wwPDB EM Validation Summary Report

Dec 10, 2022 – 09:31 am GMT

PDB ID	:	4UQ8
EMDB ID	:	EMD-2676
Title	:	Electron cryo-microscopy of bovine Complex I
Authors	:	Vinothkumar, K.R.; Zhu, J.; Hirst, J.
Deposited on	:	2014-06-21
Resolution	:	4.95 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:

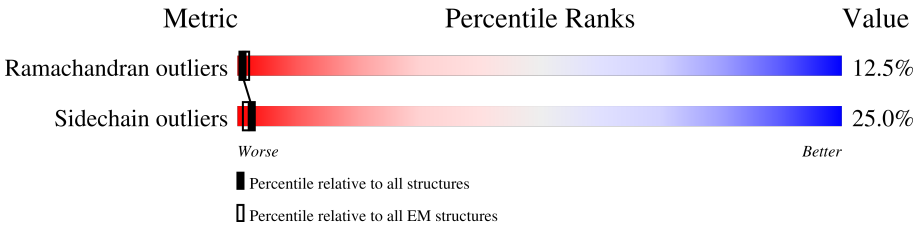
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.95 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)
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	111	75% 25%
2	B	143	97%
3	C	154	99%
4	D	384	100%
5	E	159	100%
6	F	411	8% 99%
7	G	538	96%
8	H	313	91% 9%
9	I	162	97%

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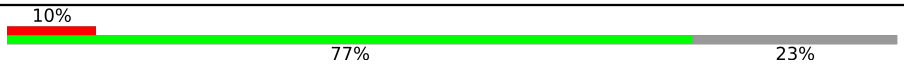
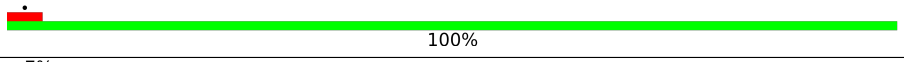
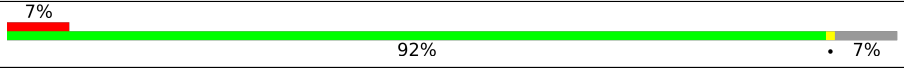
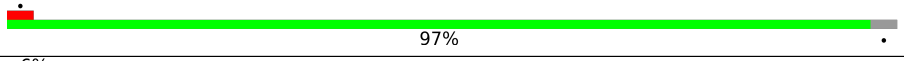
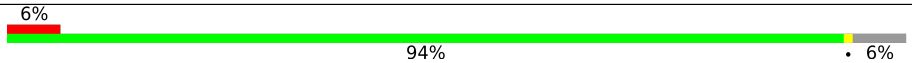
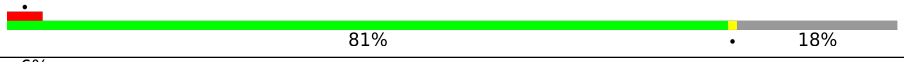
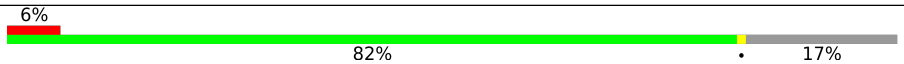
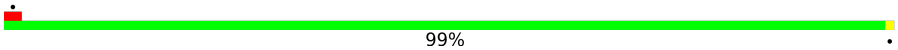
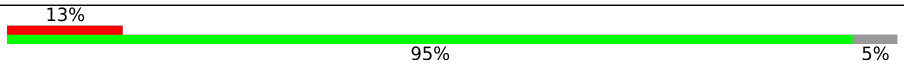
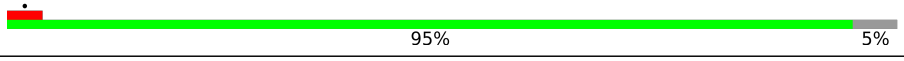
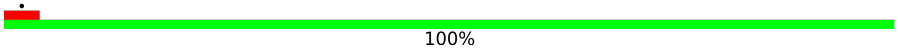
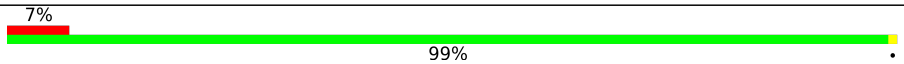
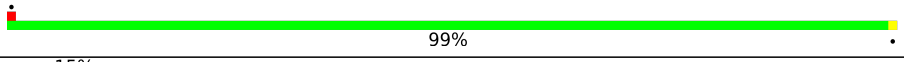
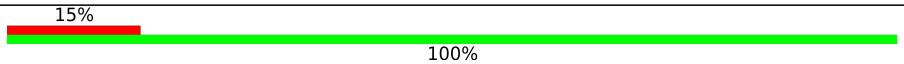
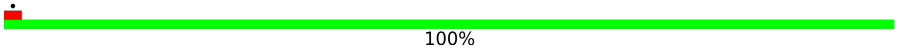
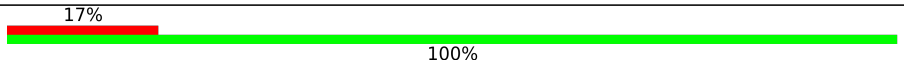
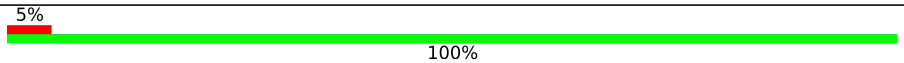
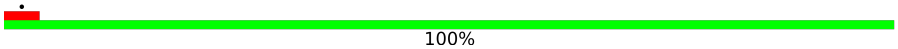
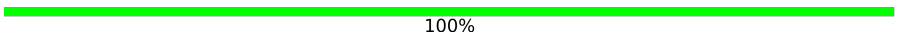
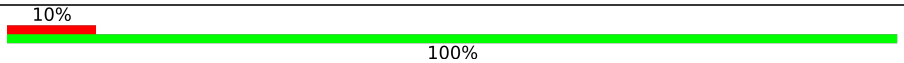
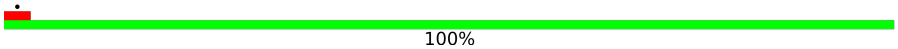
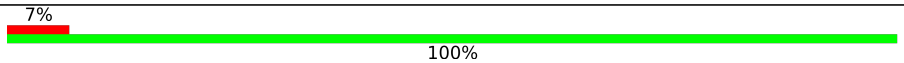
Mol	Chain	Length	Quality of chain
10	J	171	
11	K	84	
12	L	601	
13	M	453	
14	N	345	
15	O	220	
16	P	303	
17	Q	85	
18	R	47	
19	S	80	
20	T	75	
21	U	79	
22	V	71	
23	W	72	
24	X	79	
25	Y	106	
26	Z	65	
27	a	29	
28	b	42	
29	c	27	
29	w	27	
30	d	39	
31	e	20	
32	f	30	
32	h	30	

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Mol	Chain	Length	Quality of chain
32	i	30	7% 100%
33	g	22	100%
34	j	24	100%
34	l	24	100%
35	k	28	7% 100%
35	p	28	100%
35	s	28	100%
36	m	34	100%
37	n	59	100%
38	o	21	100%
39	q	25	100%
40	r	26	100%
41	t	57	100%
42	u	43	35% 65%
43	v	32	100%

2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 28647 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 UBIQUINONE OXIDOREDUCTASE CHAIN 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	83	415	249	83	83	0	0

- Molecule 2 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 7, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	143	719	429	143	143	4	0	0

- Molecule 3 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 3, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	154	770	462	154	154	0	0

- Molecule 4 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	384	1920	1152	384	384	0	0

- Molecule 5 is a protein called NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	159	799	477	159	159	4	0	0

- Molecule 6 is a protein called NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	411	Total	C	N	O	S	0	0
			2059	1233	411	411	4		

- Molecule 7 is a protein called NADH-UBIQUINONE OXIDOREDUCTASE 75 KDA SUBUNIT, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	527	Total	C	N	O	S	0	0
			2651	1584	529	527	11		

- Molecule 8 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	285	Total	C	N	O	0	0
			1425	855	285	285		

- Molecule 9 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 8, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	162	Total	C	N	O	S	0	0
			818	486	162	162	8		

- Molecule 10 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	131	Total	C	N	O	0	0
			655	393	131	131		

