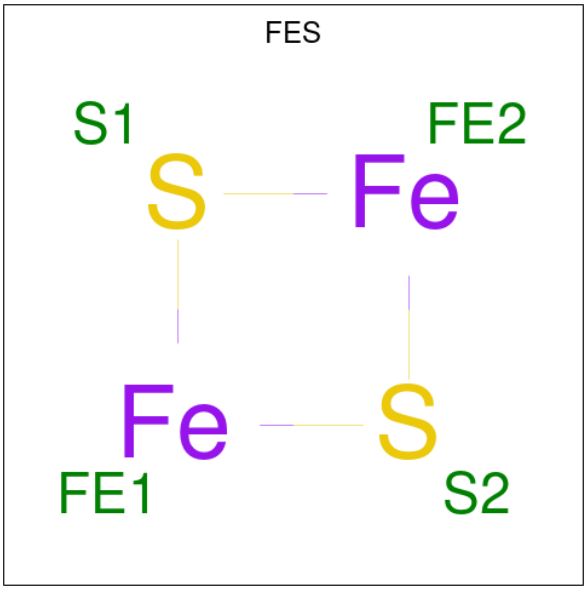
Mol	Chain	Residues	Atoms					AltConf
11	K	1	Total	C	F	H	N	0
			42	18	4	14	6	
11	T	1	Total	C	F	H	N	0
			42	18	4	14	6	

- Molecule 12 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
12	D	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
12	N	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



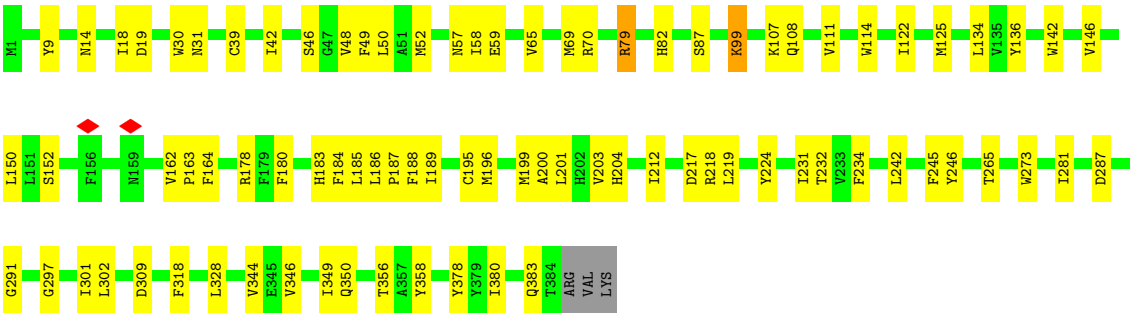
Mol	Chain	Residues	Atoms	AltConf
13	C	1	Total Fe S 4 2 2	0
13	M	1	Total Fe S 4 2 2	0

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.

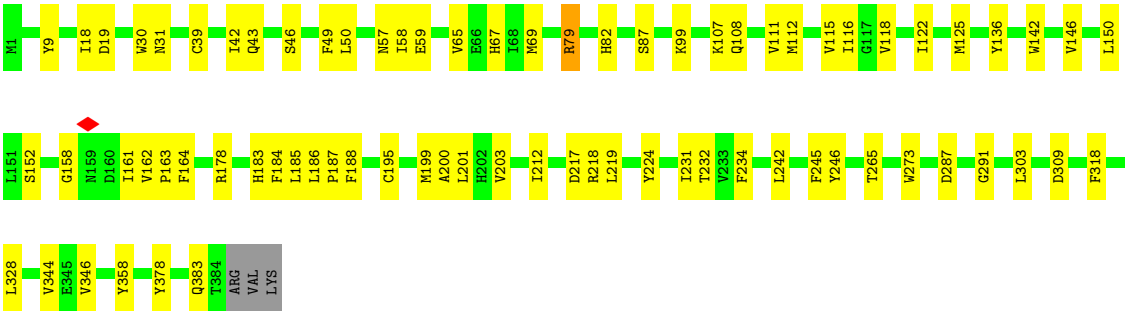
• Molecule 1: Cytochrome b

Chain K:



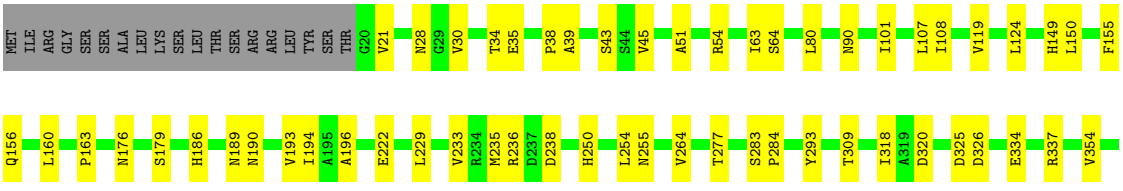
• Molecule 1: Cytochrome b

Chain T:

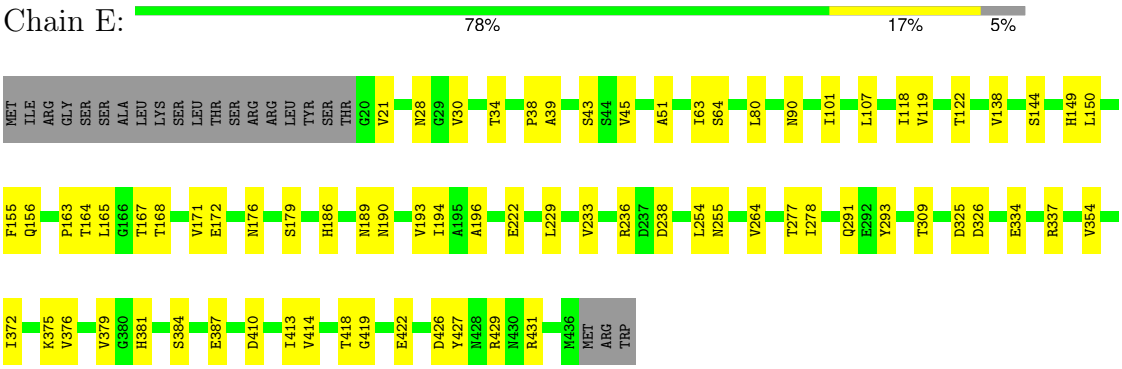


• Molecule 2: Ubiquinol--cytochrome-c reductase subunit

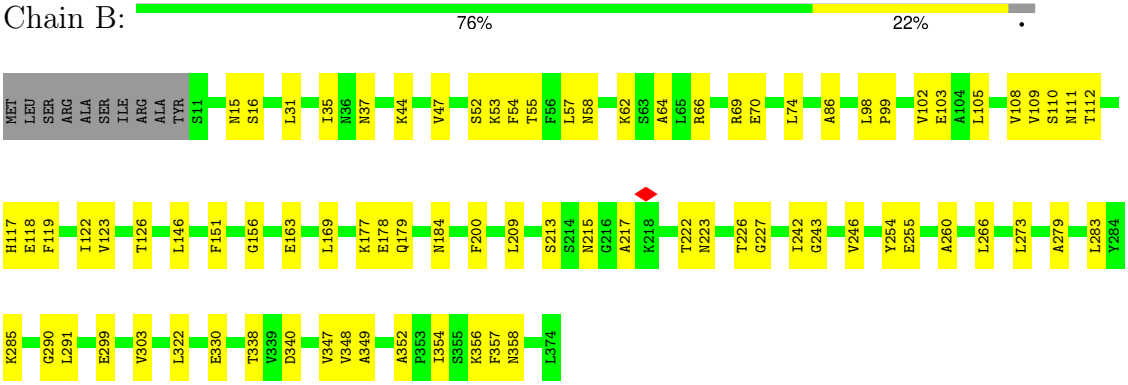
Chain A:



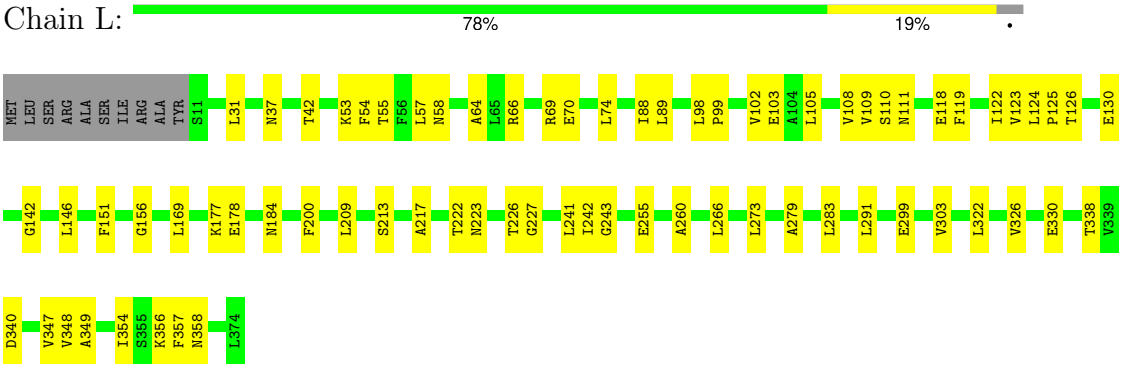
• Molecule 2: Ubiquinol--cytochrome-c reductase subunit



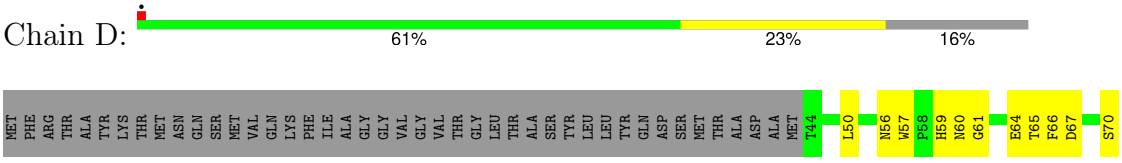
• Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

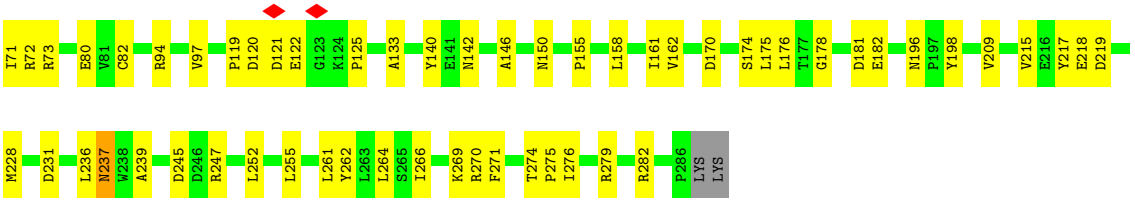


• Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

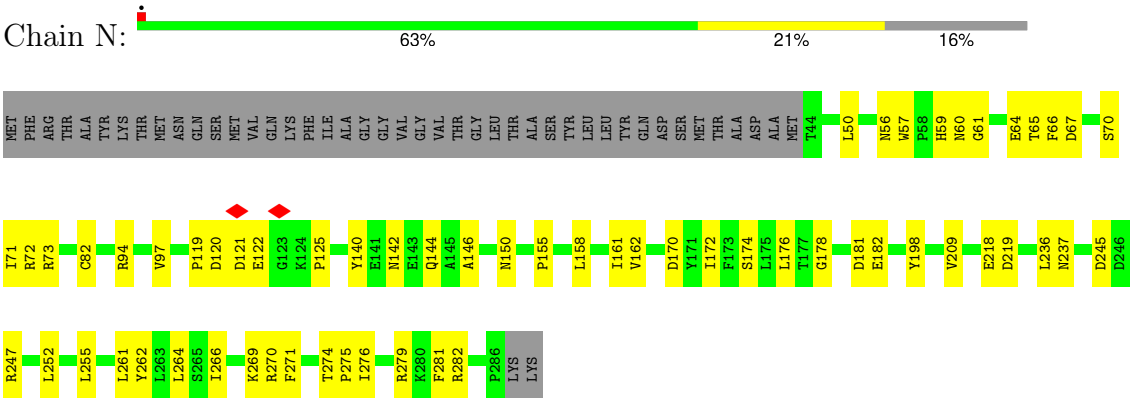


• Molecule 4: Ubiquinol--cytochrome-c reductase catalytic subunit

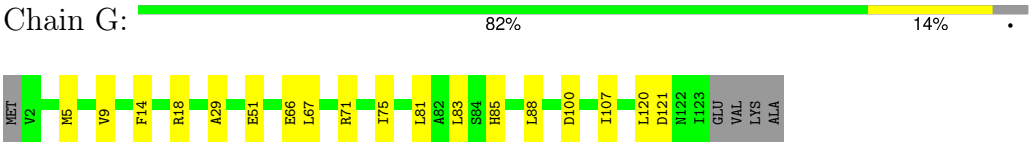




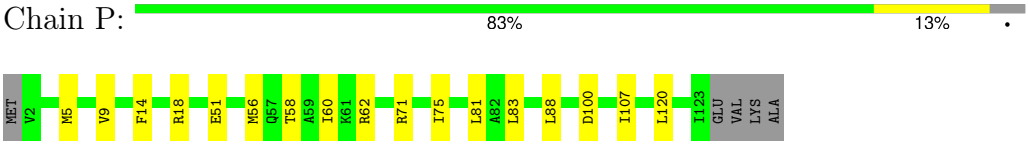
• Molecule 4: Ubiquinol--cytochrome-c reductase catalytic subunit



