wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 08:21 AM EST

PDB ID	:	7RJA
EMDB ID	:	EMD-24482
Title	:	Complex III2 from Candida albicans, inhibitor free
Authors	:	Di Trani, J.M.; Rubinstein, J.L.
Deposited on	:	2021-07-20
Resolution	:	3.00 Å(reported)

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

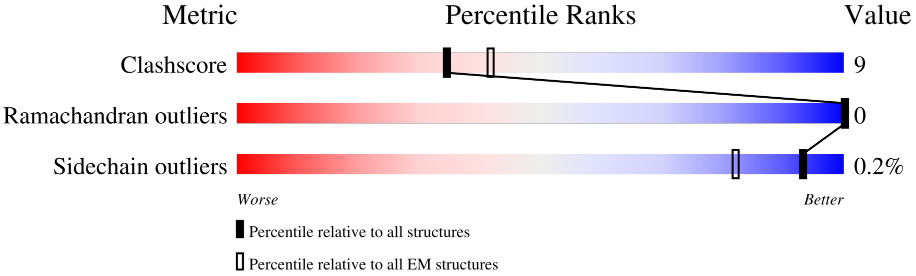
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	439	 82% 13% 5%
1	J	439	 78% 17% 5%
2	K	387	 • 75% 24% •
2	T	387	 81% 17% ••
3	D	288	 69% 15% 15%
3	N	288	 • 64% 20% 15%
4	G	127	 78% 18% •
4	Q	127	 80% 16% •

Continued on next page...

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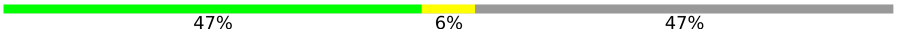
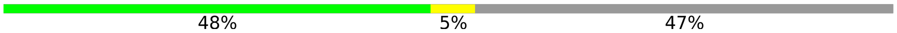
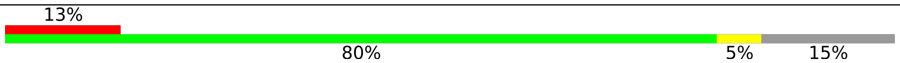
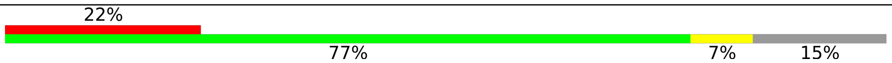
Mol	Chain	Length	Quality of chain
5	F	95	 79% 11% 11%
5	P	95	 79% 11% 11%
6	H	135	 47% 6% 47%
6	R	135	 48% 5% 47%
7	I	65	 55% 5% 40%
7	S	65	 52% 8% 40%
8	C	213	 13% 80% 5% 15%
8	M	213	 22% 77% 7% 15%
9	B	374	 80% 17%
9	L	374	 75% 22%

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
12	HEC	D	301	-	-	X	-
12	HEC	N	301	-	-	X	-
13	FES	M	301	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 57732 atoms, of which 28314 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 Ubiquinol--cytochrome-c reductase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	416	6364	2012	3166	546	636	4	0	0
1	J	416	6364	2012	3166	546	636	4	0	0

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	K	383	6146	2056	3090	478	505	17	0	0
2	T	383	6146	2056	3090	478	505	17	0	0

- Molecule 3 is a protein called Ubiquinol--cytochrome-c reductase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	244	3736	1225	1820	333	351	7	0	0
3	N	244	3736	1225	1820	333	351	7	0	0

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 7.

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

- Molecule 5 is a protein called Ubiquinol--cytochrome-c reductase subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	85	1399	466	691	119	122	1	0	0
5	P	85	1399	466	691	119	122	1	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	H	72	1148	376	544	106	116	6	0	0
6	R	72	1148	376	544	106	116	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called Ubiquinol--cytochrome-c reductase subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
7	I	39	639	220	315	54	50	0	0
7	S	39	639	220	315	54	50	0	0

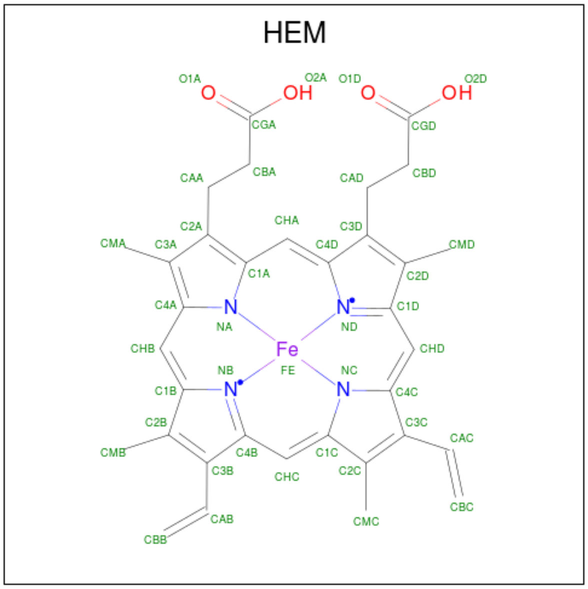
- Molecule 8 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

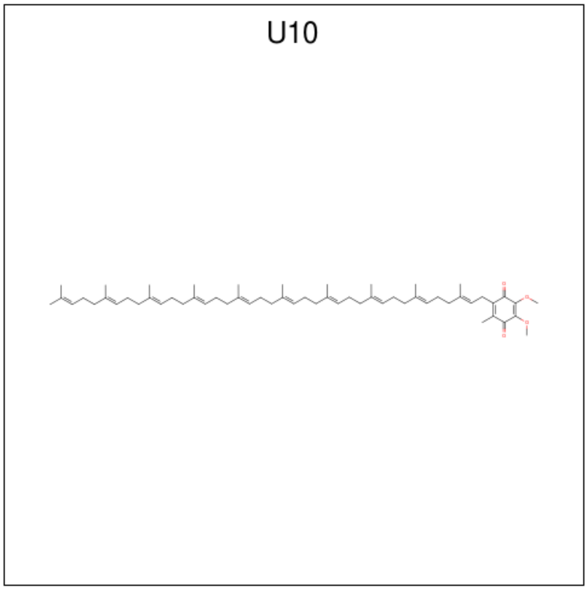
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	B	364	5392	1708	2692	443	548	1	0	0
9	L	364	5392	1708	2692	443	548	1	0	0

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



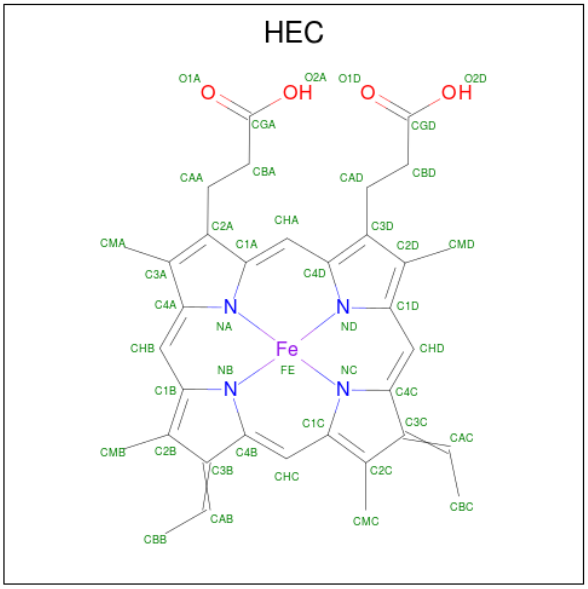
Mol	Chain	Residues	Atoms						AltConf
10	K	1	Total 146	C 68	Fe 2	H 60	N 8	O 8	0
10	K	1	Total 146	C 68	Fe 2	H 60	N 8	O 8	0
10	T	1	Total 146	C 68	Fe 2	H 60	N 8	O 8	0
10	T	1	Total 146	C 68	Fe 2	H 60	N 8	O 8	0

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



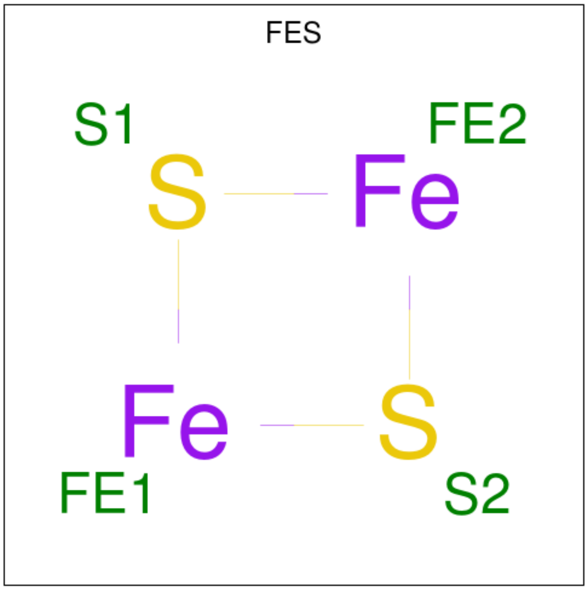
Mol	Chain	Residues	Atoms	AltConf
11	K	1	Total C H O 101 43 50 8	0
11	K	1	Total C H O 101 43 50 8	0
11	T	1	Total C H O 101 43 50 8	0
11	T	1	Total C H O 101 43 50 8	0

- 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 73	C 34	Fe 1	H 30	N 4	O 4	0
12	N	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0

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

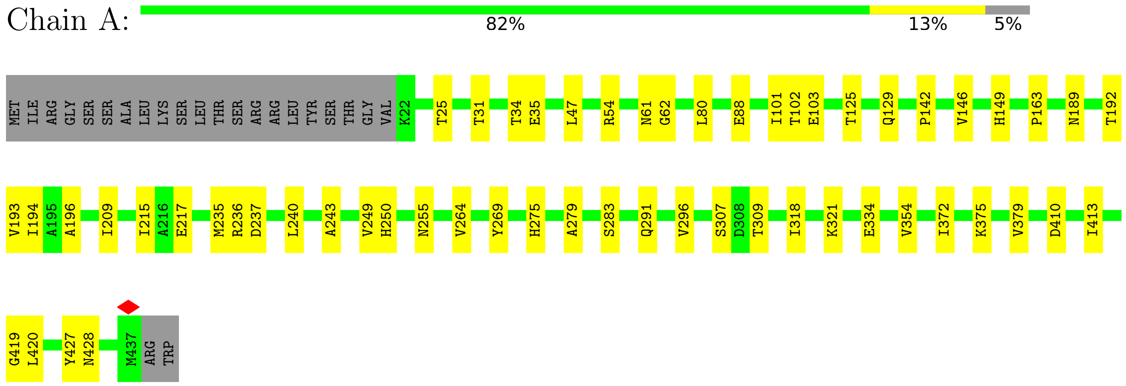


Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total 4	Fe 2	S 2	0
13	M	1	Total 4	Fe 2	S 2	0

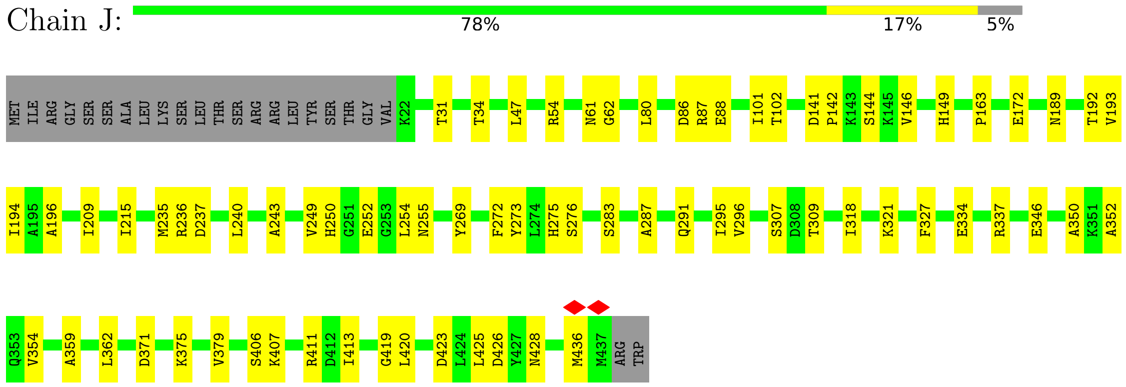
3 Residue-property plots ⓘ

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.

