



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 06:34 pm GMT

PDB ID : 6ZJY
EMDB ID : EMD-11238
Title : Respiratory complex I from *Thermus thermophilus*, NAD⁺ dataset, minor state
Authors : Kaszuba, K.; Tambalo, M.; Gallagher, G.T.; Sazanov, L.A.
Deposited on : 2020-06-29
Resolution : 5.50 Å (reported)
Based on initial model : 6Y11

This is a Full wwPDB EM Validation 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:

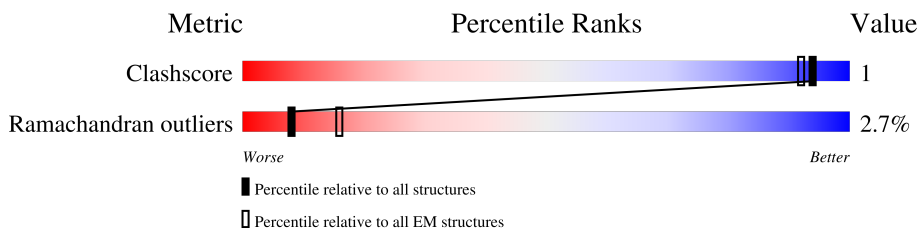
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.50 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

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 $\leq 5\%$. 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	1	438	
2	2	181	
3	3	783	
4	4	409	
5	5	207	
6	6	181	
7	9	182	
8	7	129	
9	A	119	

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Mol	Chain	Length	Quality of chain
10	J	176	
11	K	95	
12	L	606	
13	M	469	
14	N	427	
15	H	365	

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
16	SF4	1	501	-	-	X	-
16	SF4	3	803	-	-	X	-
16	SF4	9	202	-	-	X	-

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 22855 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 NADH-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	1	437	2136	1262	437	437	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	2	178	875	519	178	178	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	754	3714	2206	754	754	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	4	384	1890	1122	384	384	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	5	196	961	569	196	196	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	6	166	818	486	166	166	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	9	180	885	525	180	180	0	0

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	7	127	628	374	127	127	0	0

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	A	117	570	336	117	117	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	160	783	463	160	160	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	K	95	467	277	95	95	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	605	2955	1745	605	605	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	467	2276	1342	467	467	0	0

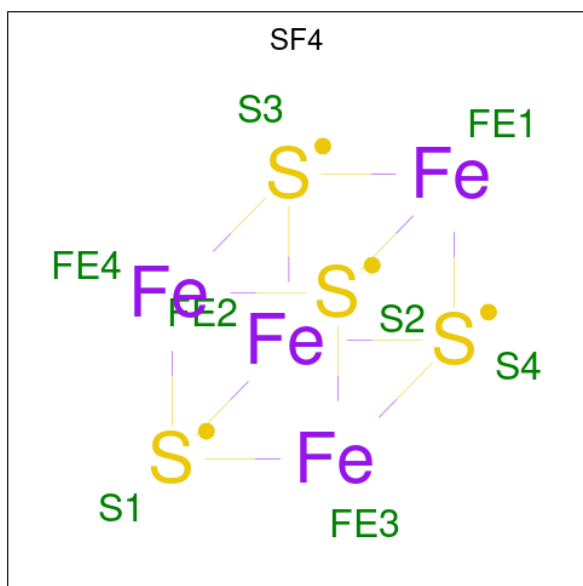
- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	N	427	2092	1238	427	427	0	0

- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 8.

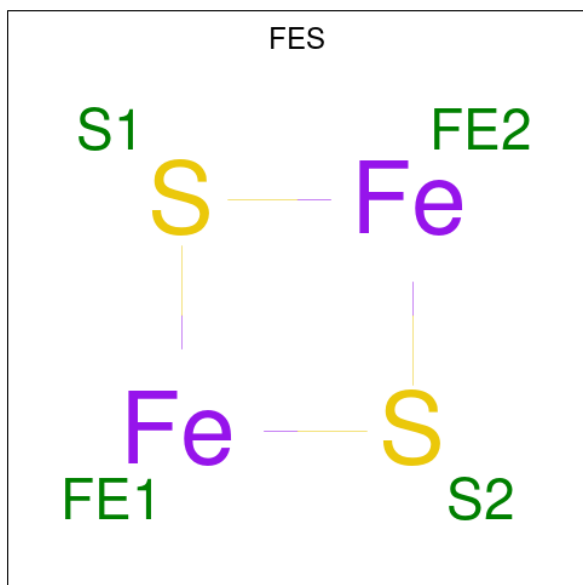
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	H	353	1741	1035	353	353	0	0

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
16	1	1	8	4	4	0
16	3	1	24	12	12	0
16	3	1	24	12	12	0
16	3	1	24	12	12	0
16	6	1	8	4	4	0
16	9	1	16	8	8	0
16	9	1	16	8	8	0

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

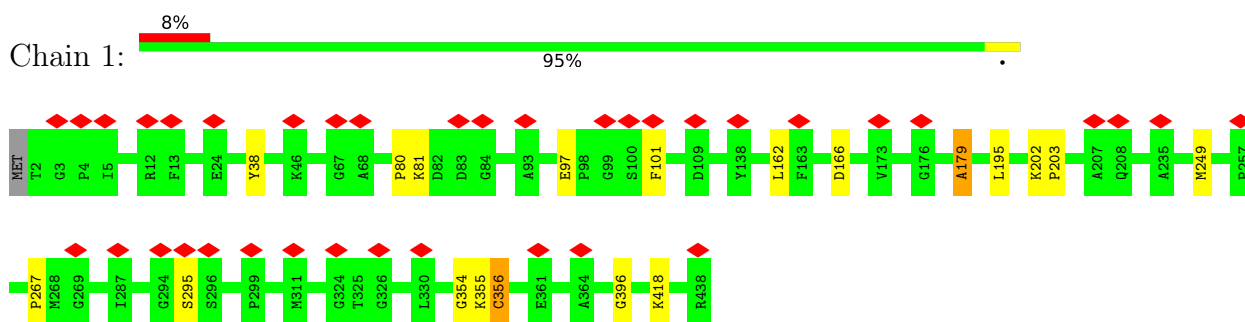


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	2	1	4	2	2	0
17	3	1	4	2	2	0

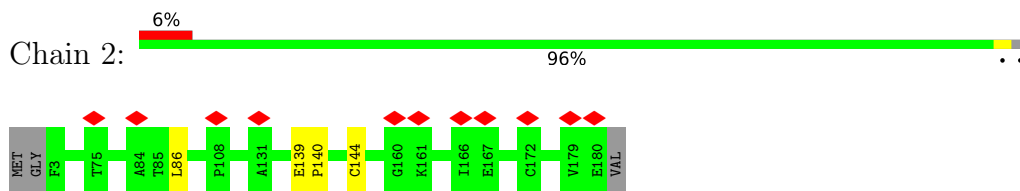
3 Residue-property plots

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.

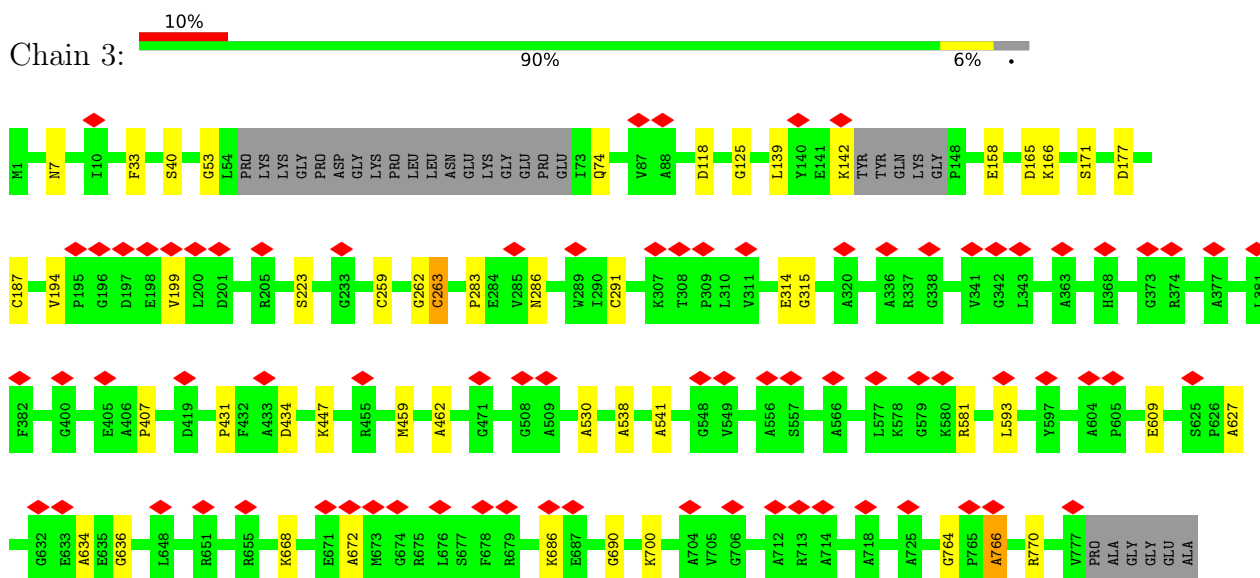
- Molecule 1: NADH-quinone oxidoreductase subunit 1