- Molecule 11 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4L.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	84	Total	C	N	O	0	0
			420	252	84	84		

- Molecule 12 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	558	Total	C	N	O	0	0
			2790	1674	558	558		

- Molecule 13 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	439	Total	C	N	O	0	0
			2195	1317	439	439		

- Molecule 14 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	326	Total	C	N	O	0	0
			1630	978	326	326		

- Molecule 15 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	181	Total	C	N	O	0	0
			905	543	181	181		

- Molecule 16 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	252	Total	C	N	O	0	0
			1260	756	252	252		

- Molecule 17 is a protein called NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	69	Total	C	N	O	0	0
			345	207	69	69		

- Molecule 18 is a protein called NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 19 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	80	Total	C	N	O	0	0
			400	240	80	80		

- Molecule 20 is a protein called ACYL CARRIER PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	71	Total 355	C 213	N 71	O 71	0	0

- Molecule 21 is a protein called NADH UBIQUINONE DEHYDROGENASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	75	Total 375	C 225	N 75	O 75	0	0

- Molecule 22 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	71	Total 355	C 213	N 71	O 71	0	0

- Molecule 23 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	72	Total 360	C 216	N 72	O 72	0	0

- Molecule 24 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	79	Total 395	C 237	N 79	O 79	0	0

- Molecule 25 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	106	Total 530	C 318	N 106	O 106	0	0

- Molecule 26 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	65	Total 325	C 195	N 65	O 65	0	0

- Molecule 27 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	29	Total 145	C 87	N 29	O 29	0	0

- Molecule 28 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	42	Total 210	C 126	N 42	O 42	0	0

- Molecule 29 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	c	27	Total 135	C 81	N 27	O 27	0	0
29	w	27	Total 135	C 81	N 27	O 27	0	0

- Molecule 30 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	d	39	Total 195	C 117	N 39	O 39	0	0

- Molecule 31 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	20	Total 100	C 60	N 20	O 20	0	0

- Molecule 32 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	f	30	Total 150	C 90	N 30	O 30	0	0
32	h	30	Total 150	C 90	N 30	O 30	0	0
32	i	30	Total 150	C 90	N 30	O 30	0	0

- Molecule 33 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	g	22	Total 110	C 66	N 22	O 22	0	0

- Molecule 34 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	j	24	Total 120	C 72	N 24	O 24	0	0
34	l	24	Total 120	C 72	N 24	O 24	0	0

- Molecule 35 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	k	28	Total 140	C 84	N 28	O 28	0	0
35	p	28	Total 140	C 84	N 28	O 28	0	0
35	s	28	Total 140	C 84	N 28	O 28	0	0

- Molecule 36 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	m	34	Total 170	C 102	N 34	O 34	0	0

- Molecule 37 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	n	59	Total 295	C 177	N 59	O 59	0	0

- Molecule 38 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	21	Total 105	C 63	N 21	O 21	0	0

- Molecule 39 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	q	25	Total	C	N	O	0	0
			125	75	25	25		

- Molecule 40 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	r	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 41 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	t	57	Total	C	N	O	0	0
			285	171	57	57		

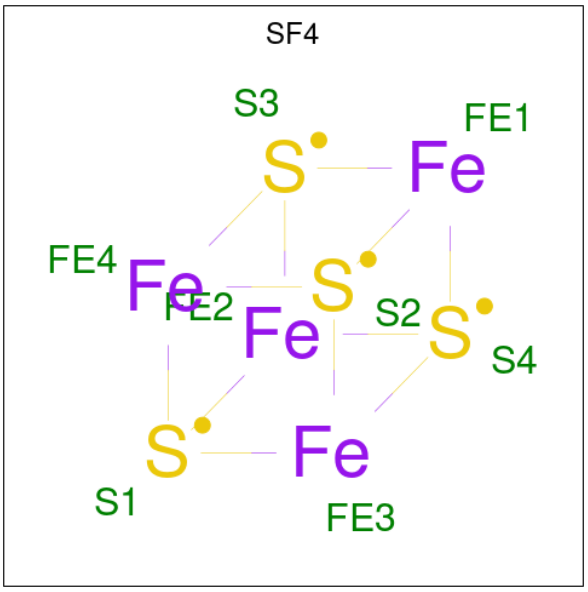
- Molecule 42 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	u	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 43 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

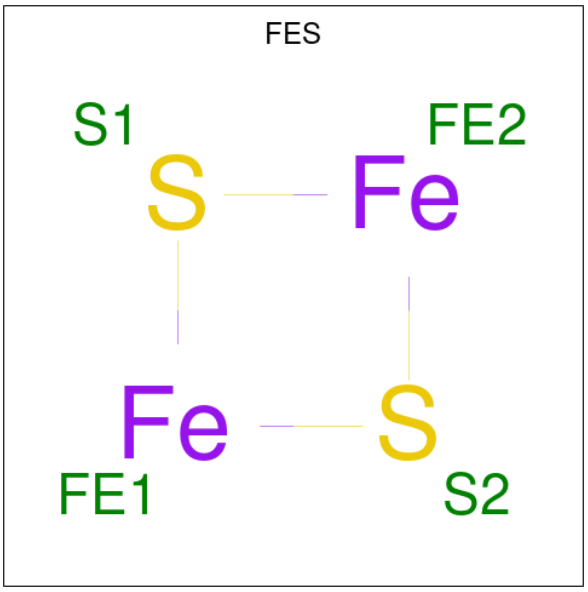
Mol	Chain	Residues	Atoms				AltConf	Trace
43	v	32	Total	C	N	O	0	0
			160	96	32	32		

- Molecule 44 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

3 Residue-property plots (i)

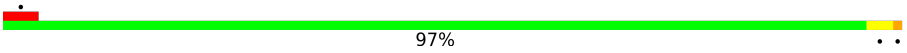
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

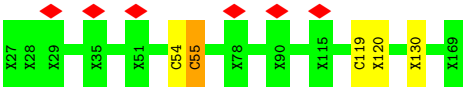
• Molecule 1: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 3

Chain A:

• Molecule 2: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 7, MITOCHONDRIAL

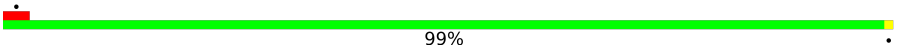
Chain B:

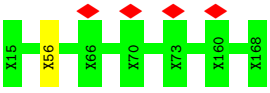




• Molecule 3: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 3, MITOCHONDRIAL

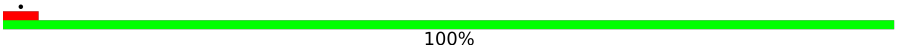
Chain C:

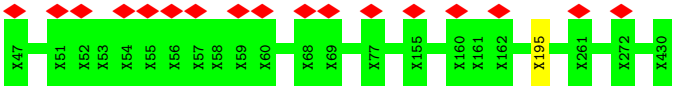




• Molecule 4: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 2, MITOCHONDRIAL

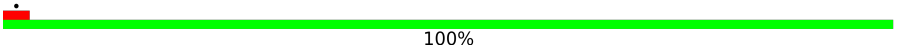
Chain D:

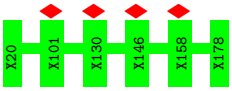




• Molecule 5: NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 2, MITOCHONDRIAL

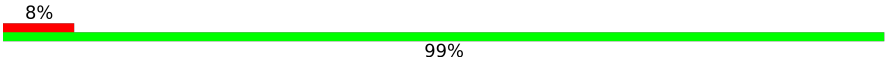
Chain E:

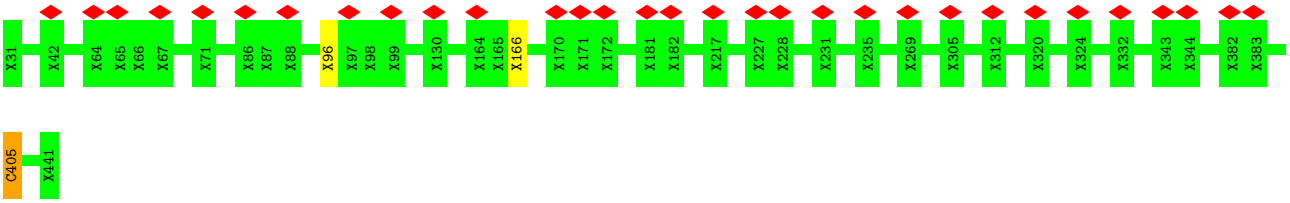




• Molecule 6: NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 1, MITOCHONDRIAL