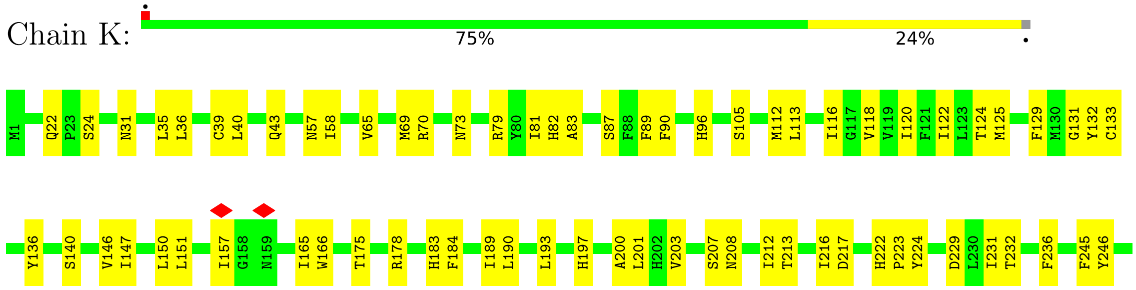
- Molecule 1: Ubiquinol--cytochrome-c reductase subunit

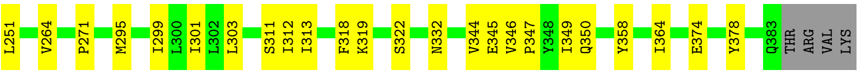


- Molecule 1: Ubiquinol--cytochrome-c reductase subunit



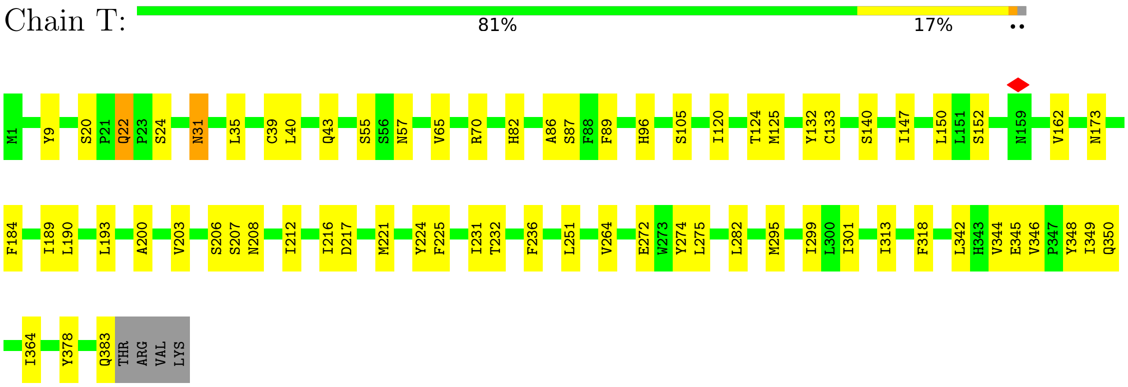
- Molecule 2: Cytochrome b





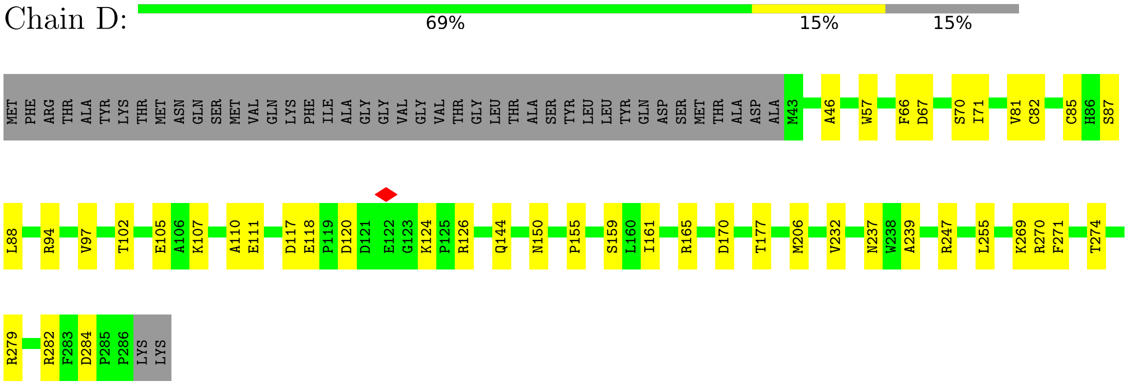
- Molecule 2: Cytochrome b

Chain T:



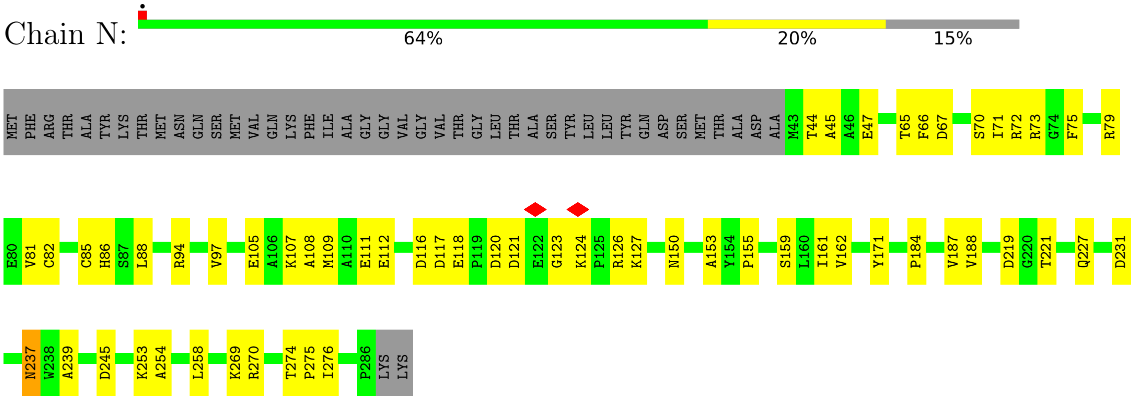
- Molecule 3: Ubiquinol--cytochrome-c reductase catalytic subunit

Chain D:



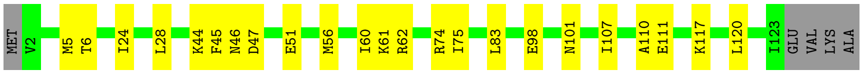
- Molecule 3: Ubiquinol--cytochrome-c reductase catalytic subunit

Chain N:



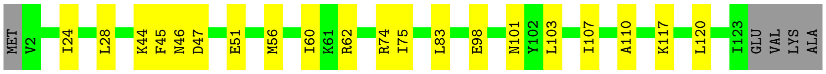
- Molecule 4: Cytochrome b-c1 complex subunit 7

Chain G:



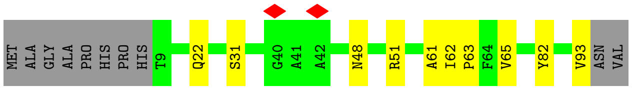
- Molecule 4: Cytochrome b-c1 complex subunit 7

Chain Q:



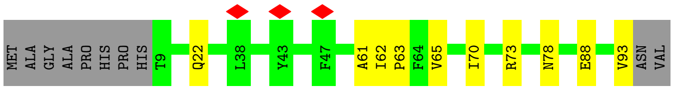
- Molecule 5: Ubiquinol--cytochrome-c reductase subunit 8

Chain F:



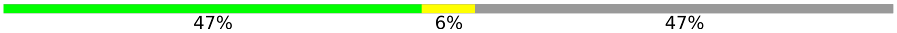
- Molecule 5: Ubiquinol--cytochrome-c reductase subunit 8

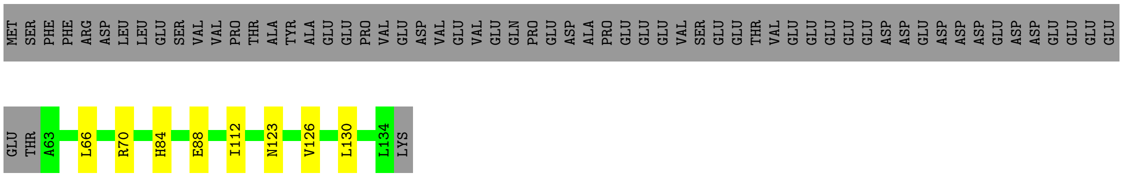
Chain P:



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

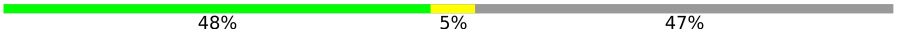
Chain H:

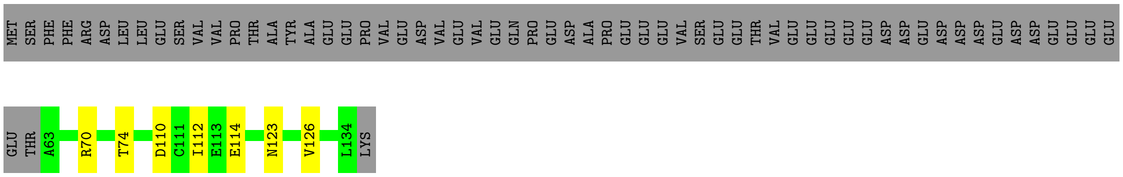




- Molecule 6: Ubiquinol--cytochrome-c reductase subunit 6

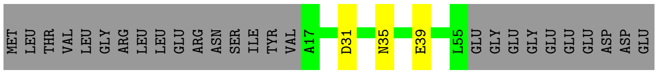
Chain R:





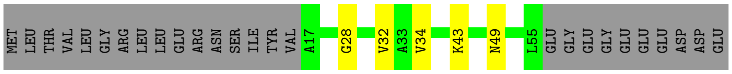
- Molecule 7: Ubiquinol--cytochrome-c reductase subunit 9

Chain I:



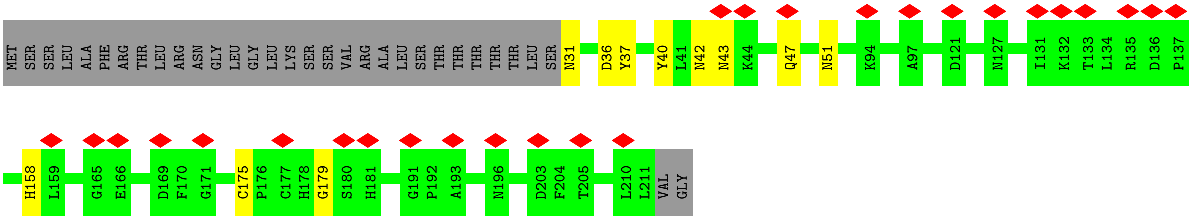
- Molecule 7: Ubiquinol--cytochrome-c reductase subunit 9

Chain S:



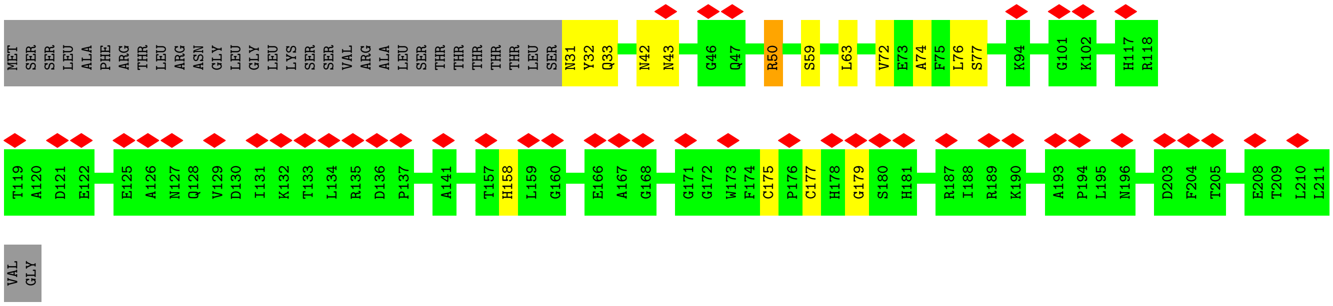
- Molecule 8: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain C:



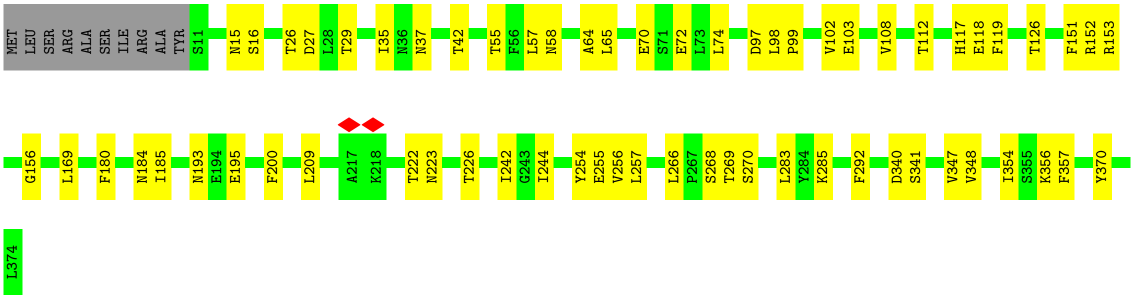
- Molecule 8: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain M:



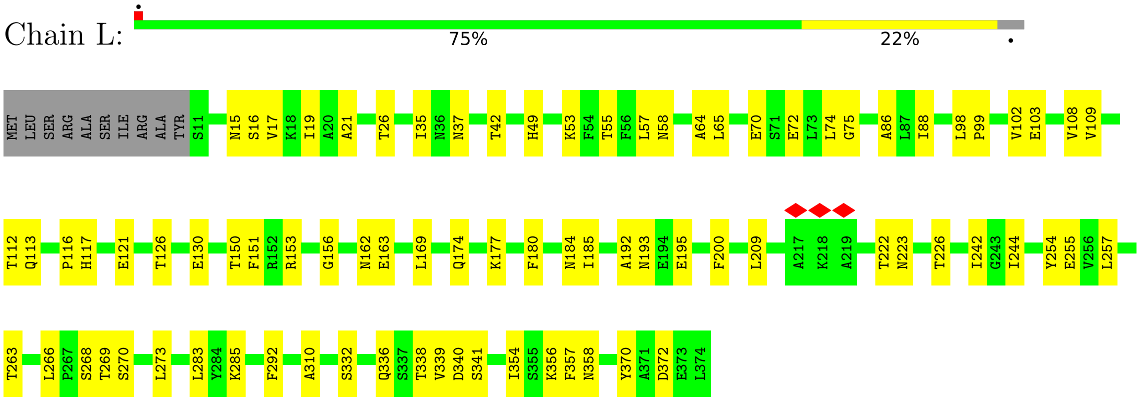
- Molecule 9: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



- Molecule 9: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain L:


75%
22%
MET
LEU
SER
ARG
ALA
SER
ILE
ARG
ALA
TYR
S11
N15
S16
V17
K18
I19
A20
A21
T26
I35
N36
N37
T42
H49
K53
F54
T55
F56
L57
N58
A64
L65
E70
S71
E72
L73
L74
G75
A86
L87
I88
L98
P99
V102
E103
V108
V109
T112
Q113
P116
H117
E121
T126
E130
T150
F151
R152
R153
G156
N162
E163
L169
Q174
K177
F180
N184
I185
A192
N193
E194
E195
F200
L209
A217
K218
A219
T222
N223
T226
I242
G243
I244
Y254
E255
V256
L257
T263
L266
P267
S268
T269
S270
L273
L283
Y284
K285
F292
A310
S332
Q336
S337
T338
V339
D340
S341
I354
S355
K356
F357
N358
Y370
A371
D372
E373
L374

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96783	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 $(e^-/\AA^2)$	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	4.587	Depositor
Minimum map value	-2.941	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.180	Depositor
Recommended contour level	0.63	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, HEM, U10, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/3254	0.47	0/4409
1	J	0.30	0/3254	0.47	0/4409
2	K	0.36	0/3158	0.46	0/4317
2	T	0.37	0/3158	0.46	0/4317
3	D	0.32	0/1978	0.47	0/2696
3	N	0.31	0/1978	0.48	0/2696
4	G	0.28	0/994	0.46	0/1346
4	Q	0.28	0/994	0.46	0/1346
5	F	0.35	0/731	0.50	0/994
5	P	0.32	0/731	0.51	0/994
6	H	0.26	0/621	0.46	0/840
6	R	0.26	0/621	0.44	0/840
7	I	0.27	0/336	0.36	0/451
7	S	0.28	0/336	0.37	0/451
8	C	0.28	0/1051	0.45	0/1441
8	M	0.27	0/1051	0.47	0/1441
9	B	0.30	0/2748	0.46	0/3735
9	L	0.29	0/2748	0.46	0/3735
All	All	0.31	0/29742	0.46	0/40458

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3198	3166	3168	43	0
1	J	3198	3166	3168	50	0
2	K	3056	3090	3090	78	0
2	T	3056	3090	3091	62	0
3	D	1916	1820	1821	48	0
3	N	1916	1820	1821	63	0
4	G	976	1002	1002	24	0
4	Q	976	1002	1002	22	0
5	F	708	691	692	7	0
5	P	708	691	692	7	0
6	H	604	544	543	6	0
6	R	604	544	543	4	0
7	I	324	315	314	2	0
7	S	324	315	314	3	0
8	C	1043	697	706	10	0
8	M	1043	697	706	16	0
9	B	2700	2692	2685	52	0
9	L	2700	2692	2685	59	0
10	K	86	60	60	17	0
10	T	86	60	60	17	0
11	K	51	50	52	8	0
11	T	51	50	54	7	0
12	D	43	30	30	24	0
12	N	43	30	30	31	0
13	C	4	0	0	1	0
13	M	4	0	0	4	0
All	All	29418	28314	28329	506	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 9.

The worst 5 of 506 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)
8:M:158:HIS:O	13:M:301:FES:S2	1.97	1.21
3:N:82:CYS:CA	12:N:301:HEC:HBB2	1.71	1.11
3:N:82:CYS:HA	12:N:301:HEC:HBB2	1.33	1.06
3:D:82:CYS:CA	12:D:301:HEC:HBB2	1.84	1.02
10:K:401:HEM:HBC2	10:K:401:HEM:HHD	1.42	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	414/439 (94%)	399 (96%)	15 (4%)	0	100	100
1	J	414/439 (94%)	398 (96%)	16 (4%)	0	100	100
2	K	381/387 (98%)	357 (94%)	24 (6%)	0	100	100
2	T	381/387 (98%)	363 (95%)	18 (5%)	0	100	100
3	D	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
3	N	242/288 (84%)	234 (97%)	8 (3%)	0	100	100
4	G	120/127 (94%)	119 (99%)	1 (1%)	0	100	100
4	Q	120/127 (94%)	119 (99%)	1 (1%)	0	100	100
5	F	83/95 (87%)	78 (94%)	5 (6%)	0	100	100
5	P	83/95 (87%)	79 (95%)	4 (5%)	0	100	100
6	H	70/135 (52%)	69 (99%)	1 (1%)	0	100	100
6	R	70/135 (52%)	69 (99%)	1 (1%)	0	100	100
7	I	37/65 (57%)	36 (97%)	1 (3%)	0	100	100
7	S	37/65 (57%)	37 (100%)	0	0	100	100
8	C	179/213 (84%)	170 (95%)	9 (5%)	0	100	100
8	M	179/213 (84%)	171 (96%)	8 (4%)	0	100	100
9	B	362/374 (97%)	347 (96%)	15 (4%)	0	100	100
9	L	362/374 (97%)	345 (95%)	17 (5%)	0	100	100
All	All	3776/4246 (89%)	3622 (96%)	154 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	345/365 (94%)	345 (100%)	0	100	100
1	J	345/365 (94%)	345 (100%)	0	100	100
2	K	333/338 (98%)	333 (100%)	0	100	100
2	T	333/338 (98%)	331 (99%)	2 (1%)	86	95
3	D	196/237 (83%)	195 (100%)	1 (0%)	88	96
3	N	196/237 (83%)	195 (100%)	1 (0%)	88	96
4	G	106/110 (96%)	106 (100%)	0	100	100
4	Q	106/110 (96%)	106 (100%)	0	100	100
5	F	71/80 (89%)	71 (100%)	0	100	100
5	P	71/80 (89%)	71 (100%)	0	100	100
6	H	67/128 (52%)	67 (100%)	0	100	100
6	R	67/128 (52%)	67 (100%)	0	100	100
7	I	30/53 (57%)	30 (100%)	0	100	100
7	S	30/53 (57%)	30 (100%)	0	100	100
8	C	48/176 (27%)	48 (100%)	0	100	100
8	M	48/176 (27%)	47 (98%)	1 (2%)	53	82
9	B	295/307 (96%)	295 (100%)	0	100	100
9	L	295/307 (96%)	295 (100%)	0	100	100
All	All	2982/3588 (83%)	2977 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	237	ASN
2	T	22	GLN
2	T	31	ASN
3	N	237	ASN
8	M	50	ARG

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

Mol	Chain	Res	Type
6	R	104	HIS
8	M	34	GLN
9	L	179	GLN
9	L	15	ASN
6	R	87	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 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	$\#\|Z\| > 2$
10	HEM	K	402	2	41,50,50	1.42	4 (9%)	45,82,82	1.47	9 (20%)
10	HEM	K	401	2	41,50,50	1.53	3 (7%)	45,82,82	1.24	3 (6%)
11	U10	K	404	2	23,23,63	2.72	9 (39%)	28,31,79	1.49	4 (14%)
10	HEM	T	401	2	41,50,50	1.49	3 (7%)	45,82,82	1.20	4 (8%)
13	FES	M	301	8	0,4,4	-	-	-		
11	U10	T	404	-	23,23,63	2.71	9 (39%)	28,31,79	1.33	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	U10	K	403	-	28,28,63	2.78	10 (35%)	34,37,79	1.46	7 (20%)
11	U10	T	403	-	28,28,63	2.77	10 (35%)	34,37,79	1.30	6 (17%)
12	HEC	D	301	3	32,50,50	2.26	4 (12%)	24,82,82	1.39	2 (8%)
10	HEM	T	402	2	41,50,50	1.40	3 (7%)	45,82,82	1.48	9 (20%)
12	HEC	N	301	3	32,50,50	2.27	4 (12%)	24,82,82	1.37	2 (8%)
13	FES	C	301	8	0,4,4	-	-	-		

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
10	HEM	K	402	2	-	2/12/54/54	-
10	HEM	K	401	2	-	5/12/54/54	-
11	U10	K	404	2	-	2/15/39/87	0/1/1/1
10	HEM	T	401	2	-	6/12/54/54	-
13	FES	M	301	8	-	-	0/1/1/1
11	U10	T	404	-	-	1/15/39/87	0/1/1/1
11	U10	K	403	-	-	3/21/45/87	0/1/1/1
11	U10	T	403	-	-	3/21/45/87	0/1/1/1
12	HEC	D	301	3	-	2/10/54/54	-
10	HEM	T	402	2	-	2/12/54/54	-
12	HEC	N	301	3	-	2/10/54/54	-
13	FES	C	301	8	-	-	0/1/1/1

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	301	HEC	C2B-C3B	-6.97	1.33	1.40
12	D	301	HEC	C2B-C3B	-6.80	1.33	1.40
12	D	301	HEC	C3C-C2C	-6.56	1.33	1.40
12	N	301	HEC	C3C-C2C	-6.48	1.34	1.40
11	T	404	U10	C8-C9	6.27	1.48	1.33

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	404	U10	C10-C9-C11	4.05	122.09	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	T	402	HEM	CHA-C4D-ND	3.53	128.74	124.38
10	K	402	HEM	CHA-C4D-ND	3.33	128.50	124.38
11	K	404	U10	C7-C8-C9	-3.31	121.28	126.79
10	T	402	HEM	CHD-C1D-ND	3.20	127.91	124.43

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	K	401	HEM	C1A-C2A-CAA-CBA
10	K	401	HEM	C3A-C2A-CAA-CBA
10	T	401	HEM	C1A-C2A-CAA-CBA
11	K	403	U10	C12-C11-C9-C8
11	K	403	U10	C12-C11-C9-C10

There are no ring outliers.