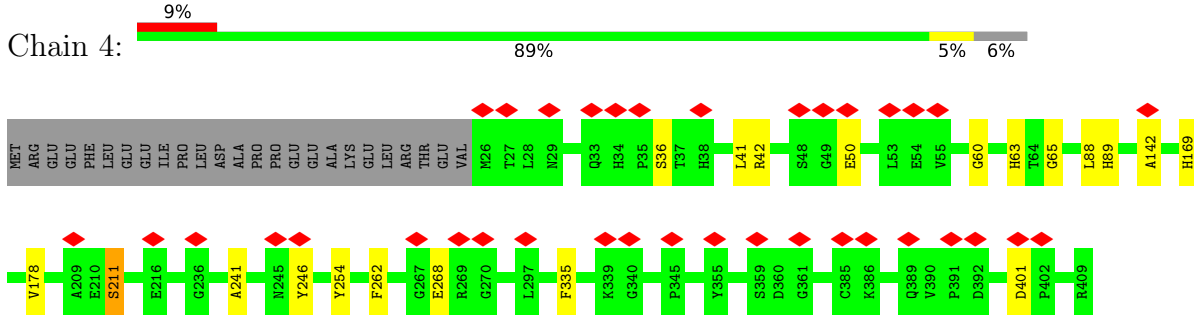
- Molecule 2: NADH-quinone oxidoreductase subunit 2



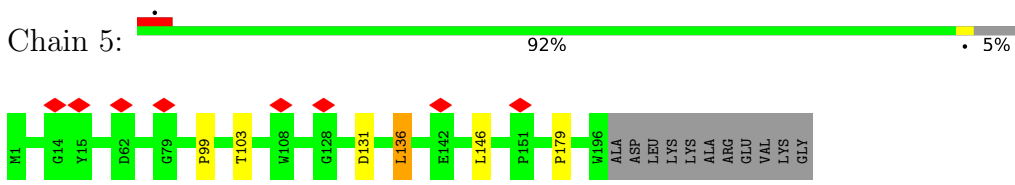
- Molecule 3: NADH-quinone oxidoreductase subunit 3



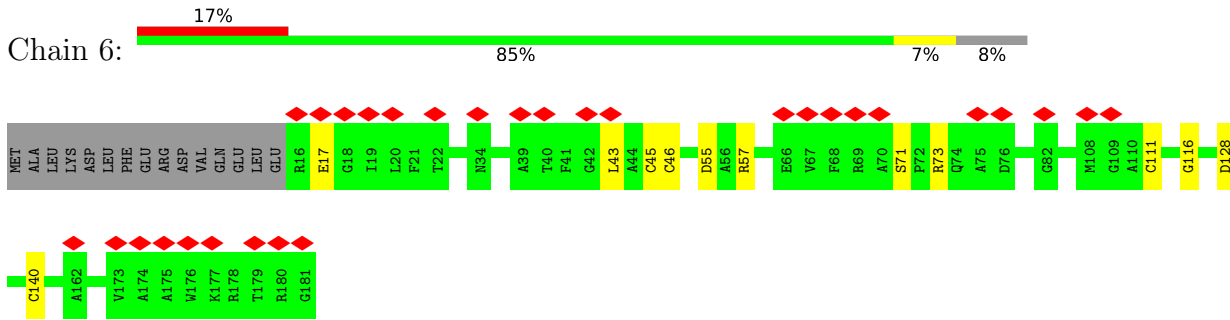
● Molecule 4: NADH-quinone oxidoreductase subunit 4



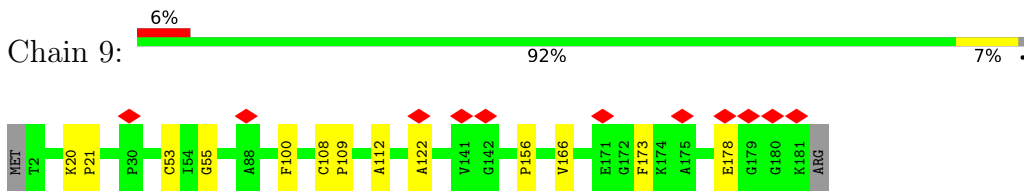
● Molecule 5: NADH-quinone oxidoreductase subunit 5



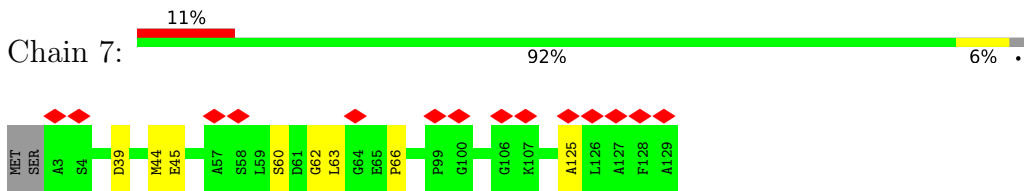
● Molecule 6: NADH-quinone oxidoreductase subunit 6



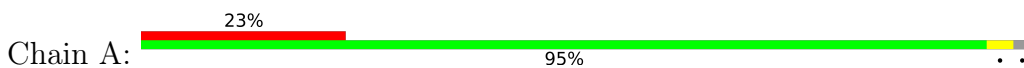
● Molecule 7: NADH-quinone oxidoreductase subunit 9