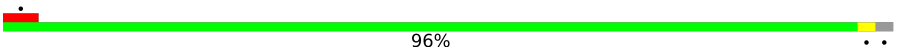
Chain F:

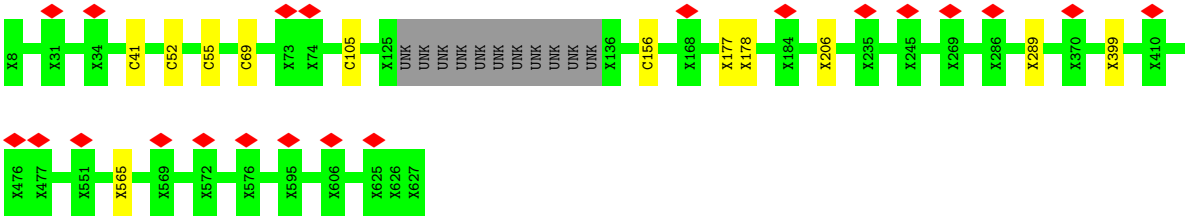




• Molecule 7: NADH-UBIQUINONE OXIDOREDUCTASE 75 KDA SUBUNIT, MITOCHONDRIAL

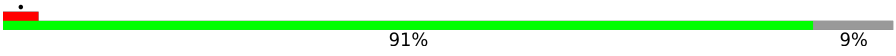
Chain G:

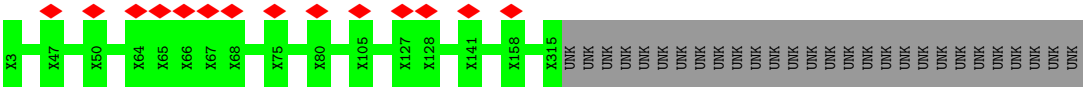




• Molecule 8: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 1

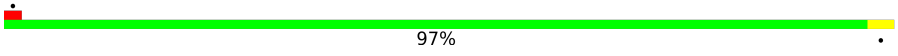
Chain H:

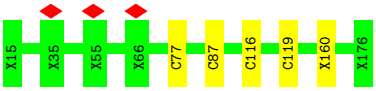




• Molecule 9: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 8, MITOCHONDRIAL

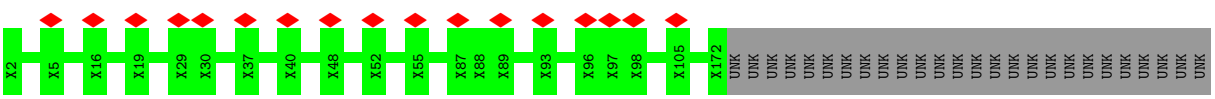
Chain I:





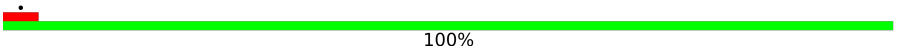
• Molecule 10: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 6

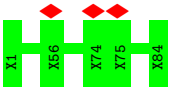
Chain J:



• Molecule 11: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4L

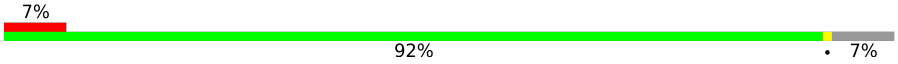
Chain K:

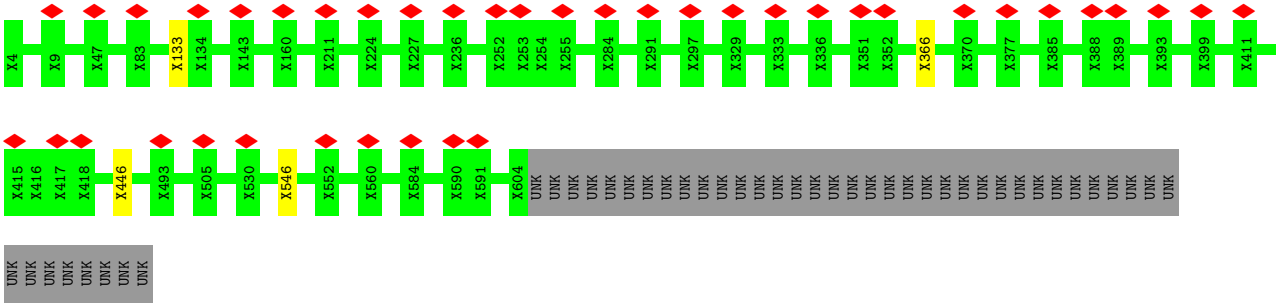




• Molecule 12: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 5

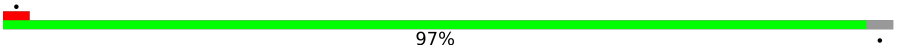
Chain L:

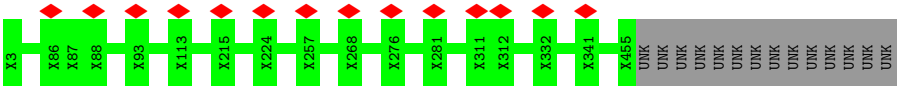




• Molecule 13: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4

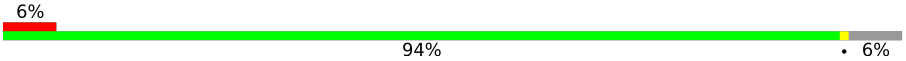
Chain M:





• Molecule 14: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 2

Chain N:

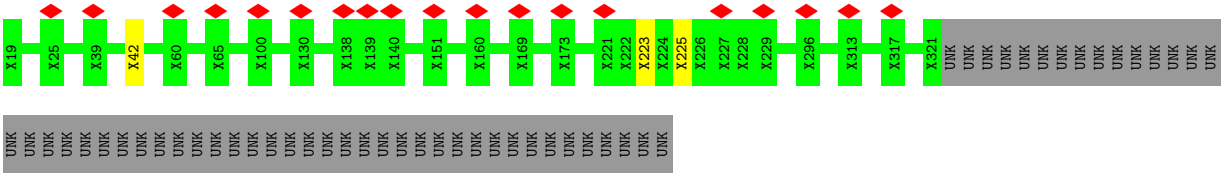


• Molecule 15: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 10

Chain O:

• Molecule 16: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 9, MITOCHONDRIAL

Chain P:



• Molecule 17: NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 4

Chain Q:

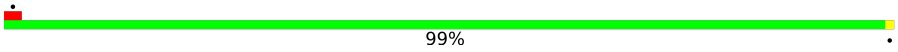
• Molecule 18: NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 6

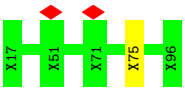
Chain R:

There are no outlier residues recorded for this chain.

• Molecule 19: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 2

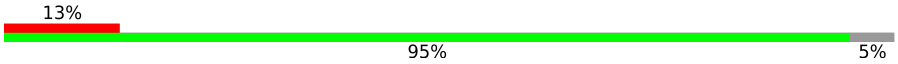
Chain S:

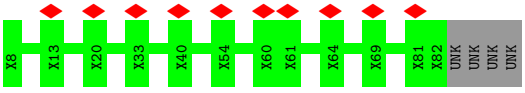




• Molecule 20: ACYL CARRIER PROTEIN, MITOCHONDRIAL

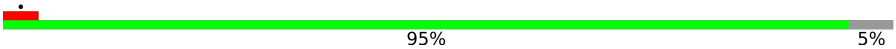
Chain T:

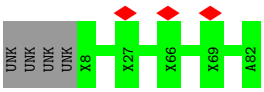




• Molecule 21: NADH UBIQUINONE DEHYDROGENASE

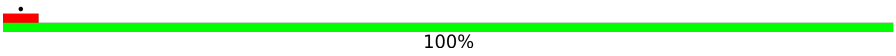
Chain U:

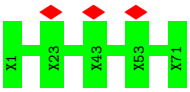




• Molecule 22: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 5

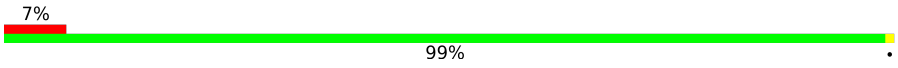
Chain V:

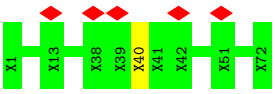




• Molecule 23: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 6

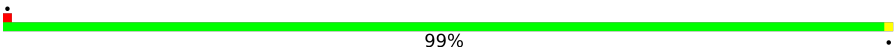
Chain W:

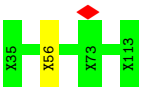




• Molecule 24: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 8

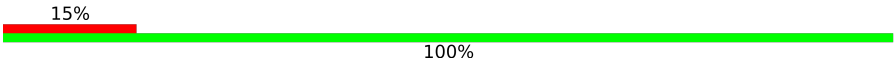
Chain X:

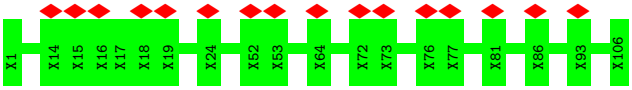




• Molecule 25: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 11

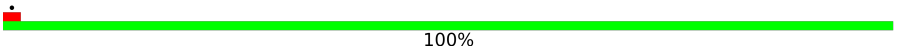
Chain Y:

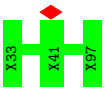




• Molecule 26: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 13

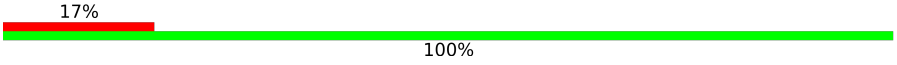
Chain Z:

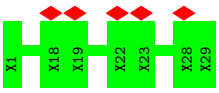




• Molecule 27: NADH UBIQUINONE OXIDOREDUCTASE

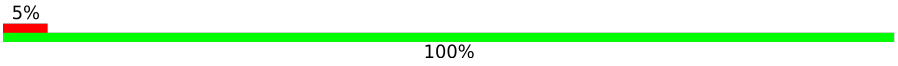
Chain a:

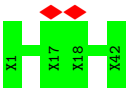




• Molecule 28: NADH UBIQUINONE OXIDOREDUCTASE

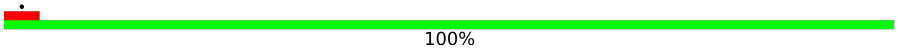
Chain b:

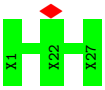




• Molecule 29: NADH UBIQUINONE OXIDOREDUCTASE

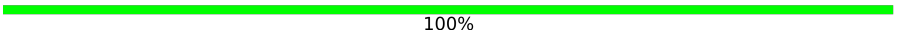
Chain c:





• Molecule 29: NADH UBIQUINONE OXIDOREDUCTASE

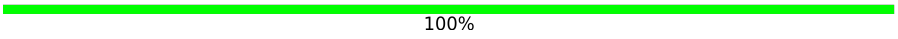
Chain w:



There are no outlier residues recorded for this chain.

• Molecule 30: NADH UBIQUINONE OXIDOREDUCTASE

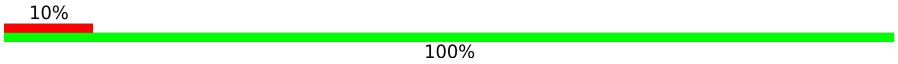
Chain d:

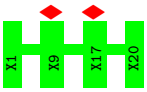


There are no outlier residues recorded for this chain.

• Molecule 31: NADH UBIQUINONE OXIDOREDUCTASE

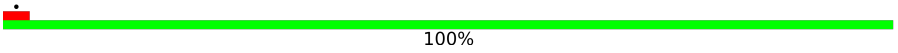
Chain e:

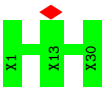




• Molecule 32: NADH UBIQUINONE OXIDOREDUCTASE

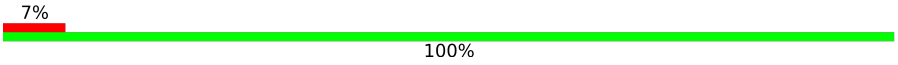
Chain f:

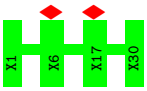




• Molecule 32: NADH UBIQUINONE OXIDOREDUCTASE

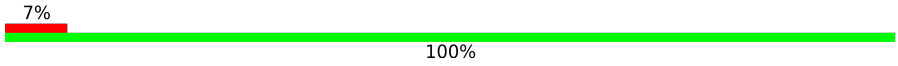
Chain h:

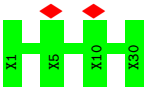




• Molecule 32: NADH UBIQUINONE OXIDOREDUCTASE

Chain i:





• Molecule 33: NADH UBIQUINONE OXIDOREDUCTASE

Chain g: 

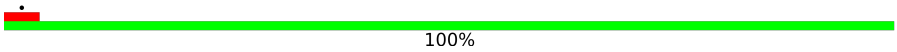
There are no outlier residues recorded for this chain.

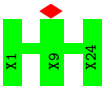
• Molecule 34: NADH UBIQUINONE OXIDOREDUCTASE

Chain j: 

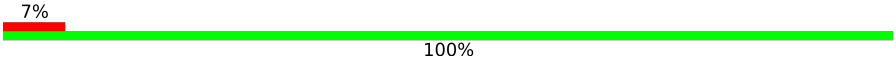
There are no outlier residues recorded for this chain.

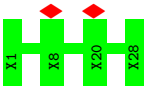
• Molecule 34: NADH UBIQUINONE OXIDOREDUCTASE

Chain l: 

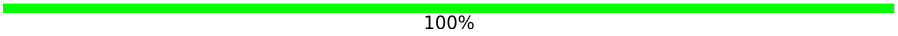


• Molecule 35: NADH UBIQUINONE OXIDOREDUCTASE

Chain k: 

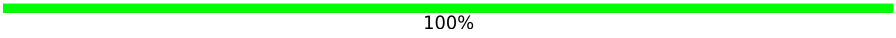


• Molecule 35: NADH UBIQUINONE OXIDOREDUCTASE

Chain p: 

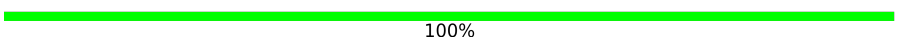
There are no outlier residues recorded for this chain.

• Molecule 35: NADH UBIQUINONE OXIDOREDUCTASE

Chain s: 

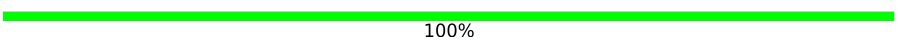
There are no outlier residues recorded for this chain.

• Molecule 36: NADH UBIQUINONE OXIDOREDUCTASE

Chain m: 

There are no outlier residues recorded for this chain.

• Molecule 37: NADH UBIQUINONE OXIDOREDUCTASE

Chain n: 

There are no outlier residues recorded for this chain.

• Molecule 38: NADH UBIQUINONE OXIDOREDUCTASE

Chain o: 100%

There are no outlier residues recorded for this chain.

• Molecule 39: NADH UBIQUINONE OXIDOREDUCTASE

Chain q: 100%

There are no outlier residues recorded for this chain.

• Molecule 40: NADH UBIQUINONE OXIDOREDUCTASE

Chain r: 100%

There are no outlier residues recorded for this chain.

• Molecule 41: NADH UBIQUINONE OXIDOREDUCTASE

Chain t: 100%

There are no outlier residues recorded for this chain.