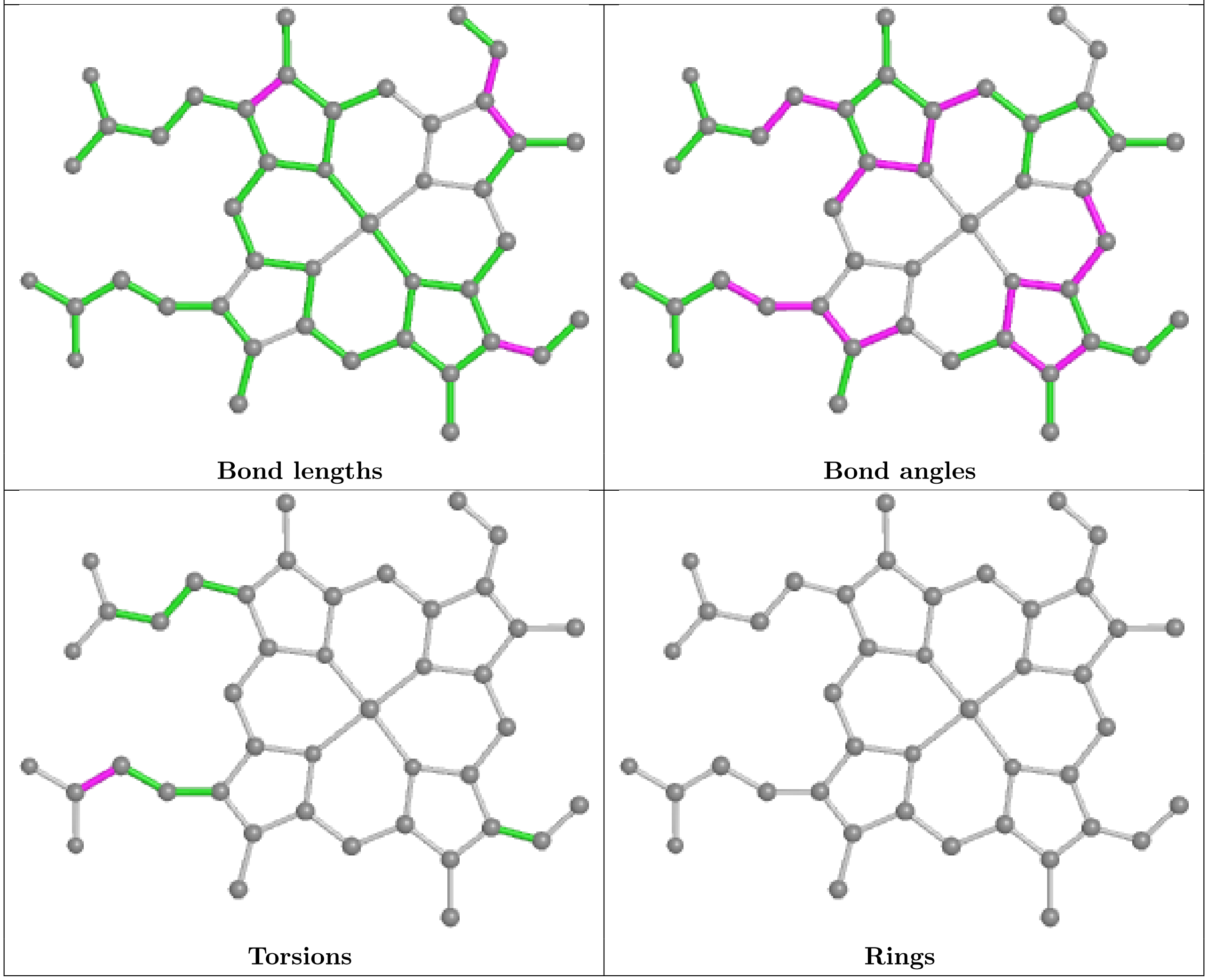
12 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	402	HEM	7	0
10	K	401	HEM	10	0
11	K	404	U10	1	0
10	T	401	HEM	10	0
13	M	301	FES	4	0
11	T	404	U10	2	0
11	K	403	U10	7	0
11	T	403	U10	5	0
12	D	301	HEC	24	0
10	T	402	HEM	7	0
12	N	301	HEC	31	0
13	C	301	FES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM K 402



