wwPDB EM Validation Summary Report

Mar 27, 2023 – 10:58 AM EDT

PDB ID	:	8E9I
EMDB ID	:	EMD-27965
Title	:	Mycobacterial respiratory complex I, semi-inserted quinone
Authors	:	Liang, Y.; Rubinstein, J.L.
Deposited on	:	2022-08-26
Resolution	:	2.80 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:

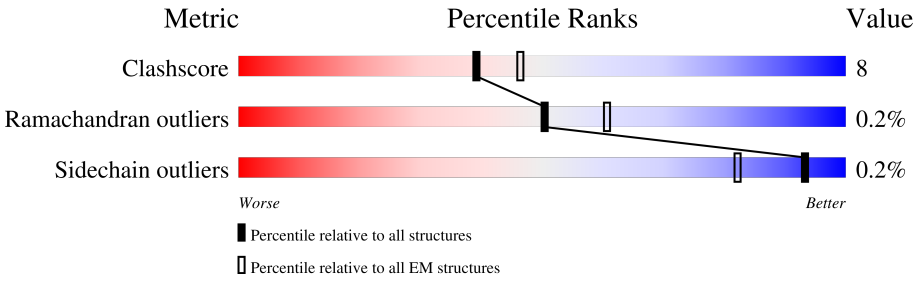
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.80 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	O	132	80% 14% 6%
2	B	184	78% 21% •
3	A	122	• 73% 26% •
4	C	238	82% 11% 8%
5	D	442	74% 18% 8%
6	E	245	80% 14% • 5%
7	G	794	• 84% 15% •
8	F	443	• 84% 14% •

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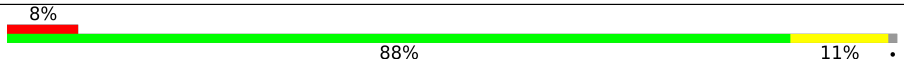
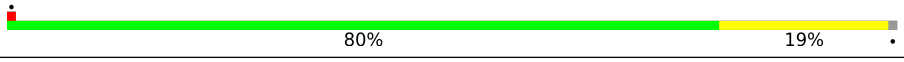
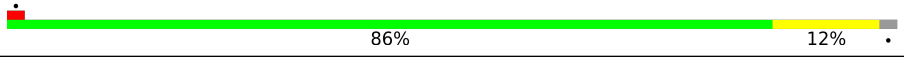
Mol	Chain	Length	Quality of chain
9	I	180	
10	H	408	
11	J	252	
12	K	99	
13	L	629	
14	N	521	
15	M	529	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 35471 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 Two-component system response regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	O	124	878	564	158	152	4	0	0

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	183	1304	846	230	214	14	0	0

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	121	925	631	149	141	4	0	0

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	219	1623	1050	297	271	5	0	0

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	407	2971	1900	543	505	23	0	0

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	232	1564	995	278	282	9	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	780	Total	C	N	O	S	0	0
			5374	3419	997	929	29		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	435	Total	C	N	O	S	0	0
			3105	2000	556	536	13		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	166	Total	C	N	O	S	0	0
			1183	753	209	208	13		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	395	Total	C	N	O	S	0	0
			2847	1901	466	468	12		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	230	Total	C	N	O	S	0	0
			1585	1043	269	269	4		

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	99	Total	C	N	O	S	0	0
			736	478	128	122	8		

- Molecule 13 is a protein called NADH-quinone oxidoreductase, L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	621	Total	C	N	O	S	0	0
			3784	2399	678	697	10		

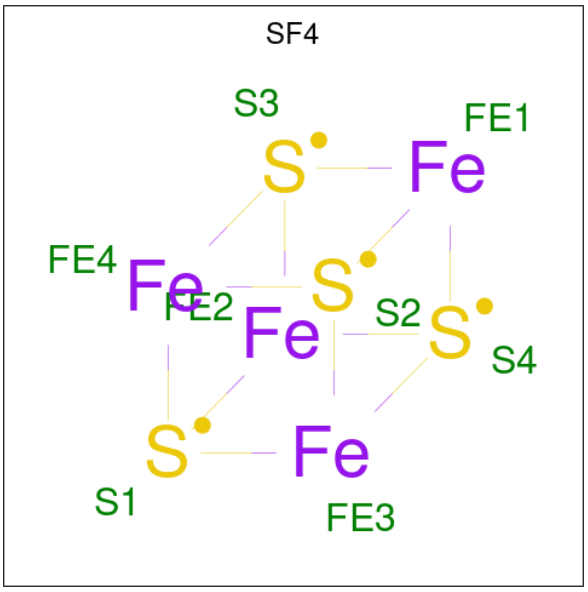
- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	518	Total	C	N	O	S	0	0
			3618	2402	584	619	13		

- Molecule 15 is a protein called NADH-quinone oxidoreductase, M subunit.

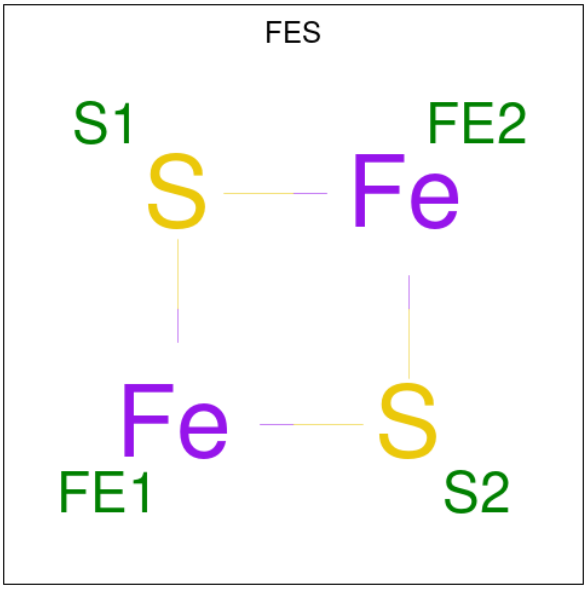
Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	518	Total	C	N	O	S	0	0
			3712	2501	592	604	15		

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



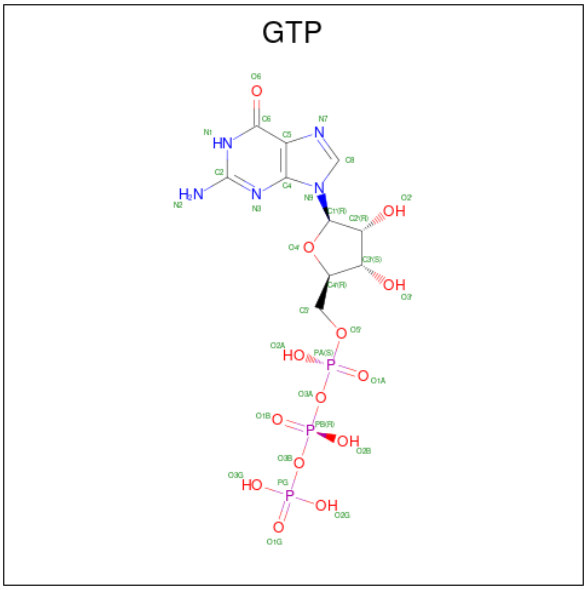
Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	Fe	S	0
			8	4	4	
16	G	1	Total	Fe	S	0
			8	4	4	
16	G	1	Total	Fe	S	0
			8	4	4	
16	G	1	Total	Fe	S	0
			8	4	4	
16	F	1	Total	Fe	S	0
			8	4	4	
16	I	1	Total	Fe	S	0
			8	4	4	
16	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



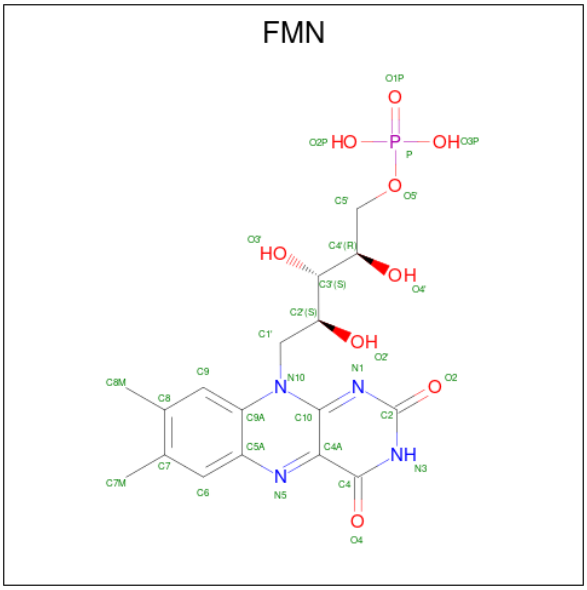
Mol	Chain	Residues	Atoms	AltConf
17	E	1	Total Fe S 4 2 2	0
17	G	1	Total Fe S 4 2 2	0

- Molecule 18 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	G	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 19 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

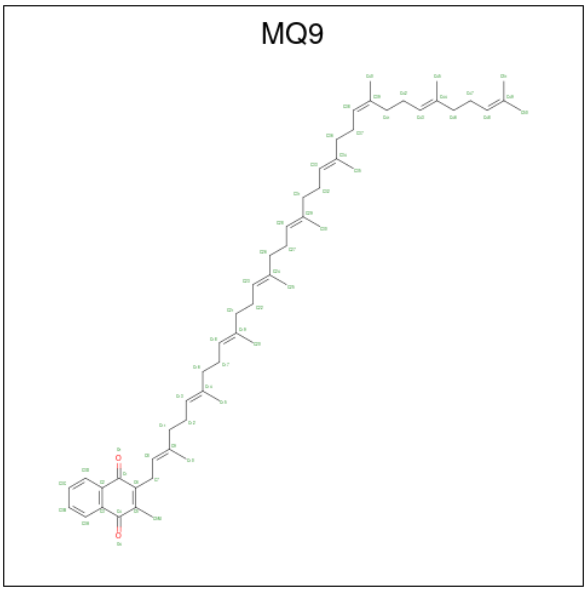


Mol	Chain	Residues	Atoms					AltConf
19	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

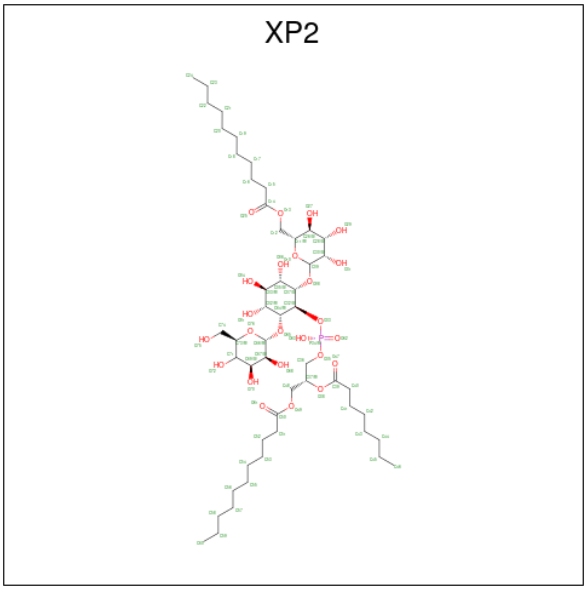
Mol	Chain	Residues	Atoms		AltConf
20	F	1	Total	Zn	0
			1	1	

- Molecule 21 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	H	1	Total	C	O	0
			58	56	2	

- Molecule 22 is (2R)-3-{[(R)-hydroxy({(1S,2R,3R,4R,5S,6S)-3,4,5-trihydroxy-2-(alpha-D-mannopyranosyloxy)-6-[(6-O-undecanoyl-beta-D-mannopyranosyl)oxy]cyclohexyl}oxy)phosphoryl]oxy}-2-(octanoyloxy)propyl undecanoate (three-letter code: XP2) (formula: $C_{51}H_{93}O_{24}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	L	1	Total	C	O	P	0
			76	51	24	1	

3 Residue-property plots (i)

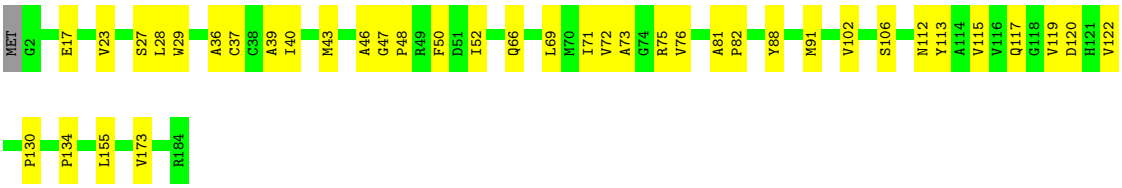
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Two-component system response regulator

Chain O:

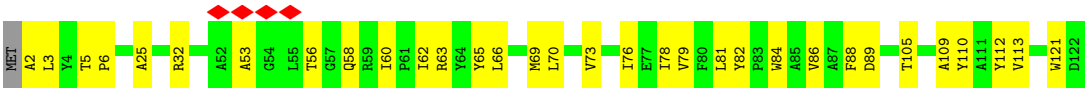
• Molecule 2: NADH-quinone oxidoreductase subunit B

Chain B:



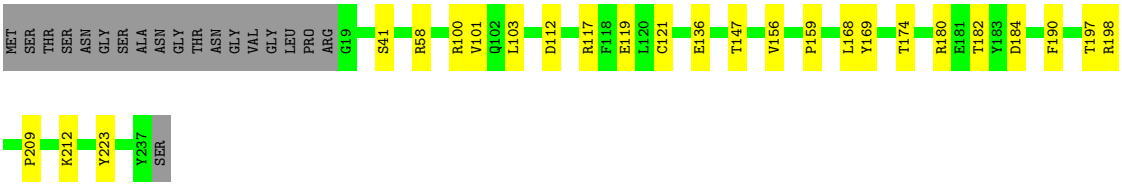
• Molecule 3: NADH-quinone oxidoreductase subunit A

Chain A:



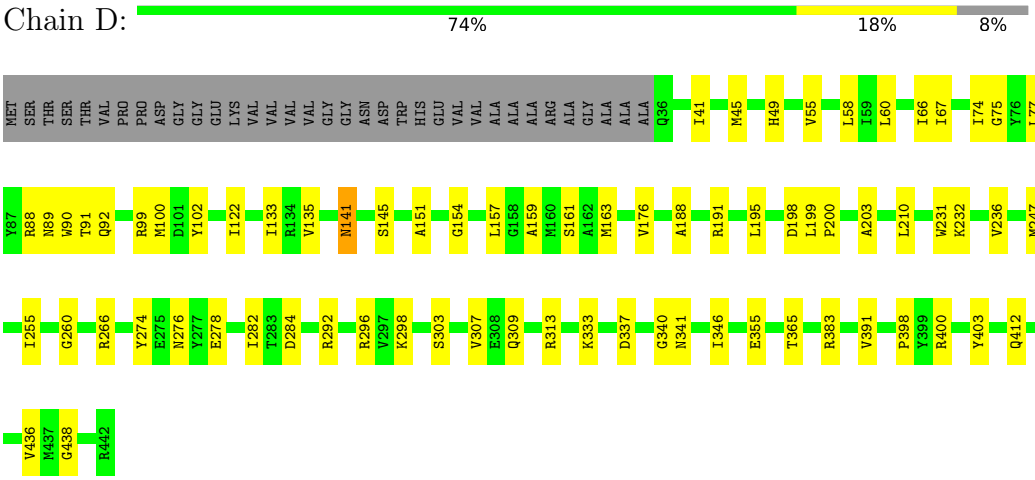
• Molecule 4: NADH-quinone oxidoreductase subunit C

Chain C:



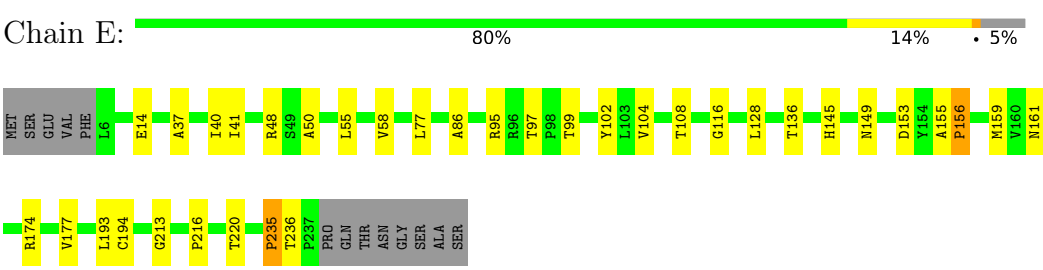
• Molecule 5: NADH-quinone oxidoreductase subunit D

Chain D:



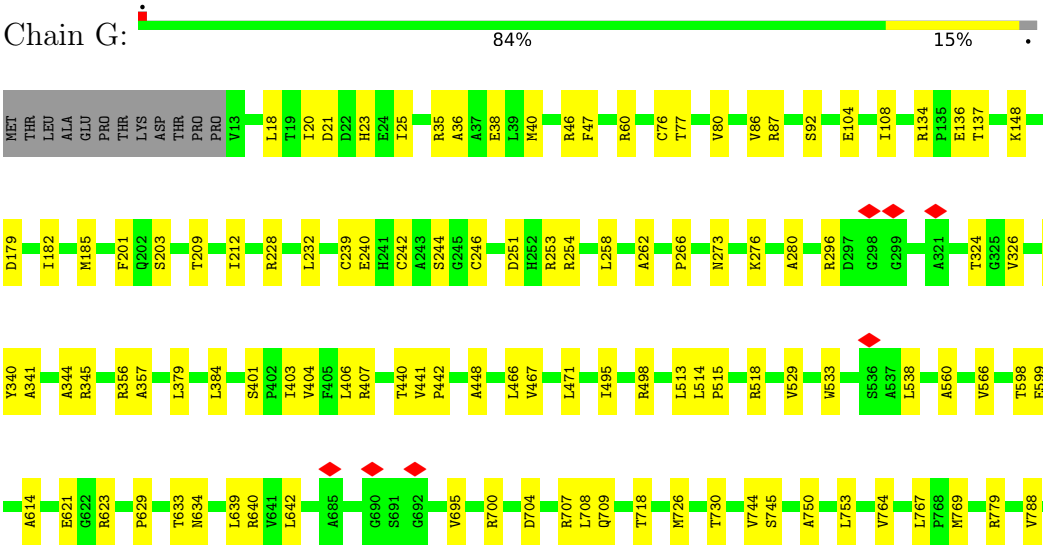
• Molecule 6: NADH-quinone oxidoreductase subunit E

Chain E:



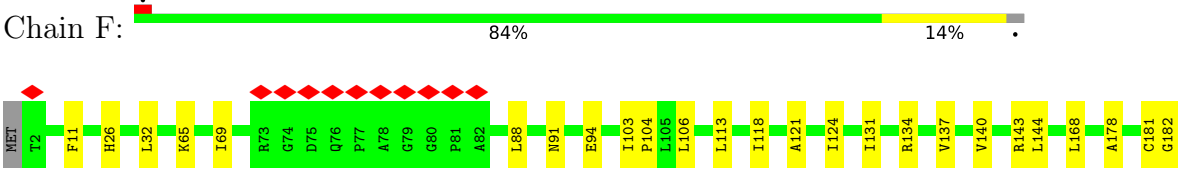
• Molecule 7: NADH-quinone oxidoreductase subunit G

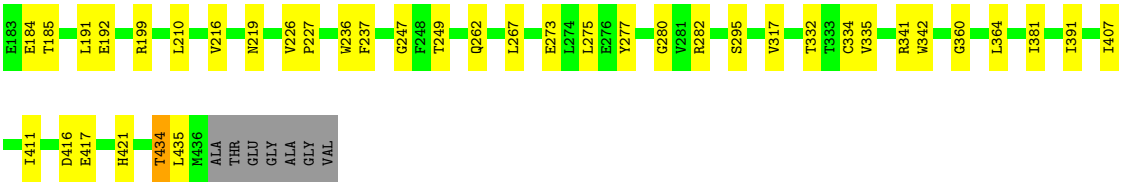
Chain G:



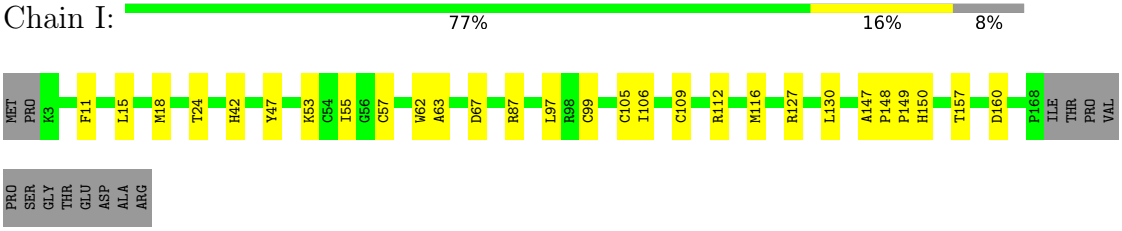
• Molecule 8: NADH-quinone oxidoreductase subunit F

Chain F:

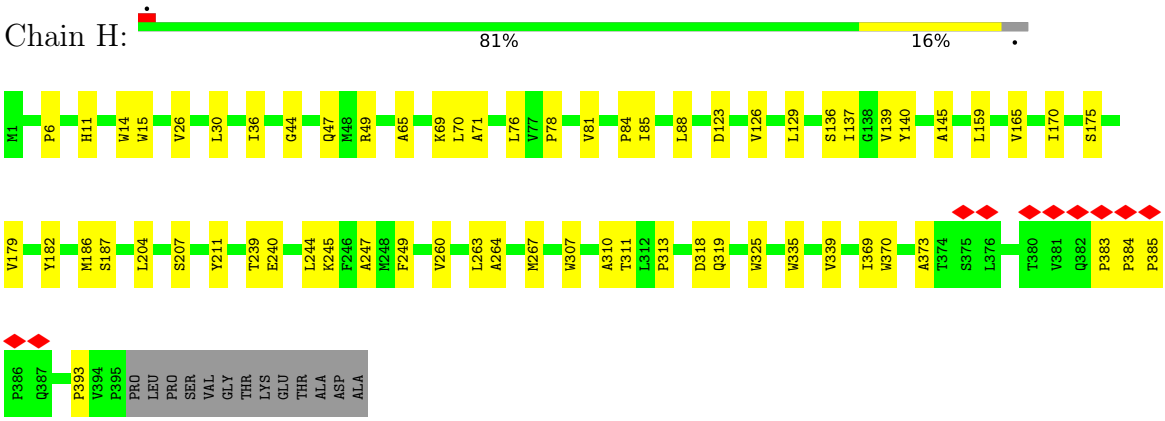




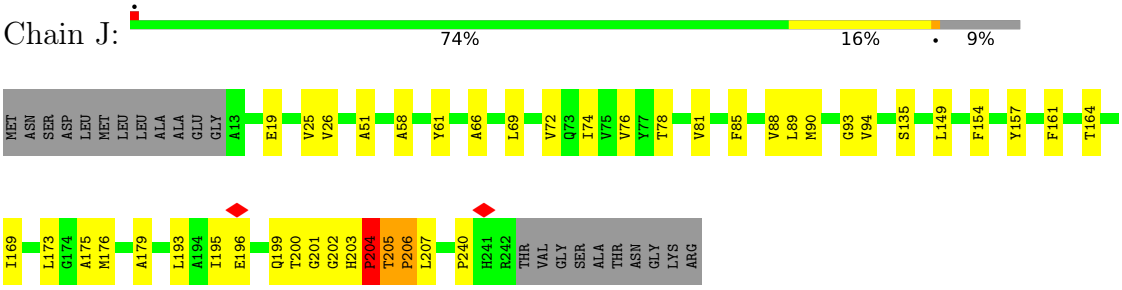
• Molecule 9: NADH-quinone oxidoreductase subunit I



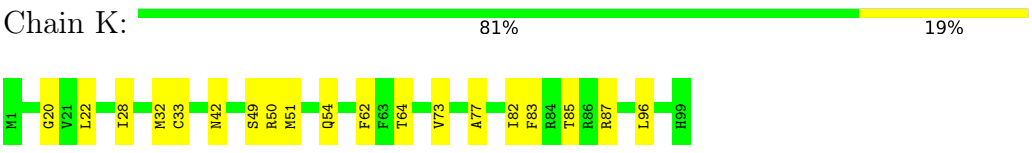
• Molecule 10: NADH-quinone oxidoreductase subunit H



• Molecule 11: NADH-quinone oxidoreductase subunit J

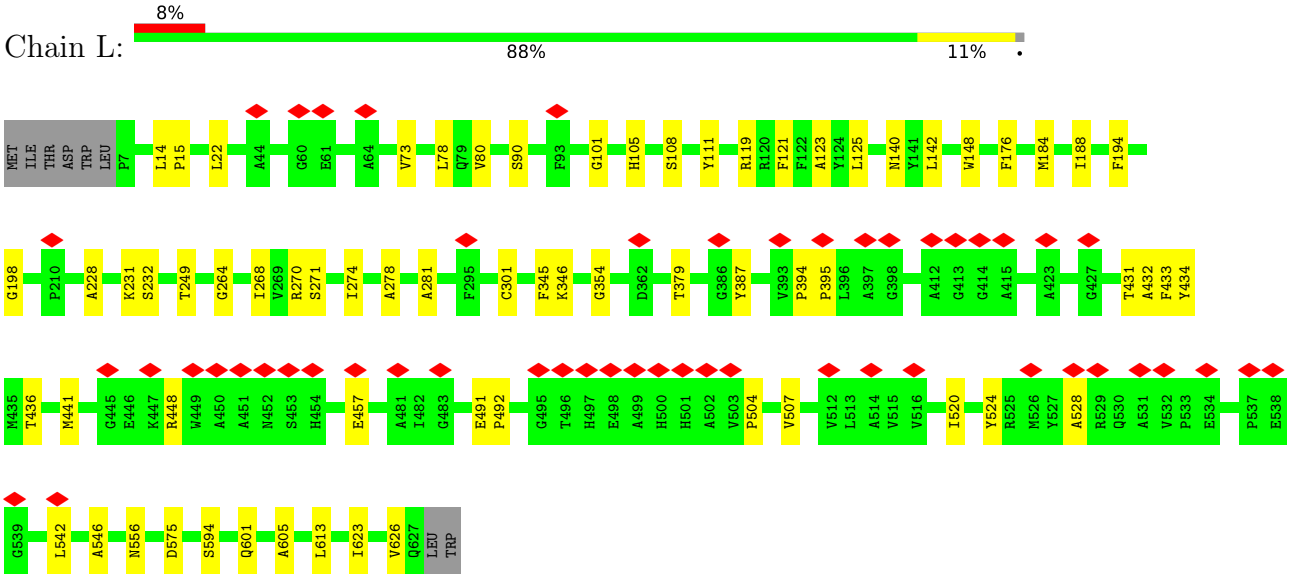


• Molecule 12: NADH-quinone oxidoreductase subunit K



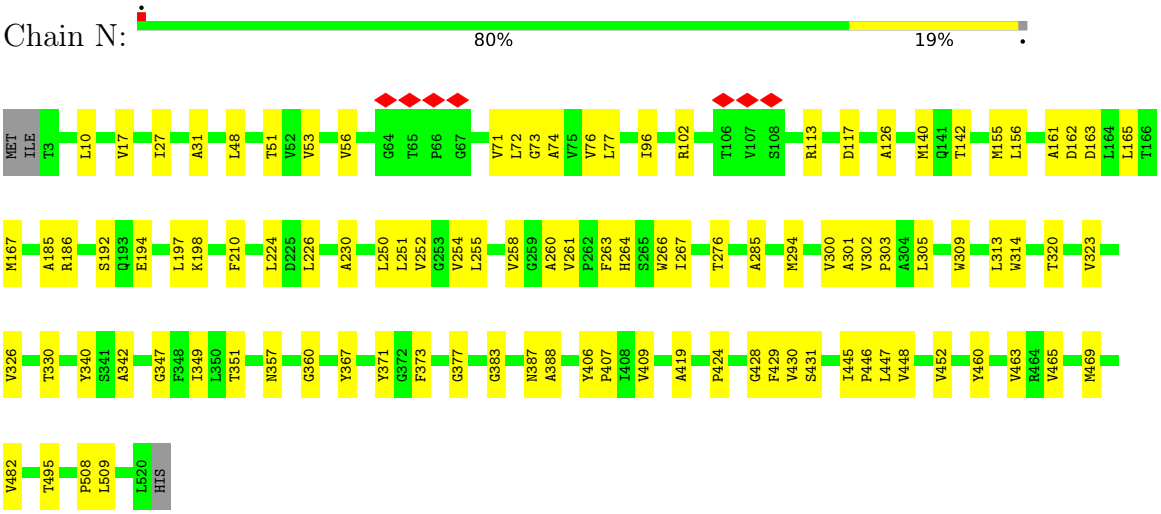
• Molecule 13: NADH-quinone oxidoreductase, L subunit