• Molecule 42: NADH UBIQUINONE OXIDOREDUCTASE

Chain u: 35% 65%

X1 X15 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

• Molecule 43: NADH UBIQUINONE OXIDOREDUCTASE

Chain v: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25492	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81495	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.635	Depositor
Minimum map value	-0.698	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	480.76, 480.76, 480.76	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.717, 1.717, 1.717	Depositor

5 Model quality

5.1 Standard geometry

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
2	B	1.57	1/21 (4.8%)	2.68	2/23 (8.7%)
5	E	0.77	0/20	1.59	0/20
6	F	2.57	1/20 (5.0%)	2.24	0/20
7	G	1.04	0/65	1.60	0/67
9	I	2.32	2/40 (5.0%)	1.47	0/40
21	U	0.08	0/4	0.20	0/4
All	All	1.68	4/170 (2.4%)	1.82	2/174 (1.1%)

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
2	B	0	2
3	C	0	1
4	D	0	1
6	F	0	2
7	G	0	6
9	I	0	1
12	L	0	4
14	N	0	2
15	O	0	2
16	P	0	3
17	Q	0	1
19	S	0	1
23	W	0	1
24	X	0	1
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	405	CYS	CA-CB	-8.99	1.34	1.53
9	I	87	CYS	CA-CB	7.91	1.71	1.53
9	I	77	CYS	CA-CB	6.99	1.69	1.53
2	B	55	CYS	CA-CB	5.36	1.65	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	55	CYS	CA-CB-SG	-9.60	96.72	114.00
2	B	55	CYS	CB-CA-C	-5.16	100.09	110.40

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	120	UNK	Peptide
2	B	130	UNK	Peptide
3	C	56	UNK	Peptide
4	D	195	UNK	Peptide
6	F	96	UNK	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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
2	B	4/143 (3%)	3 (75%)	0	1 (25%)	0 1
5	E	4/159 (2%)	3 (75%)	1 (25%)	0	100 100
6	F	4/411 (1%)	4 (100%)	0	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	12/538 (2%)	9 (75%)	1 (8%)	2 (17%)	0 3
9	I	8/162 (5%)	7 (88%)	0	1 (12%)	0 5
All	All	32/1413 (2%)	26 (81%)	2 (6%)	4 (12%)	1 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	119	CYS
7	G	105	CYS
9	I	116	CYS
7	G	156	CYS

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
2	B	4/4 (100%)	2 (50%)	2 (50%)	0 0
5	E	4/4 (100%)	4 (100%)	0	100 100
6	F	4/4 (100%)	3 (75%)	1 (25%)	0 4
7	G	12/12 (100%)	8 (67%)	4 (33%)	0 2
9	I	8/8 (100%)	7 (88%)	1 (12%)	4 21
All	All	32/32 (100%)	24 (75%)	8 (25%)	2 4

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	119	CYS
7	G	69	CYS
7	G	52	CYS
7	G	41	CYS
7	G	55	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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)

8 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	$\#\|Z\| > 2$
44	SF4	I	222	9	0,12,12	-	-	-		
44	SF4	B	201	2	0,12,12	-	-	-		
44	SF4	G	802	7	0,12,12	-	-	-		
45	FES	E	201	5	0,4,4	-	-	-		
44	SF4	G	801	7	0,12,12	-	-	-		
44	SF4	I	223	9	0,12,12	-	-	-		
44	SF4	F	508	6	0,12,12	-	-	-		
45	FES	G	804	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
44	SF4	I	222	9	-	-	0/6/5/5
44	SF4	B	201	2	-	-	0/6/5/5
44	SF4	G	802	7	-	-	0/6/5/5
45	FES	E	201	5	-	-	0/1/1/1
44	SF4	G	801	7	-	-	0/6/5/5
44	SF4	I	223	9	-	-	0/6/5/5
44	SF4	F	508	6	-	-	0/6/5/5
45	FES	G	804	7	-	-	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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	G	6
12	L	5
15	O	3
10	J	2
16	P	2
8	H	2
20	T	2
1	A	1
14	N	1
13	M	1
17	Q	1

The worst 5 of 26 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	23:UNK	C	52:UNK	N	39.81
1	J	107:UNK	C	140:UNK	N	30.90
1	N	300:UNK	C	320:UNK	N	26.56
1	P	250:UNK	C	285:UNK	N	26.48
1	L	466:UNK	C	487:UNK	N	23.59

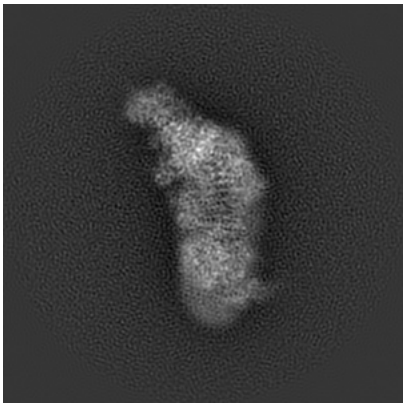
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2676. These allow visual inspection of the internal detail of the map and identification of artifacts.

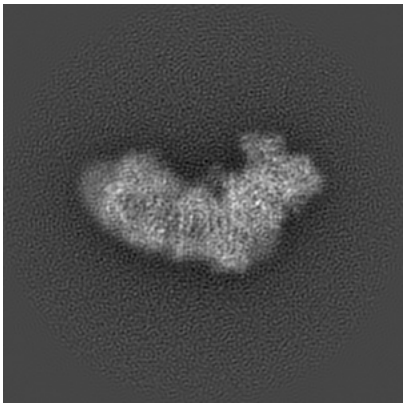
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

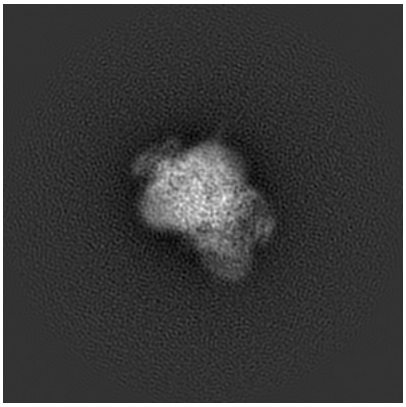
6.1.1 Primary map



X



Y

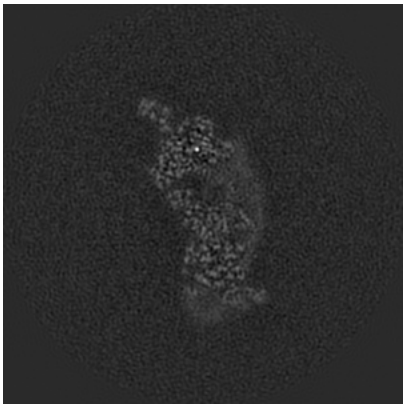


Z

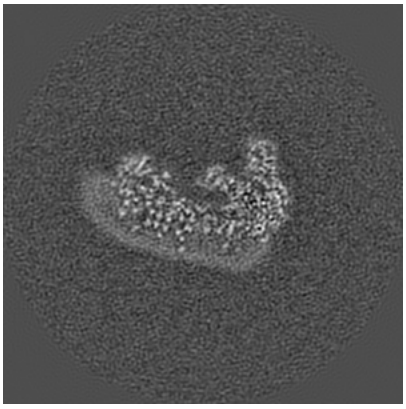
The images above show the map projected in three orthogonal directions.

6.2 Central slices

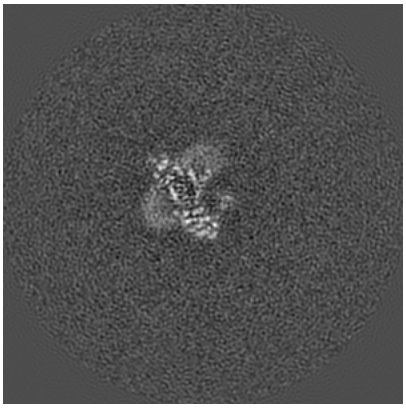
6.2.1 Primary map



X Index: 140



Y Index: 140

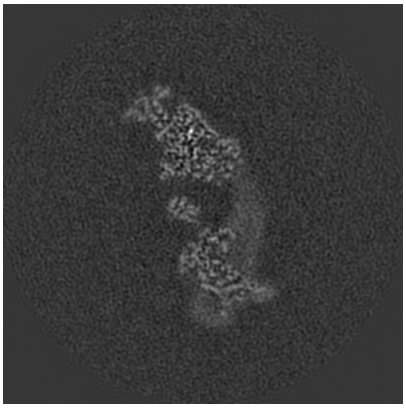


Z Index: 140

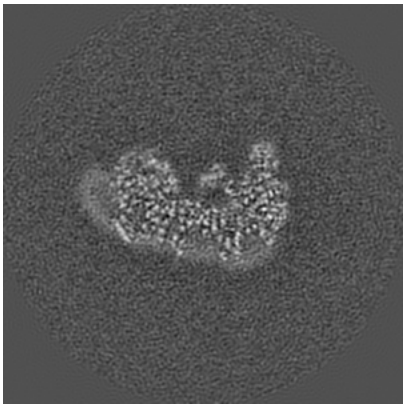
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