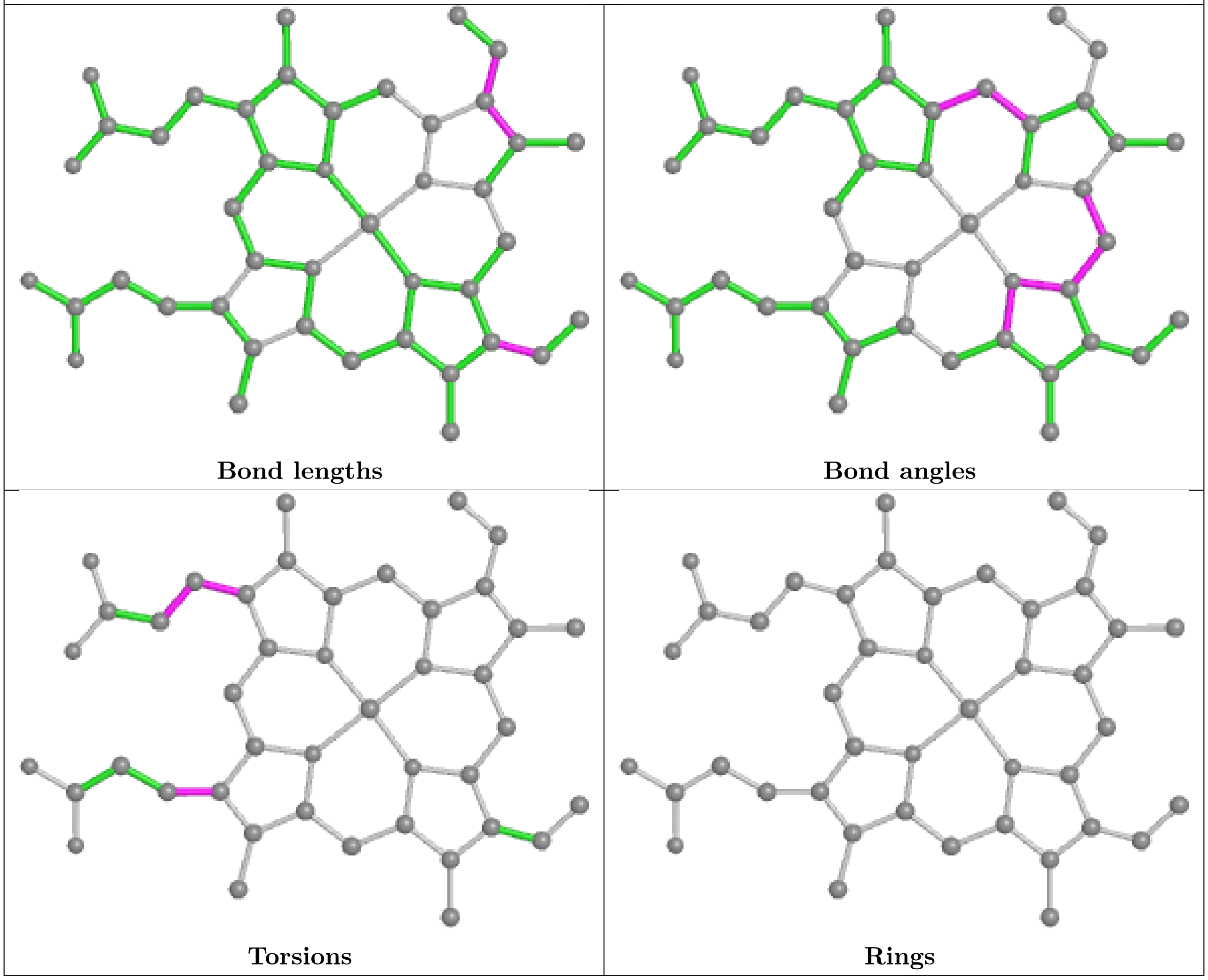
Bond lengths

Bond angles

Torsions

Rings

Ligand HEM K 401



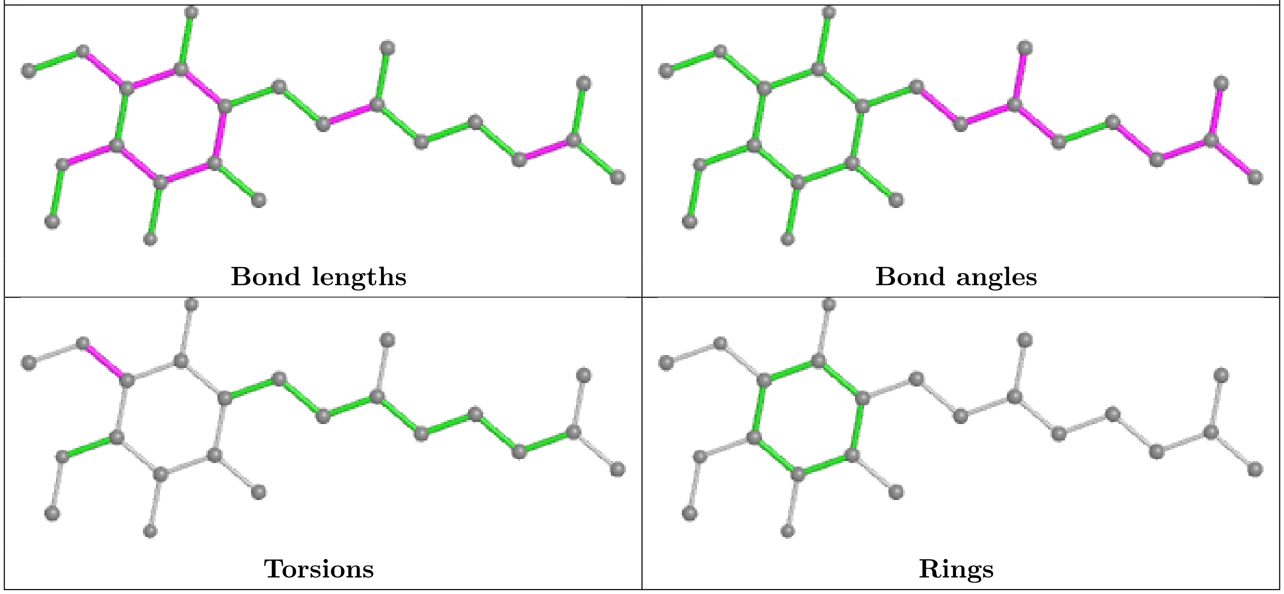
Bond lengths

Bond angles

Torsions

Rings

Ligand U10 K 404



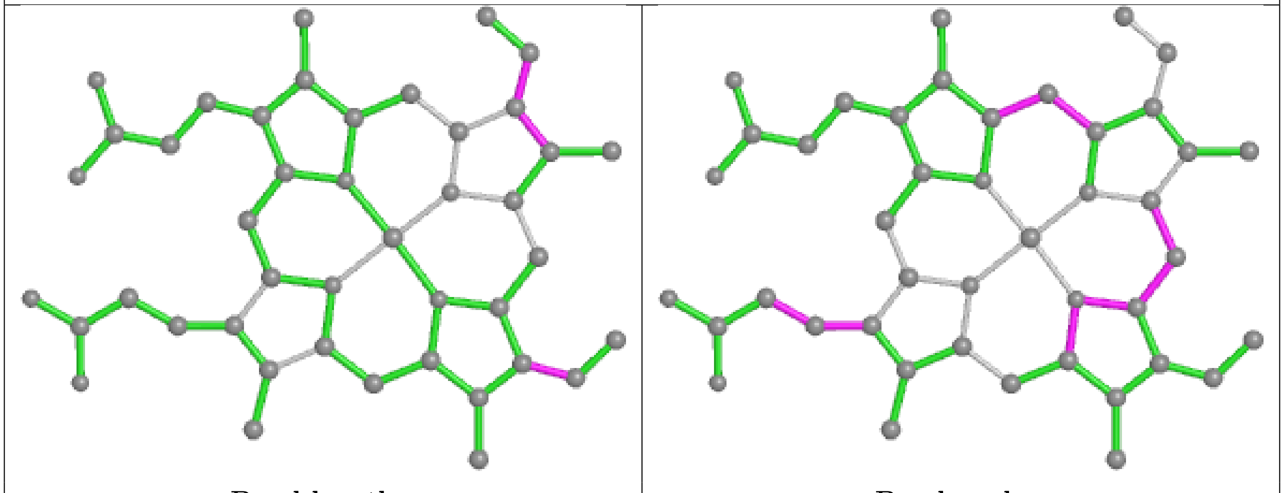
Bond lengths

Bond angles

Torsions

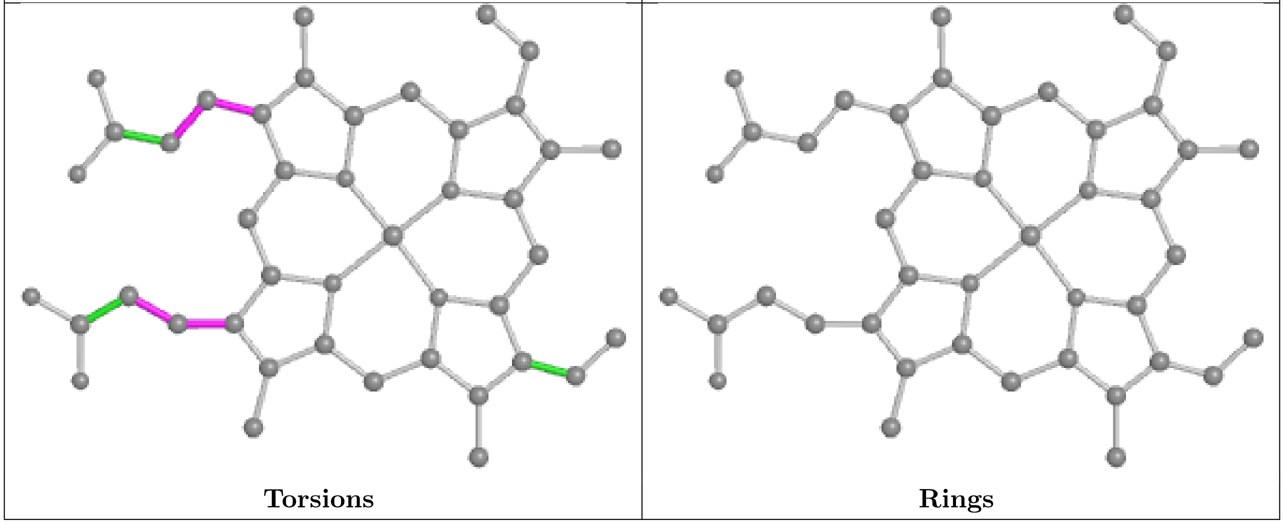
Rings

Ligand HEM T 401



Bond lengths

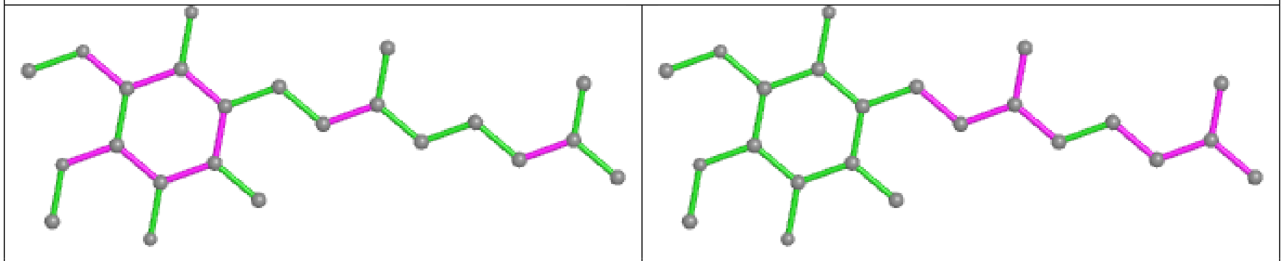
Bond angles



Torsions

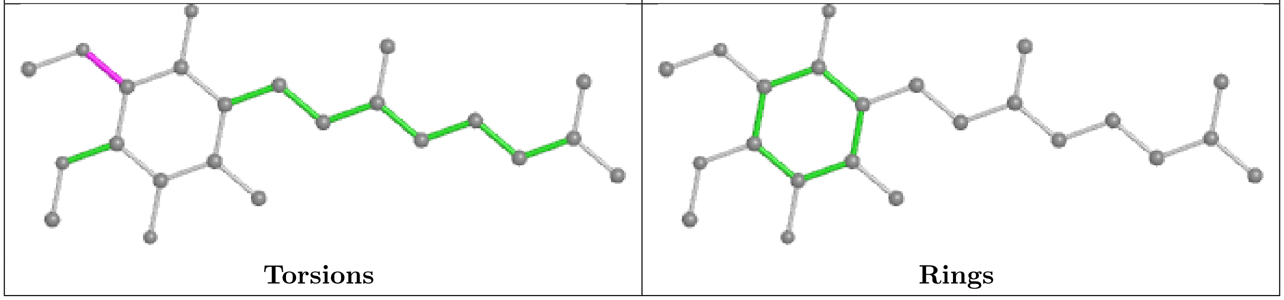
Rings

Ligand U10 T 404



Bond lengths

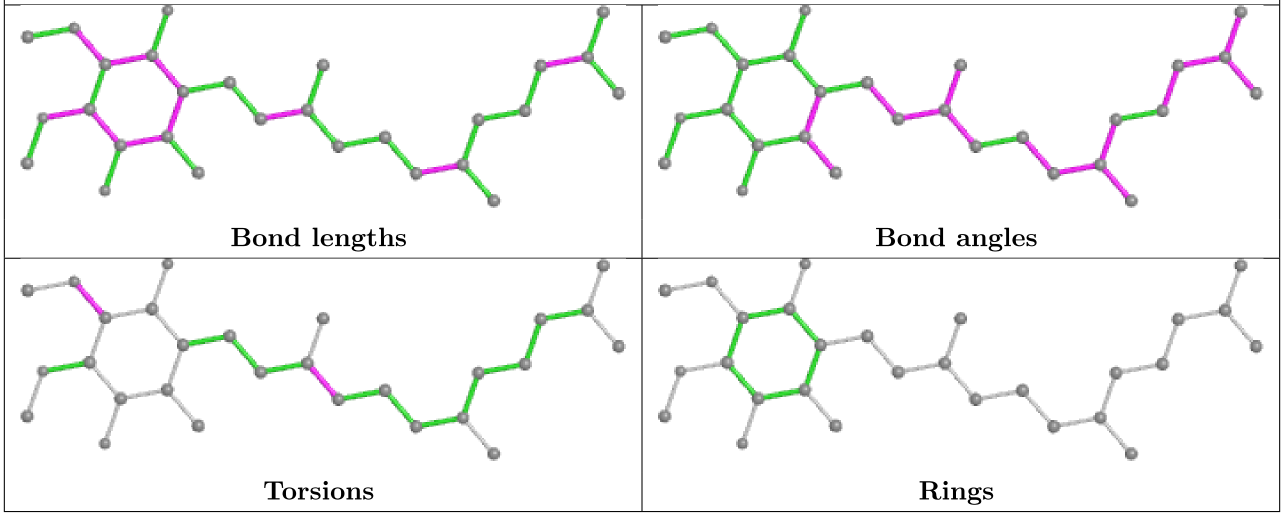
Bond angles



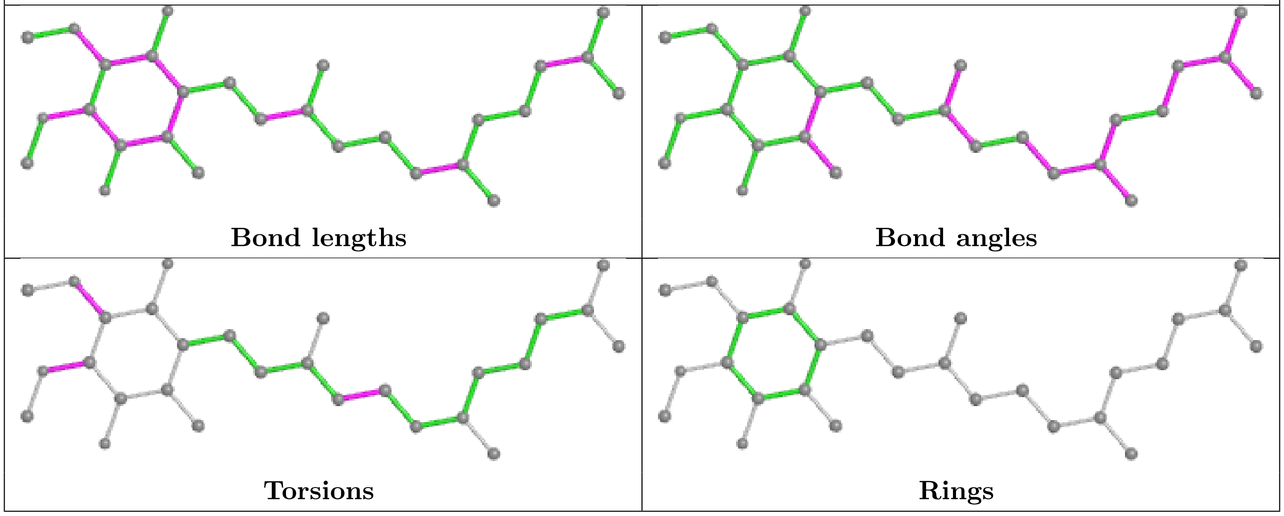
Torsions

Rings

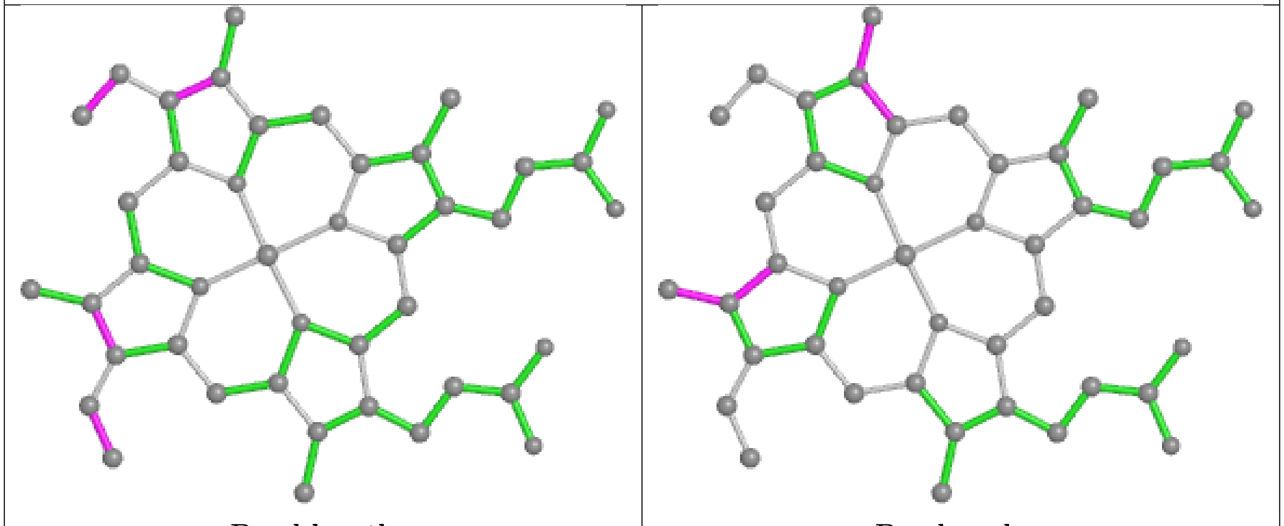
Ligand U10 K 403



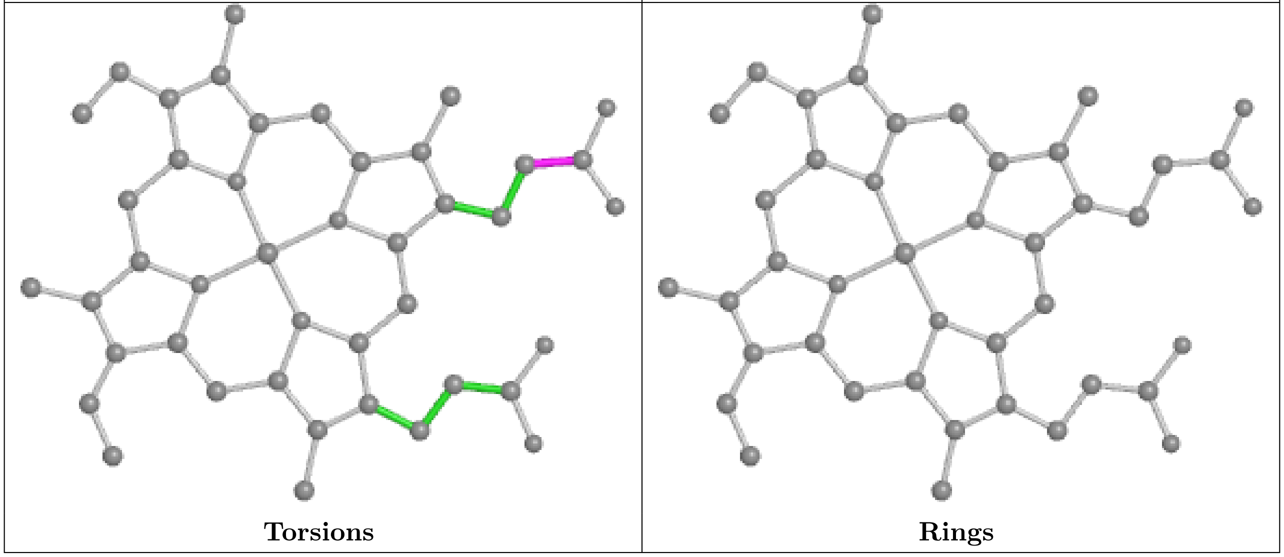
Ligand U10 T 403



Ligand HEC D 301

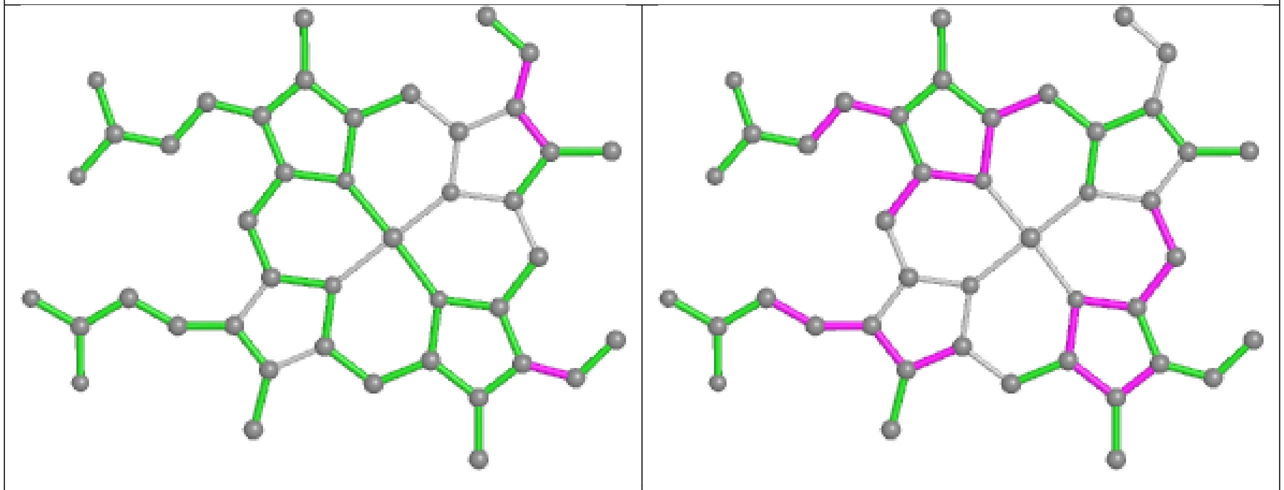