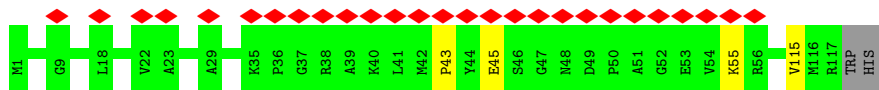


● Molecule 8: NADH-quinone oxidoreductase subunit 15

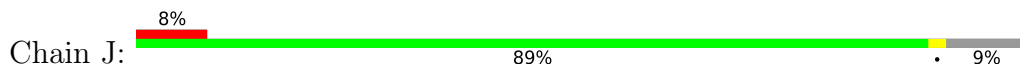


● Molecule 9: NADH-quinone oxidoreductase subunit 7

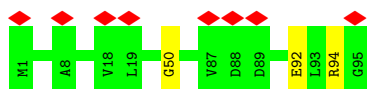




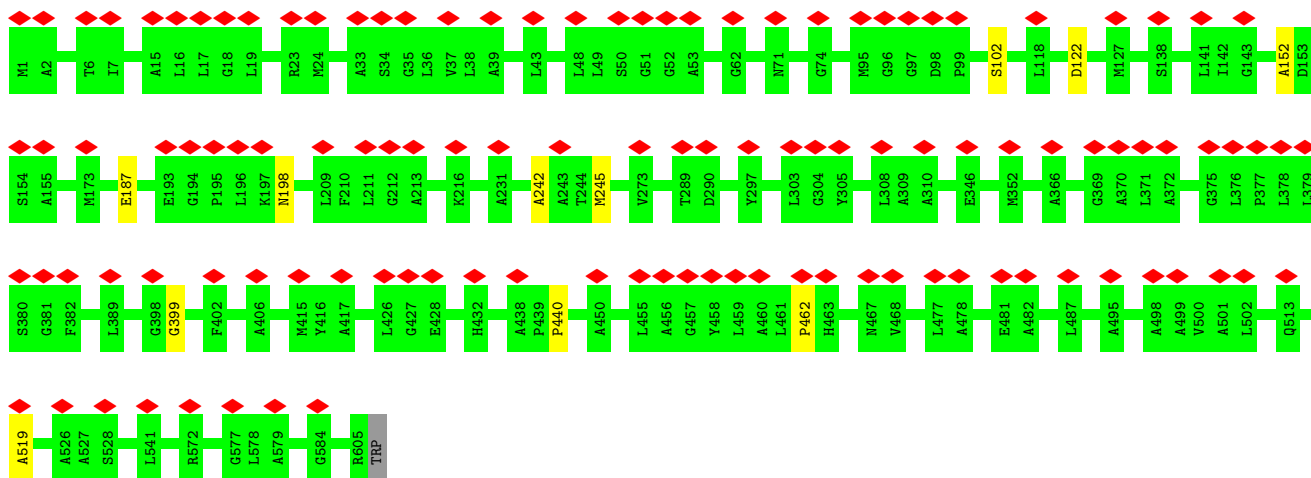
- Molecule 10: NADH-quinone oxidoreductase subunit 10



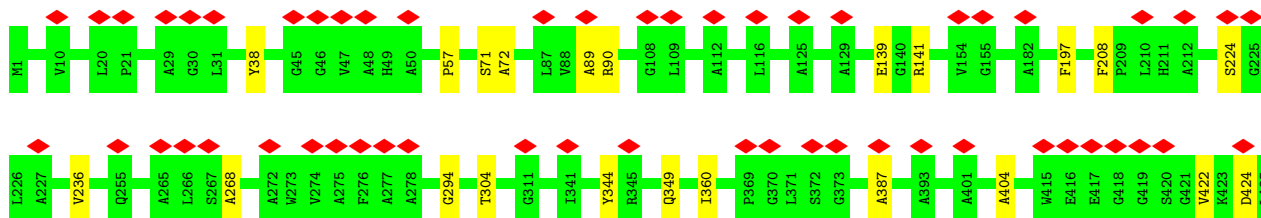
- Molecule 11: NADH-quinone oxidoreductase subunit 11

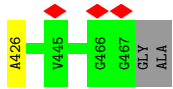


- Molecule 12: NADH-quinone oxidoreductase subunit 12

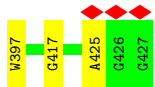
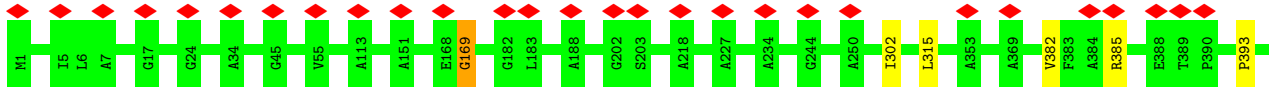


- Molecule 13: NADH-quinone oxidoreductase subunit 13

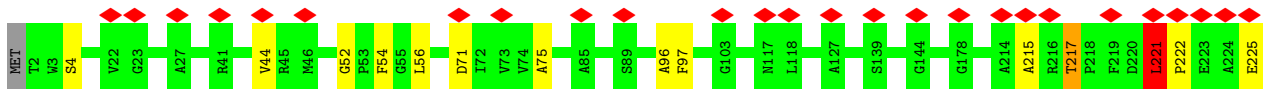
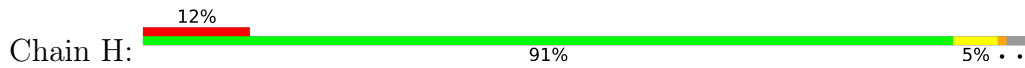




• Molecule 14: NADH-quinone oxidoreductase subunit 14



• Molecule 15: NADH-quinone oxidoreductase subunit 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29000	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 ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.705	Depositor
Minimum map value	-0.223	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.147	Depositor
Map size (Å)	880.64, 880.64, 880.64	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES

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	1	1.07	0/2135	1.16	3/2958 (0.1%)
2	2	1.03	0/874	1.10	0/1213
3	3	1.06	0/3711	1.22	6/5157 (0.1%)
4	4	1.09	0/1889	1.16	5/2625 (0.2%)
5	5	1.05	0/960	1.16	0/1331
6	6	1.14	0/817	1.25	3/1135 (0.3%)
7	9	1.12	0/884	1.22	0/1227
8	7	1.10	0/627	1.21	2/872 (0.2%)
9	A	0.97	0/569	1.00	0/786
10	J	1.05	0/782	1.07	1/1083 (0.1%)
11	K	1.01	0/466	1.00	0/646
12	L	0.98	0/2954	1.08	3/4092 (0.1%)
13	M	1.04	0/2275	1.08	3/3148 (0.1%)
14	N	1.04	0/2091	0.99	0/2900
15	H	1.06	0/1740	1.13	5/2420 (0.2%)
All	All	1.05	0/22774	1.13	31/31593 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
2	2	0	1
4	4	0	3
6	6	0	1
7	9	0	4
9	A	0	1
10	J	0	1
11	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	1
14	N	0	1
15	H	0	2
All	All	0	19

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	288	PHE	CB-CA-C	-6.59	97.21	110.40
4	4	211	SER	N-CA-C	-6.54	93.34	111.00
4	4	65	GLY	N-CA-C	-6.53	96.77	113.10
1	1	179	ALA	N-CA-CB	6.39	119.04	110.10
15	H	314	PHE	N-CA-CB	6.22	121.80	110.60
3	3	187	CYS	N-CA-CB	6.11	121.60	110.60
12	L	187	GLU	CB-CA-C	-6.03	98.35	110.40
1	1	356	CYS	C-N-CA	5.96	136.60	121.70
6	6	46	CYS	CB-CA-C	-5.88	98.64	110.40
15	H	71	ASP	N-CA-C	-5.82	95.29	111.00
6	6	45	CYS	CB-CA-C	5.74	121.88	110.40
15	H	269	MET	N-CA-C	-5.66	95.72	111.00
3	3	142	LYS	N-CA-C	-5.59	95.92	111.00
13	M	197	PHE	CB-CA-C	-5.55	99.31	110.40
4	4	211	SER	N-CA-CB	5.53	118.79	110.50
13	M	38	TYR	CB-CA-C	-5.49	99.42	110.40
4	4	42	ARG	N-CA-C	-5.41	96.40	111.00
3	3	171	SER	CB-CA-C	-5.39	99.86	110.10
8	7	125	ALA	N-CA-CB	5.39	117.64	110.10
4	4	241	ALA	N-CA-CB	5.36	117.60	110.10
10	J	79	GLY	N-CA-C	-5.32	99.81	113.10
12	L	242	ALA	N-CA-CB	5.31	117.53	110.10
3	3	766	ALA	N-CA-CB	5.29	117.50	110.10
6	6	140	CYS	N-CA-CB	5.20	119.96	110.60
3	3	33	PHE	CB-CA-C	-5.15	100.11	110.40
1	1	162	LEU	N-CA-C	-5.12	97.18	111.00
3	3	291	CYS	N-CA-CB	5.10	119.78	110.60
13	M	38	TYR	N-CA-CB	5.09	119.77	110.60
8	7	62	GLY	N-CA-C	-5.07	100.42	113.10
12	L	152	ALA	N-CA-CB	5.06	117.18	110.10
15	H	96	ALA	N-CA-CB	5.02	117.13	110.10

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	166	ASP	Peptide
1	1	203	PRO	Peptide
1	1	396	GLY	Peptide
2	2	139	GLU	Peptide
4	4	142	ALA	Peptide
4	4	254	TYR	Peptide
4	4	36	SER	Peptide
6	6	55	ASP	Peptide
7	9	100	PHE	Mainchain
7	9	178	GLU	Peptide
7	9	20	LYS	Peptide
7	9	21	PRO	Peptide
9	A	115	VAL	Peptide
15	H	217	THR	Peptide
15	H	221	LEU	Peptide
10	J	83	PHE	Peptide
11	K	50	GLY	Peptide
13	M	71	SER	Peptide
14	N	169	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2136	0	989	7	0
2	2	875	0	398	0	0
3	3	3714	0	1785	14	0
4	4	1890	0	833	1	0
5	5	961	0	427	1	0
6	6	818	0	388	2	0
7	9	885	0	406	8	0
8	7	628	0	300	1	0
9	A	570	0	280	0	0
10	J	783	0	409	0	0
11	K	467	0	248	0	0
12	L	2955	0	1499	0	0
13	M	2276	0	1200	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	2092	0	1120	1	0
15	H	1741	0	818	3	0
16	1	8	0	0	6	0
16	3	24	0	0	6	0
16	6	8	0	0	1	0
16	9	16	0	0	8	0
17	2	4	0	0	0	0
17	3	4	0	0	0	0
All	All	22855	0	11100	39	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 1.