Chain L:



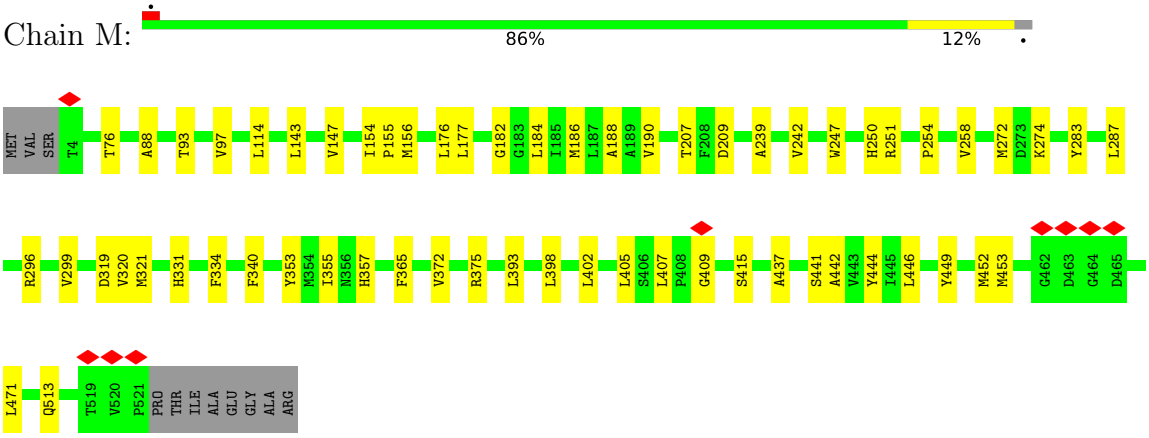
• Molecule 14: NADH-quinone oxidoreductase subunit N

Chain N:



• Molecule 15: NADH-quinone oxidoreductase, M subunit

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14385	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 ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.526	Depositor
Minimum map value	-0.957	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	1.6	Depositor
Map size (Å)	453.19986, 453.19986, 453.19986	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.180208, 1.180208, 1.180208	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XP2, SF4, GTP, ZN, FES, FMN, MQ9

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	O	0.29	0/896	0.52	0/1230
2	B	0.35	0/1333	0.51	0/1819
3	A	0.34	0/952	0.49	0/1303
4	C	0.35	0/1674	0.54	0/2298
5	D	0.35	0/3033	0.53	0/4129
6	E	0.31	0/1603	0.51	0/2215
7	G	0.33	0/5489	0.54	0/7535
8	F	0.33	0/3191	0.50	0/4368
9	I	0.38	0/1216	0.52	0/1667
10	H	0.33	0/2930	0.47	0/4026
11	J	0.33	0/1617	0.53	1/2223 (0.0%)
12	K	0.31	0/747	0.49	0/1012
13	L	0.27	0/3859	0.43	0/5316
14	N	0.33	0/3700	0.49	0/5081
15	M	0.31	0/3810	0.45	0/5241
All	All	0.33	0/36050	0.50	1/49463 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	J	204	PRO	N-CA-CB	-5.50	96.55	102.60

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	O	878	0	875	14	0
2	B	1304	0	1310	30	0
3	A	925	0	944	33	0
4	C	1623	0	1525	15	0
5	D	2971	0	2933	71	0
6	E	1564	0	1462	31	0
7	G	5374	0	5240	82	0
8	F	3105	0	2949	44	0
9	I	1183	0	1076	24	0
10	H	2847	0	2770	48	0
11	J	1585	0	1578	54	0
12	K	736	0	756	17	0
13	L	3784	0	3098	43	0
14	N	3618	0	3664	80	0
15	M	3712	0	3754	41	0
16	B	8	0	0	1	0
16	F	8	0	0	0	0
16	G	24	0	0	1	0
16	I	16	0	0	2	0
17	E	4	0	0	0	0
17	G	4	0	0	1	0
18	G	32	0	12	4	0
19	F	31	0	19	5	0
20	F	1	0	0	0	0
21	H	58	0	80	8	0
22	L	76	0	0	1	0
All	All	35471	0	34045	543	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 8.

The worst 5 of 543 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:D:249:LEU:HD22	11:J:205:THR:HG23	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:49:SER:OG	12:K:54:GLN:O	1.90	0.90
11:J:205:THR:HB	11:J:206:PRO:HD3	1.54	0.88
8:F:191:LEU:HD22	8:F:210:LEU:HD11	1.55	0.88
3:A:110:TYR:OH	10:H:325:TRP:O	1.94	0.85

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	O	122/132 (92%)	114 (93%)	8 (7%)	0	100	100
2	B	181/184 (98%)	169 (93%)	12 (7%)	0	100	100
3	A	119/122 (98%)	110 (92%)	9 (8%)	0	100	100
4	C	217/238 (91%)	206 (95%)	10 (5%)	1 (0%)	29	61
5	D	405/442 (92%)	389 (96%)	16 (4%)	0	100	100
6	E	230/245 (94%)	215 (94%)	13 (6%)	2 (1%)	17	46
7	G	778/794 (98%)	739 (95%)	39 (5%)	0	100	100
8	F	433/443 (98%)	401 (93%)	32 (7%)	0	100	100
9	I	164/180 (91%)	154 (94%)	10 (6%)	0	100	100
10	H	393/408 (96%)	364 (93%)	25 (6%)	4 (1%)	15	44
11	J	228/252 (90%)	207 (91%)	18 (8%)	3 (1%)	12	36
12	K	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
13	L	619/629 (98%)	586 (95%)	33 (5%)	0	100	100
14	N	516/521 (99%)	489 (95%)	27 (5%)	0	100	100
15	M	516/529 (98%)	495 (96%)	21 (4%)	0	100	100
All	All	5018/5218 (96%)	4734 (94%)	274 (6%)	10 (0%)	50	78

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	58	ARG
6	E	156	PRO
10	H	383	PRO
10	H	384	PRO
11	J	204	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	O	82/103 (80%)	82 (100%)	0	100	100
2	B	125/149 (84%)	125 (100%)	0	100	100
3	A	86/98 (88%)	86 (100%)	0	100	100
4	C	150/201 (75%)	150 (100%)	0	100	100
5	D	287/361 (80%)	286 (100%)	1 (0%)	92	98
6	E	138/190 (73%)	138 (100%)	0	100	100
7	G	484/610 (79%)	482 (100%)	2 (0%)	91	97
8	F	283/347 (82%)	282 (100%)	1 (0%)	91	97
9	I	105/145 (72%)	105 (100%)	0	100	100
10	H	261/330 (79%)	261 (100%)	0	100	100
11	J	143/191 (75%)	142 (99%)	1 (1%)	84	95
12	K	74/80 (92%)	74 (100%)	0	100	100
13	L	225/452 (50%)	225 (100%)	0	100	100
14	N	337/387 (87%)	337 (100%)	0	100	100
15	M	349/412 (85%)	349 (100%)	0	100	100
All	All	3129/4056 (77%)	3124 (100%)	5 (0%)	93	98

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

Mol	Chain	Res	Type
5	D	141	ASN
7	G	148	LYS
7	G	356	ARG
8	F	434	THR
11	J	204	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	D	78	HIS
7	G	248	GLN
8	F	262	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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	$\#\|Z\| > 2$
18	GTP	G	802	-	26,34,34	1.19	1 (3%)	32,54,54	1.61	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	SF4	G	803	7	0,12,12	-	-	-		
16	SF4	B	1000	2	0,12,12	-	-	-		
22	XP2	L	701	-	78,78,78	1.42	11 (14%)	101,103,103	1.13	5 (4%)
17	FES	E	1000	6	0,4,4	-	-	-		
19	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.26	7 (14%)
21	MQ9	H	501	-	59,59,59	0.41	1 (1%)	72,75,75	0.48	1 (1%)
16	SF4	I	202	9	0,12,12	-	-	-		
16	SF4	I	201	9	0,12,12	-	-	-		
16	SF4	G	805	7	0,12,12	-	-	-		
16	SF4	G	804	7	0,12,12	-	-	-		
16	SF4	F	503	8	0,12,12	-	-	-		
17	FES	G	801	7	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
18	GTP	G	802	-	-	2/18/38/38	0/3/3/3
16	SF4	G	803	7	-	-	0/6/5/5
16	SF4	B	1000	2	-	-	0/6/5/5
22	XP2	L	701	-	-	25/62/126/126	0/3/3/3
19	FMN	F	501	-	-	6/18/18/18	0/3/3/3
17	FES	E	1000	6	-	-	0/1/1/1
21	MQ9	H	501	-	-	14/53/73/73	0/2/2/2
16	SF4	I	202	9	-	-	0/6/5/5
16	SF4	I	201	9	-	-	0/6/5/5
16	SF4	G	804	7	-	-	0/6/5/5
16	SF4	G	805	7	-	-	0/6/5/5
16	SF4	F	503	8	-	-	0/6/5/5
17	FES	G	801	7	-	-	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	802	GTP	C5-C6	-4.14	1.39	1.47
22	L	701	XP2	O49-C50	3.88	1.44	1.33
22	L	701	XP2	O10-C09	3.72	1.51	1.41
22	L	701	XP2	O13-C14	3.67	1.44	1.33
22	L	701	XP2	O38-C39	3.61	1.44	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	802	GTP	PA-O3A-PB	-3.94	119.29	132.83
22	L	701	XP2	C66-O65-C64	-3.92	108.27	117.96
22	L	701	XP2	O38-C39-C40	3.86	119.82	111.50
22	L	701	XP2	C09-O08-C07	-3.82	108.50	117.96
18	G	802	GTP	PB-O3B-PG	-3.67	120.22	132.83

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	F	501	FMN	N10-C1'-C2'-O2'
19	F	501	FMN	N10-C1'-C2'-C3'
21	H	501	MQ9	C5-C6-C7-C8
21	H	501	MQ9	C1-C6-C7-C8
21	H	501	MQ9	C7-C8-C9-C10

There are no ring outliers.

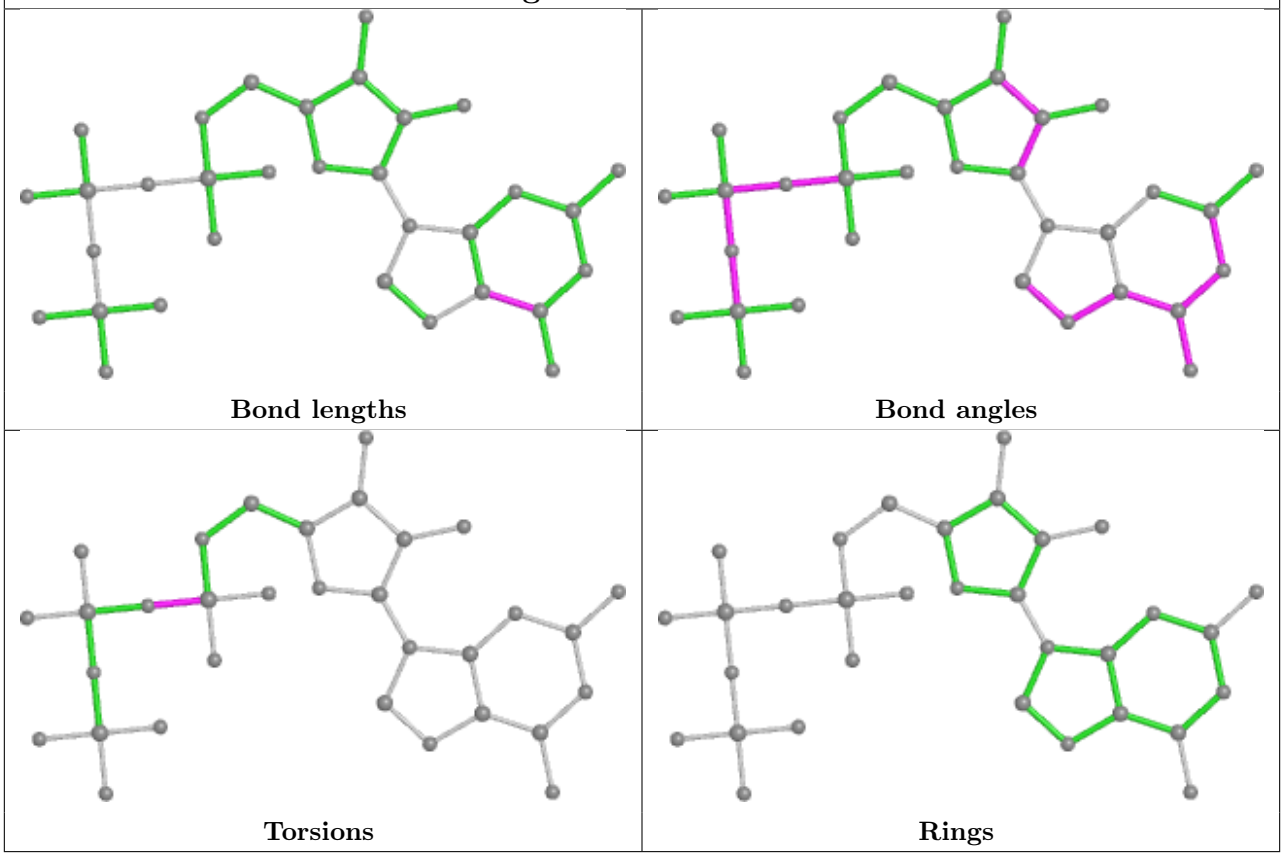
9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	802	GTP	4	0
16	B	1000	SF4	1	0
22	L	701	XP2	1	0
19	F	501	FMN	5	0
21	H	501	MQ9	8	0
16	I	202	SF4	1	0
16	I	201	SF4	1	0
16	G	805	SF4	1	0
17	G	801	FES	1	0