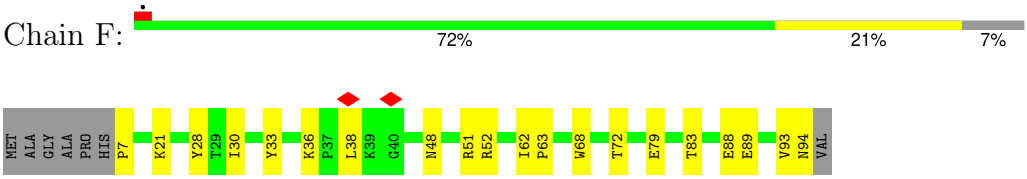
• Molecule 5: Cytochrome b-c1 complex subunit 7



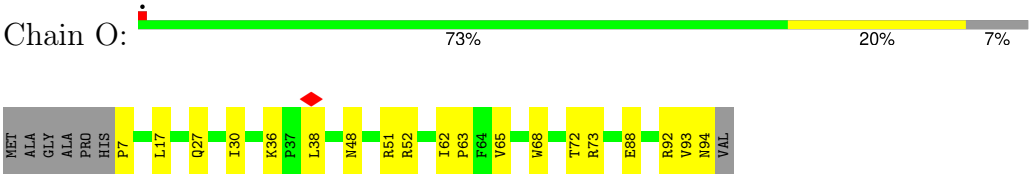
• Molecule 5: Cytochrome b-c1 complex subunit 7



• Molecule 6: Ubiquinol--cytochrome-c reductase subunit 8

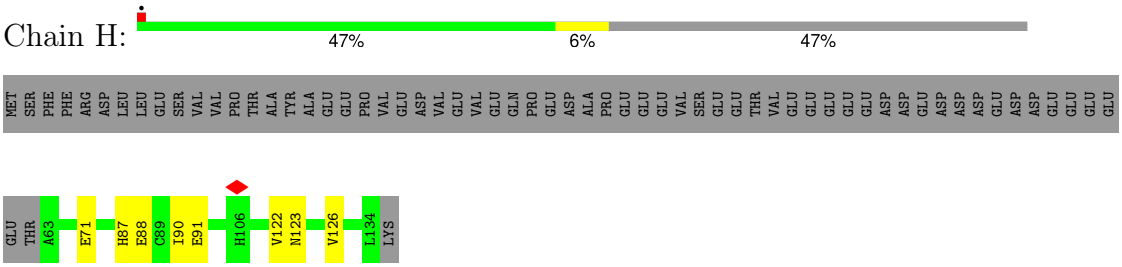


• Molecule 6: Ubiquinol--cytochrome-c reductase subunit 8



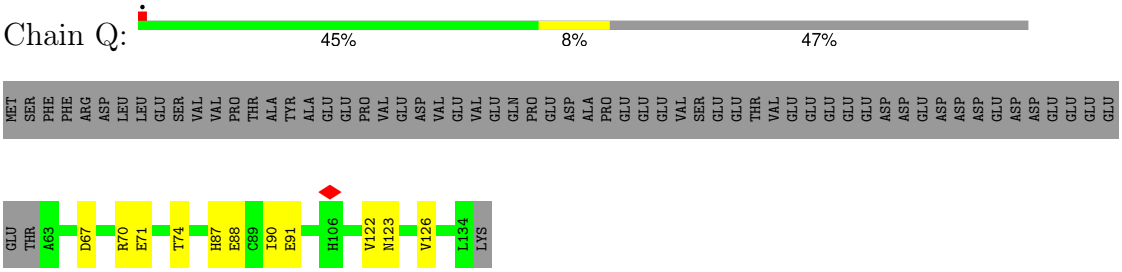
• Molecule 7: Ubiquinol--cytochrome-c reductase subunit 6

Chain H:



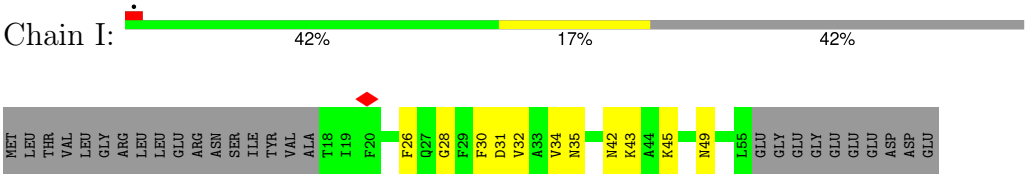
• Molecule 7: Ubiquinol--cytochrome-c reductase subunit 6

Chain Q:



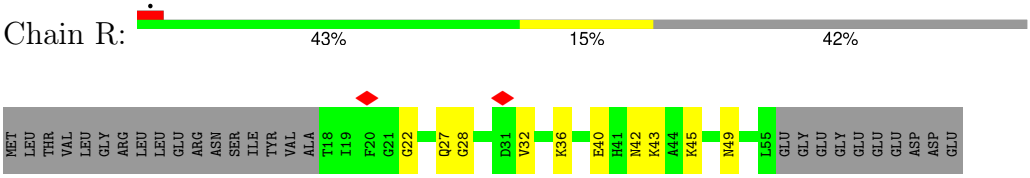
• Molecule 8: Ubiquinol--cytochrome-c reductase subunit 9

Chain I:



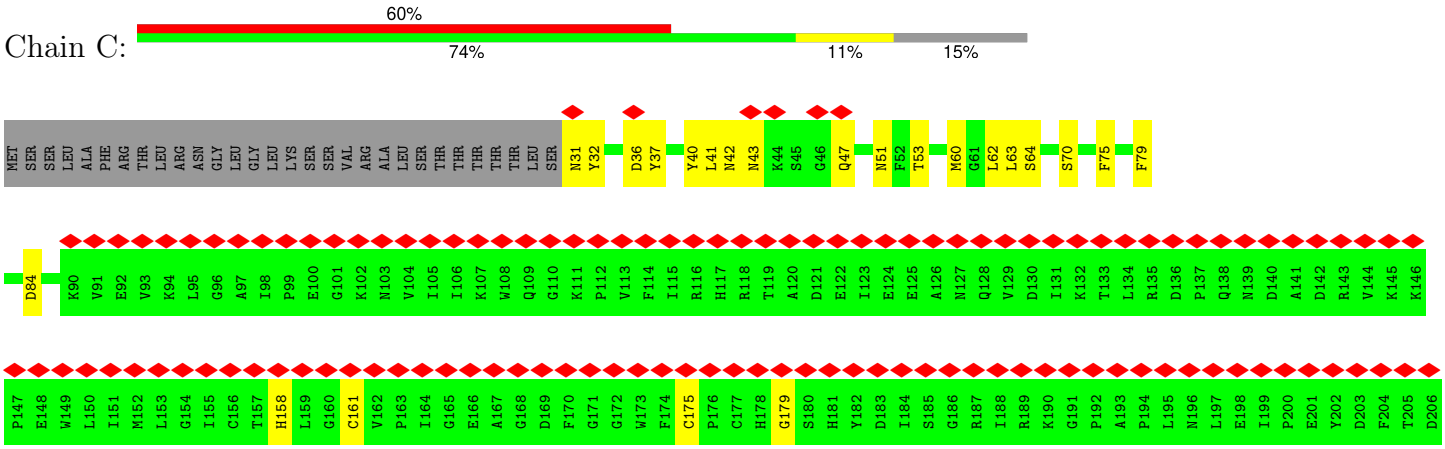
• Molecule 8: Ubiquinol--cytochrome-c reductase subunit 9

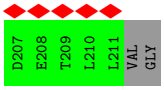
Chain R:



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

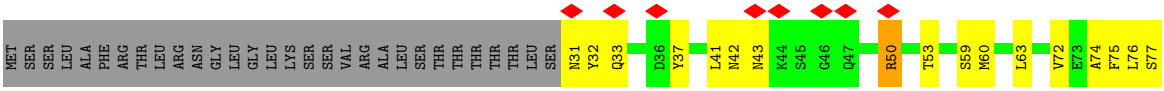
Chain C:

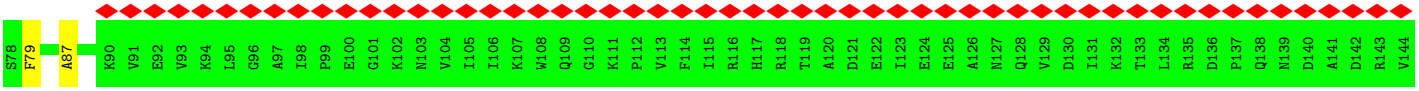


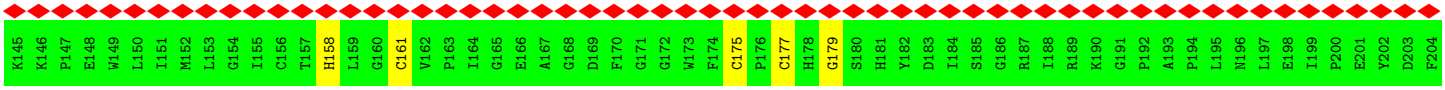


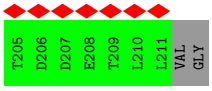
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain M:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.718	Depositor
Minimum map value	-2.127	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.52	Depositor
Map size (Å)	296.63998, 296.63998, 296.63998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, HEC, HEM, ZL5

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	K	0.30	0/3161	0.46	0/4323
1	T	0.30	0/3161	0.46	0/4323
2	A	0.27	0/3253	0.45	0/4409
2	E	0.27	0/3253	0.45	0/4409
3	B	0.27	0/2748	0.48	2/3735 (0.1%)
3	L	0.27	0/2748	0.48	2/3735 (0.1%)
4	D	0.30	0/1961	0.50	2/2672 (0.1%)
4	N	0.28	0/1961	0.50	2/2672 (0.1%)
5	G	0.26	0/994	0.45	0/1346
5	P	0.26	0/994	0.45	0/1346
6	F	0.32	0/747	0.51	0/1018
6	O	0.30	0/747	0.50	0/1018
7	H	0.25	0/598	0.46	0/810
7	Q	0.26	0/598	0.47	0/810
8	I	0.24	0/324	0.36	0/435
8	R	0.25	0/324	0.36	0/435
9	C	0.28	0/1051	0.45	0/1441
9	M	0.27	0/1051	0.47	0/1441
All	All	0.28	0/29674	0.47	8/40378 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	217	ALA	CB-CA-C	7.22	120.93	110.10
3	L	217	ALA	CB-CA-C	7.21	120.92	110.10
4	N	119	PRO	N-CA-CB	5.95	110.44	103.30
4	D	125	PRO	N-CA-CB	5.92	110.41	103.30
4	N	125	PRO	N-CA-CB	5.92	110.41	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3058	3088	3088	76	0
1	T	3058	3088	3088	75	0
2	A	3197	3162	3167	72	0
2	E	3197	3162	3167	62	0
3	B	2700	2692	2685	57	0
3	L	2700	2692	2685	51	0
4	D	1901	1812	1798	64	0
4	N	1901	1812	1798	65	0
5	G	976	1002	1002	14	0
5	P	976	1002	1002	14	0
6	F	723	687	695	23	0
6	O	723	687	695	19	0
7	H	582	522	522	6	0
7	Q	582	522	522	6	0
8	I	313	300	302	8	0
8	R	313	300	302	7	0
9	C	1043	697	706	53	0
9	M	1043	697	706	67	0
10	K	86	60	60	19	0
10	T	86	60	60	17	0
11	K	28	14	0	0	0
11	T	28	14	0	0	0
12	D	43	30	32	10	0
12	N	43	30	32	10	0
13	C	4	0	0	1	0
13	M	4	0	0	4	0
All	All	29308	28132	28114	593	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 10.