All (39) 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)
3:3:262:GLY:N	16:3:803:SF4:S2	2.05	1.26
1:1:355:LYS:N	16:1:501:SF4:S3	2.36	0.97
3:3:262:GLY:CA	16:3:803:SF4:S2	2.52	0.96
1:1:356:CYS:O	16:1:501:SF4:S3	2.27	0.91
1:1:354:GLY:C	16:1:501:SF4:S3	2.49	0.91
7:9:112:ALA:HB3	16:9:202:SF4:S4	2.15	0.86
7:9:55:GLY:CA	16:9:202:SF4:S1	2.64	0.85
7:9:55:GLY:HA2	16:9:202:SF4:S1	2.17	0.84
3:3:259:CYS:N	16:3:803:SF4:S3	2.61	0.73
3:3:609:GLU:HA	3:3:627:ALA:H	1.55	0.69
1:1:354:GLY:N	16:1:501:SF4:S3	2.66	0.68
7:9:55:GLY:C	16:9:202:SF4:S1	2.63	0.67
3:3:262:GLY:HA2	16:3:803:SF4:S2	2.33	0.67
3:3:459:MET:HA	3:3:462:ALA:HB3	1.80	0.63
3:3:700:LYS:HA	3:3:764:GLY:H	1.63	0.62
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.81	0.61
1:1:354:GLY:CA	16:1:501:SF4:S3	2.92	0.58
7:9:108:CYS:HA	16:9:202:SF4:S3	2.46	0.56
7:9:108:CYS:CB	16:9:202:SF4:S3	2.95	0.55
7:9:112:ALA:CB	16:9:202:SF4:S4	2.92	0.55
8:7:60:SER:HA	8:7:66:PRO:HA	1.90	0.54
3:3:263:CYS:N	16:3:803:SF4:S2	2.81	0.53
7:9:53:CYS:HA	16:9:202:SF4:S2	2.50	0.52
3:3:166:LYS:HA	3:3:177:ASP:HA	1.93	0.50
1:1:249:MET:HA	1:1:267:PRO:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:221:LEU:H	15:H:222:PRO:HA	1.75	0.50
1:1:355:LYS:CB	16:1:501:SF4:S2	3.01	0.49
6:6:111:CYS:N	16:6:201:SF4:S3	2.83	0.48
3:3:125:GLY:N	16:3:801:SF4:S3	2.77	0.47
13:M:268:ALA:HB2	13:M:294:GLY:HA3	1.98	0.46
15:H:221:LEU:H	15:H:222:PRO:CA	2.29	0.45
3:3:40:SER:HA	3:3:434:ASP:H	1.82	0.44
15:H:52:GLY:HA2	15:H:56:LEU:H	1.82	0.44
3:3:53:GLY:HA2	3:3:74:GLN:O	2.19	0.43
3:3:690:GLY:H	3:3:770:ARG:CB	2.32	0.42
6:6:71:SER:C	6:6:73:ARG:H	2.22	0.41
13:M:139:GLU:C	13:M:141:ARG:H	2.24	0.41
4:4:60:GLY:HA3	5:5:136:LEU:HA	2.02	0.41
14:N:315:LEU:H	14:N:382:VAL:HA	1.85	0.41

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	1	435/438 (99%)	387 (89%)	38 (9%)	10 (2%)	6	34
2	2	176/181 (97%)	160 (91%)	13 (7%)	3 (2%)	9	41
3	3	748/783 (96%)	650 (87%)	73 (10%)	25 (3%)	4	26
4	4	382/409 (93%)	339 (89%)	30 (8%)	13 (3%)	3	26
5	5	194/207 (94%)	173 (89%)	15 (8%)	6 (3%)	4	27
6	6	164/181 (91%)	134 (82%)	25 (15%)	5 (3%)	4	28
7	9	178/182 (98%)	155 (87%)	18 (10%)	5 (3%)	5	30
8	7	125/129 (97%)	109 (87%)	12 (10%)	4 (3%)	4	26
9	A	115/119 (97%)	104 (90%)	8 (7%)	3 (3%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	158/176 (90%)	133 (84%)	23 (15%)	2 (1%)	12	47
11	K	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	6	35
12	L	603/606 (100%)	540 (90%)	55 (9%)	8 (1%)	12	47
13	M	465/469 (99%)	408 (88%)	41 (9%)	16 (3%)	3	26
14	N	425/427 (100%)	378 (89%)	40 (9%)	7 (2%)	9	43
15	H	351/365 (96%)	306 (87%)	31 (9%)	14 (4%)	3	23
All	All	4612/4767 (97%)	4061 (88%)	428 (9%)	123 (3%)	8	31

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	101	PHE
1	1	179	ALA
3	3	165	ASP
3	3	263	CYS
3	3	634	ALA
3	3	672	ALA
4	4	211	SER
4	4	262	PHE
4	4	335	PHE
6	6	43	LEU
9	A	43	PRO
12	L	122	ASP
13	M	72	ALA
13	M	349	GLN
13	M	424	ASP
14	N	425	ALA
15	H	217	THR
15	H	221	LEU
15	H	225	GLU
2	2	86	LEU
3	3	7	ASN
3	3	139	LEU
3	3	158	GLU
3	3	314	GLU
3	3	668	LYS
3	3	766	ALA
4	4	41	LEU
4	4	63	HIS
4	4	88	LEU

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Mol	Chain	Res	Type
4	4	89	HIS
5	5	103	THR
5	5	146	LEU
6	6	57	ARG
6	6	116	GLY
6	6	128	ASP
7	9	156	PRO
8	7	45	GLU
8	7	63	LEU
10	J	78	GLN
12	L	462	PRO
13	M	90	ARG
13	M	224	SER
13	M	426	ALA
15	H	4	SER
15	H	54	PHE
15	H	215	ALA
15	H	226	GLN
1	1	80	PRO
1	1	195	LEU
1	1	295	SER
2	2	140	PRO
3	3	199	VAL
3	3	315	GLY
3	3	447	LYS
3	3	593	LEU
4	4	50	GLU
4	4	178	VAL
4	4	246	TYR
4	4	268	GLU
5	5	179	PRO
7	9	122	ALA
8	7	39	ASP
11	K	94	ARG
12	L	399	GLY
13	M	89	ALA
14	N	393	PRO
15	H	97	PHE
15	H	267	TRP
15	H	333	PRO
2	2	144	CYS
3	3	283	PRO

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Mol	Chain	Res	Type
3	3	286	ASN
3	3	407	PRO
3	3	431	PRO
3	3	530	ALA
3	3	581	ARG
5	5	136	LEU
6	6	17	GLU
8	7	44	MET
9	A	55	LYS
10	J	84	ASP
11	K	92	GLU
12	L	245	MET
12	L	519	ALA
13	M	387	ALA
13	M	404	ALA
14	N	385	ARG
15	H	75	ALA
15	H	275	PRO
1	1	81	LYS
1	1	97	GLU
1	1	418	LYS
3	3	118	ASP
3	3	223	SER
3	3	636	GLY
3	3	686	LYS
4	4	169	HIS
4	4	401	ASP
5	5	131	ASP
7	9	109	PRO
7	9	173	PHE
9	A	45	GLU
12	L	102	SER
12	L	198	ASN
13	M	304	THR
14	N	169	GLY
14	N	397	TRP
14	N	417	GLY
1	1	38	TYR
3	3	194	VAL
5	5	99	PRO
12	L	440	PRO
13	M	236	VAL