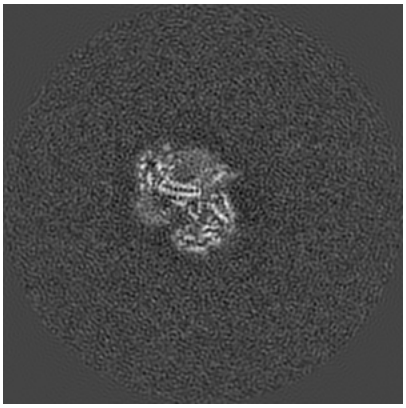
6.3.1 Primary map



X Index: 148



Y Index: 144



Z Index: 160

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

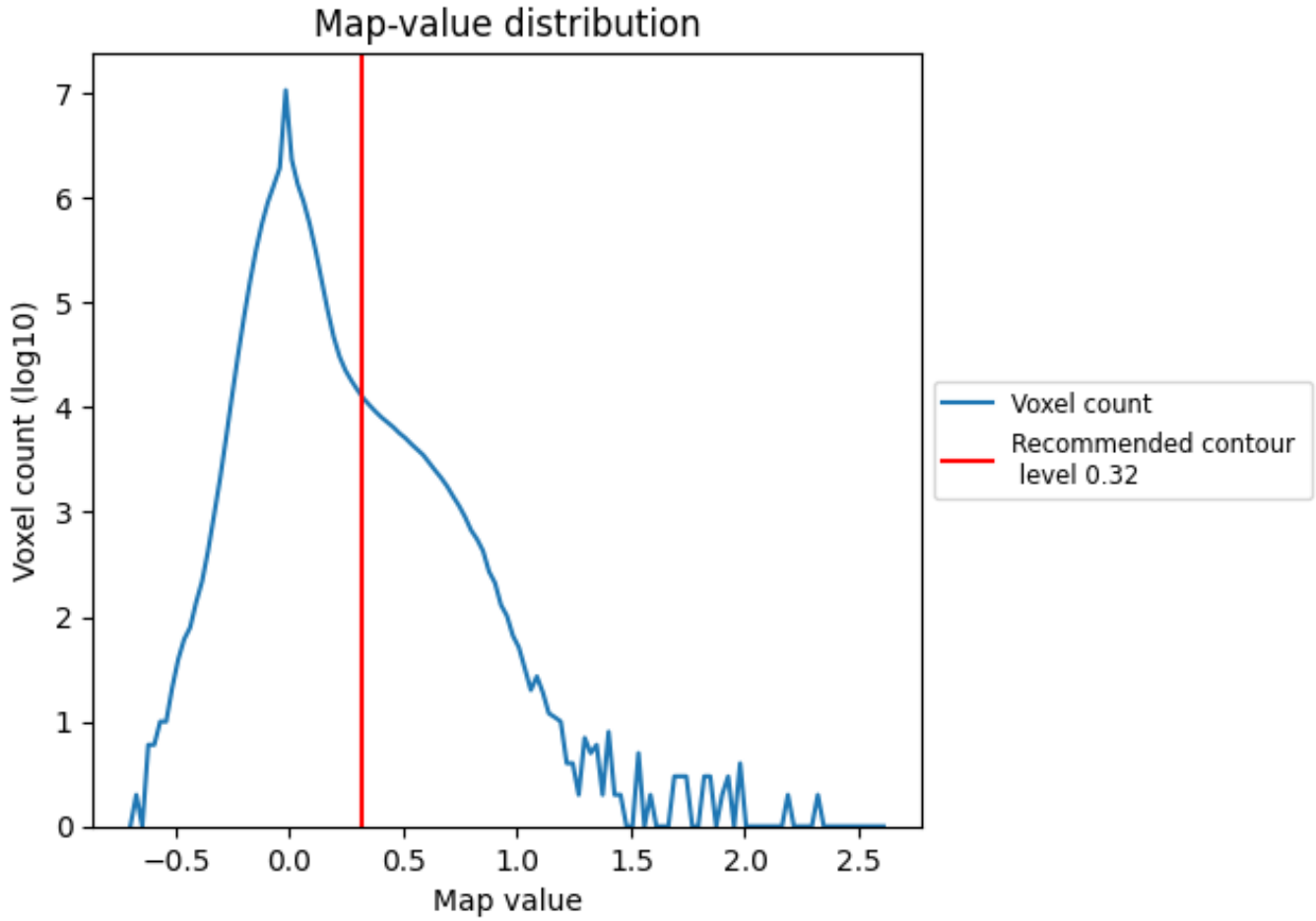
6.5 Mask visualisation (i)

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

7 Map analysis

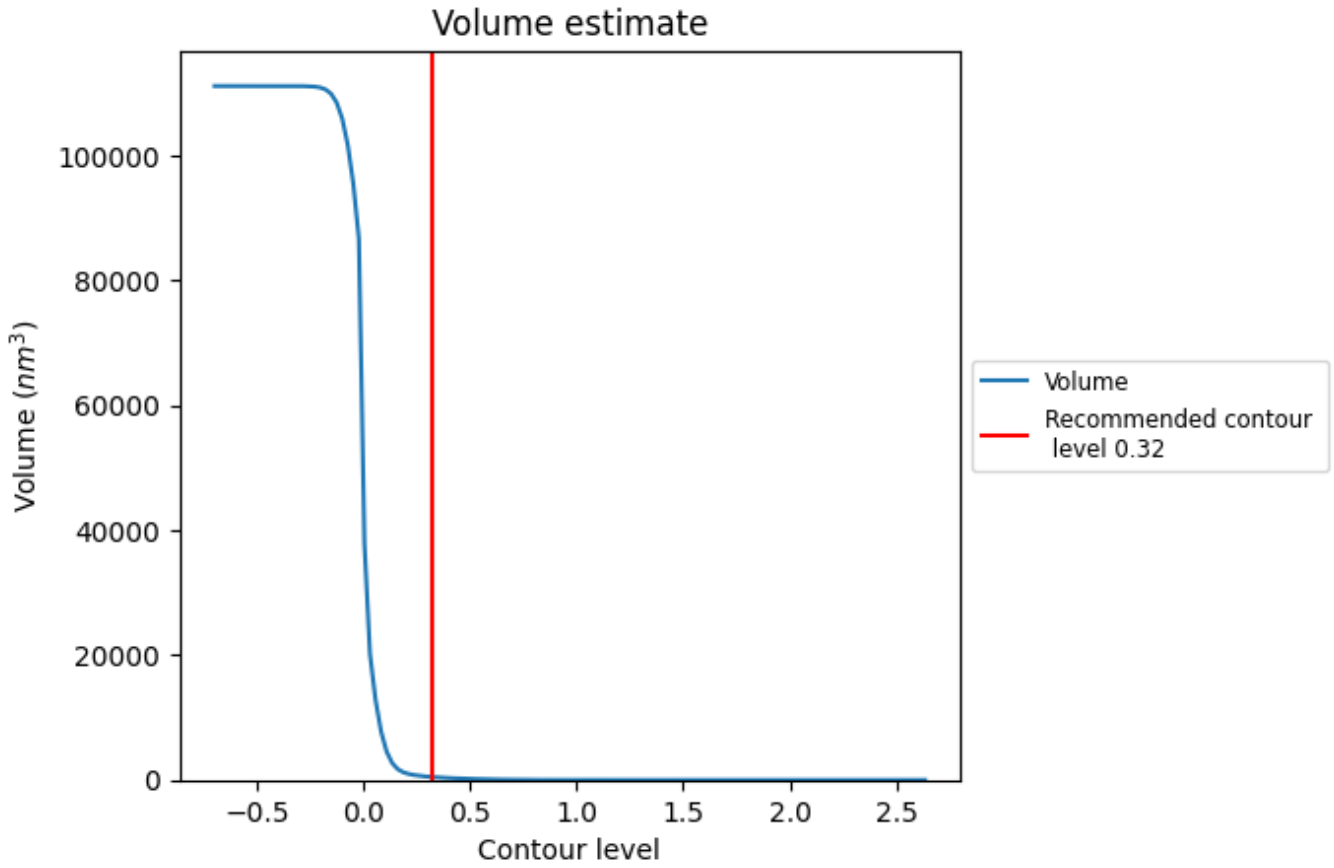
This section contains the results of statistical analysis of the map.

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.