The worst 5 of 593 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:149:HIS:CD2	9:M:31:ASN:HD22	1.44	1.32
2:A:410:ASP:OD2	9:M:50:ARG:NE	1.67	1.25
6:F:30:ILE:HD11	9:M:37:TYR:CG	1.72	1.25
6:O:30:ILE:HD11	9:C:37:TYR:CD1	1.73	1.23
9:M:158:HIS:O	13:M:301:FES:S2	1.97	1.21

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	K	382/387 (99%)	367 (96%)	15 (4%)	0	100	100
1	T	382/387 (99%)	368 (96%)	14 (4%)	0	100	100
2	A	415/439 (94%)	401 (97%)	14 (3%)	0	100	100
2	E	415/439 (94%)	401 (97%)	14 (3%)	0	100	100
3	B	362/374 (97%)	345 (95%)	17 (5%)	0	100	100
3	L	362/374 (97%)	342 (94%)	20 (6%)	0	100	100
4	D	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
4	N	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
5	G	120/127 (94%)	119 (99%)	1 (1%)	0	100	100
5	P	120/127 (94%)	119 (99%)	1 (1%)	0	100	100
6	F	86/95 (90%)	83 (96%)	3 (4%)	0	100	100
6	O	86/95 (90%)	84 (98%)	2 (2%)	0	100	100
7	H	70/135 (52%)	70 (100%)	0	0	100	100
7	Q	70/135 (52%)	70 (100%)	0	0	100	100
8	I	36/65 (55%)	36 (100%)	0	0	100	100
8	R	36/65 (55%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	179/213 (84%)	170 (95%)	9 (5%)	0	100	100
9	M	179/213 (84%)	171 (96%)	8 (4%)	0	100	100
All	All	3782/4246 (89%)	3649 (96%)	133 (4%)	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	K	332/338 (98%)	329 (99%)	3 (1%)	75	85
1	T	332/338 (98%)	329 (99%)	3 (1%)	75	85
2	A	344/365 (94%)	344 (100%)	0	100	100
2	E	344/365 (94%)	343 (100%)	1 (0%)	91	94
3	B	295/307 (96%)	295 (100%)	0	100	100
3	L	295/307 (96%)	295 (100%)	0	100	100
4	D	192/237 (81%)	191 (100%)	1 (0%)	86	91
4	N	192/237 (81%)	192 (100%)	0	100	100
5	G	106/110 (96%)	106 (100%)	0	100	100
5	P	106/110 (96%)	106 (100%)	0	100	100
6	F	72/80 (90%)	72 (100%)	0	100	100
6	O	72/80 (90%)	72 (100%)	0	100	100
7	H	62/128 (48%)	62 (100%)	0	100	100
7	Q	62/128 (48%)	62 (100%)	0	100	100
8	I	29/53 (55%)	29 (100%)	0	100	100
8	R	29/53 (55%)	29 (100%)	0	100	100
9	C	48/176 (27%)	48 (100%)	0	100	100
9	M	48/176 (27%)	47 (98%)	1 (2%)	48	70
All	All	2960/3588 (82%)	2951 (100%)	9 (0%)	90	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	291	GLN
9	M	50	ARG
1	T	79	ARG
1	T	99	LYS
1	T	383	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
9	C	31	ASN
8	R	27	GLN
2	A	291	GLN
2	A	149	HIS
4	N	237	ASN

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)

10 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	$\#\|Z\|>2$
13	FES	C	301	9	0,4,4	-	-	-		
13	FES	M	301	9	0,4,4	-	-	-		
10	HEM	T	402	1	42,50,50	1.57	4 (9%)	46,82,82	1.32	7 (15%)
10	HEM	K	401	1	42,50,50	1.46	4 (9%)	46,82,82	1.22	3 (6%)
10	HEM	T	401	1	42,50,50	1.47	4 (9%)	46,82,82	1.24	1 (2%)
12	HEC	N	301	4	32,50,50	2.18	4 (12%)	30,82,82	1.42	4 (13%)
11	ZL5	K	403	-	26,31,31	4.62	12 (46%)	32,47,47	1.52	5 (15%)
10	HEM	K	402	1	42,50,50	1.58	4 (9%)	46,82,82	1.32	7 (15%)
12	HEC	D	301	4	32,50,50	2.17	4 (12%)	30,82,82	1.42	4 (13%)
11	ZL5	T	403	-	26,31,31	4.62	12 (46%)	32,47,47	1.51	5 (15%)

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
13	FES	C	301	9	-	-	0/1/1/1
13	FES	M	301	9	-	-	0/1/1/1
10	HEM	T	402	1	-	4/12/54/54	-
10	HEM	K	401	1	-	6/12/54/54	-
10	HEM	T	401	1	-	5/12/54/54	-
12	HEC	N	301	4	-	2/10/54/54	-
11	ZL5	K	403	-	-	2/12/14/14	0/4/4/4
10	HEM	K	402	1	-	1/12/54/54	-
12	HEC	D	301	4	-	2/10/54/54	-
11	ZL5	T	403	-	-	2/12/14/14	0/4/4/4

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	403	ZL5	C07-N19	-13.73	1.23	1.35
11	K	403	ZL5	C07-N19	-13.73	1.23	1.35
11	T	403	ZL5	C09-C10	9.03	1.52	1.39
11	K	403	ZL5	C09-C10	8.94	1.52	1.39
11	K	403	ZL5	C16-C15	8.70	1.52	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	403	ZL5	C22-N23-N24	4.19	108.56	104.33
11	K	403	ZL5	C22-N23-N24	4.18	108.55	104.33
11	K	403	ZL5	C09-C08-C17	3.04	119.58	115.98
11	T	403	ZL5	C09-C08-C17	2.95	119.47	115.98
11	K	403	ZL5	C26-N25-N24	2.82	126.19	122.66

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	403	ZL5	N20-C21-C22-N27
10	K	401	HEM	C3D-CAD-CBD-CGD
10	T	401	HEM	C3D-CAD-CBD-CGD
10	K	401	HEM	C2D-C3D-CAD-CBD
10	T	401	HEM	C2D-C3D-CAD-CBD

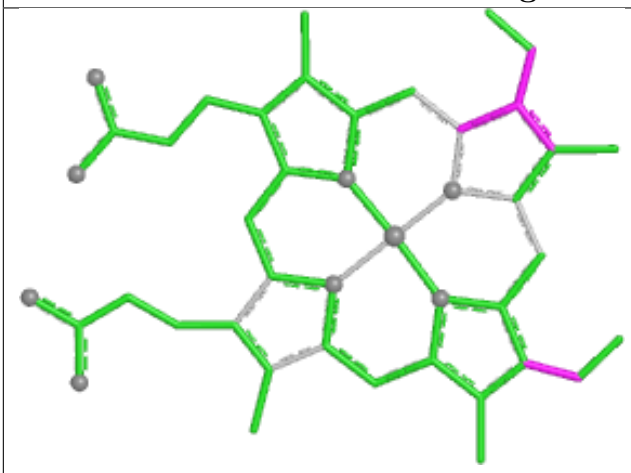
There are no ring outliers.

8 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	301	FES	1	0
13	M	301	FES	4	0
10	T	402	HEM	5	0
10	K	401	HEM	13	0
10	T	401	HEM	12	0
12	N	301	HEC	10	0
10	K	402	HEM	6	0
12	D	301	HEC	10	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 T 402



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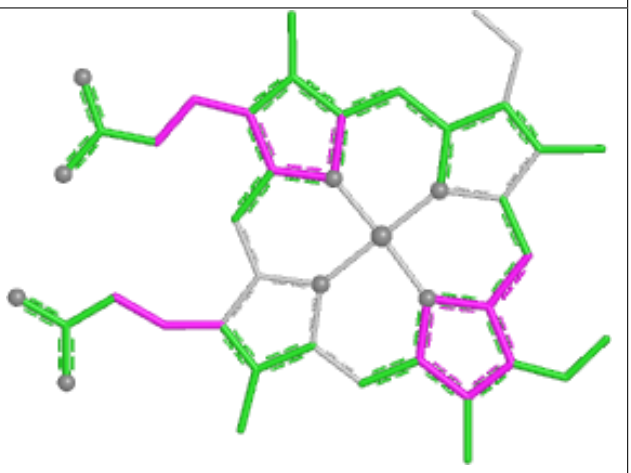

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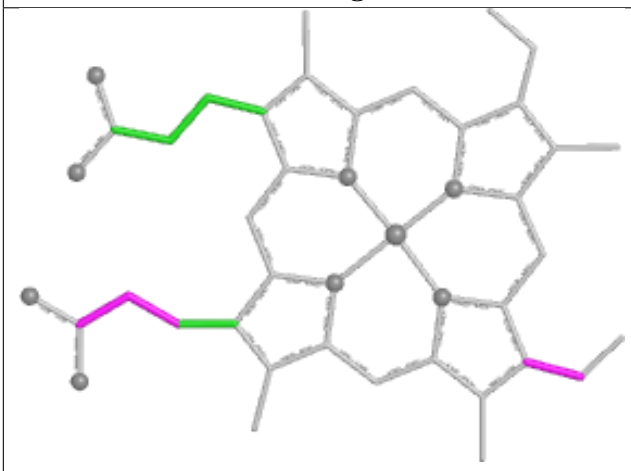

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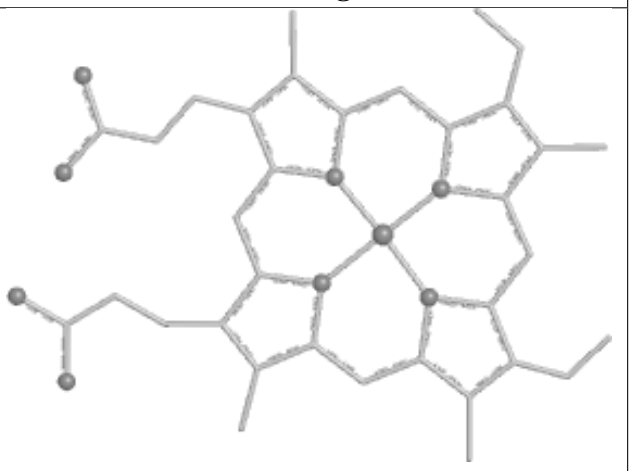
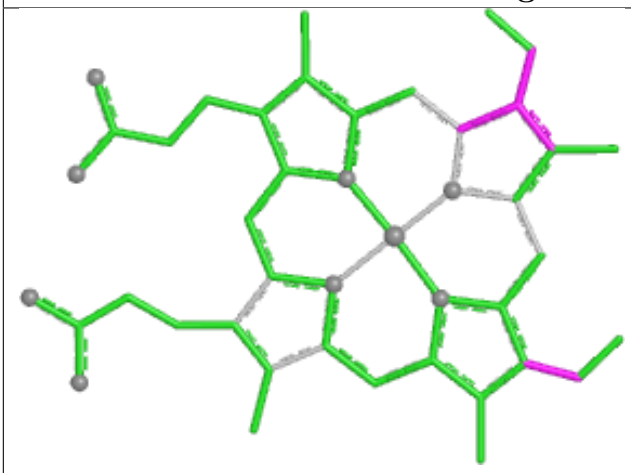