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Mol	Chain	Res	Type
13	M	344	TYR
15	H	269	MET
1	1	202	LYS
7	9	166	VAL
13	M	57	PRO
13	M	360	ILE
14	N	302	ILE
13	M	422	VAL
15	H	44	VAL
13	M	208	PHE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

9 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
16	SF4	3	803	-	0,12,12	-	-	-		
17	FES	3	804	-	0,4,4	-	-	-		
16	SF4	3	801	-	0,12,12	-	-	-		
16	SF4	9	201	7	0,12,12	-	-	-		
16	SF4	9	202	7	0,12,12	-	-	-		
16	SF4	6	201	-	0,12,12	-	-	-		
16	SF4	3	802	3	0,12,12	-	-	-		
16	SF4	1	501	1	0,12,12	-	-	-		
17	FES	2	201	-	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
16	SF4	3	803	-	-	-	0/6/5/5
17	FES	3	804	-	-	-	0/1/1/1
16	SF4	3	801	-	-	-	0/6/5/5
16	SF4	9	201	7	-	-	0/6/5/5
16	SF4	9	202	7	-	-	0/6/5/5
16	SF4	6	201	-	-	-	0/6/5/5
16	SF4	3	802	3	-	-	0/6/5/5
16	SF4	1	501	1	-	-	0/6/5/5
17	FES	2	201	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	3	803	SF4	5	0
16	3	801	SF4	1	0
16	9	202	SF4	8	0
16	6	201	SF4	1	0
16	1	501	SF4	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

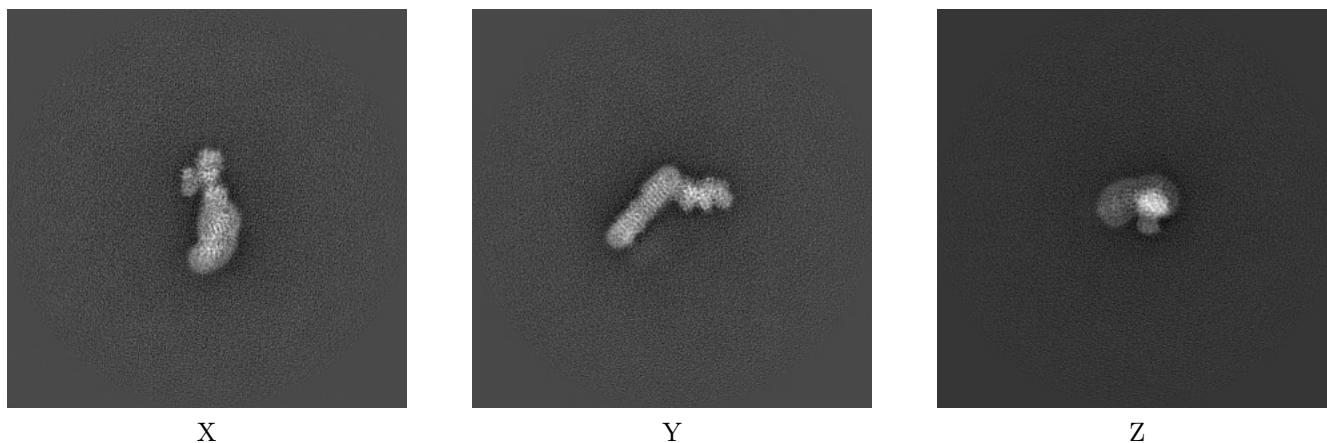
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11238. 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 [i](#)

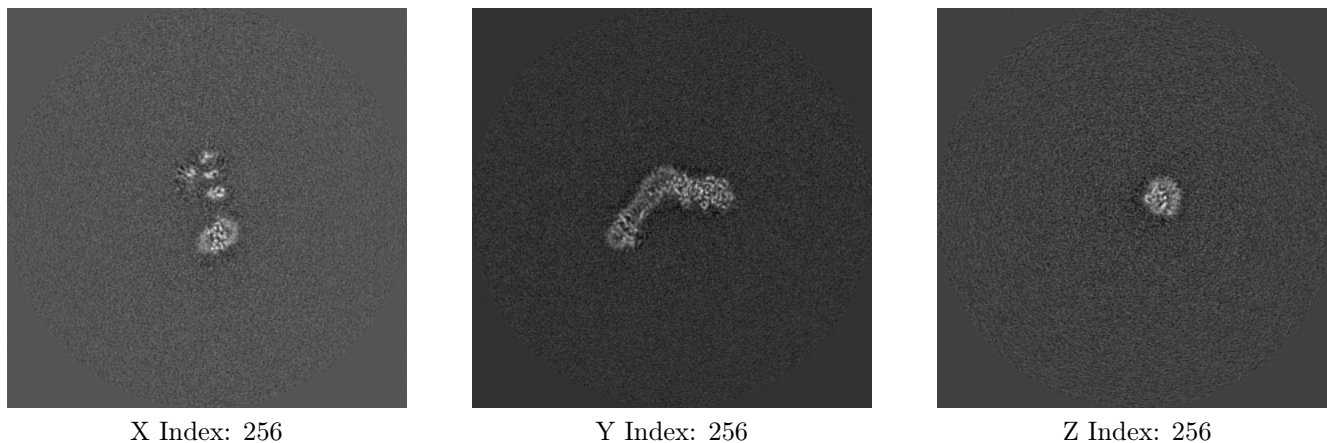
6.1.1 Primary map



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

6.2 Central slices [i](#)

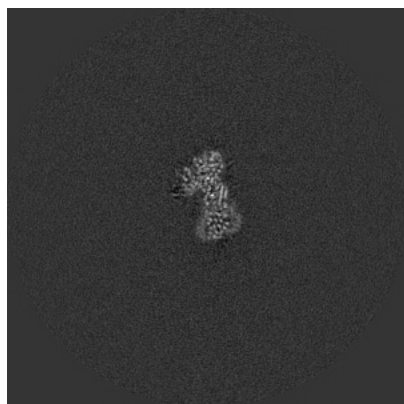
6.2.1 Primary map



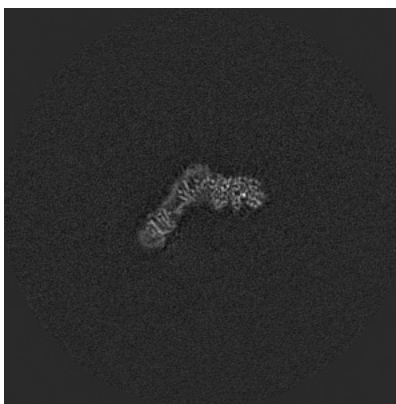
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

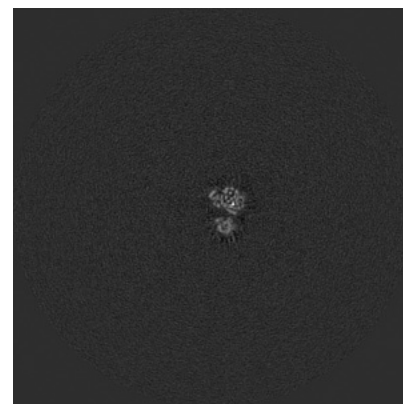
6.3.1 Primary map



X Index: 278



Y Index: 259



Z Index: 279

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.147. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