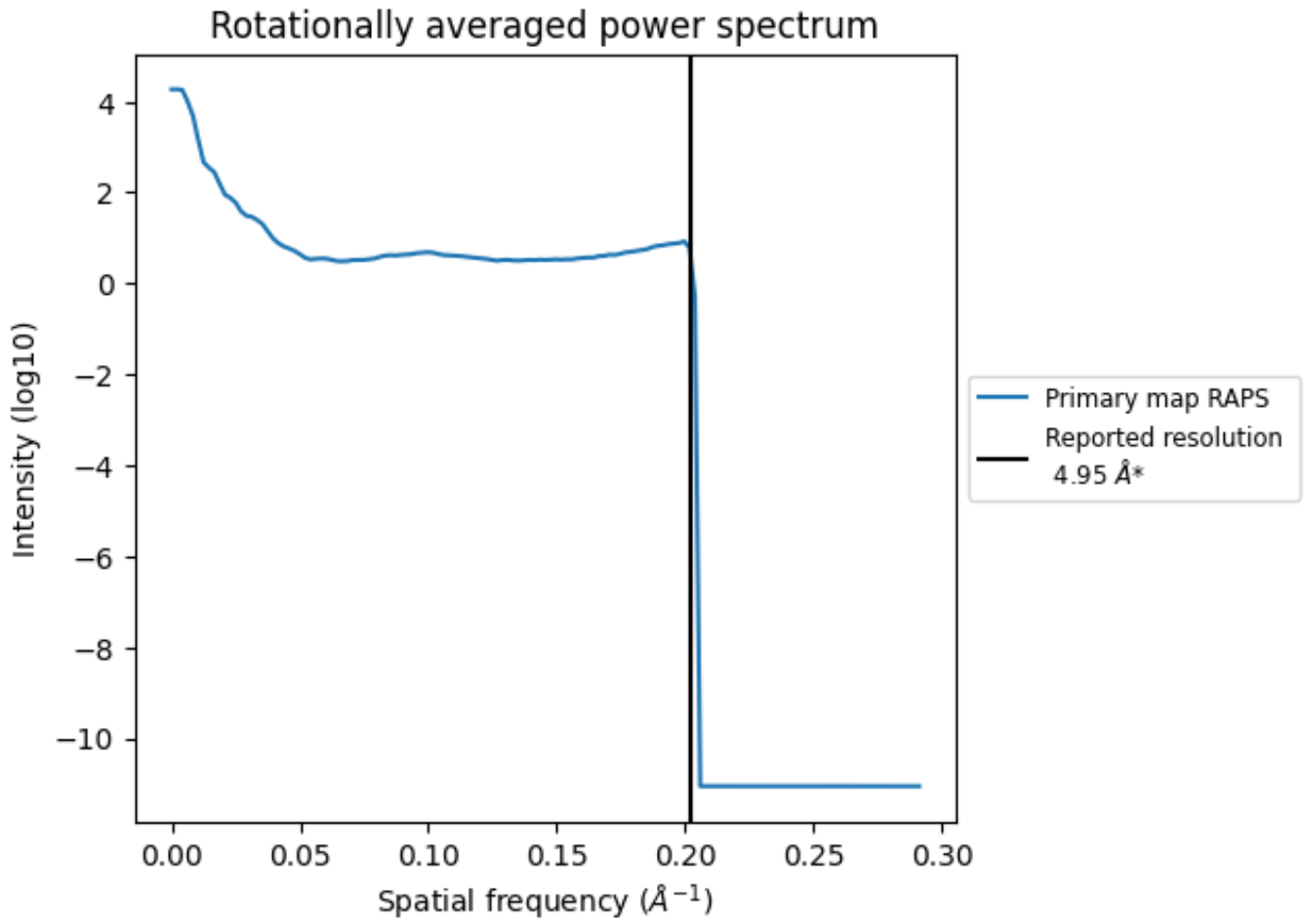
7.2 Volume estimate (i)



The volume at the recommended contour level is 480 nm^3; this corresponds to an approximate mass of 433 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)

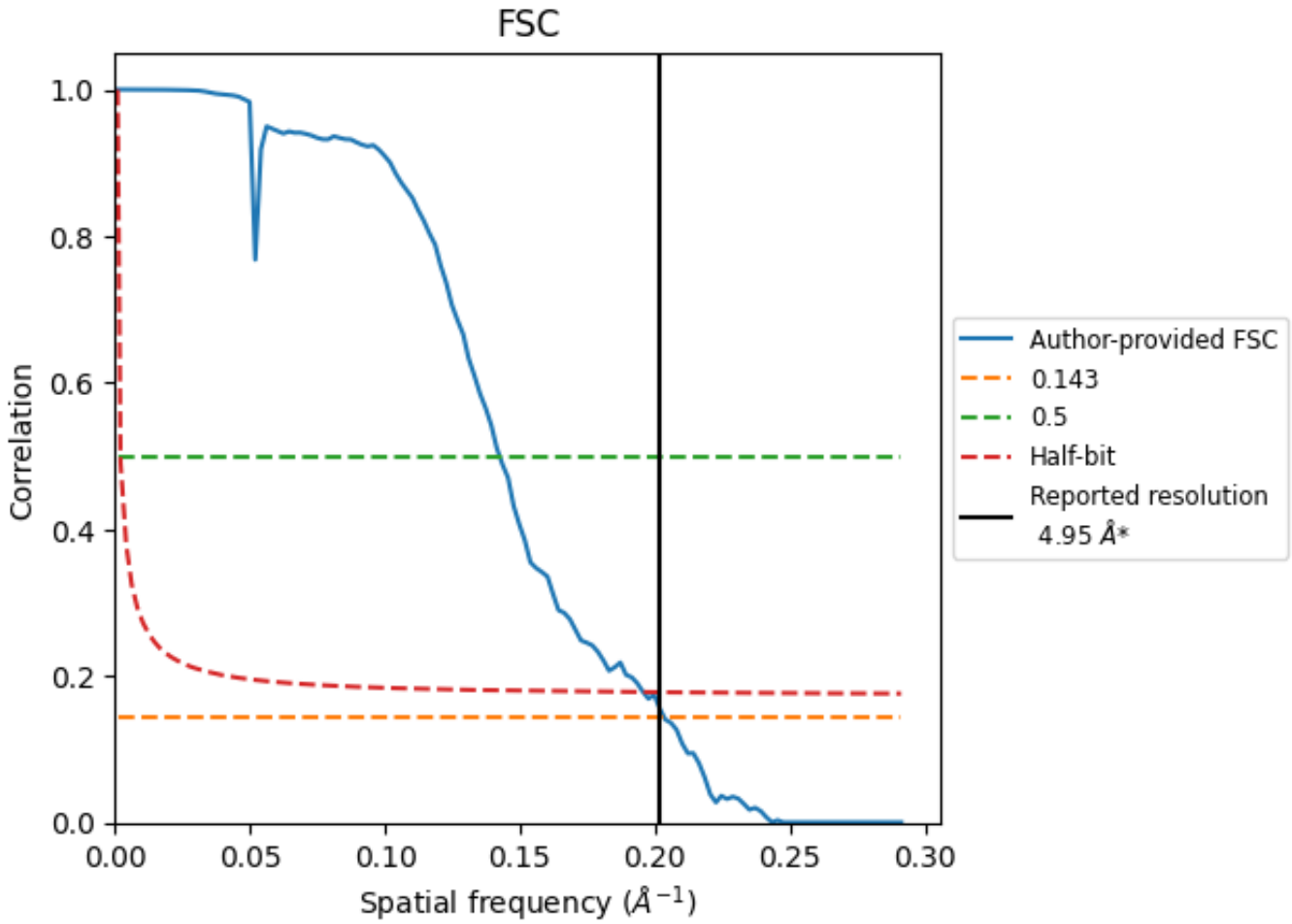


*Reported resolution corresponds to spatial frequency of 0.202 Å^{-1}

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 0.202 Å^{-1}

8.2 Resolution estimates (i)

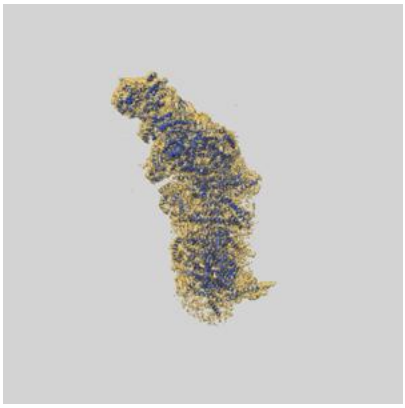
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	4.91	7.02	5.11
Unmasked-calculated*	-	-	-

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

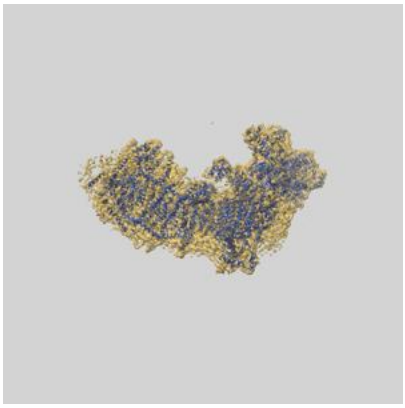
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2676 and PDB model 4UQ8. Per-residue inclusion information can be found in section 3 on page 14.