Rings

Ligand HEM K 401



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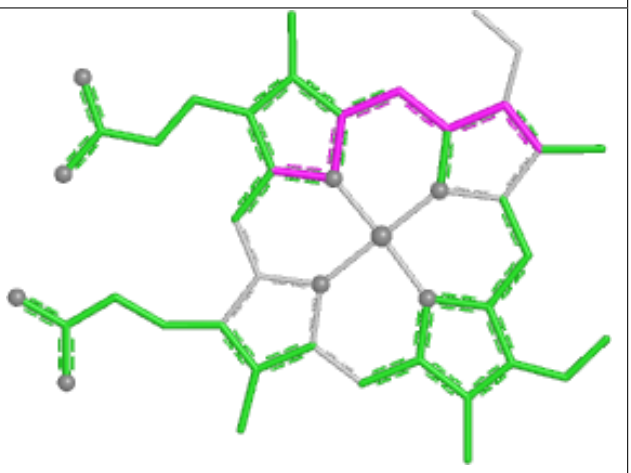

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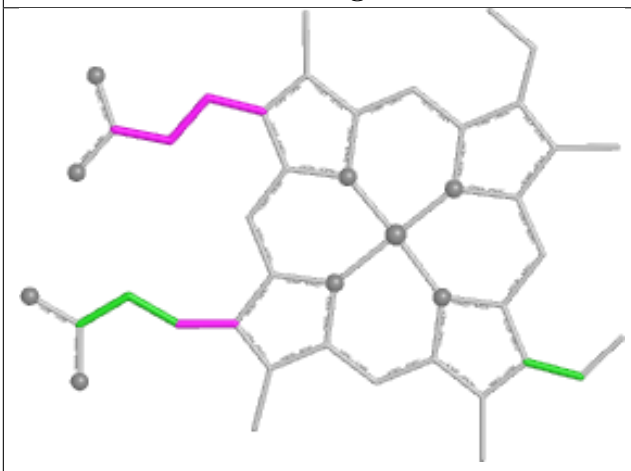

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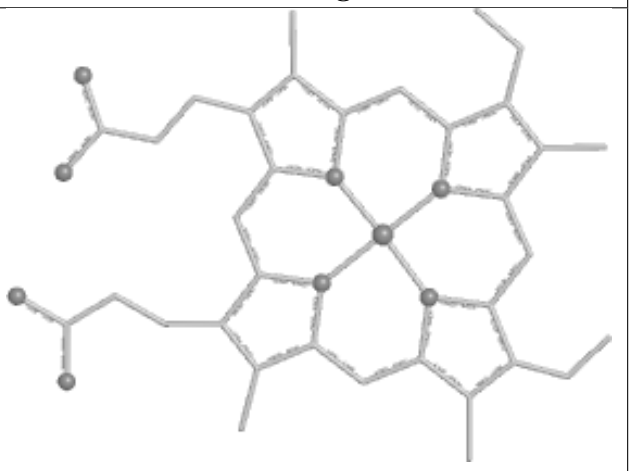

Rings

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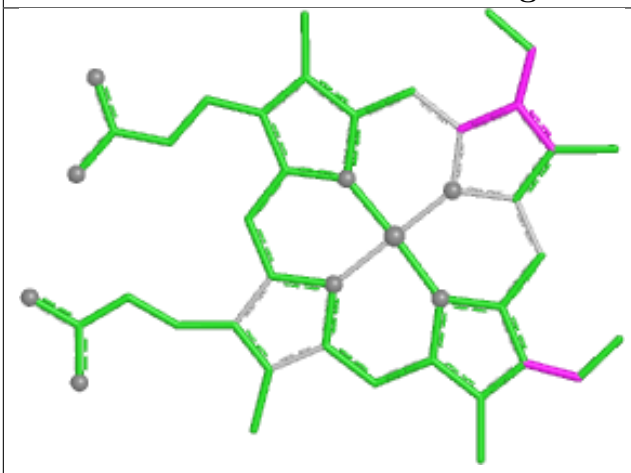

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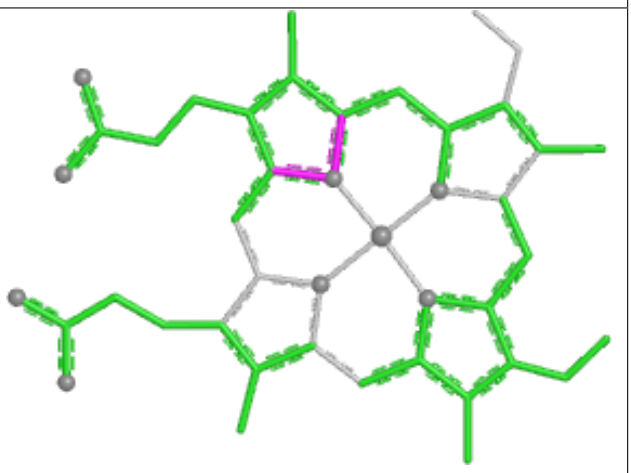

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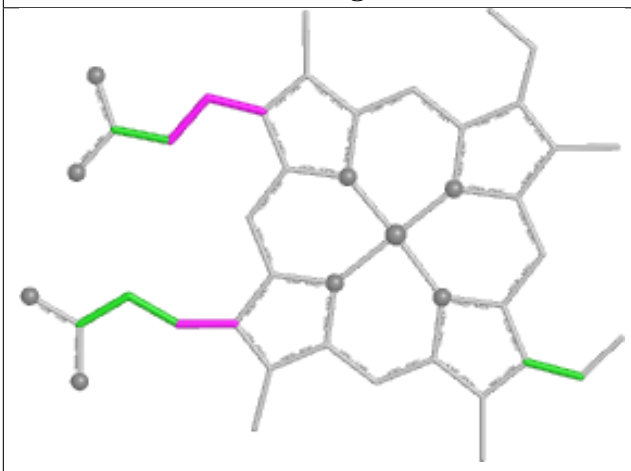

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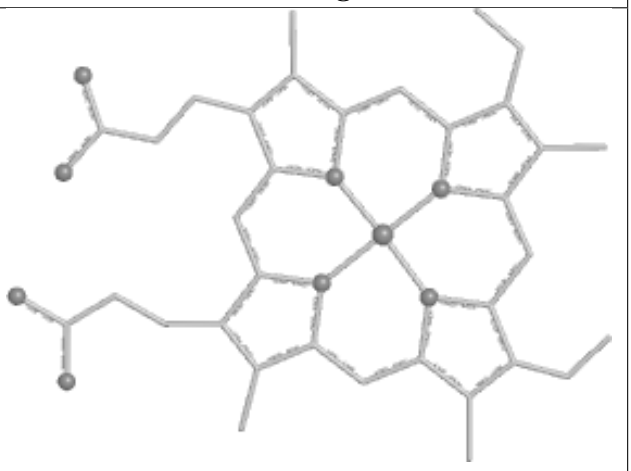
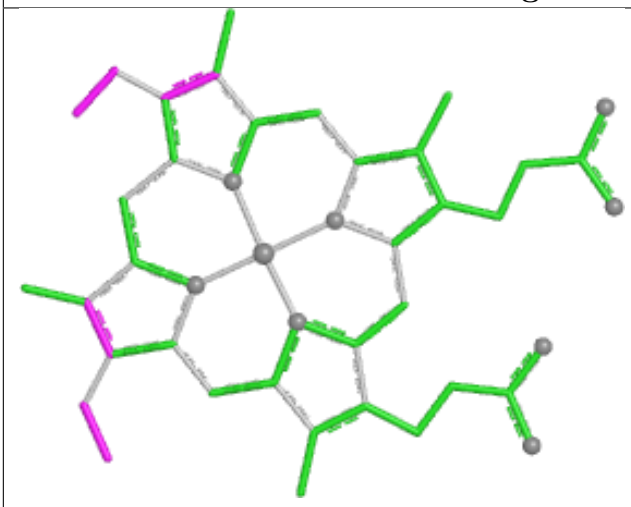


Rings

Ligand HEC N 301



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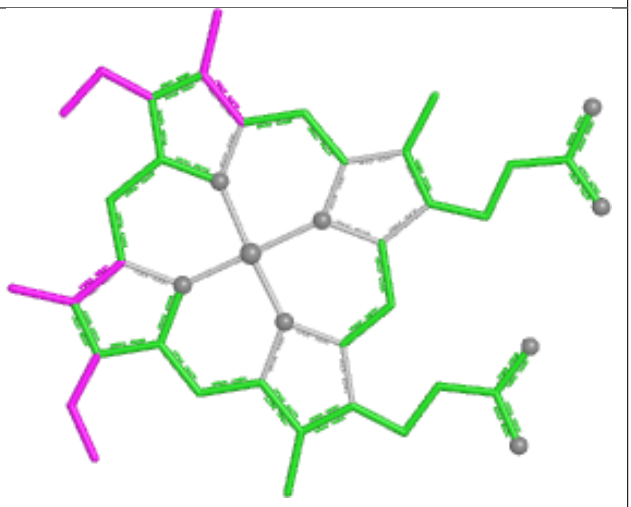

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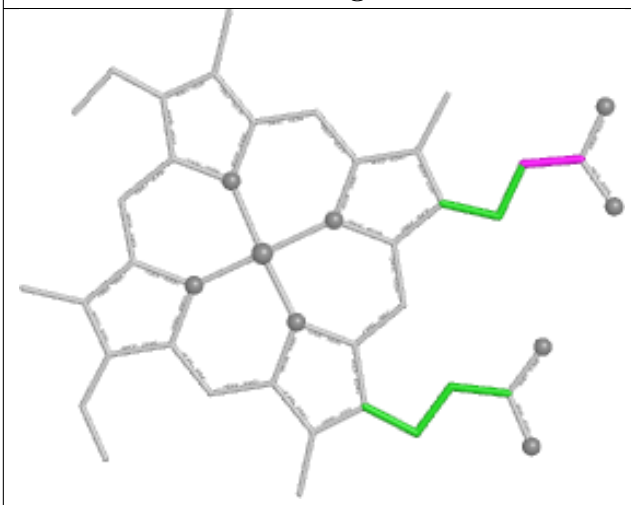

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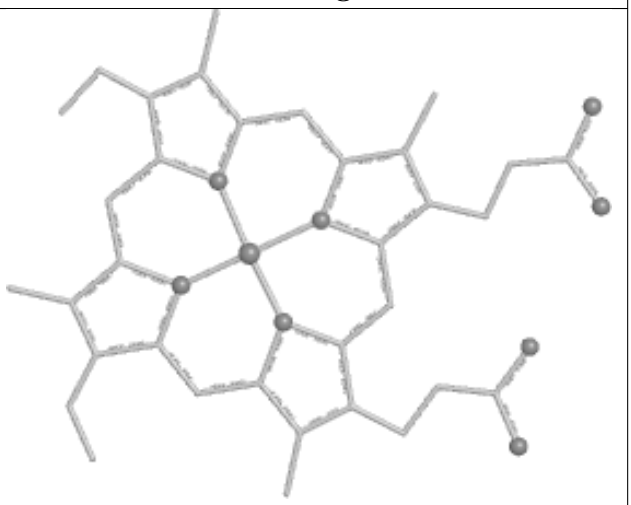