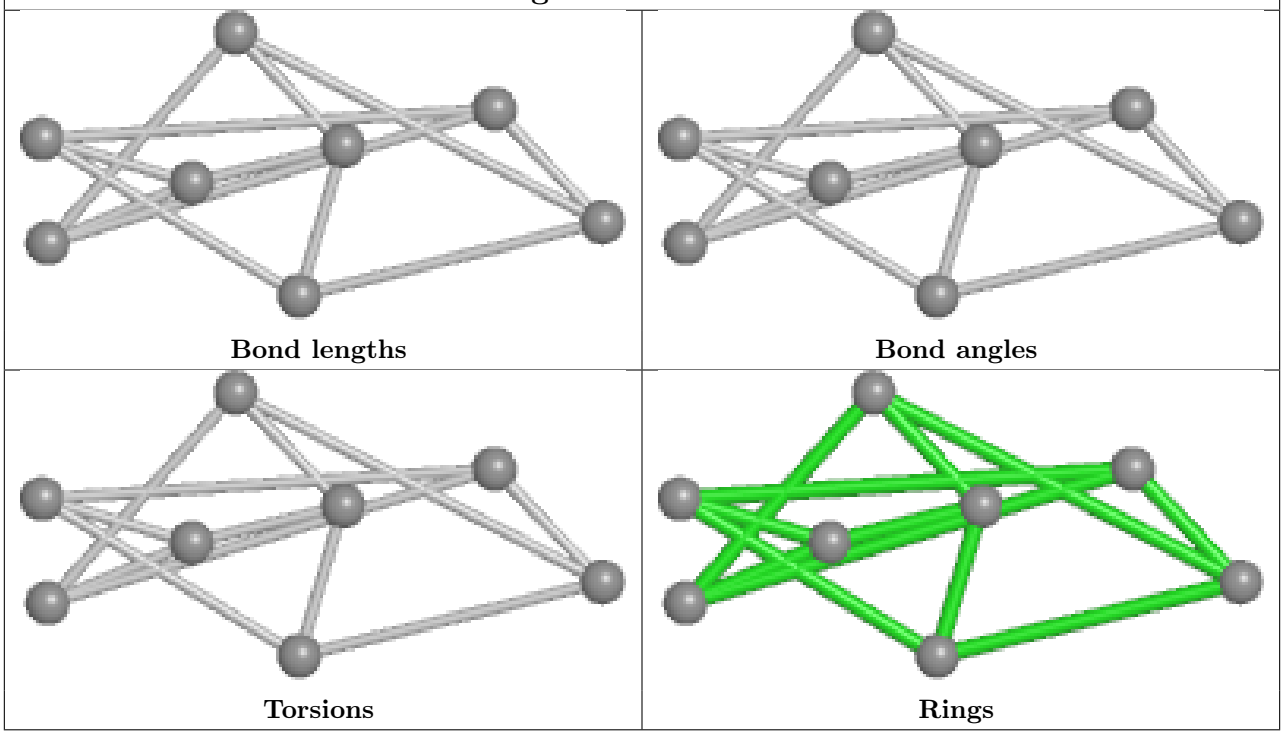
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

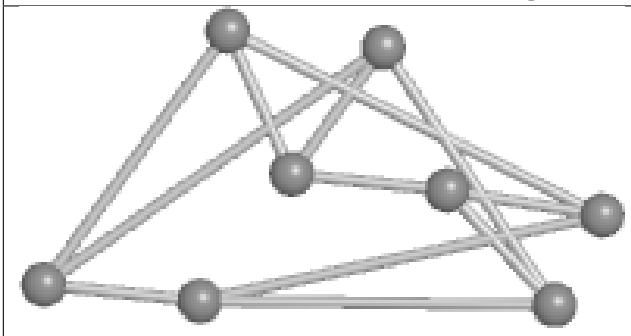
Ligand GTP G 802



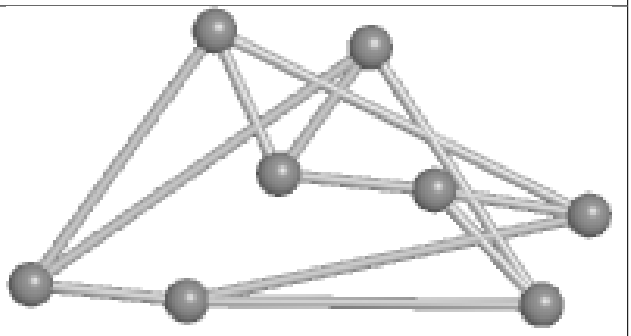
Ligand SF4 G 803



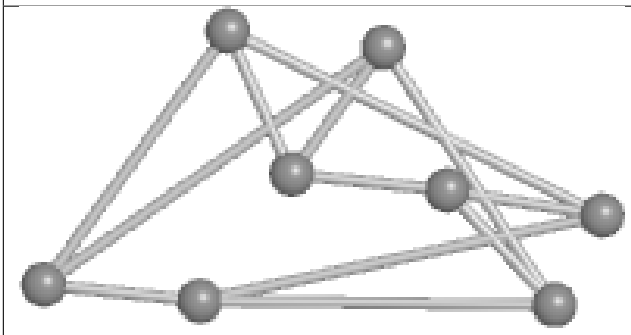
Ligand SF4 B 1000



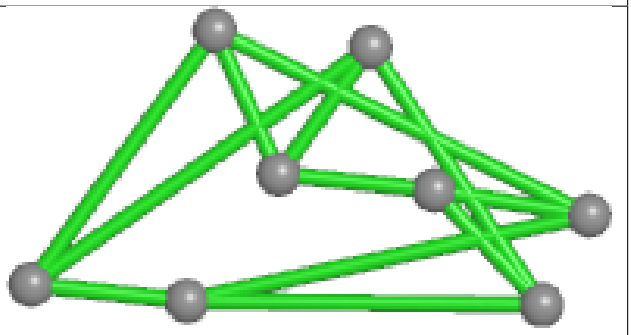
Bond lengths



Bond angles

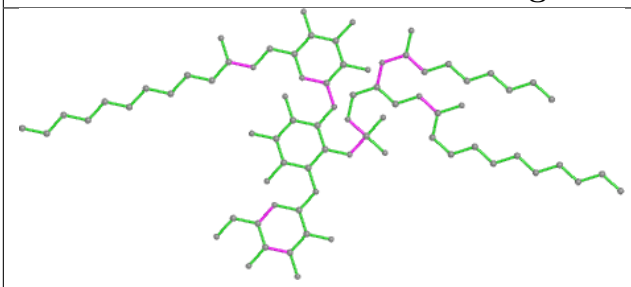


Torsions



Rings

Ligand XP2 L 701



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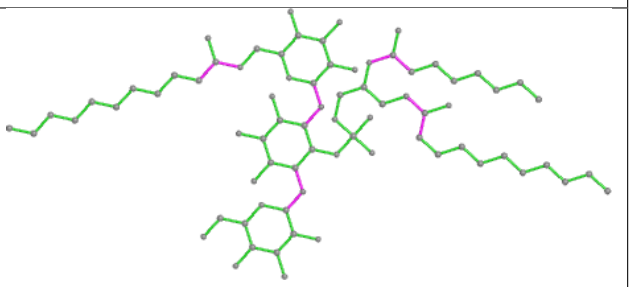

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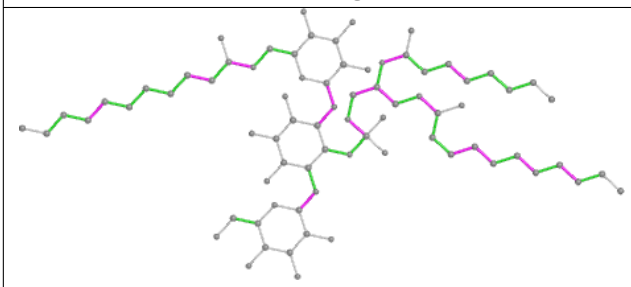

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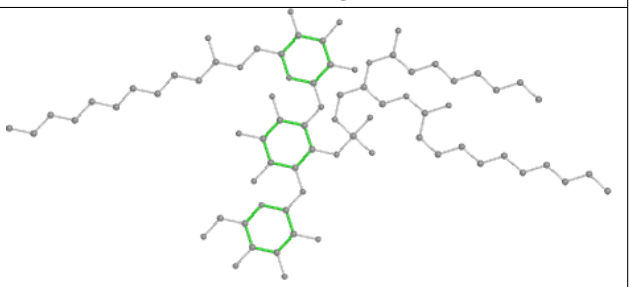
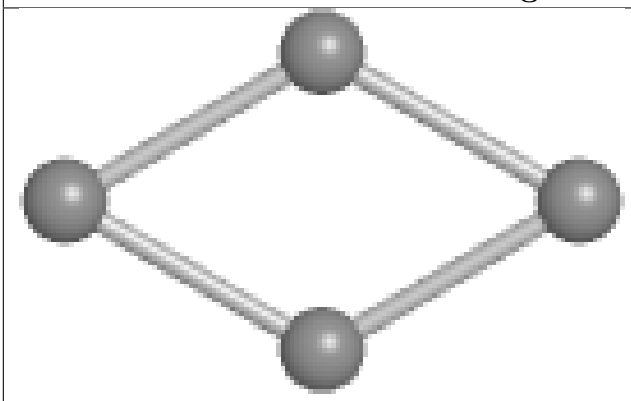


Rings

Ligand FES E 1000



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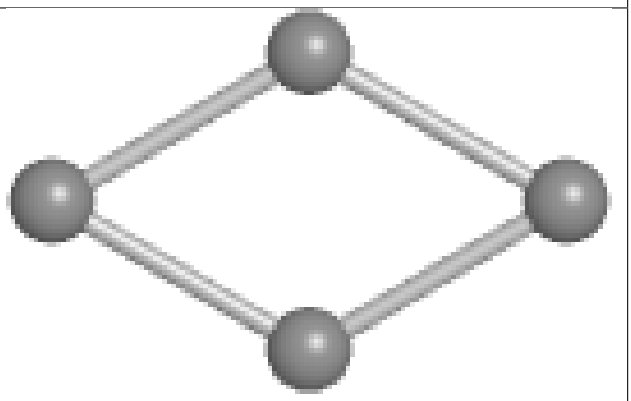

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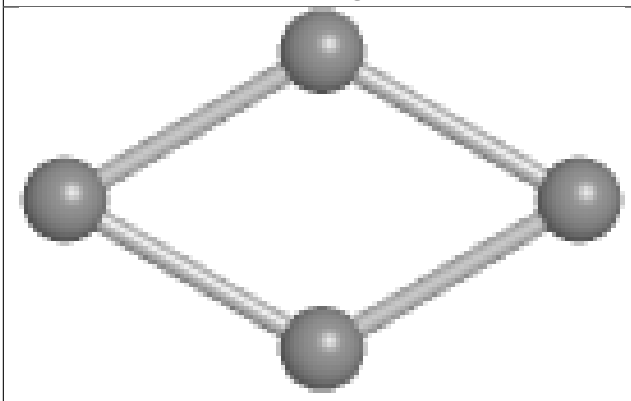

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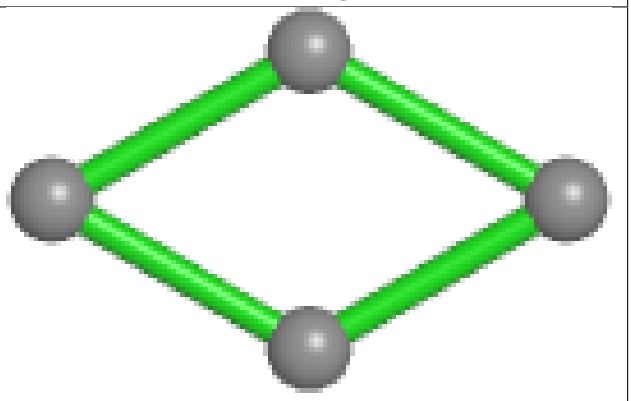
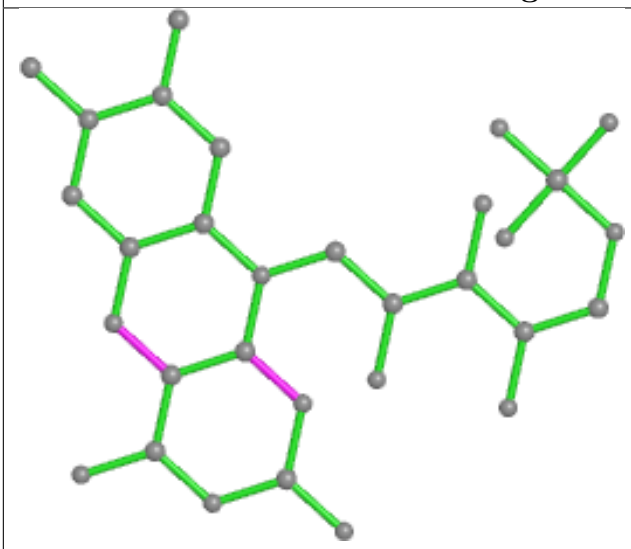


Rings

Ligand FMN F 501



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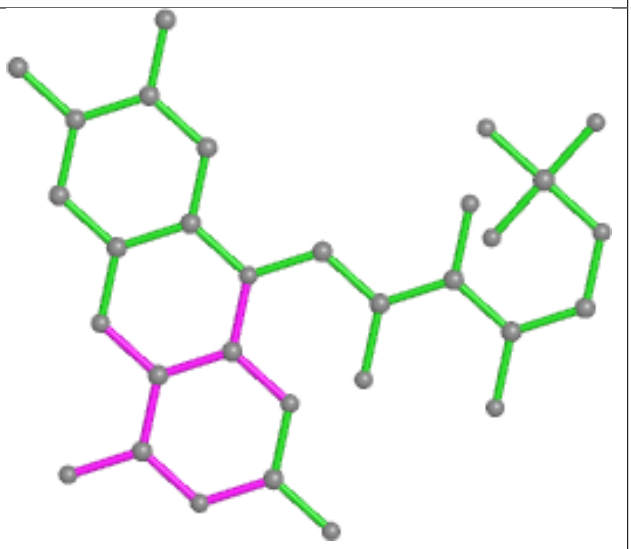