Bond lengths **Bond angles**

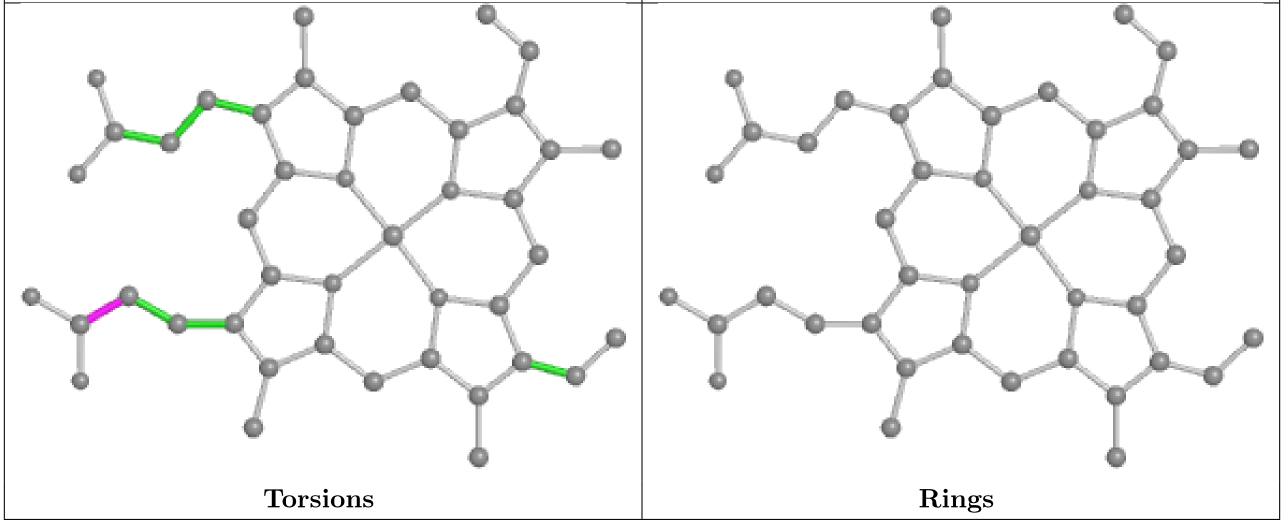


Torsions **Rings**

Ligand HEM T 402

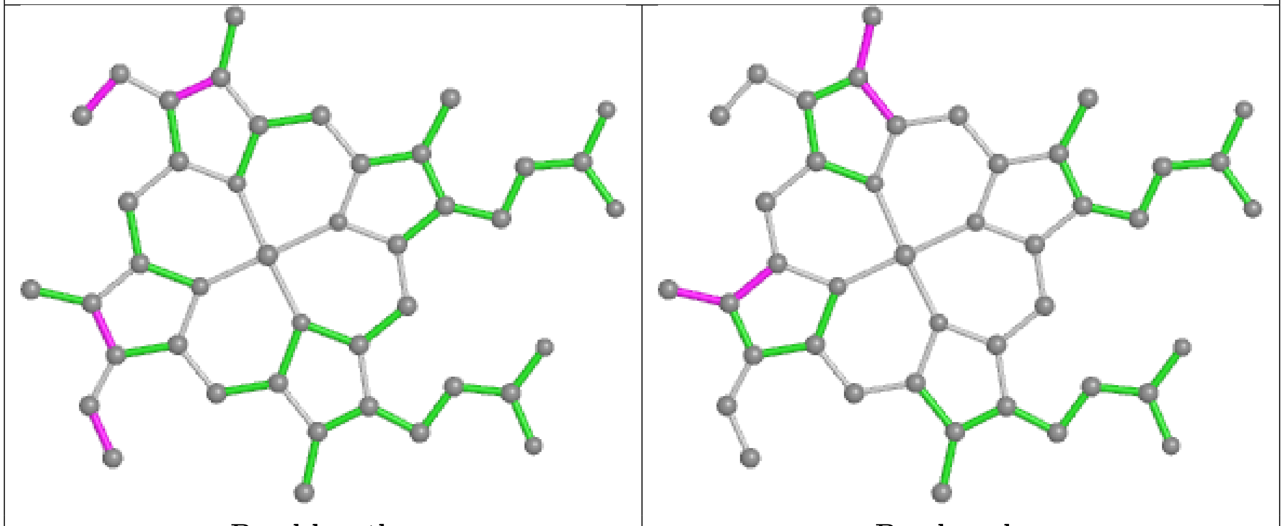


Bond lengths **Bond angles**

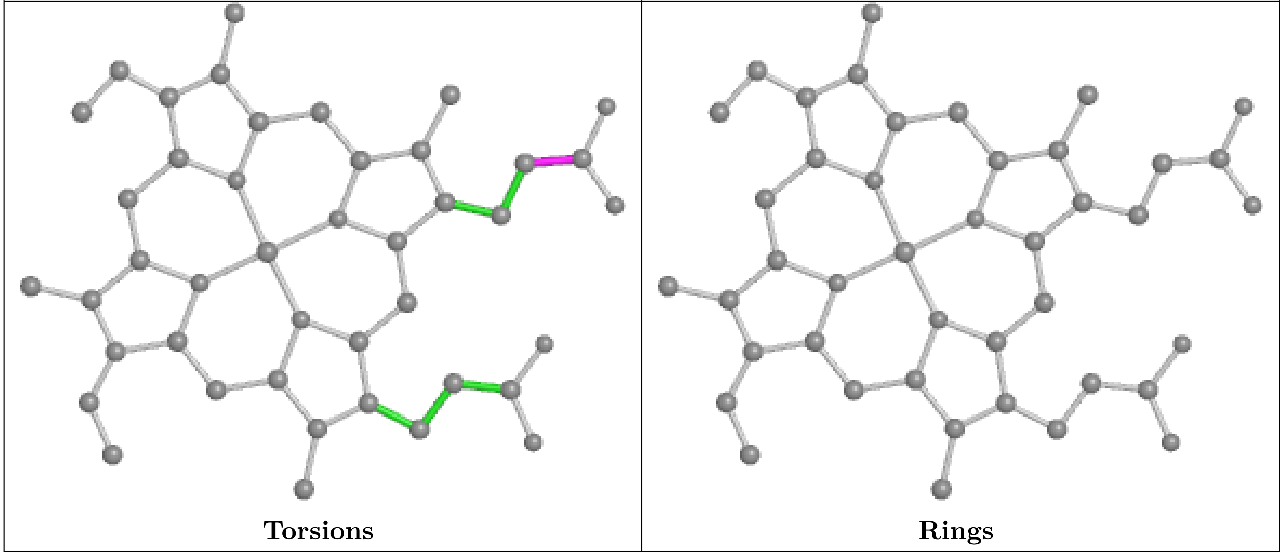


Torsions **Rings**

Ligand HEC N 301



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.

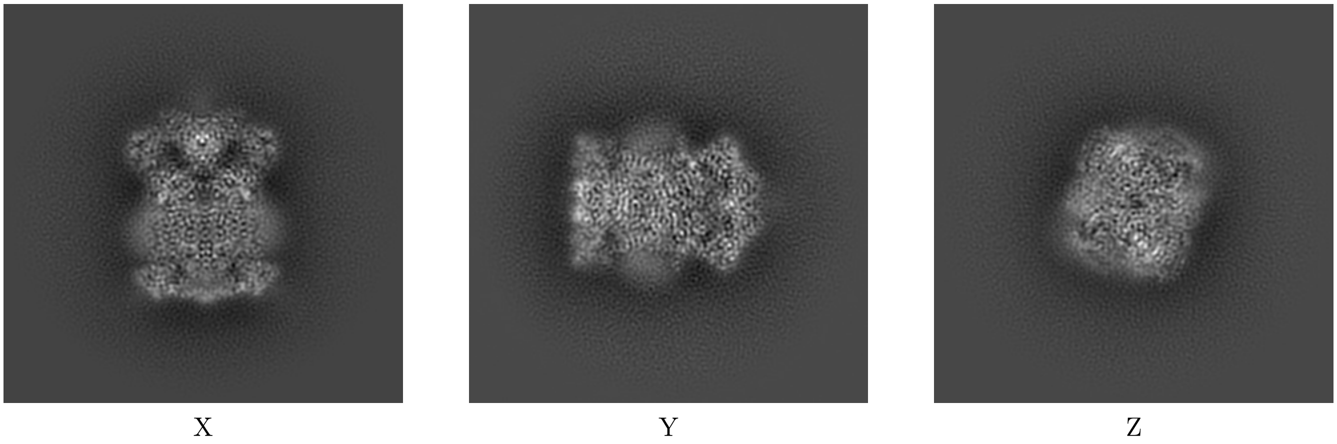
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24482. 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

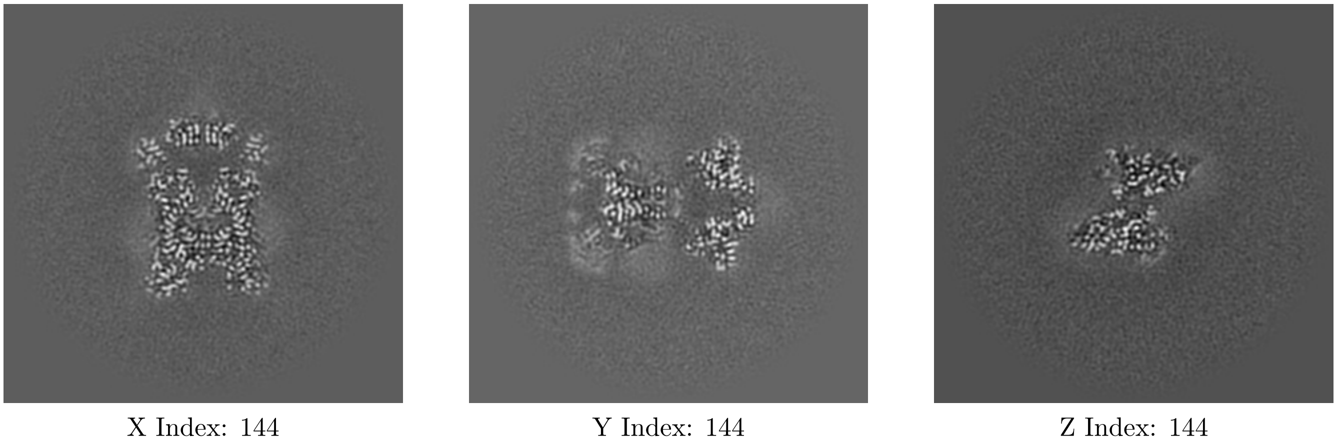
6.1.1 Primary map


X Y Z

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

6.2 Central slices

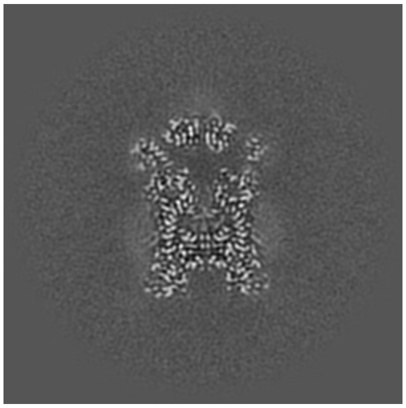
6.2.1 Primary map


X Index: 144 Y Index: 144 Z Index: 144

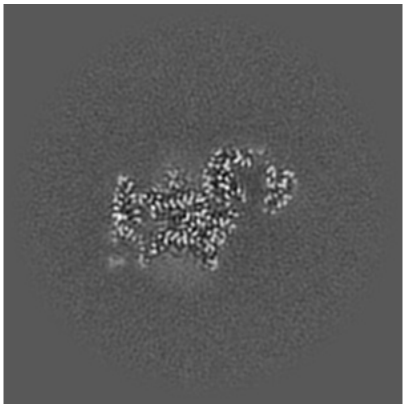
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