Rings

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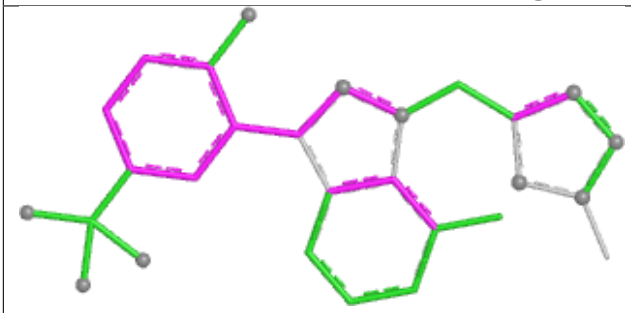
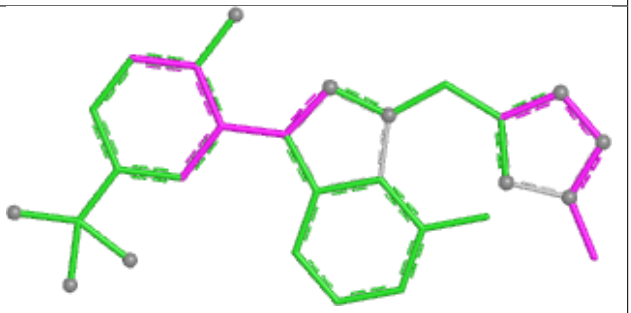
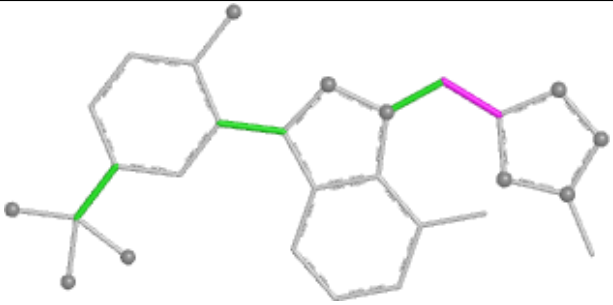
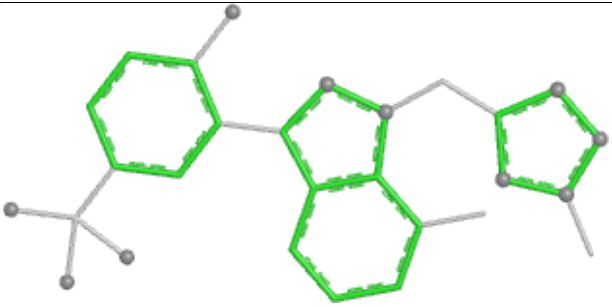
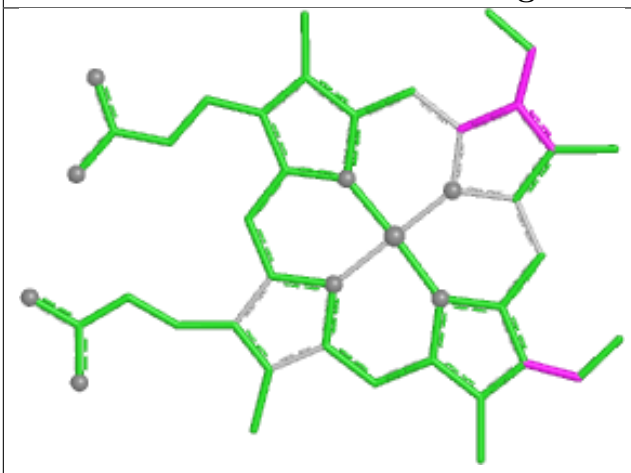
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand HEM K 402



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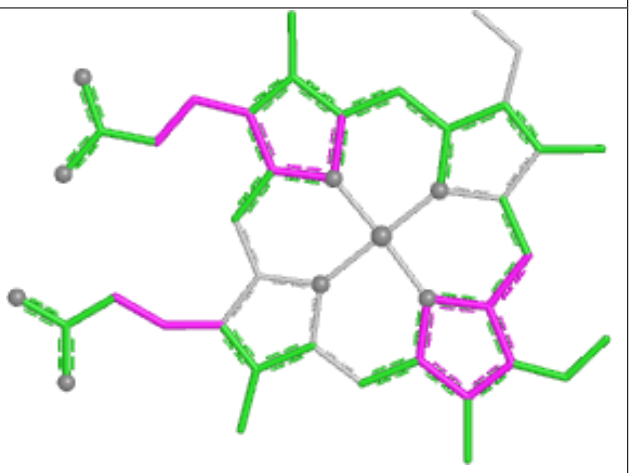

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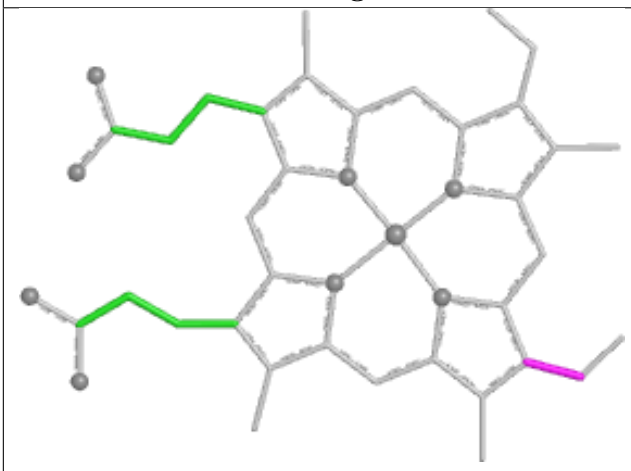

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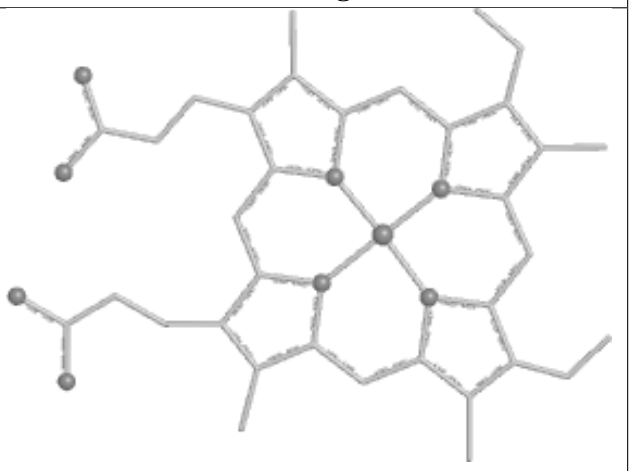
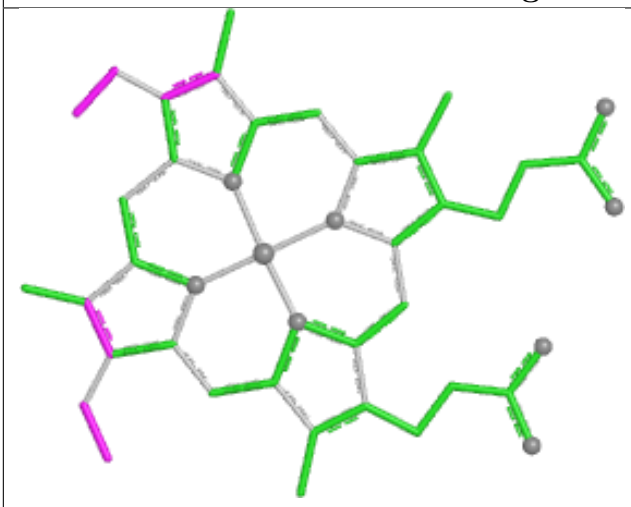
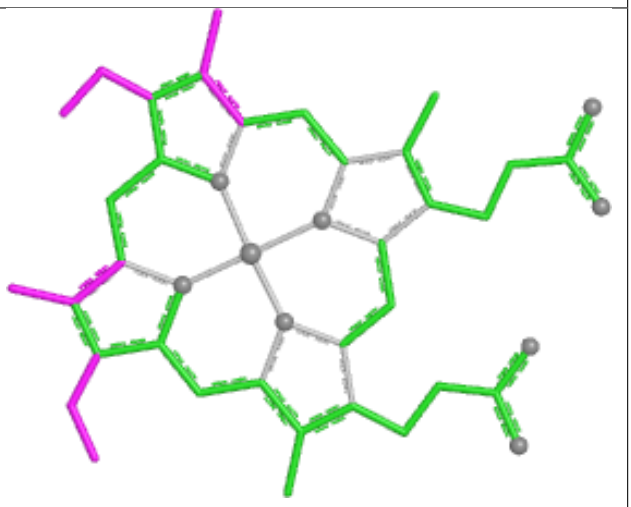