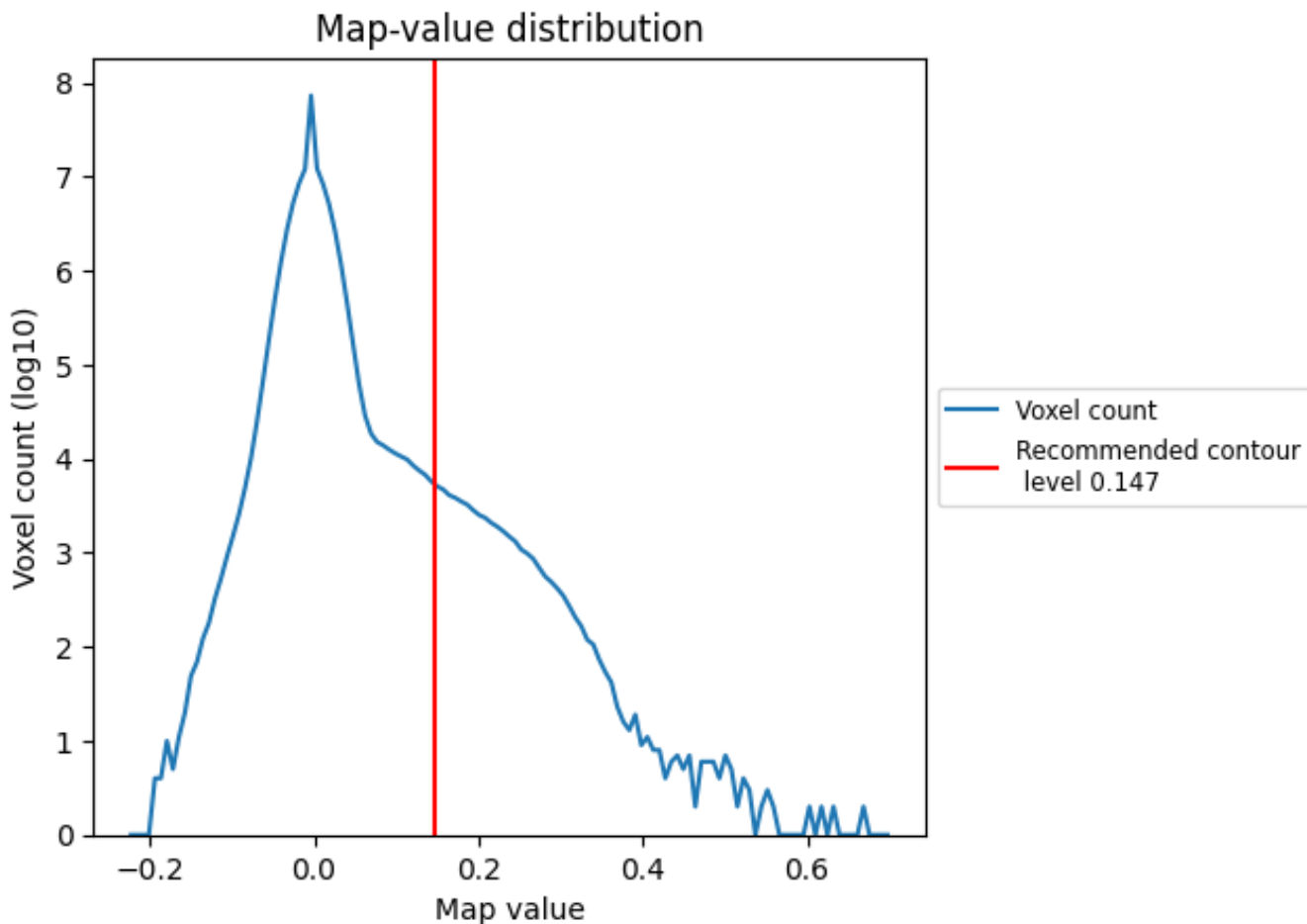
6.5 Mask visualisation

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

7 Map analysis [i](#)

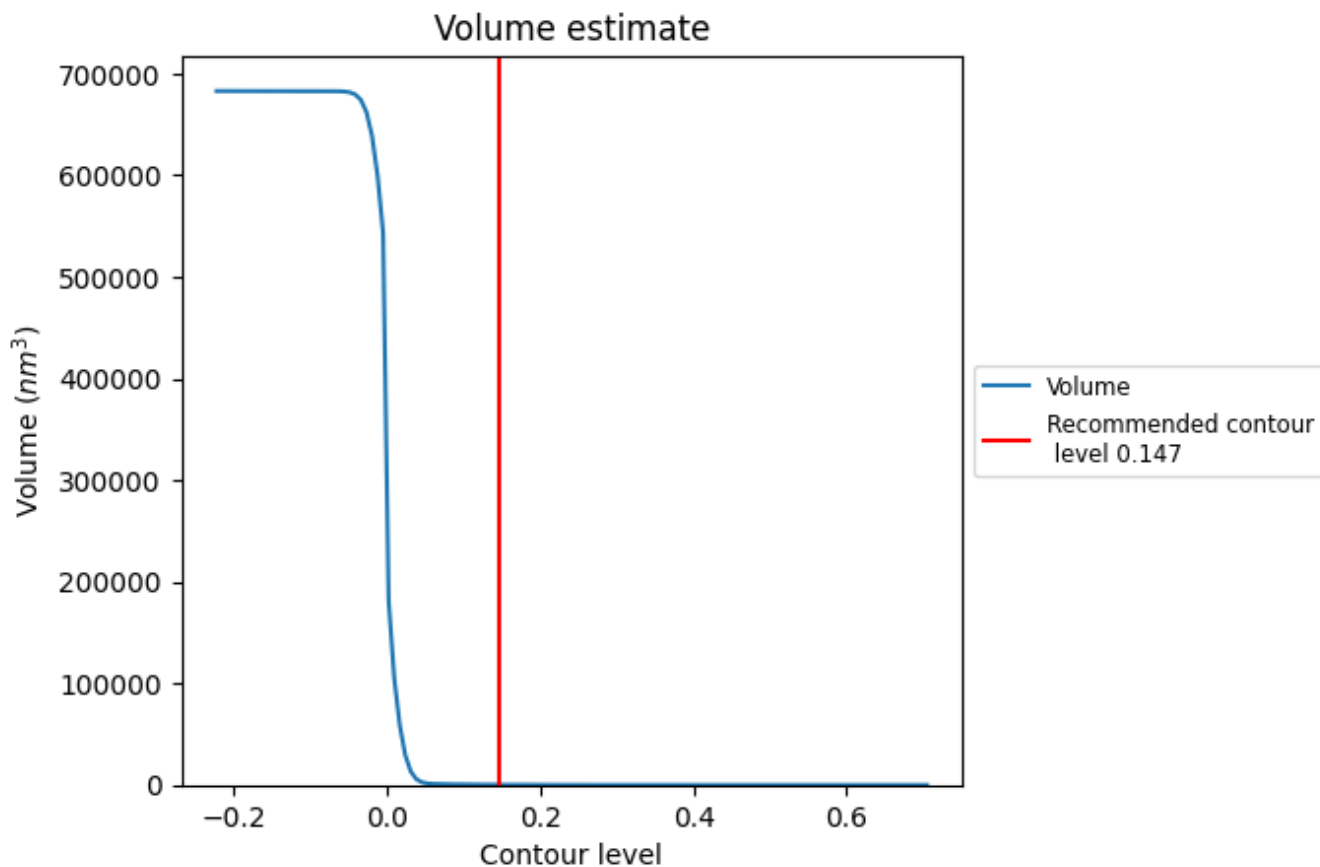
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