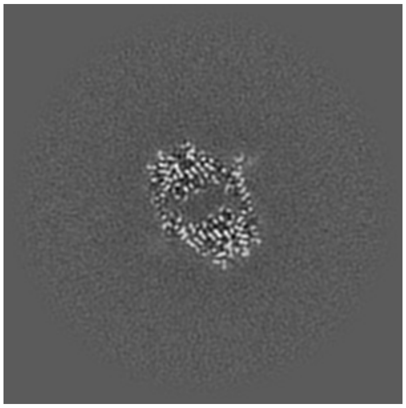
6.3.1 Primary map



X Index: 145



Y Index: 121

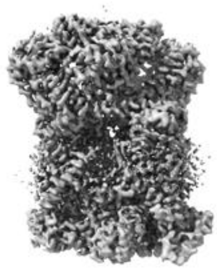


Z Index: 161

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

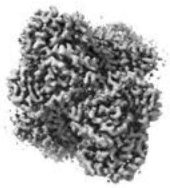
6.4 Orthogonal surface views

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.63. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

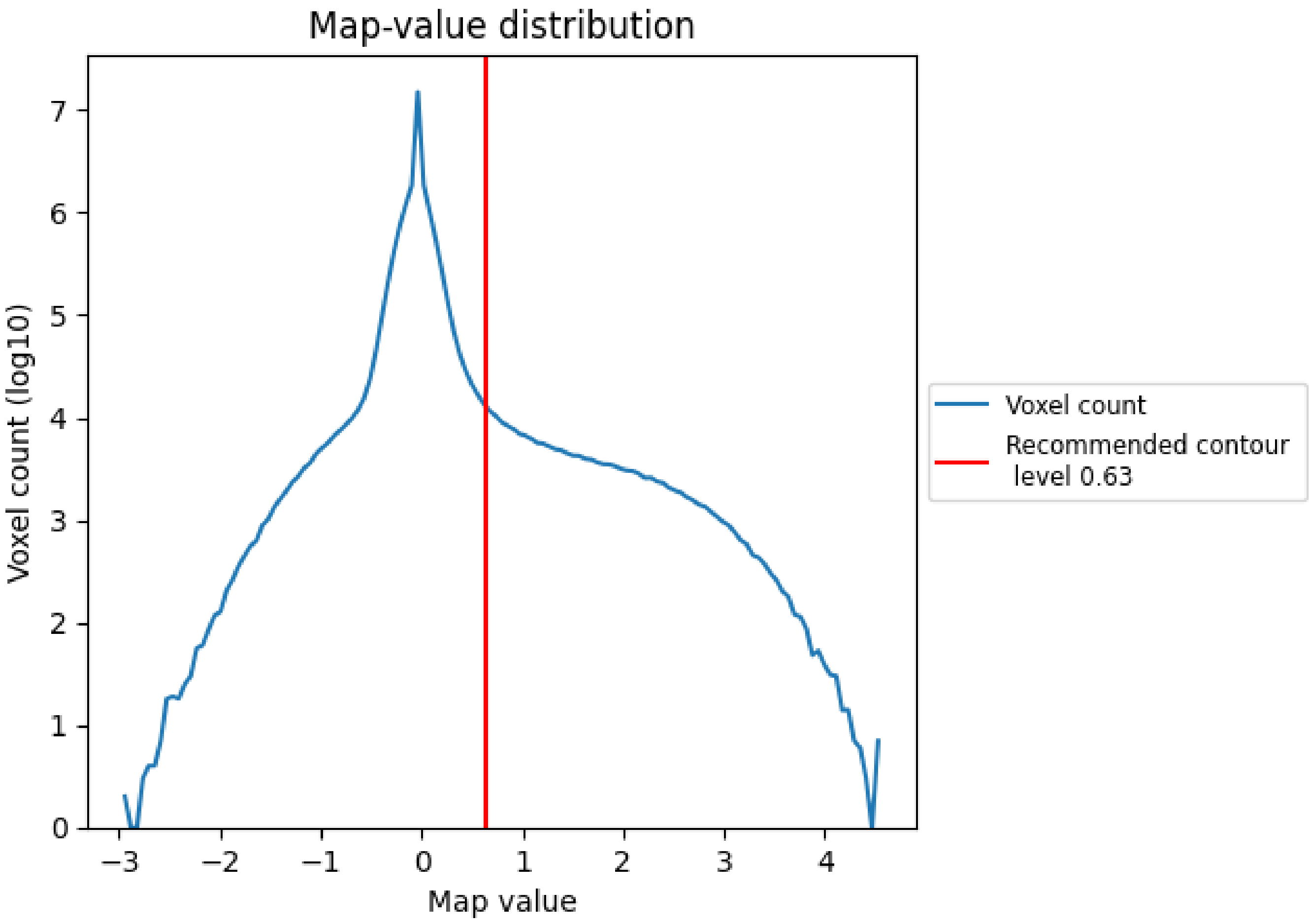
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

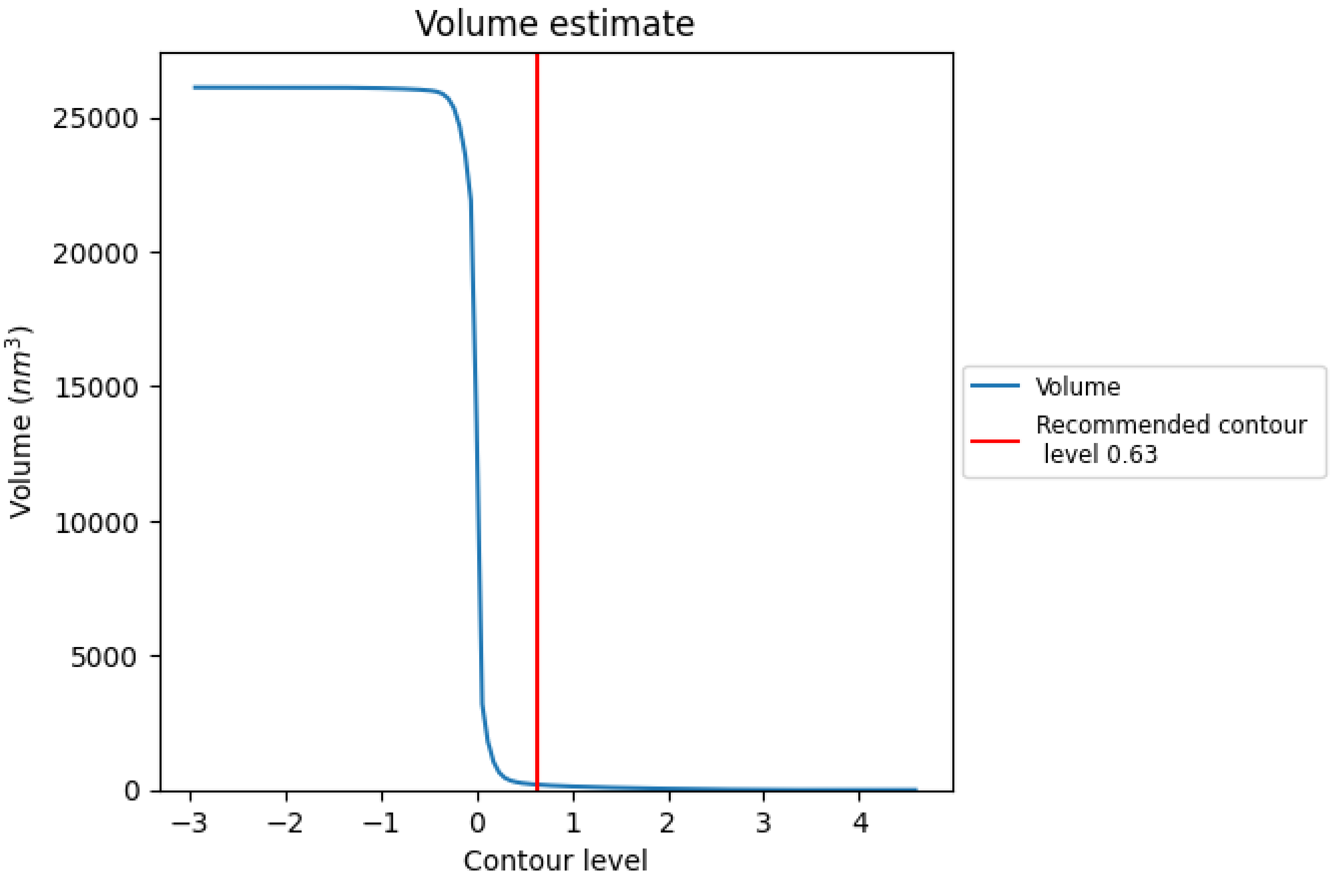
This section contains the results of statistical analysis of the map.

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.

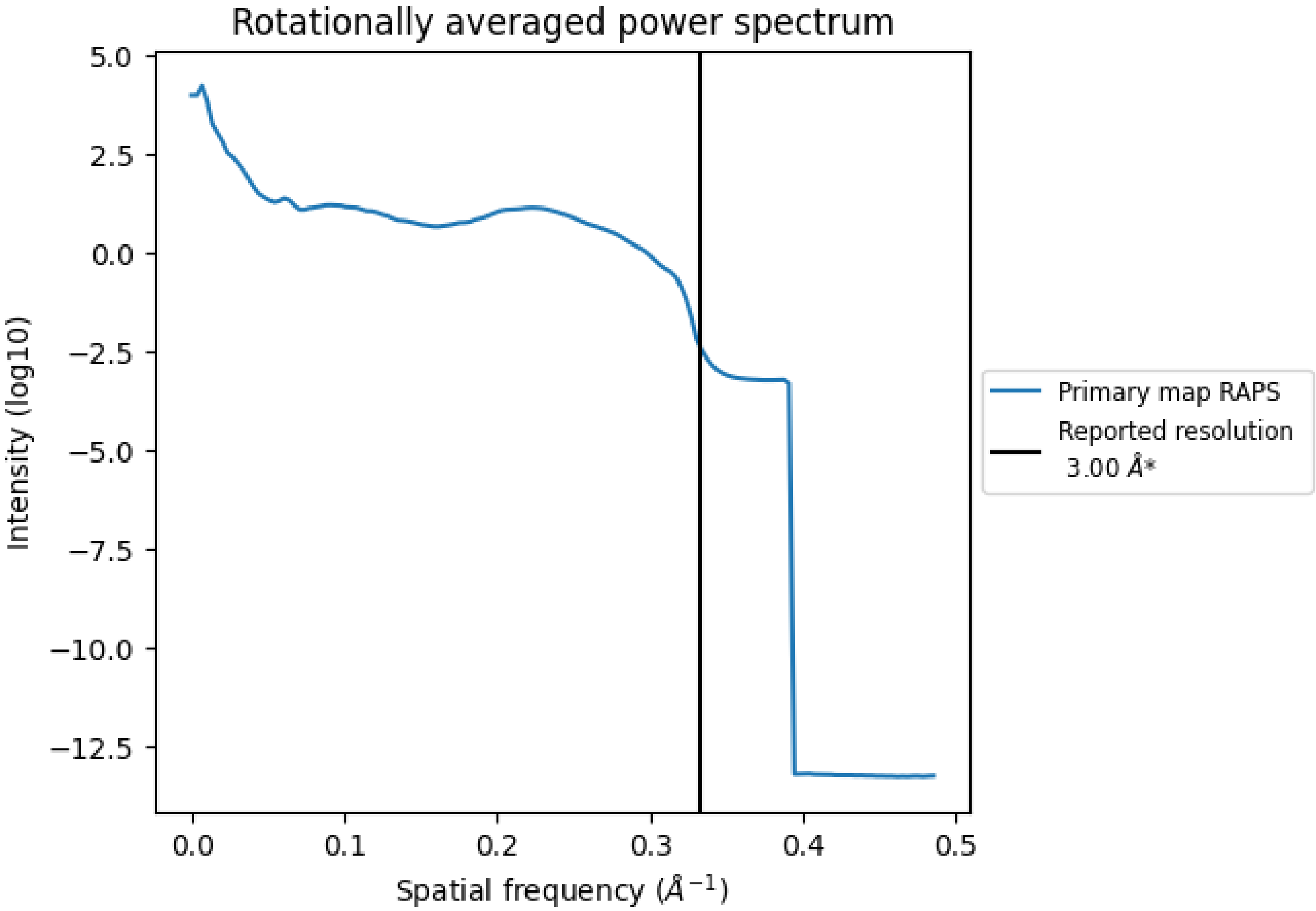
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 198 nm^3; this corresponds to an approximate mass of 179 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 ⓘ