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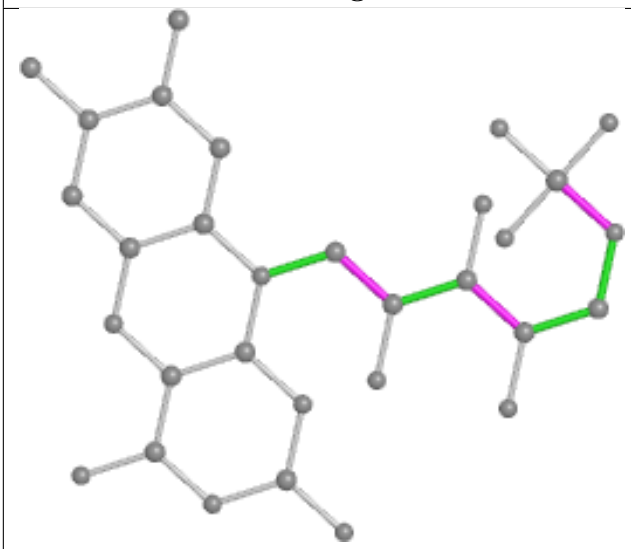

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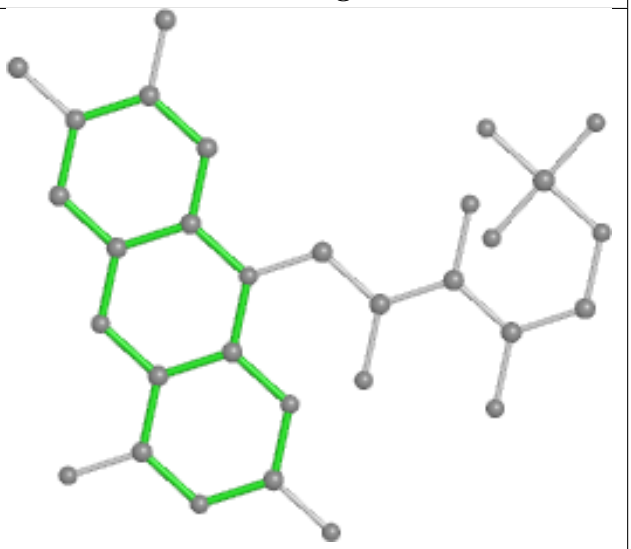
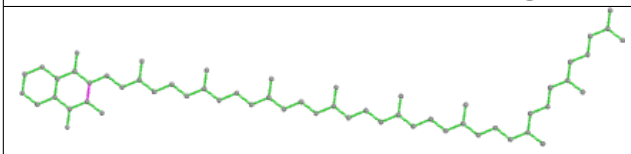
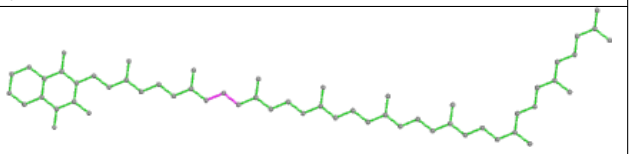


Rings

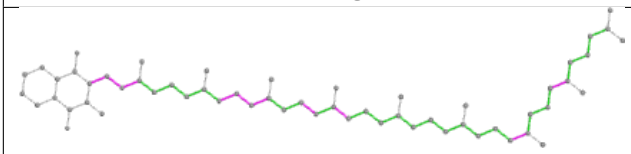
Ligand MQ9 H 501



Bond lengths



Bond angles



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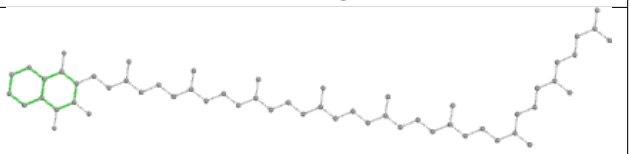
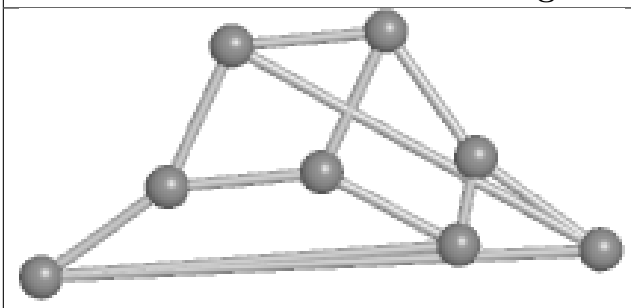
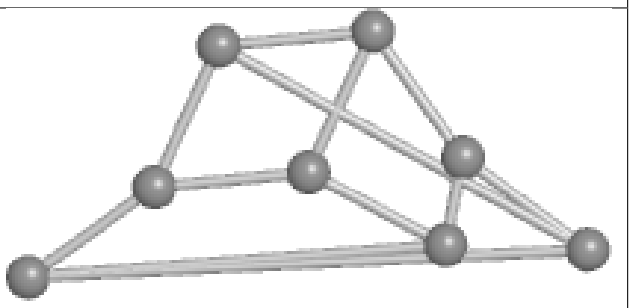


Rings

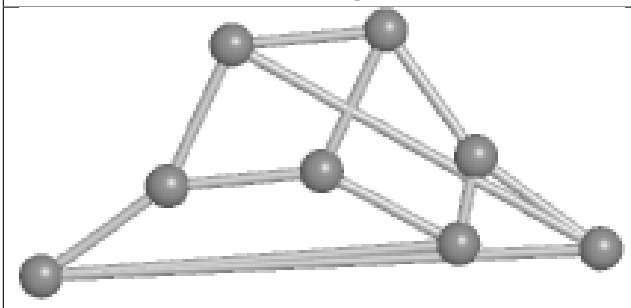
Ligand SF4 I 202



Bond lengths



Bond angles



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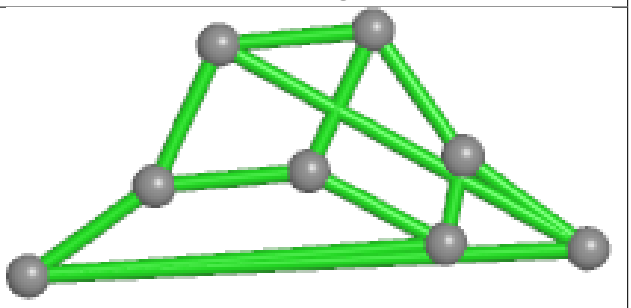
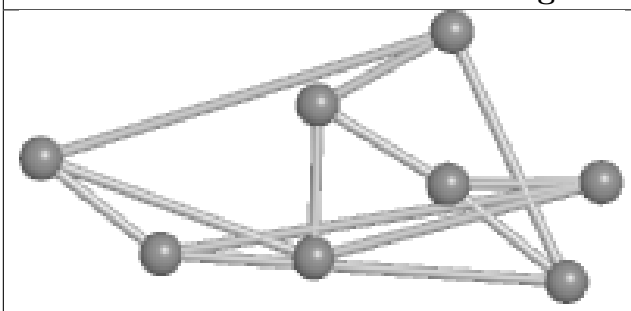


Rings

Ligand SF4 I 201



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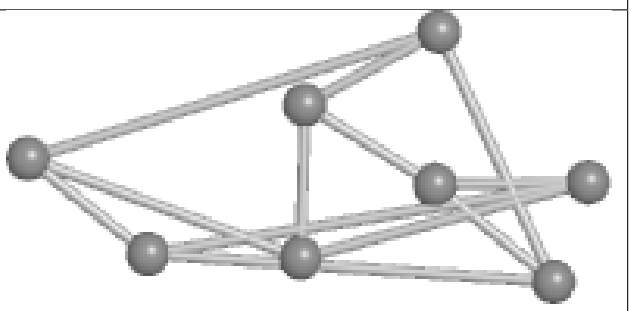
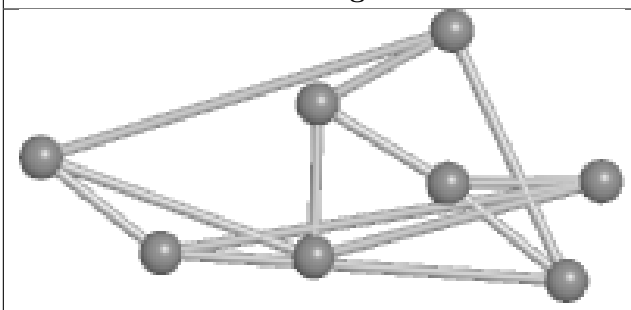
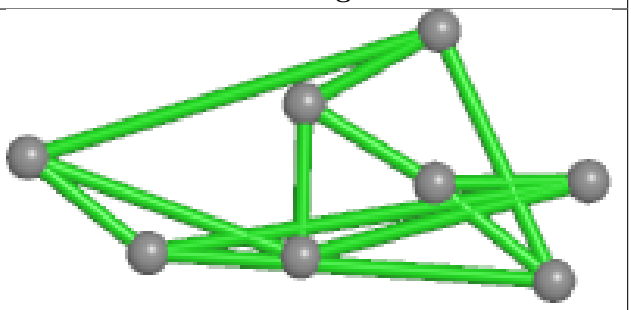