Rings

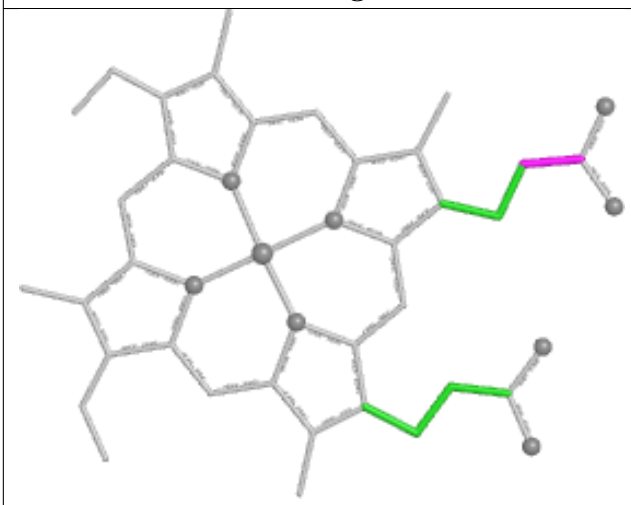
Ligand HEC D 301



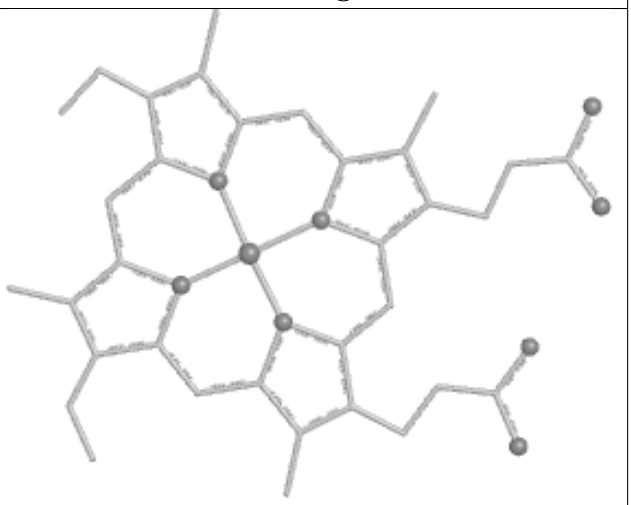
Bond lengths



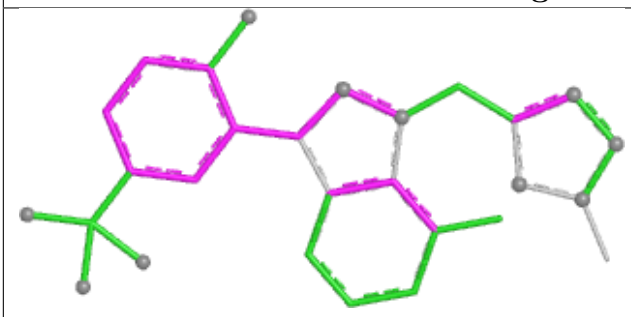
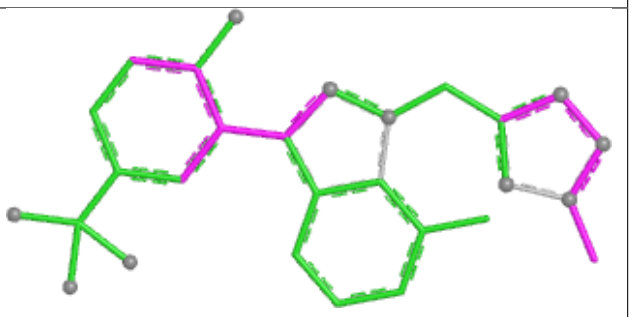
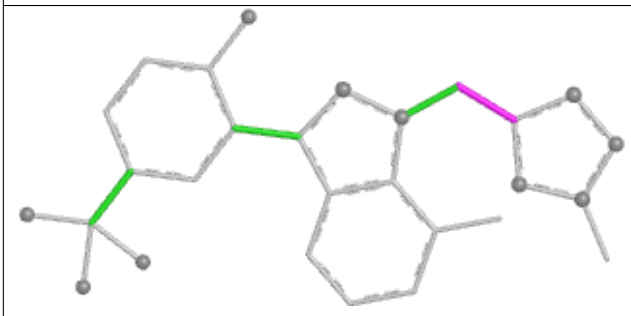
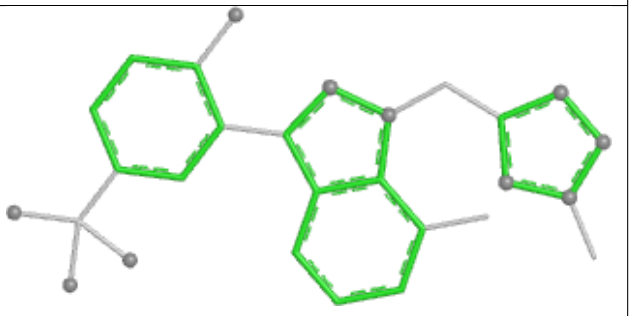
Bond angles



Torsions



Rings

Ligand ZL5 T 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

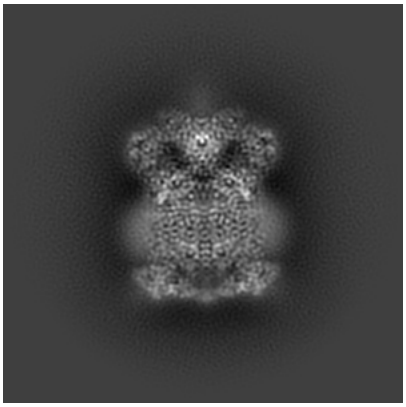
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24486. These allow visual inspection of the internal detail of the map and identification of artifacts.

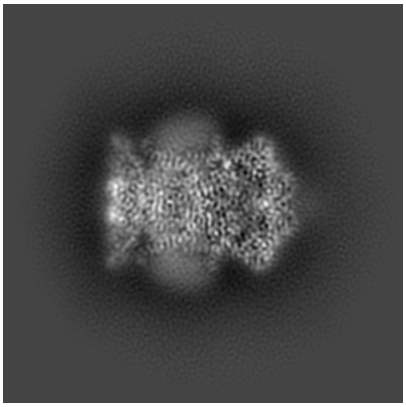
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

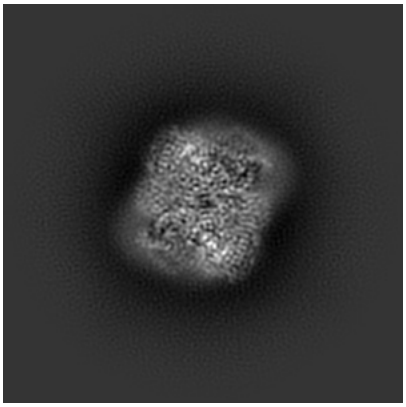
6.1.1 Primary map



X



Y

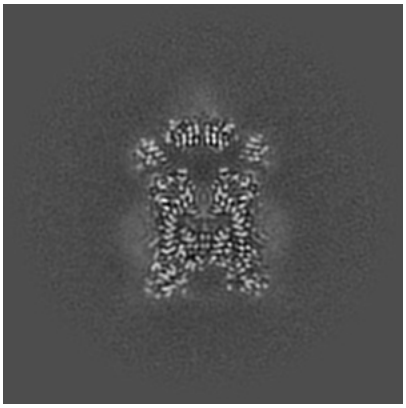


Z

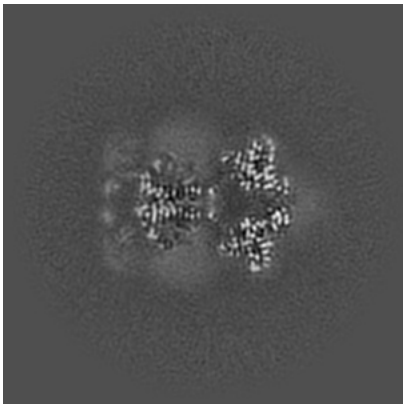
The images above show the map projected in three orthogonal directions.

6.2 Central slices

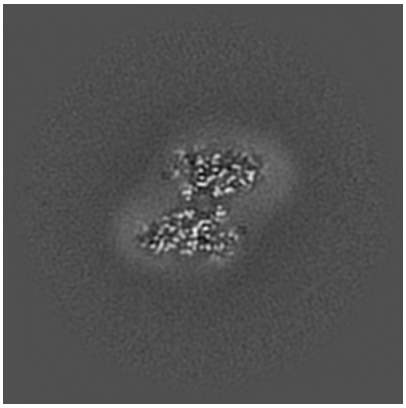
6.2.1 Primary map



X Index: 144



Y Index: 144

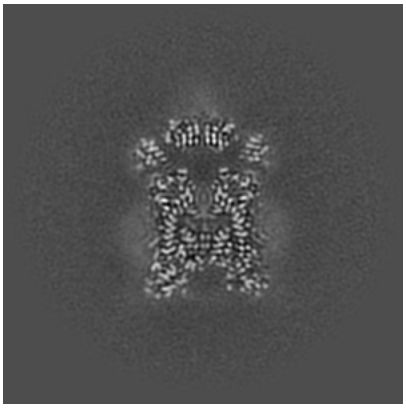


Z Index: 144

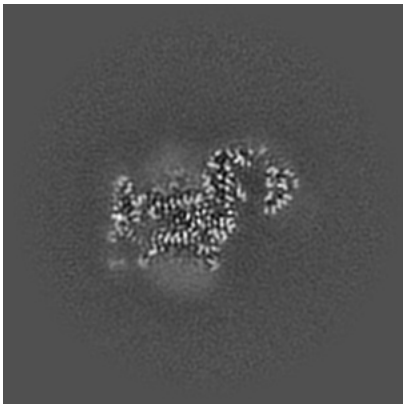
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

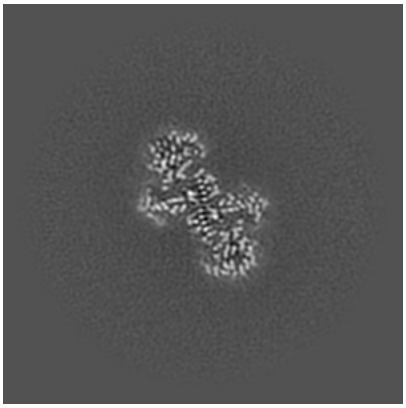
6.3.1 Primary map



X Index: 144



Y Index: 122

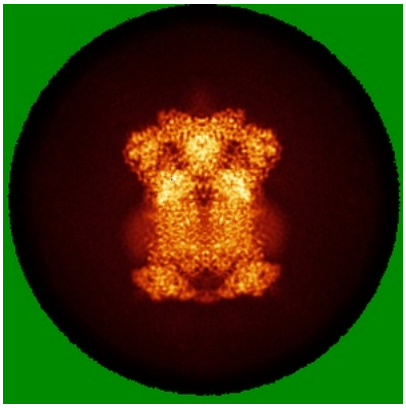


Z Index: 191

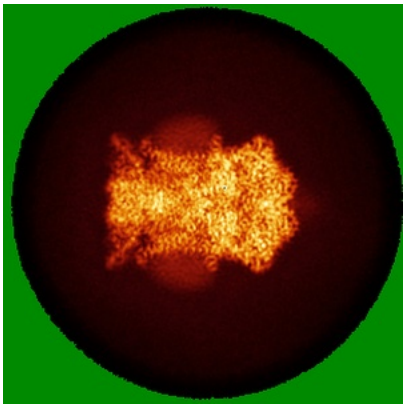
The images above show the largest variance slices of the map in three orthogonal directions.

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

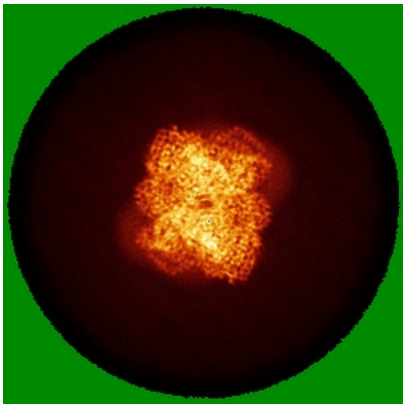
6.4.1 Primary map



X



Y

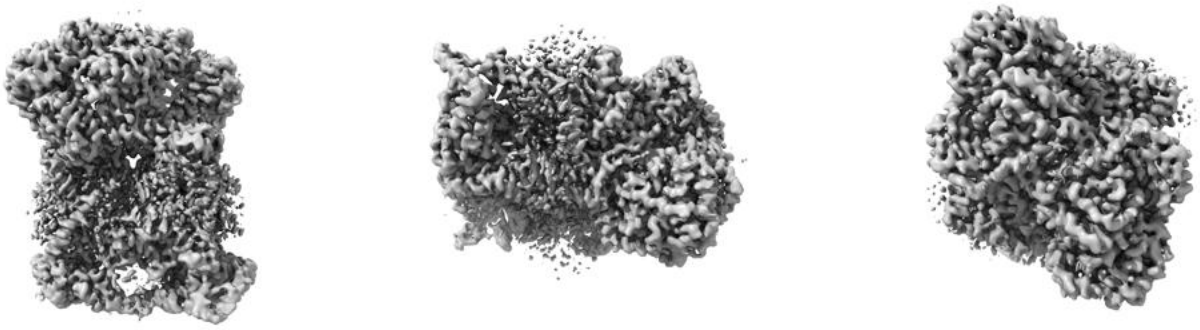


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.52. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