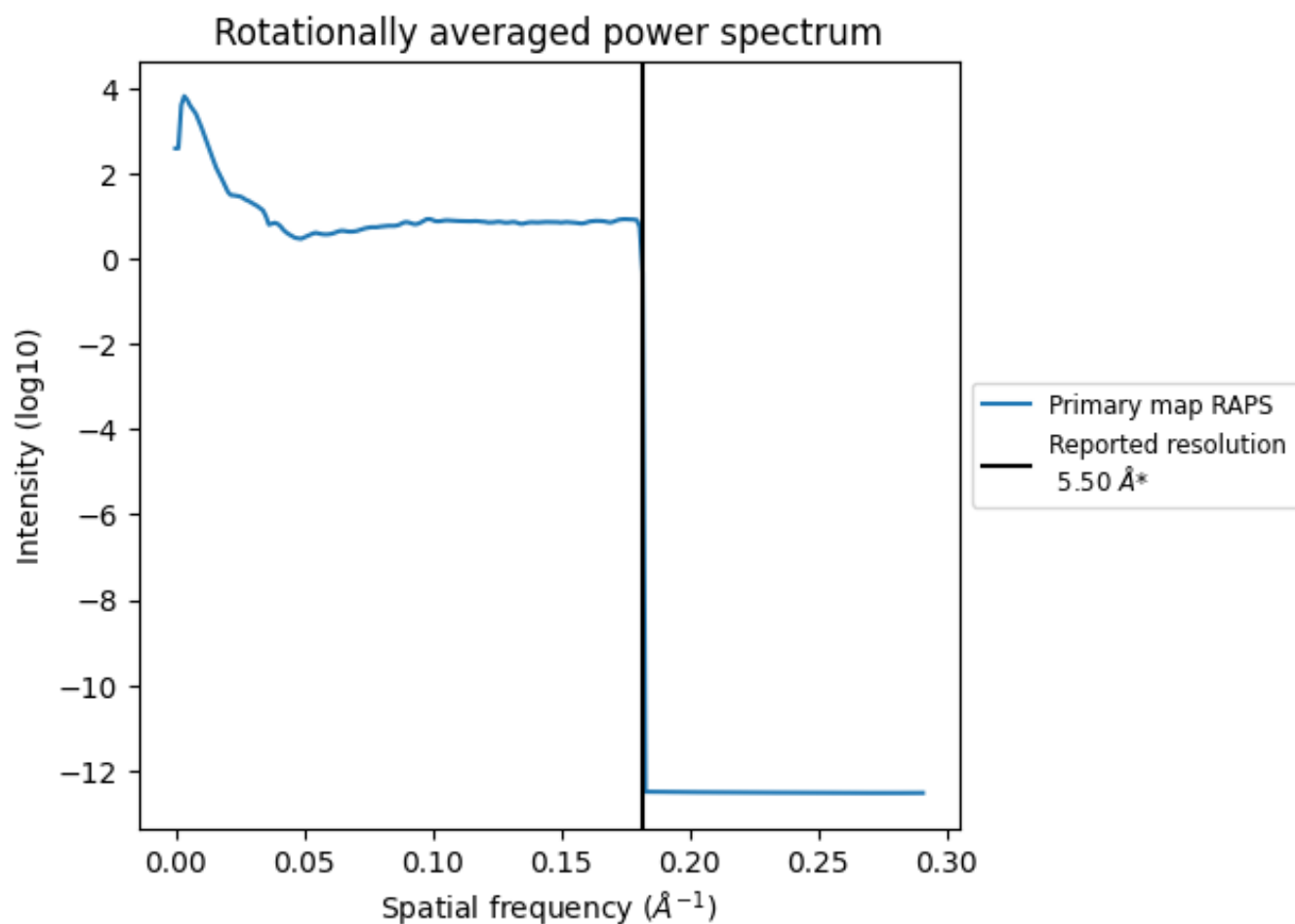
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm^3 ; this corresponds to an approximate mass of 228 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 [\(i\)](#)

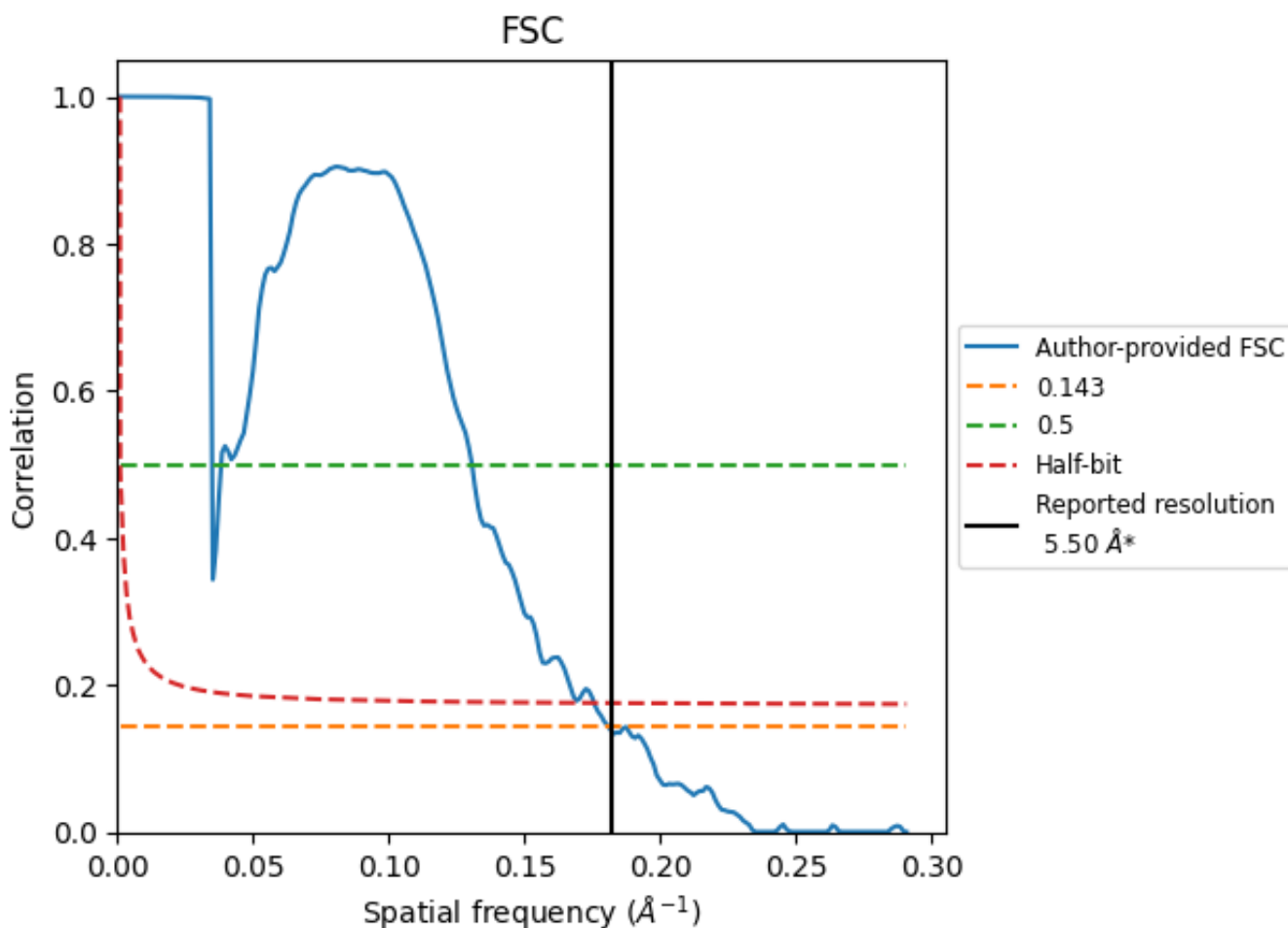


*Reported resolution corresponds to spatial frequency of 0.182\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.182 Å⁻¹

8.2 Resolution estimates [i](#)

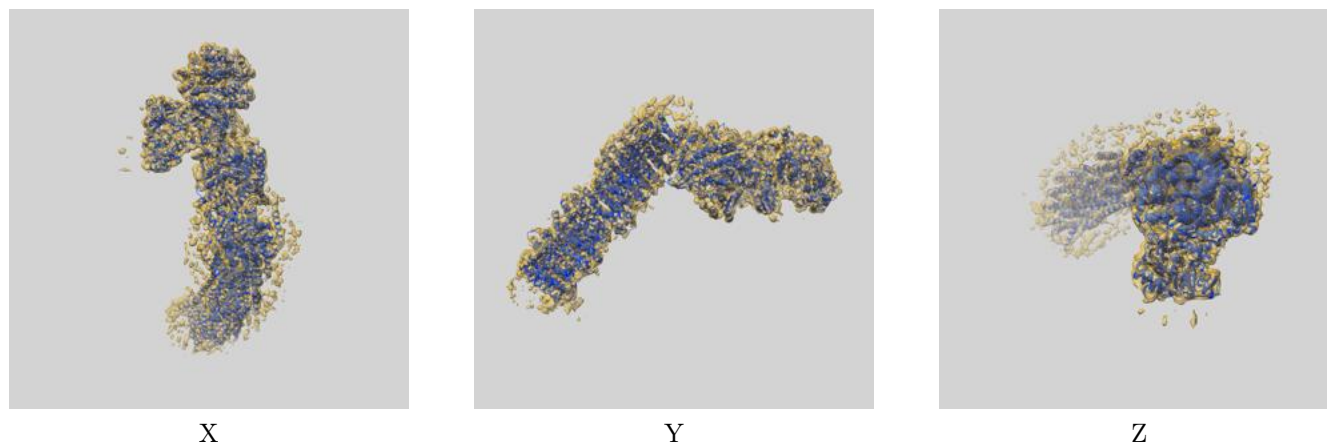
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	5.53	28.65	5.69
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