Bond angles

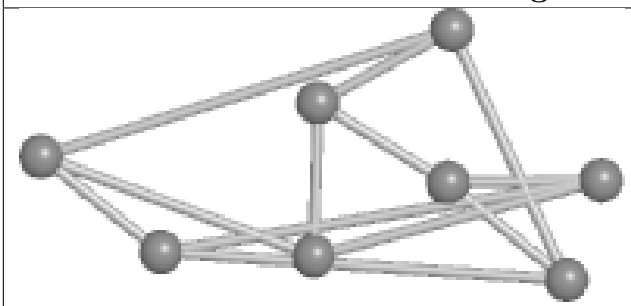


Torsions

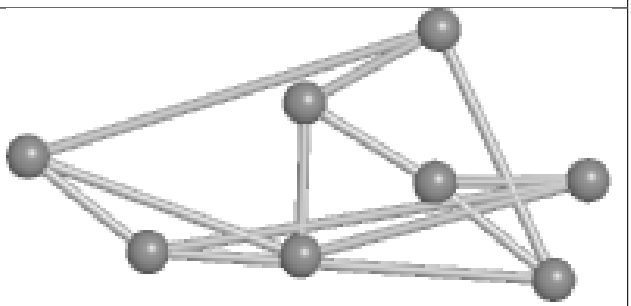


Rings

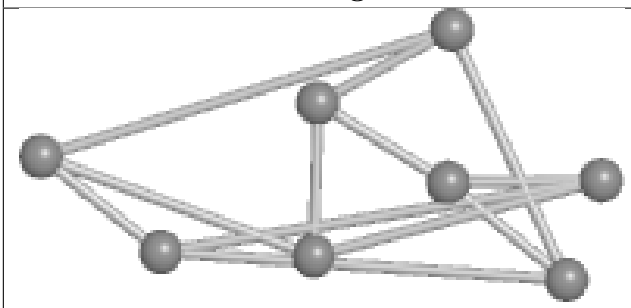
Ligand SF4 G 805



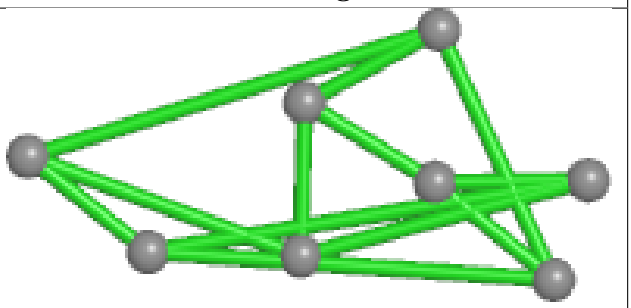
Bond lengths



Bond angles

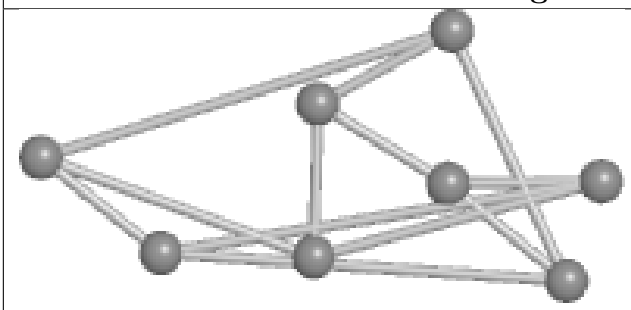


Torsions

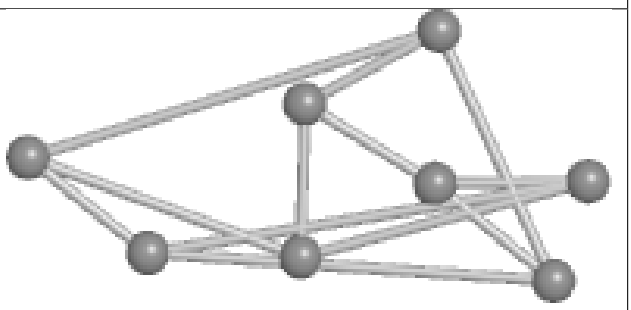


Rings

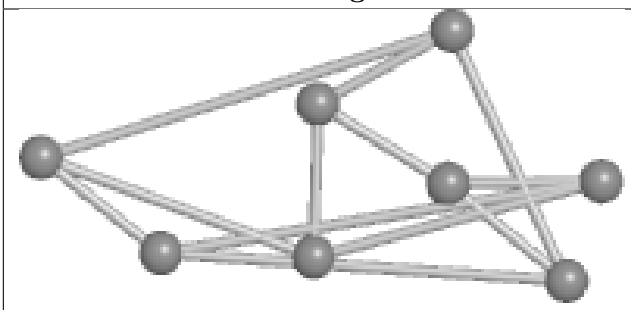
Ligand SF4 G 804



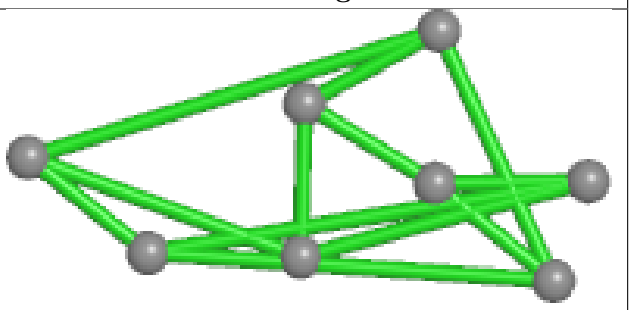
Bond lengths



Bond angles

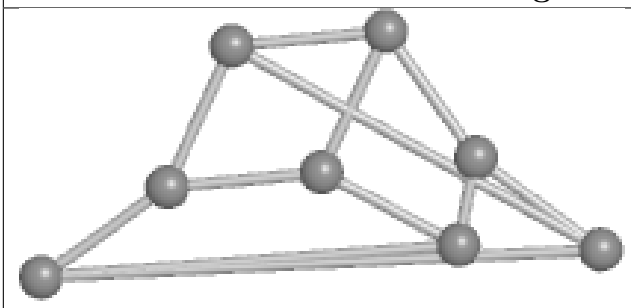


Torsions

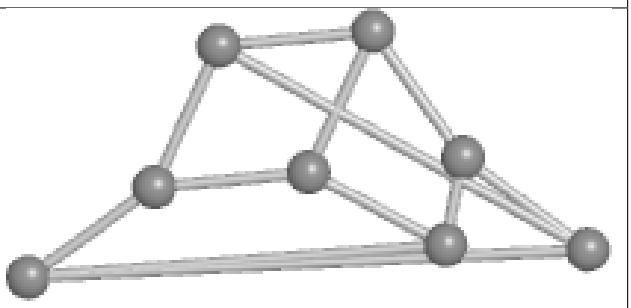


Rings

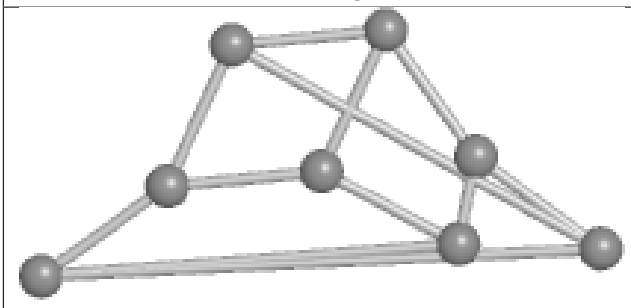
Ligand SF4 F 503



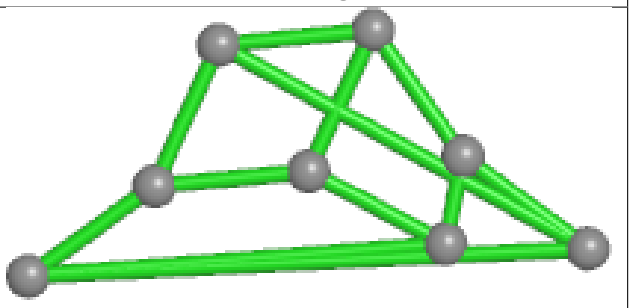
Bond lengths



Bond angles

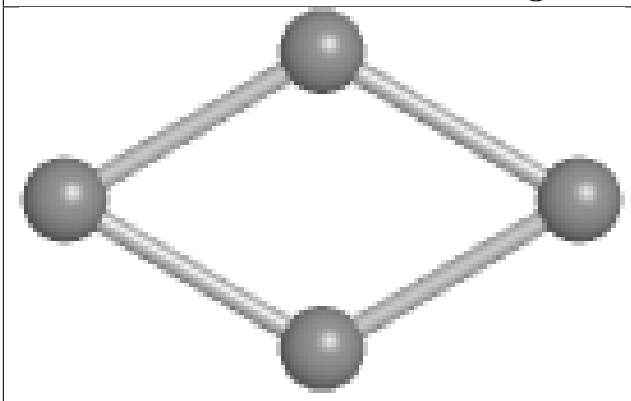


Torsions

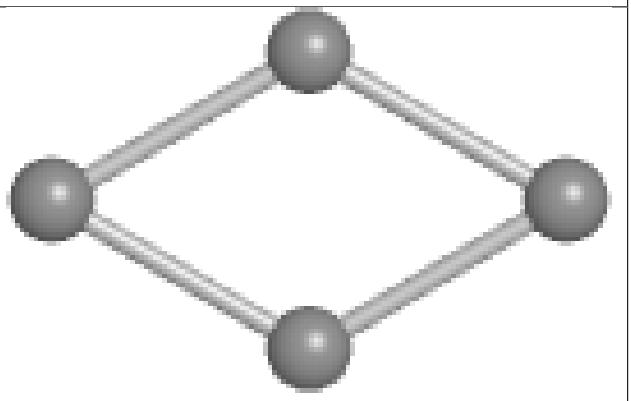


Rings

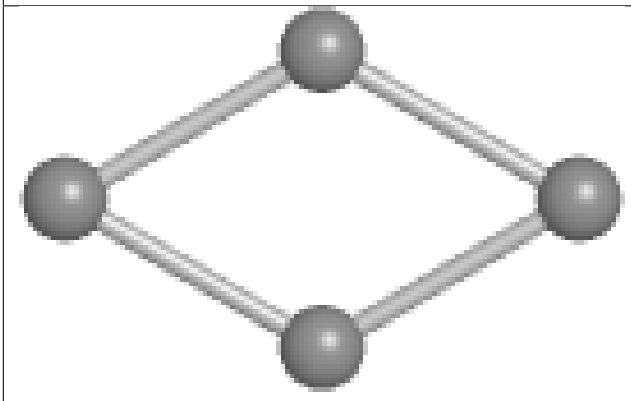
Ligand FES G 801



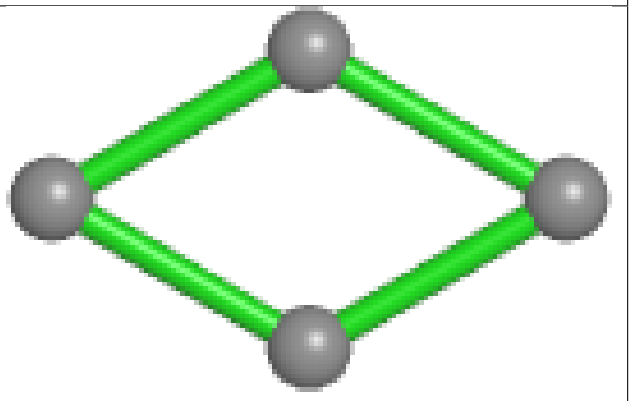
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

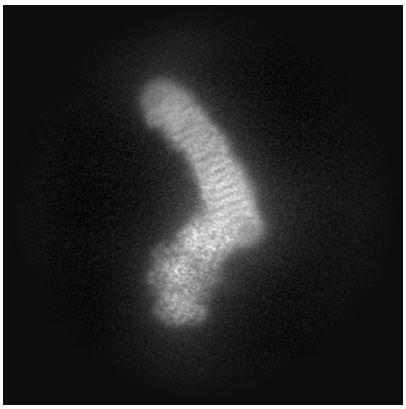
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27965. These allow visual inspection of the internal detail of the map and identification of artifacts.

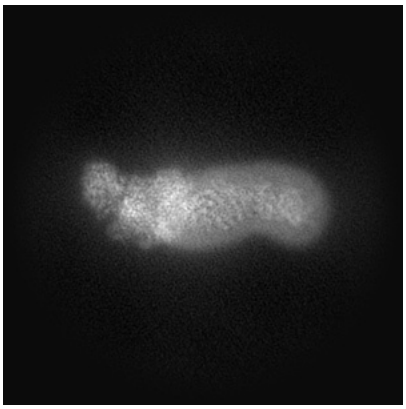
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

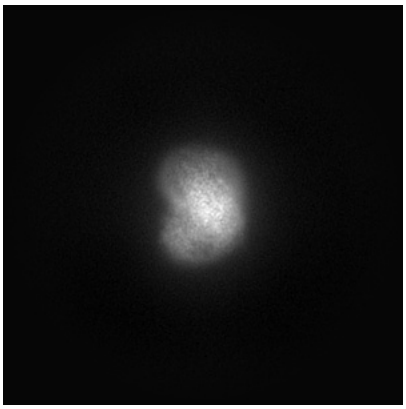
6.1.1 Primary map



X

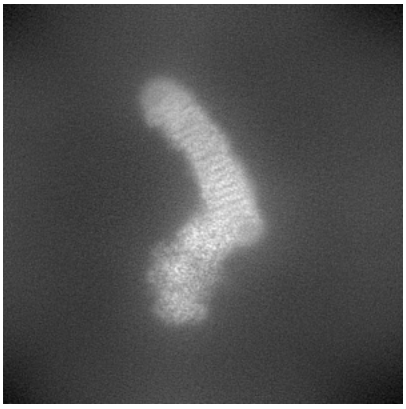


Y

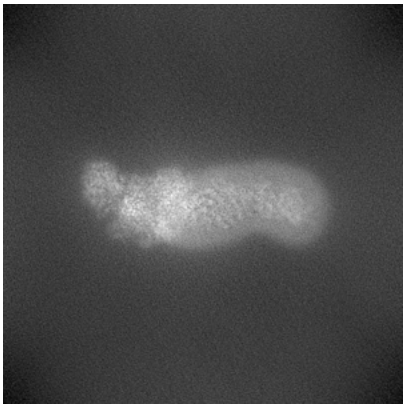


Z

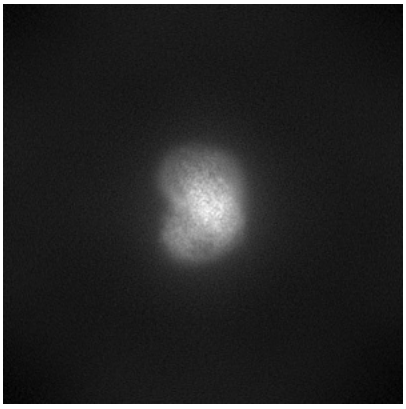
6.1.2 Raw map



X



Y

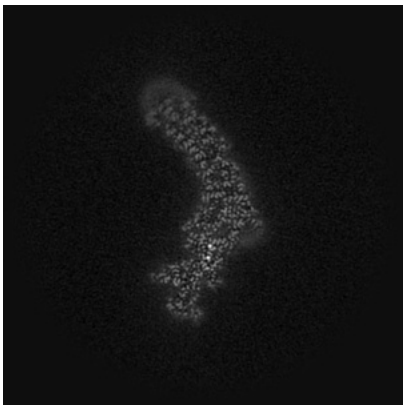


Z

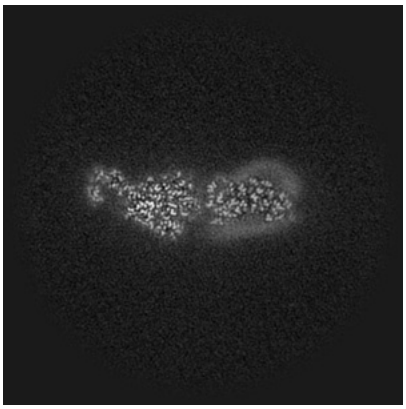
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

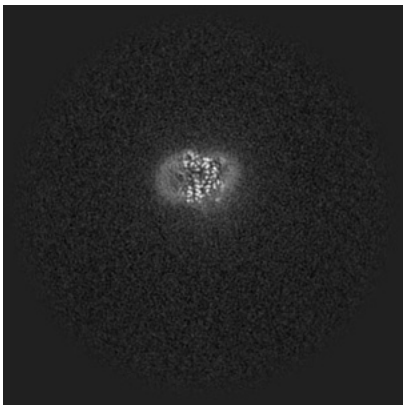
6.2.1 Primary map



X Index: 192

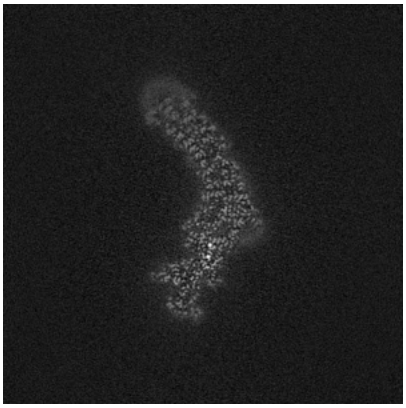


Y Index: 192

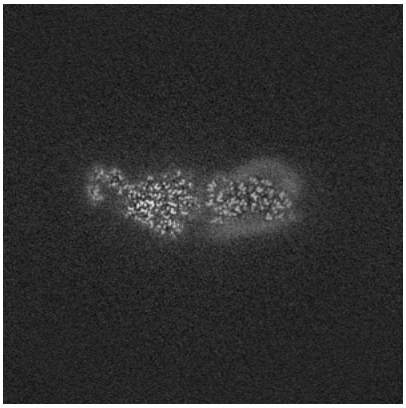


Z Index: 192

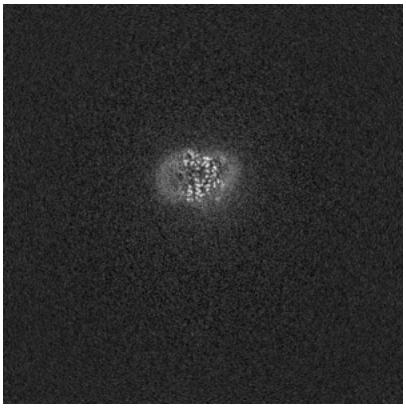
6.2.2 Raw map



X Index: 192



Y Index: 192

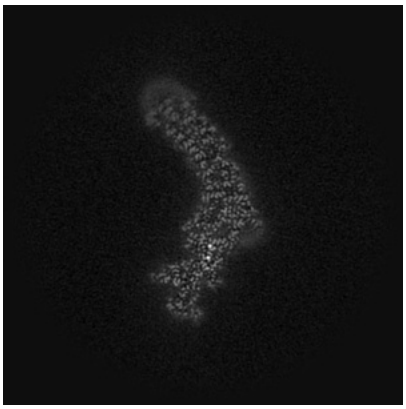


Z Index: 192

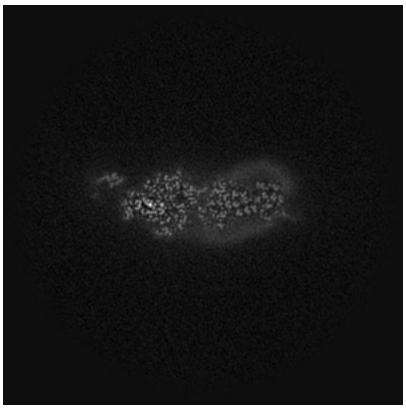
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