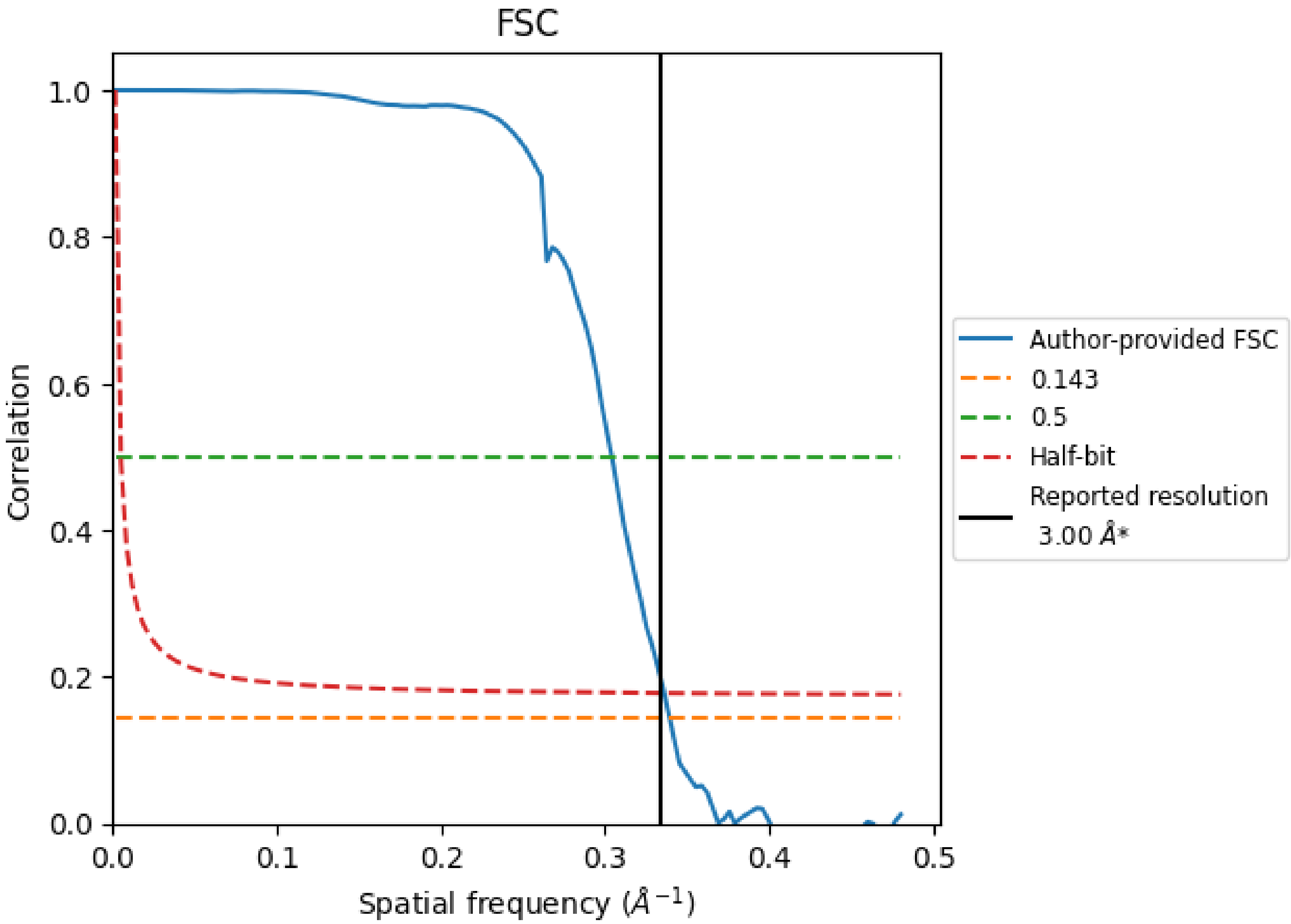


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



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

8.2 Resolution estimates ⓘ

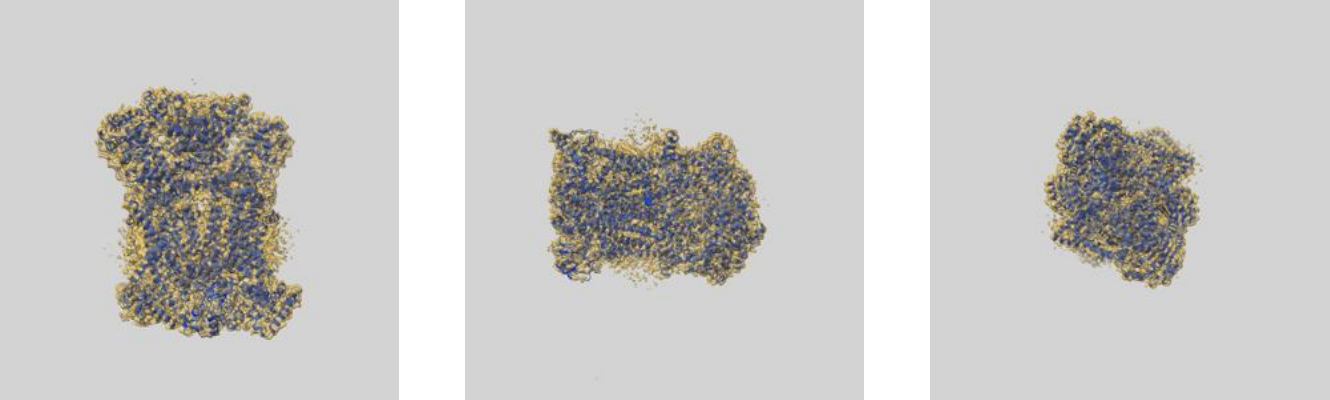
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.95	3.29	2.97
Unmasked-calculated*	-	-	-

*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-24482 and PDB model 7RJA. Per-residue inclusion information can be found in section 3 on page 9.

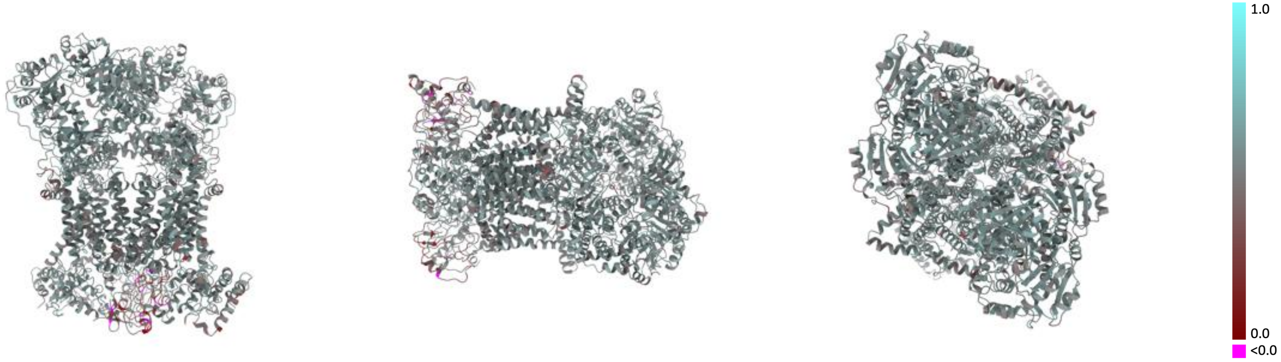
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.63 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.

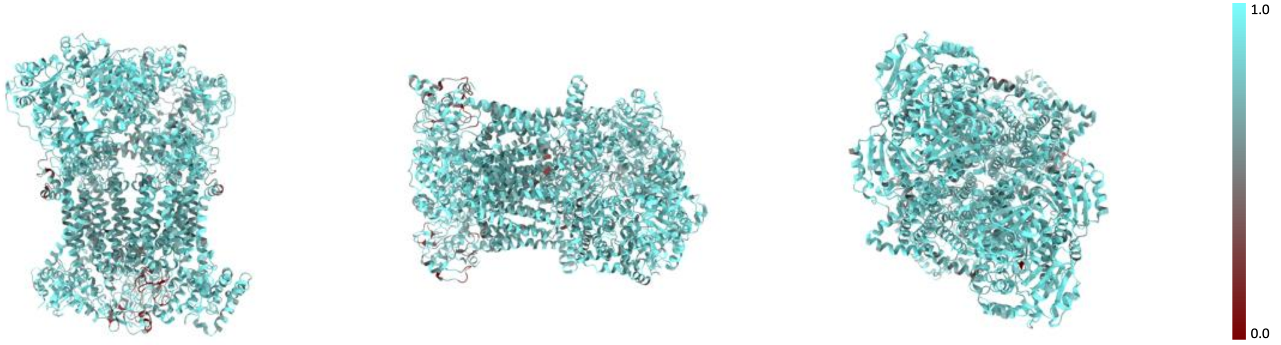
9.2 Q-score mapped to coordinate model ⓘ



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.

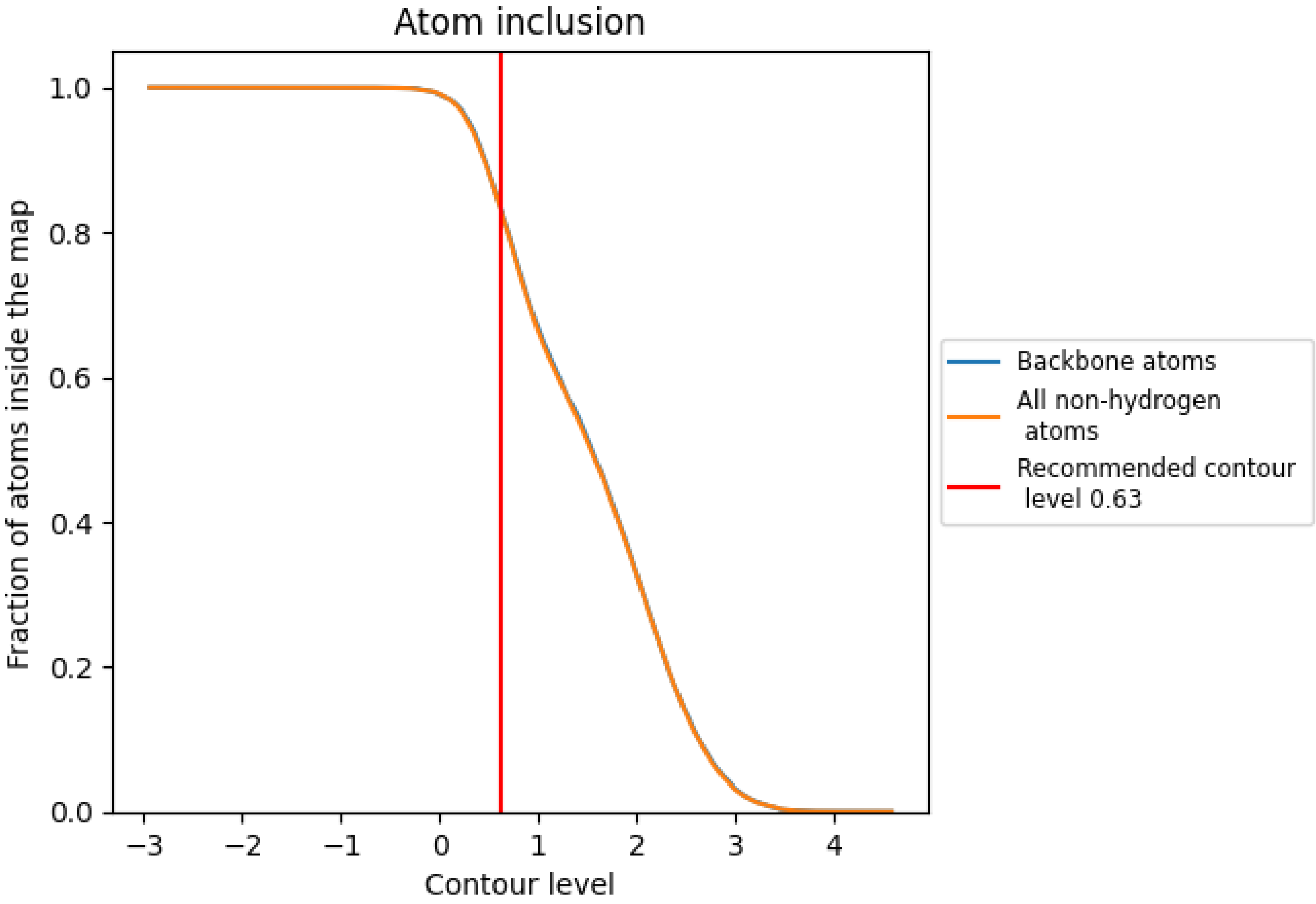
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.63).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.63) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	▬ 0.8279	▬ 0.5230
A	▬ 0.8615	▬ 0.5410
B	▬ 0.8555	▬ 0.5350
C	▬ 0.7022	▬ 0.4340
D	▬ 0.8690	▬ 0.5370
F	▬ 0.8114	▬ 0.5100
G	▬ 0.8512	▬ 0.5380
H	▬ 0.8215	▬ 0.4910
I	▬ 0.8411	▬ 0.5160
J	▬ 0.8586	▬ 0.5380
K	▬ 0.8358	▬ 0.5400
L	▬ 0.8533	▬ 0.5330
M	▬ 0.6311	▬ 0.3950
N	▬ 0.8570	▬ 0.5270
P	▬ 0.7939	▬ 0.5120
Q	▬ 0.8169	▬ 0.5220
R	▬ 0.7946	▬ 0.4760
S	▬ 0.8318	▬ 0.5120
T	▬ 0.8189	▬ 0.5300