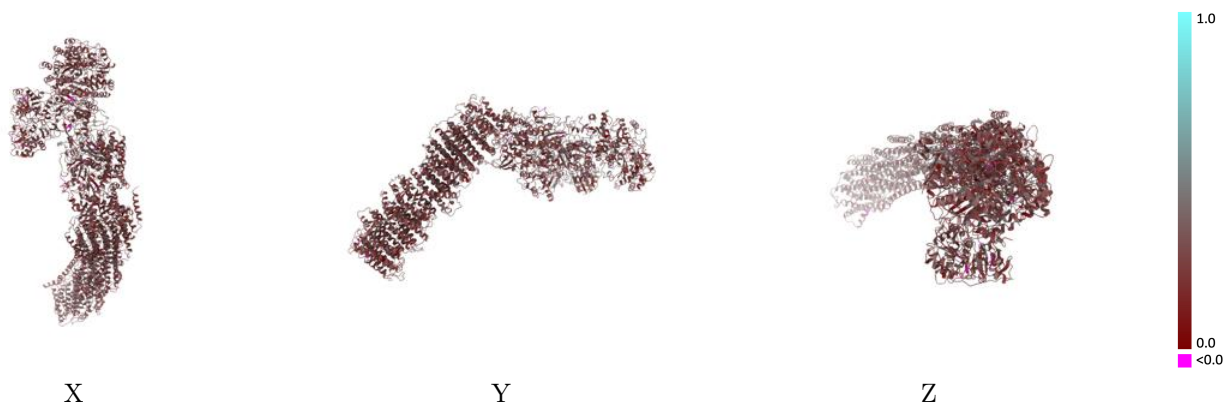
This section contains information regarding the fit between EMDB map EMD-11238 and PDB model 6ZJY. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



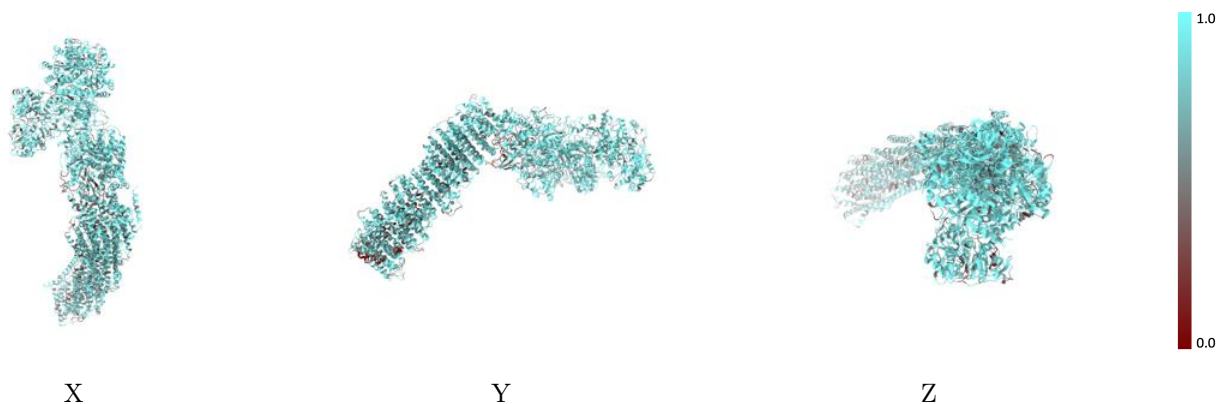
The images above show the 3D surface view of the map at the recommended contour level 0.147 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



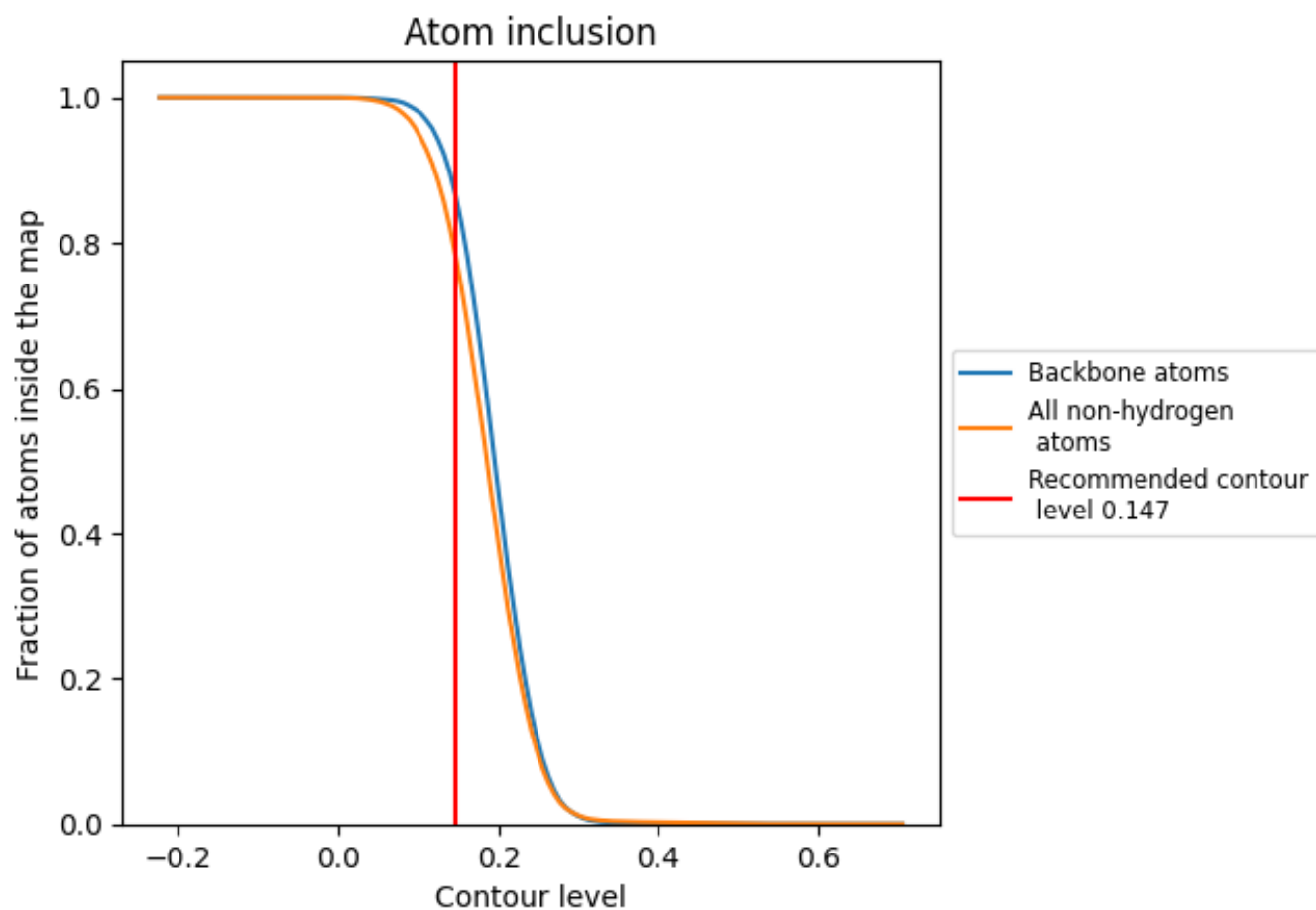
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.147).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.147) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7809	 0.2890
1	 0.8298	 0.2820
2	 0.8476	 0.2920
3	 0.7974	 0.2950
4	 0.7963	 0.3020
5	 0.8398	 0.3270
6	 0.7312	 0.2730
7	 0.7994	 0.2920
9	 0.8324	 0.3190
A	 0.6456	 0.2820
H	 0.7679	 0.2820
J	 0.7778	 0.2920
K	 0.7794	 0.2990
L	 0.7161	 0.2640
M	 0.7654	 0.2780
N	 0.7820	 0.2930