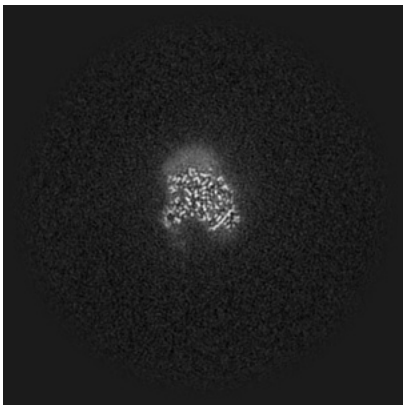
6.3.1 Primary map



X Index: 192

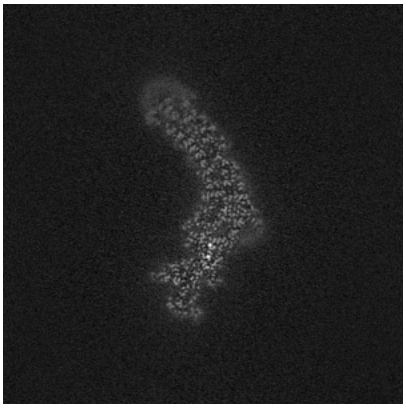


Y Index: 197

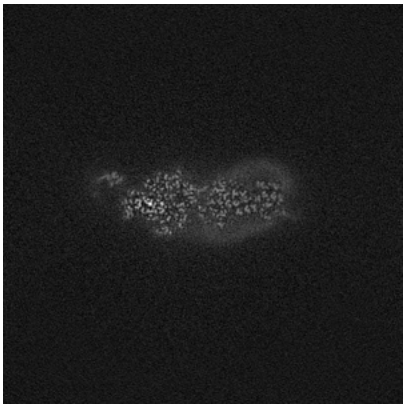


Z Index: 158

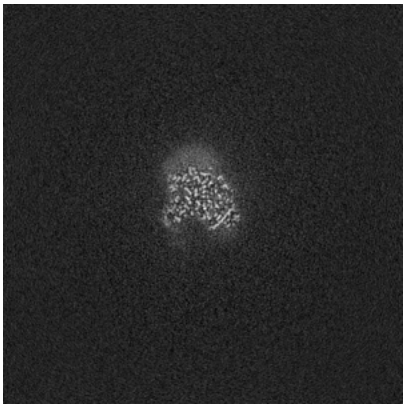
6.3.2 Raw map



X Index: 192



Y Index: 197

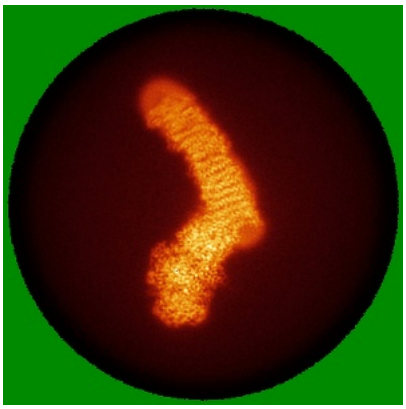


Z Index: 158

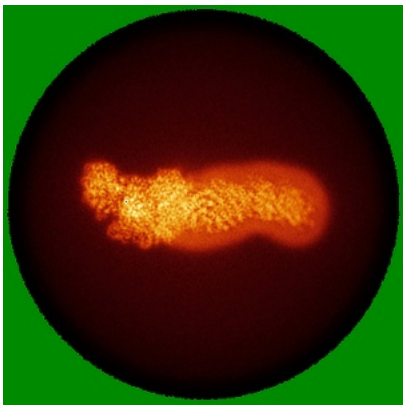
The images above show the largest variance slices of the map in three orthogonal directions.

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

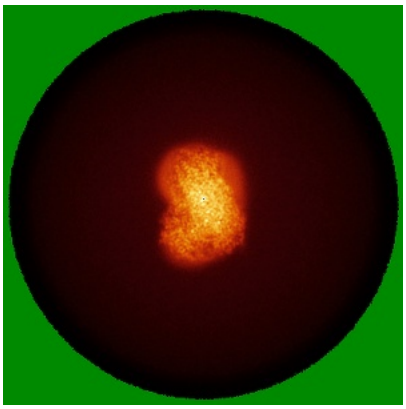
6.4.1 Primary map



X

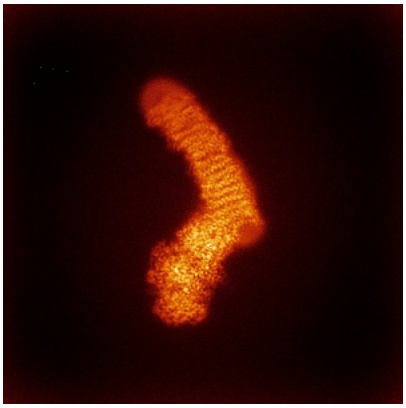


Y

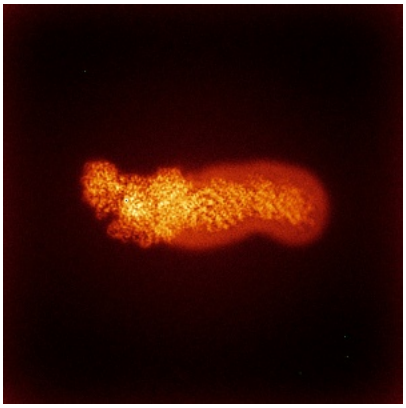


Z

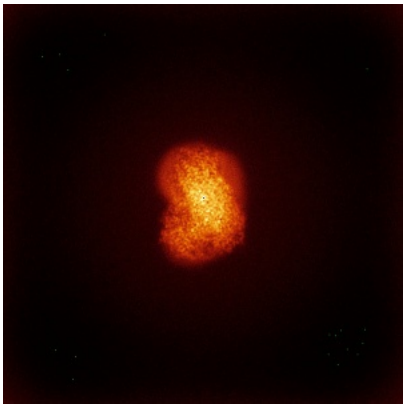
6.4.2 Raw map



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 1.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

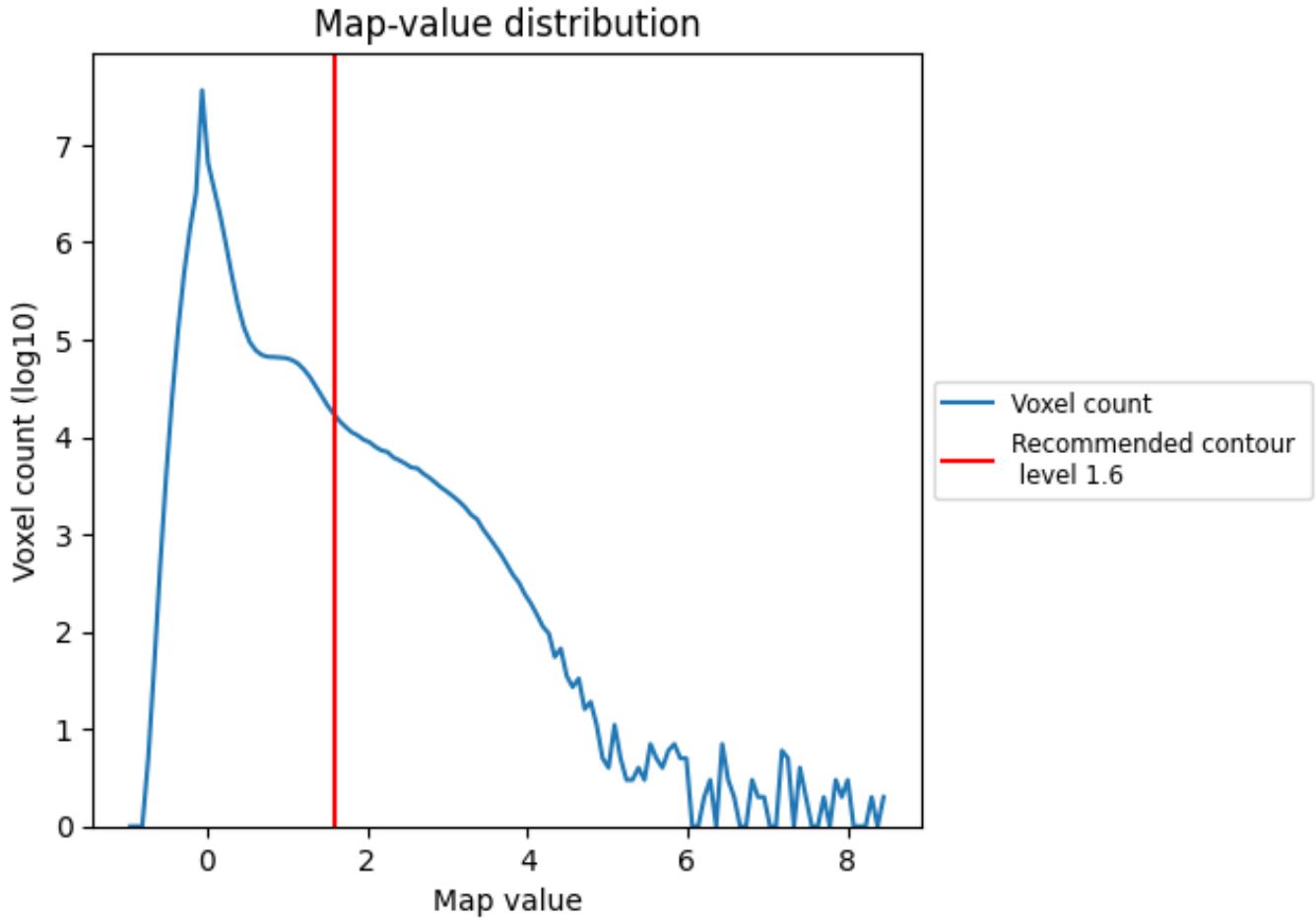
6.6 Mask visualisation (i)

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

7 Map analysis

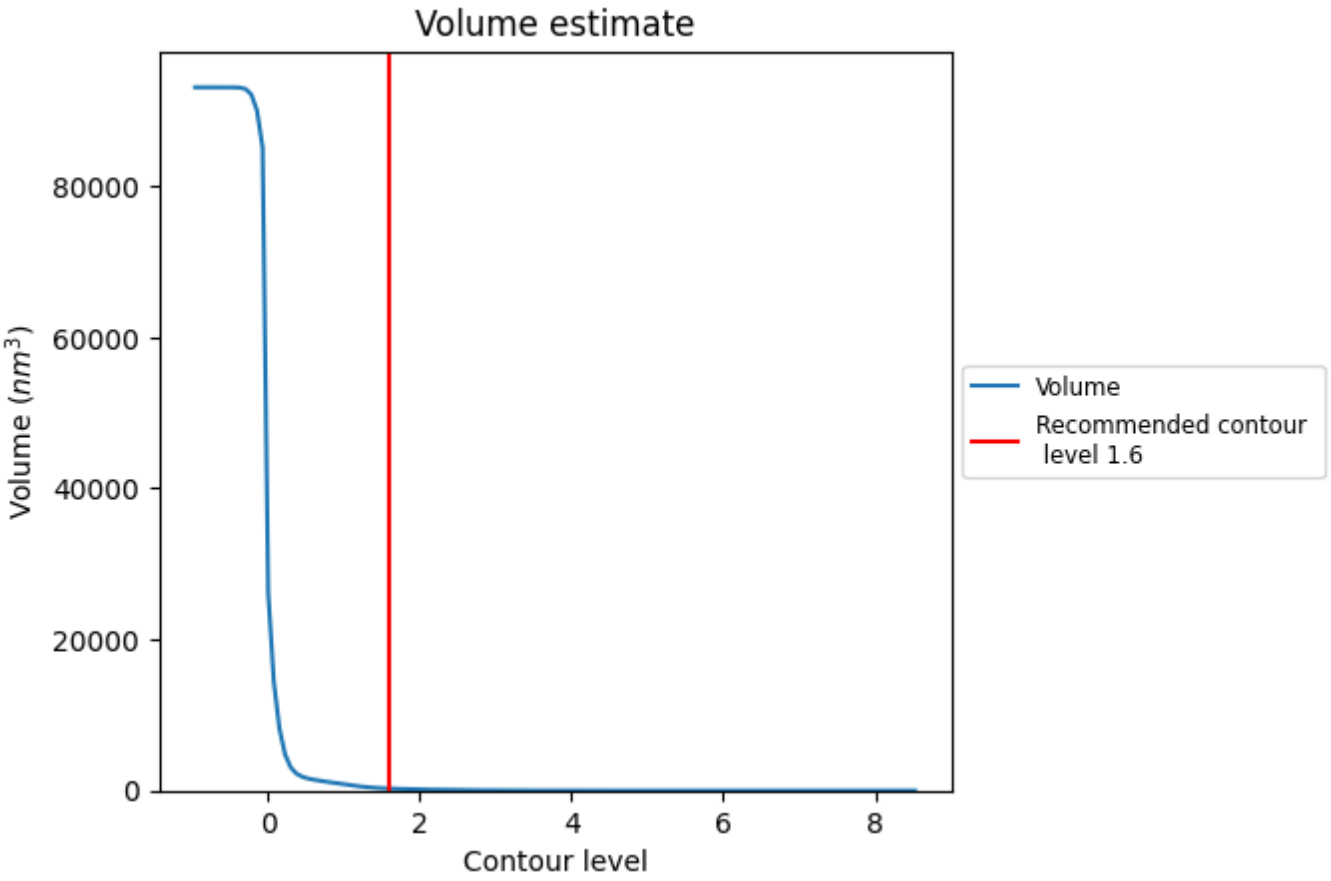
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