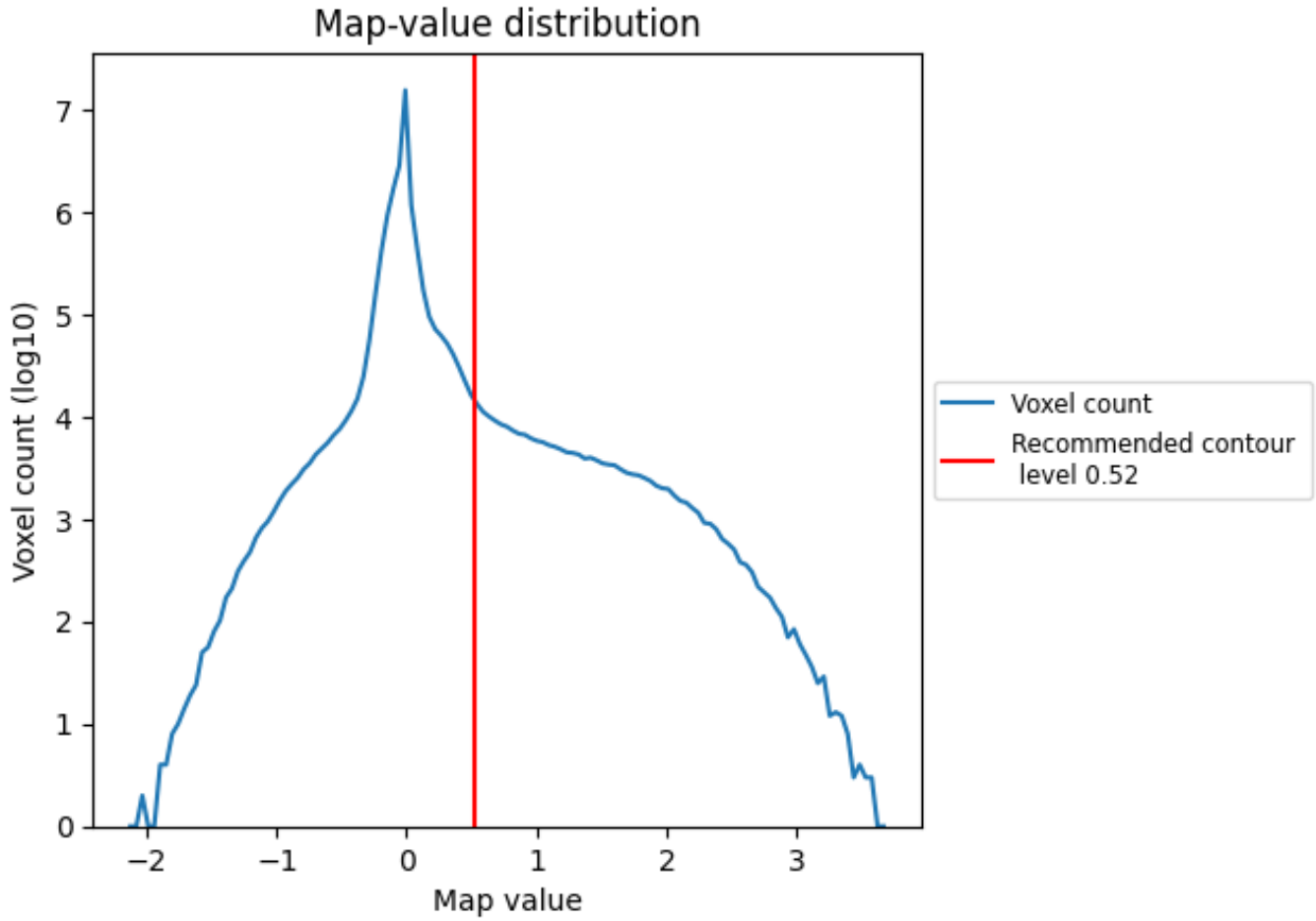
6.6 Mask visualisation (i)

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

7 Map analysis

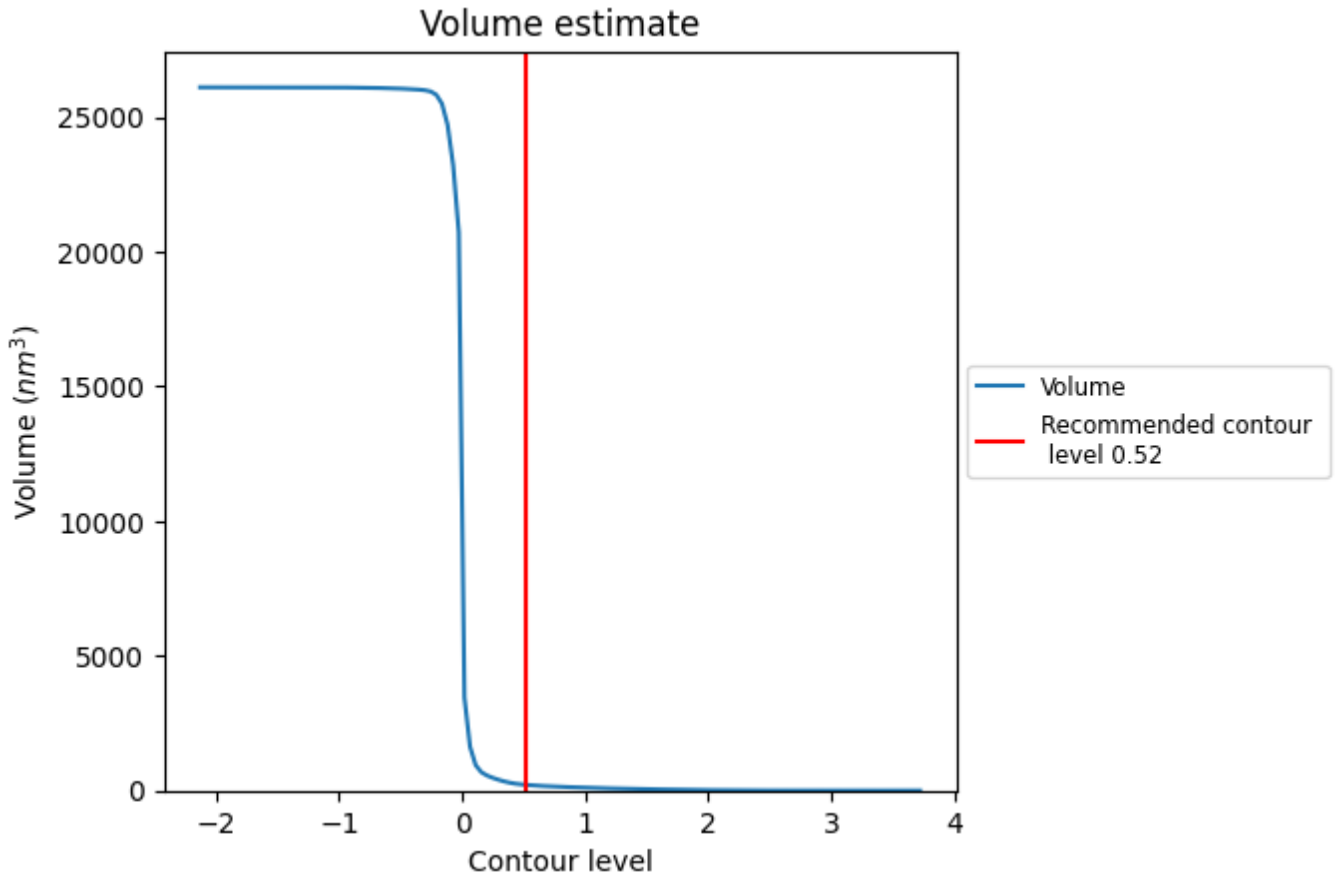
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

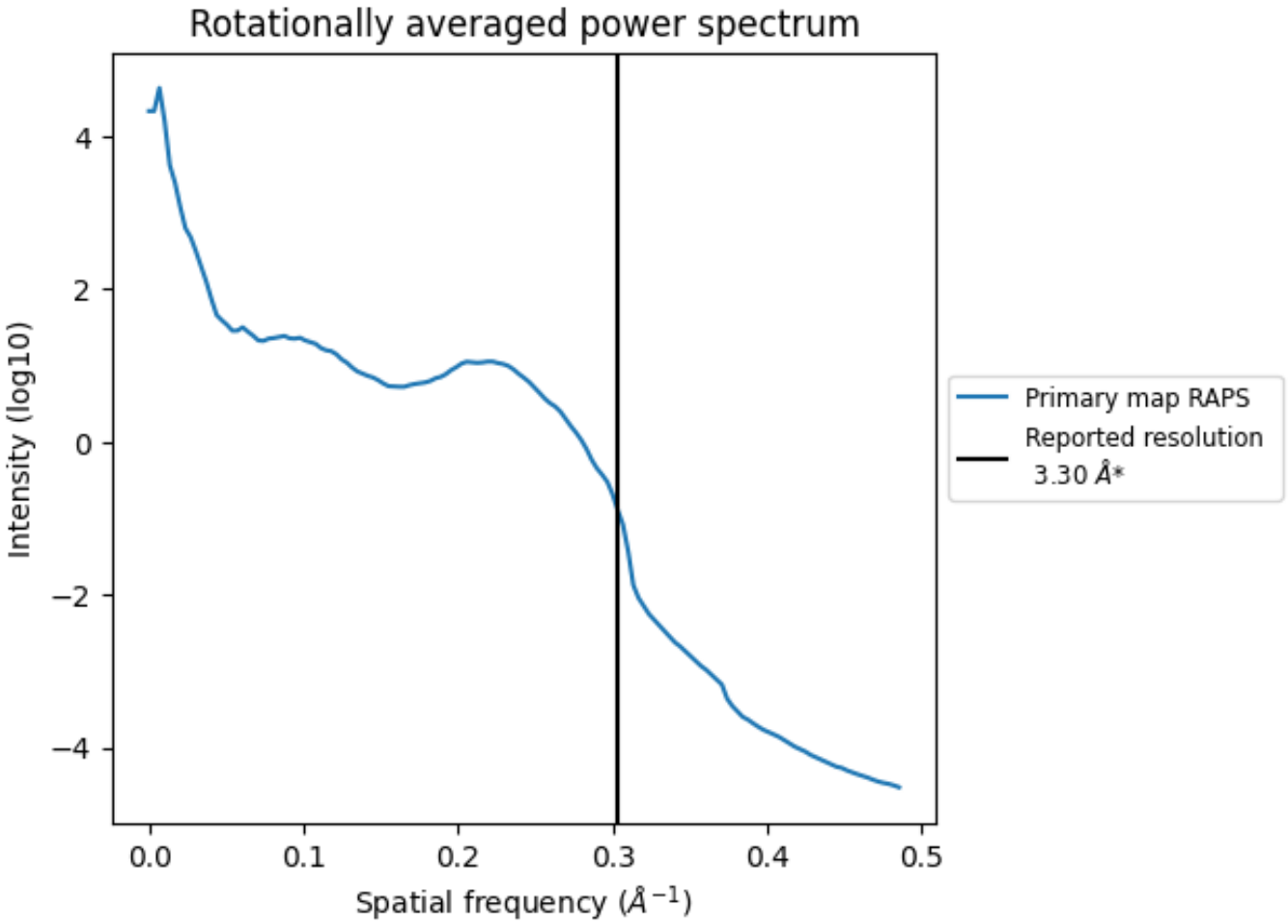
7.2 Volume estimate (i)



The volume at the recommended contour level is 210 nm^3; this corresponds to an approximate mass of 190 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)