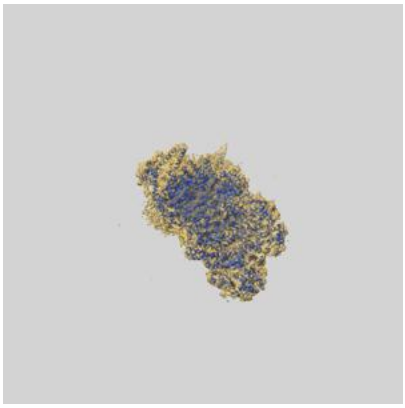
9.1 Map-model overlay



X



Y



Z

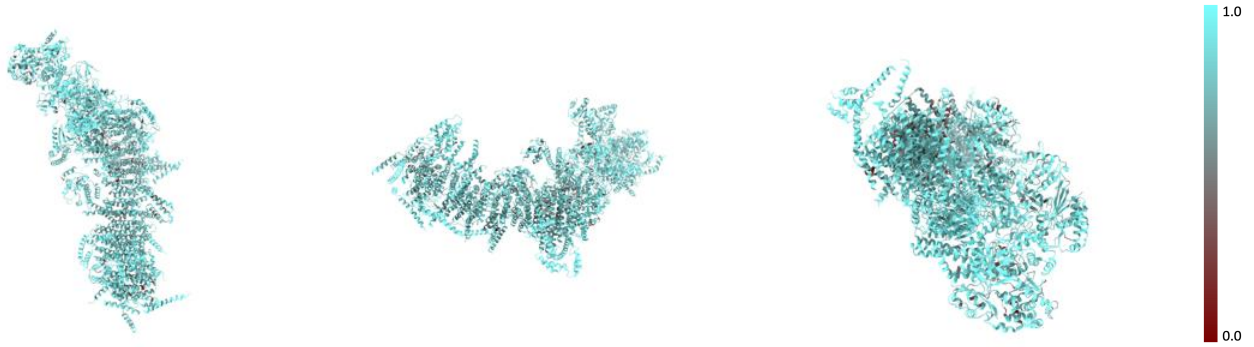
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

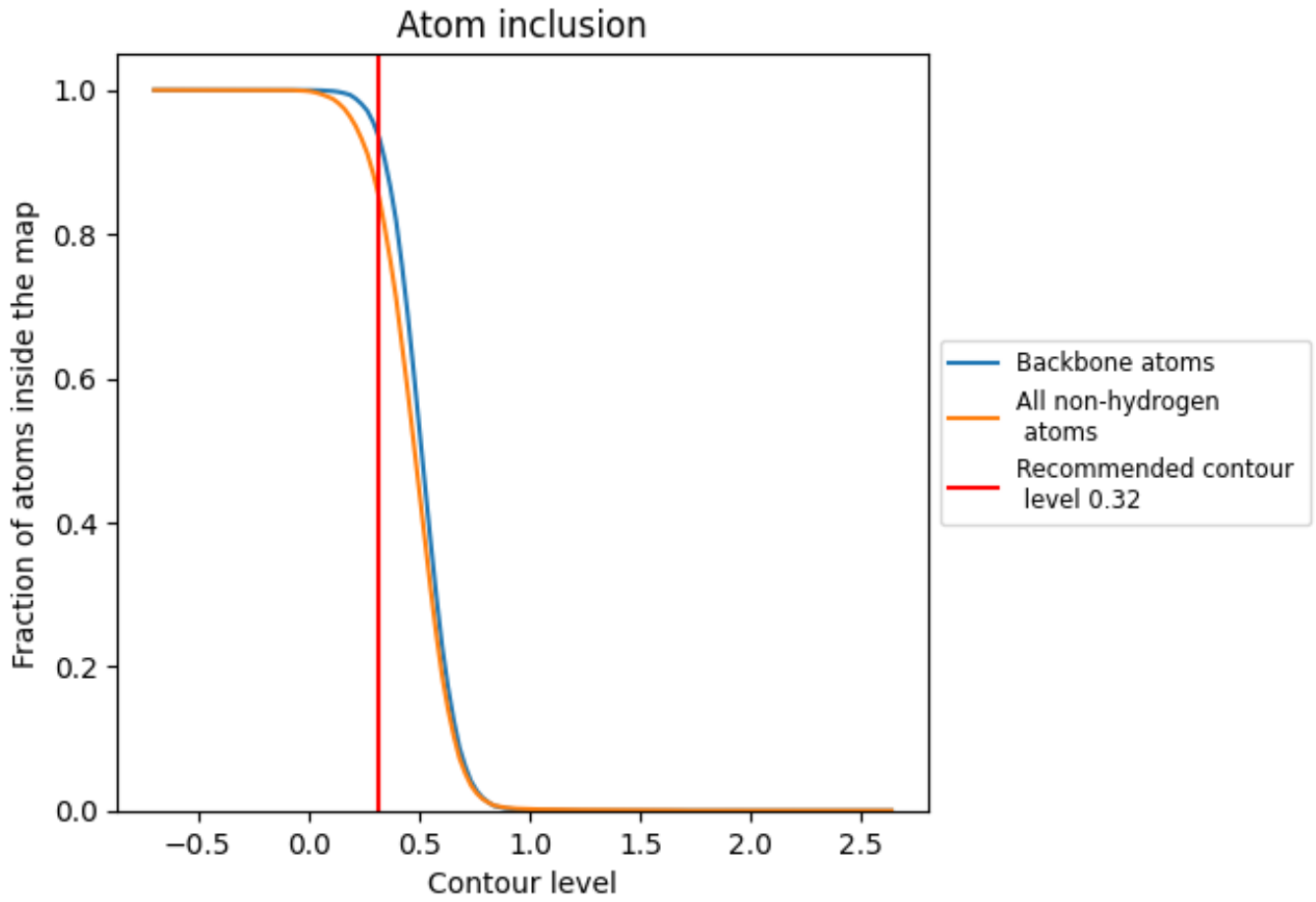
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.32).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 85% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8495	0.3380
A	0.8265	0.3350
B	0.8514	0.3690
C	0.8831	0.3740
D	0.8589	0.3640
E	0.8842	0.3210
F	0.8326	0.3090
G	0.8577	0.3450
H	0.8379	0.3480
I	0.8813	0.3560
J	0.7588	0.3100
K	0.8286	0.3460
L	0.8201	0.3330
M	0.8601	0.3680
N	0.8301	0.3350
O	0.8519	0.3390
P	0.8135	0.3160
Q	0.8928	0.3930
R	0.8809	0.3670
S	0.8675	0.2910
T	0.7831	0.2790
U	0.8320	0.3170
V	0.8930	0.3260
W	0.8361	0.3030
X	0.9165	0.3250
Y	0.7509	0.2980
Z	0.9046	0.3250
a	0.7793	0.3300
b	0.8571	0.3410
c	0.8741	0.3360
d	0.9077	0.3510
e	0.7700	0.3010
f	0.8667	0.3110
g	0.9273	0.3790
h	0.8333	0.3380

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Chain	Atom inclusion	Q-score
i	0.8667	0.3190
j	0.8917	0.3340
k	0.7929	0.2940
l	0.8750	0.3140
m	0.8706	0.3350
n	0.9119	0.3390
o	0.9333	0.3190
p	0.9357	0.3420
q	0.8960	0.3080
r	0.9615	0.3830
s	0.9429	0.3610
t	0.9298	0.3620
u	0.9600	0.3750
v	0.9375	0.3070
w	0.9111	0.3270