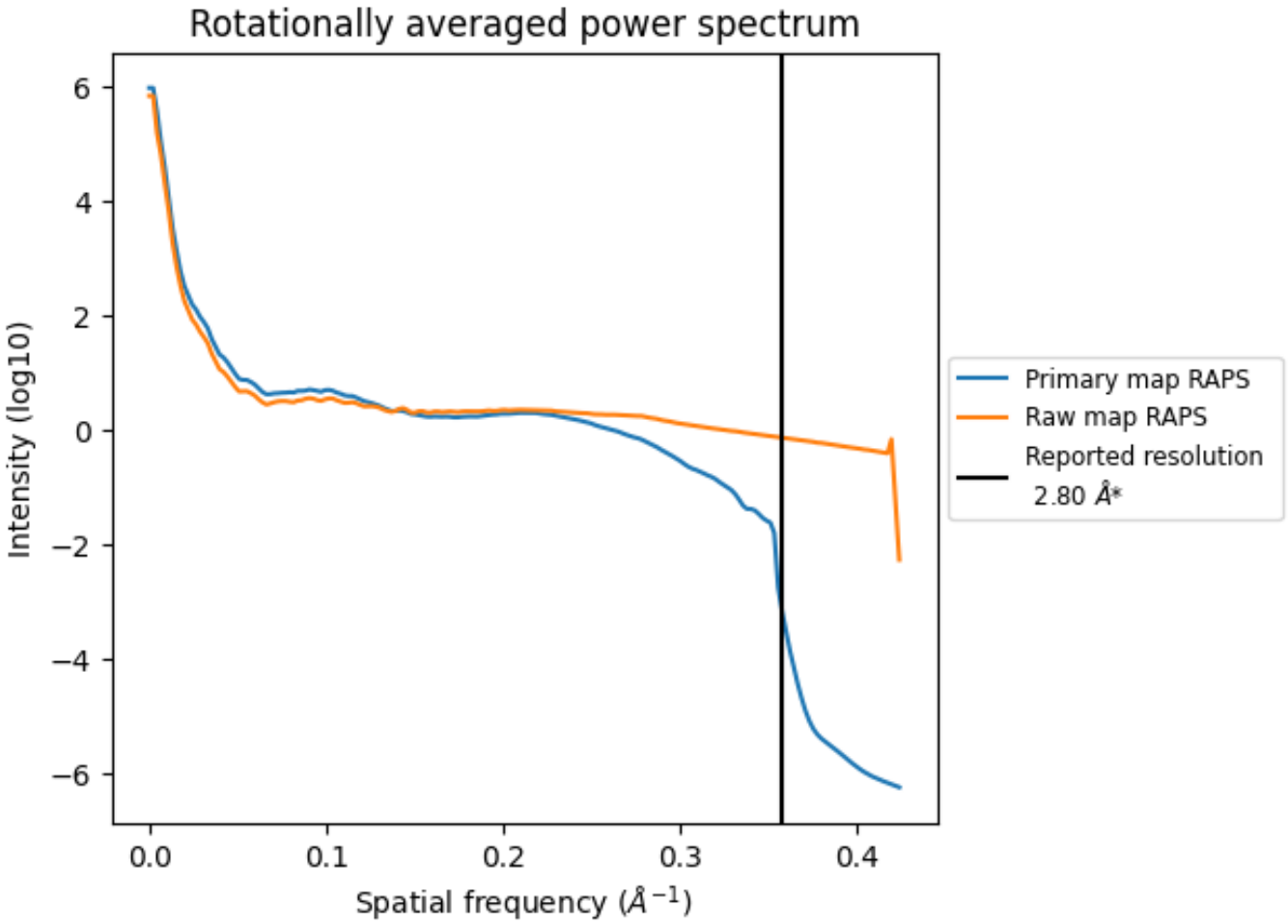
7.2 Volume estimate (i)



The volume at the recommended contour level is 267 nm^3; this corresponds to an approximate mass of 241 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)

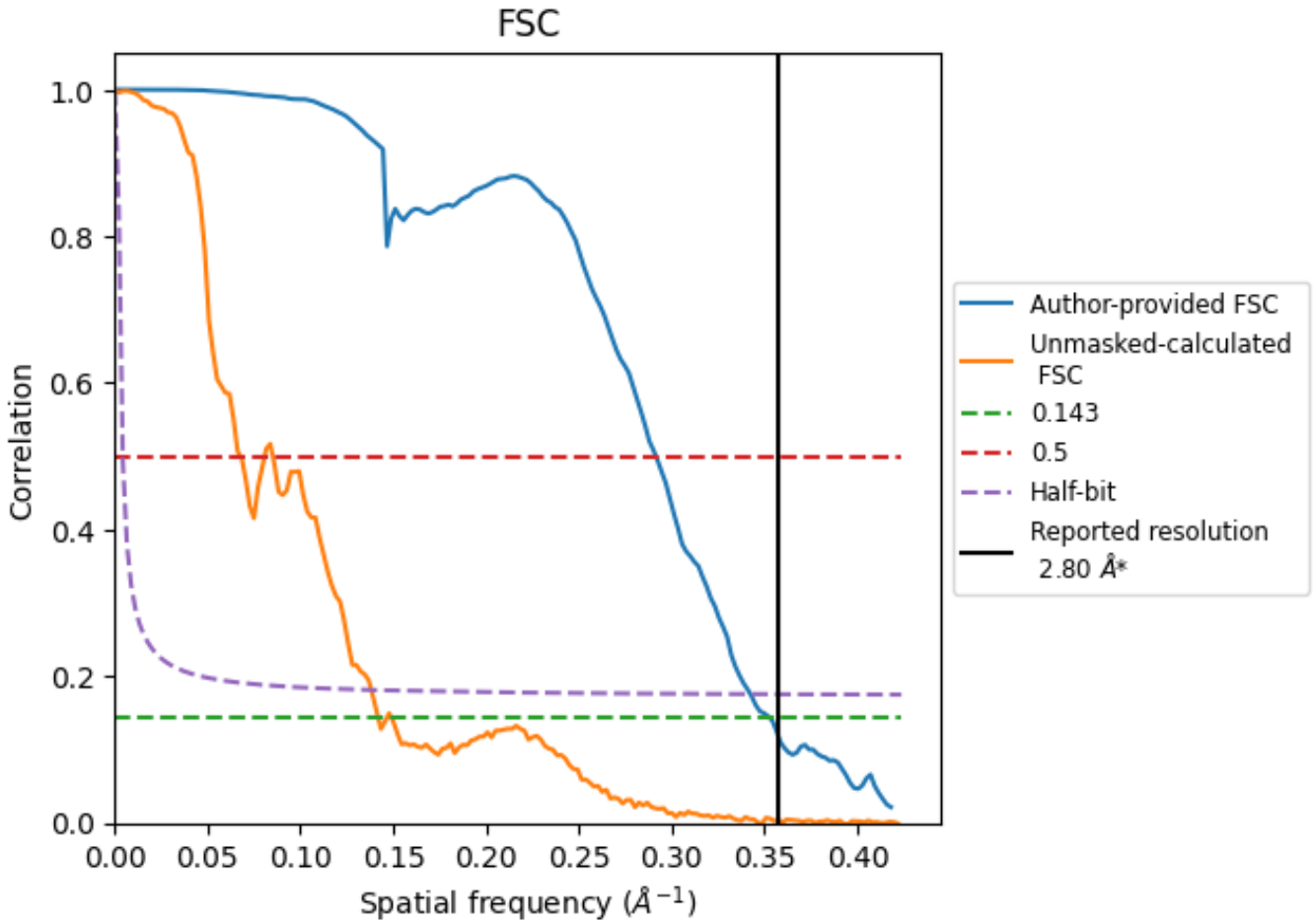


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

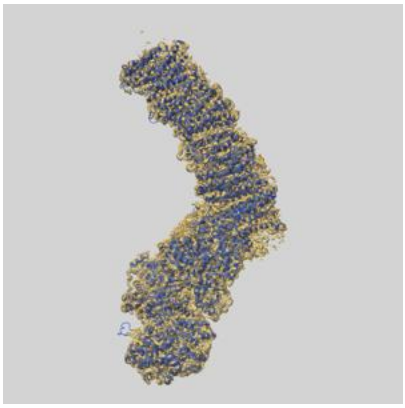
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.43	2.92
Unmasked-calculated*	7.05	14.75	7.24

*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 7.05 differs from the reported value 2.8 by more than 10 %

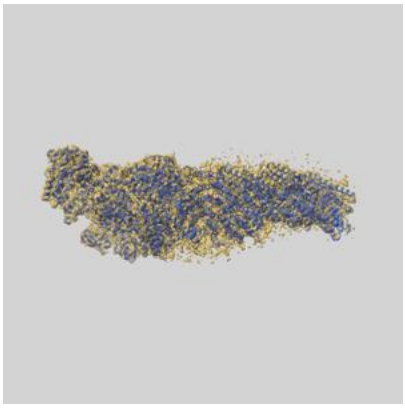
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27965 and PDB model 8E9I. Per-residue inclusion information can be found in section 3 on page 10.

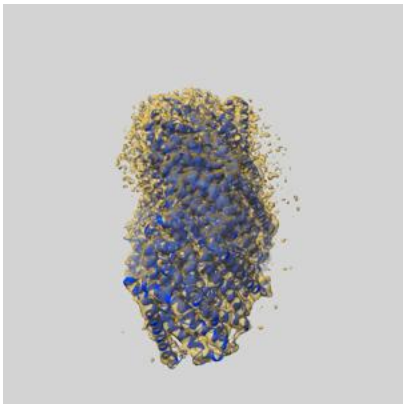
9.1 Map-model overlay



X



Y



Z

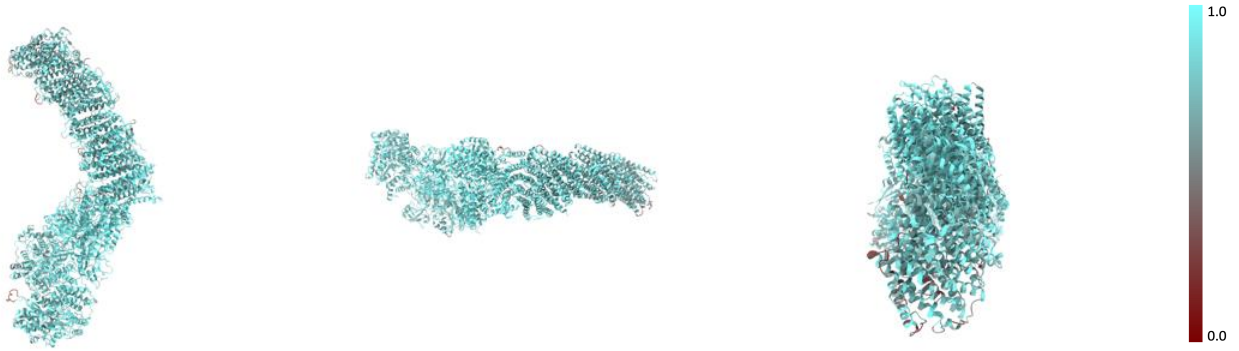
The images above show the 3D surface view of the map at the recommended contour level 1.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

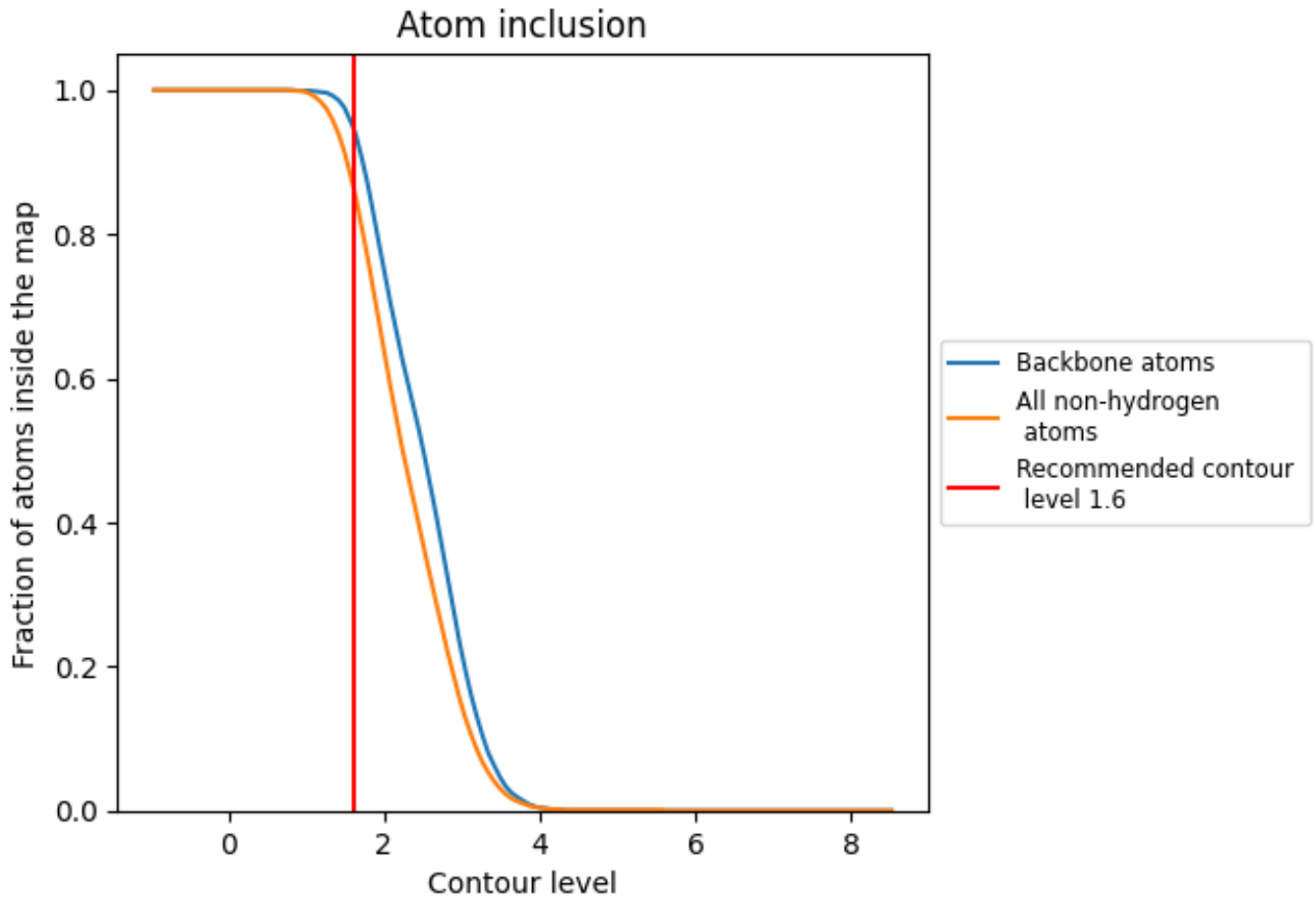
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.6).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (1.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.5090
A	0.8810	0.5170
B	0.9440	0.5380
C	0.9240	0.5440
D	0.9530	0.5460
E	0.8570	0.5060
F	0.8490	0.5090
G	0.8760	0.5300
H	0.8990	0.5140
I	0.9430	0.5490
J	0.8970	0.5110
K	0.9020	0.5130
L	0.7380	0.4240
M	0.8090	0.4900
N	0.8780	0.5100
O	0.8900	0.5260