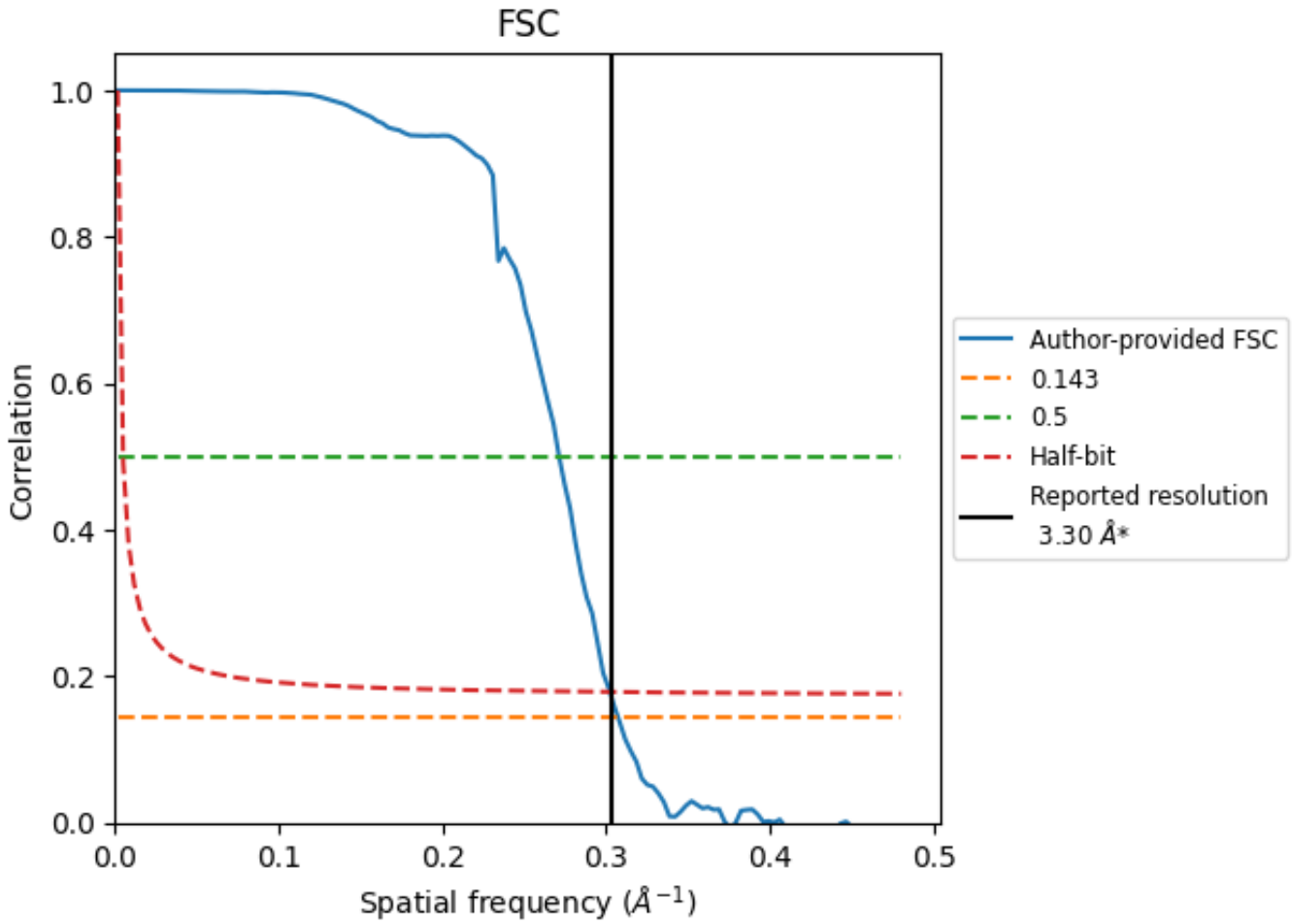


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

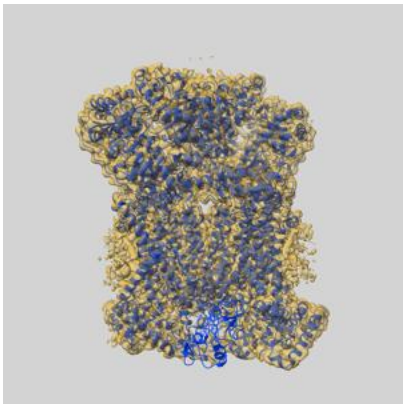
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.68	3.31
Unmasked-calculated*	-	-	-

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

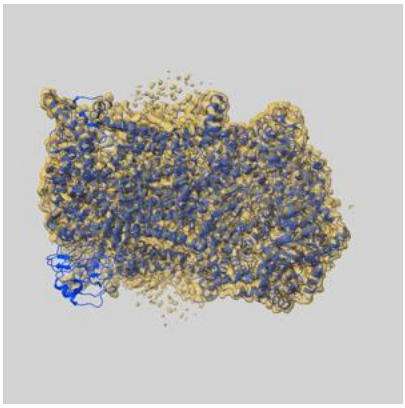
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24486 and PDB model 7RJE. Per-residue inclusion information can be found in section 3 on page 9.

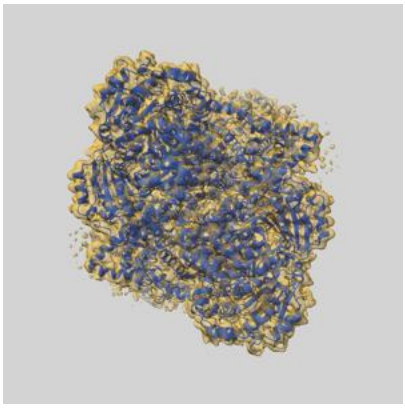
9.1 Map-model overlay



X



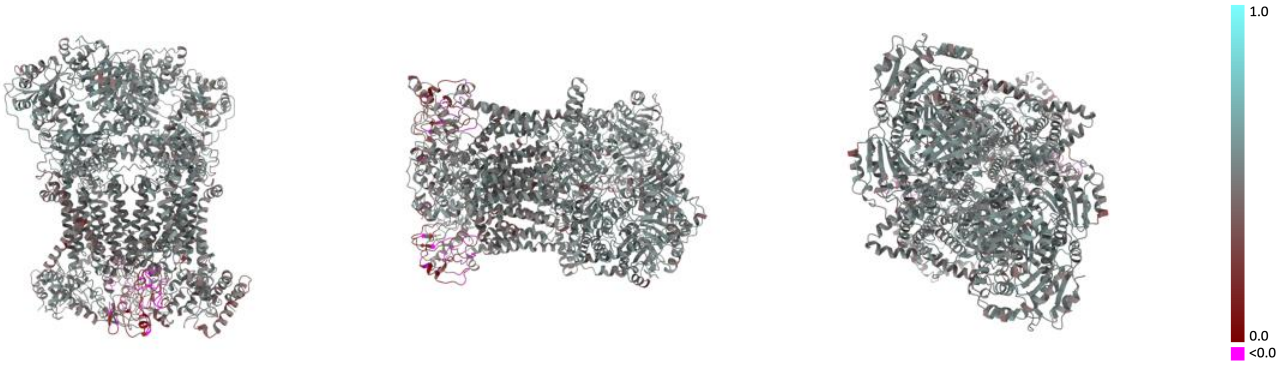
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.52 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

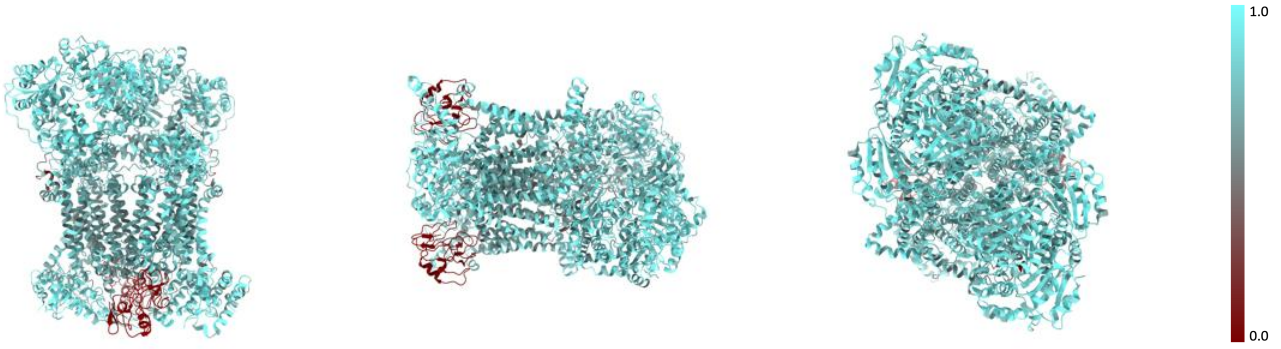
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

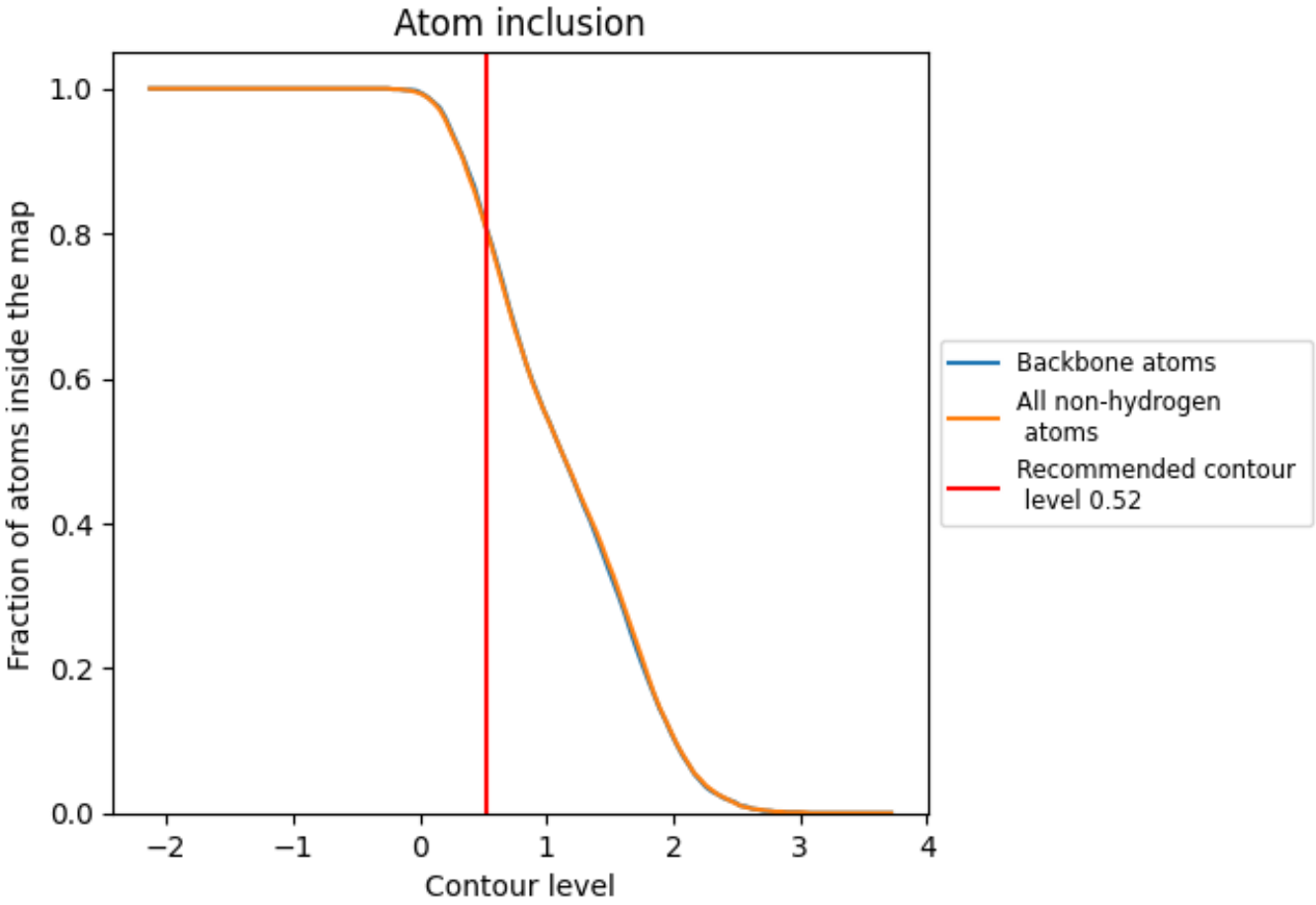
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.52).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.4860
A	0.8740	0.5170
B	0.8720	0.5130
C	0.2810	0.2890
D	0.8650	0.4920
E	0.8740	0.5150
F	0.8080	0.4760
G	0.8460	0.5090
H	0.8290	0.4320
I	0.8000	0.4520
K	0.8140	0.5000
L	0.8720	0.5140
M	0.2680	0.2890
N	0.8740	0.4940
O	0.8210	0.4810
P	0.8370	0.5060
Q	0.8240	0.4260
R	0.8100	0.4550
T	0.8190	0.5020