

Full wwPDB EM Validation Report (i)

Dec 17, 2022 – 06:40 pm GMT

PDB ID : 6ZJN

EMDB ID : EMD-11237

Title: Respiratory complex I from Thermus thermophilus, NADH dataset, minor

state

Authors : Kaszuba, K.; Tambalo, M.; Gallagher, G.T.; Sazanov, L.A.

Deposited on : 2020-06-29

Resolution : 6.10 Å(reported)

Based on initial model : 6Y11

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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 (i)) 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)

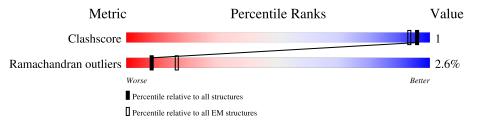
Validation Pipeline (wwPDB-VP) : 2.31.3

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 6.10 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
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 <=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	96%	·
2	2	181	96%	
3	3	783	91%	5% •
4	4	409	90%	• 6%
5	5	207	91%	• 5%
6	6	181	86%	6% • 8%
7	9	182	90%	7% ••
8	7	129	92%	6% •
9	A	119	28%	

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Mol	Chain	Length	Quality of chain	
10	т	176	6%	
10	J	176	87%	9%
11	K	95	98%	
			19%	
12	L	606	97%	•
	3.5		12%	
13	M	469	96%	•
			9%	
14	N	427	97%	•
			11%	
15	Н	365	91%	5% • •

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	3	802	-	-	X	-
16	SF4	6	201	-	-	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.

\mathbf{Mol}	Chain	Residues		Ator	$\mathbf{n}\mathbf{s}$		AltConf	Trace
1	1	437	Total 2136	C 1262	N 437	O 437	0	0

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

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

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

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

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

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

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

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

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

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



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

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

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

Mol	Chain	Residues		Ato	ms		AltConf	Trace
8	7	127	Total	С	N	О	0	0
	'	121	628	374	127	127		

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

\mathbf{Mol}	Chain	Residues		Ato	ms		AltConf	Trace
9	A	117	Total 570	C 336	N 117	O 117	0	0

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

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

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

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

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

Mol	Chain	Residues		Ator	$\mathbf{n}\mathbf{s}$		AltConf	Trace
12	L	605	Total 2955	C 1745	N 605	O 605	0	0

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

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

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

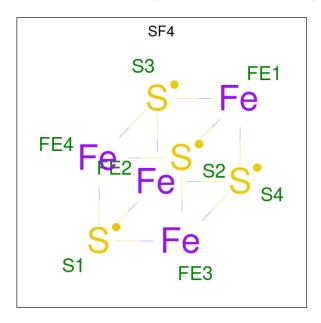


Mol	Chain	Residues		Ator	$\mathbf{n}\mathbf{s}$		AltConf	Trace
14	N	427	Total 2092	C 1238	N 427	O 427	0	0

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

I	Mol	Chain	Residues		Ator	ns		AltConf	Trace
	15	Н	353	Total 1741	C 1035	N 353	O 353	0	0

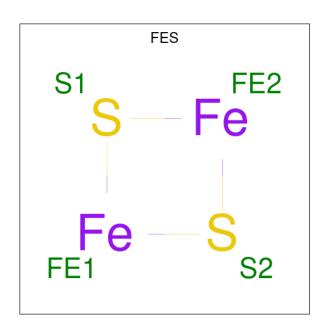
 \bullet Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

 $\bullet \ \ \ \ Molecule\ 17\ is\ FE2/S2\ (INORGANIC)\ CLUSTER\ (three-letter\ code:\ FES)\ (formula:\ Fe_2S_2).$





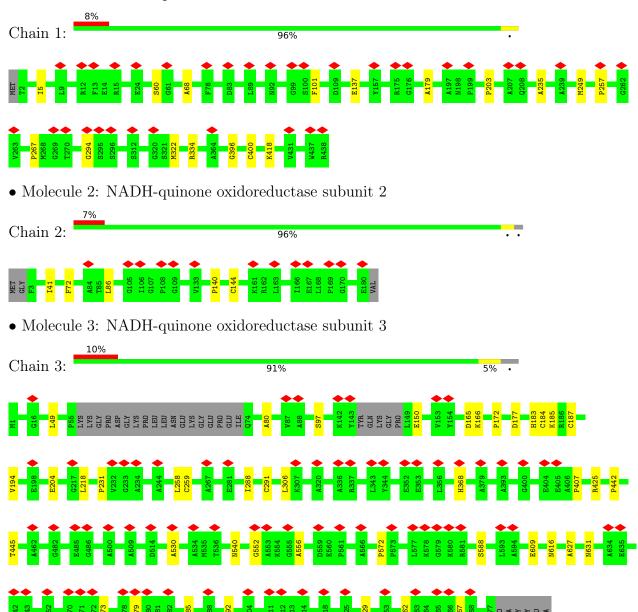
Mol	Chain	Residues	Atoms	AltConf
17	9	1	Total Fe S	0
11	2	1	$4 \qquad 2 2$	0
17	2	1	Total Fe S	0
11	3	1	$4 \qquad 2 2$	0



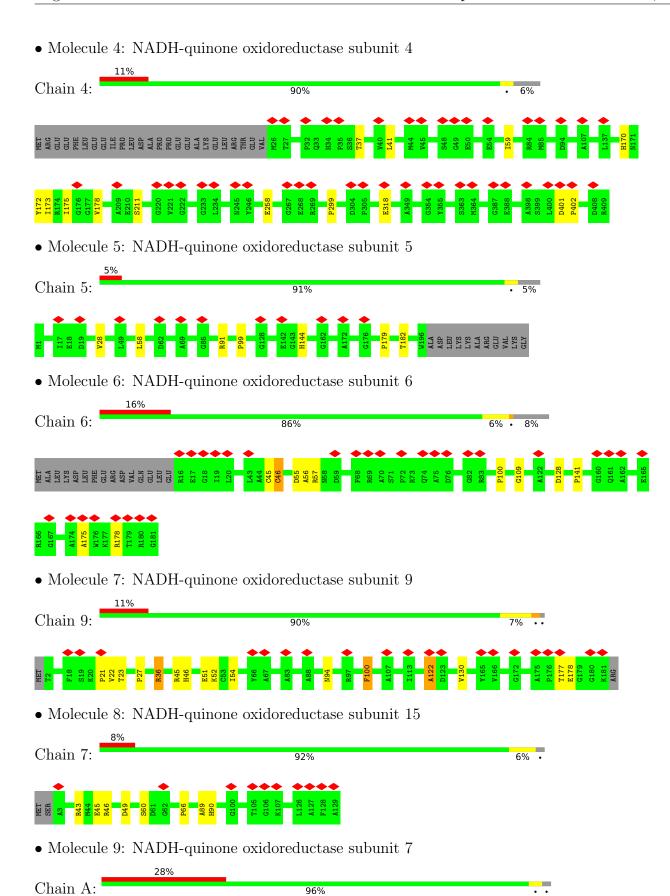
3 Residue-property plots (i)

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

• Molecule 1: NADH-quinone oxidoreductase subunit 1





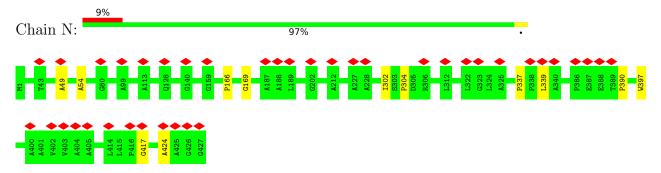




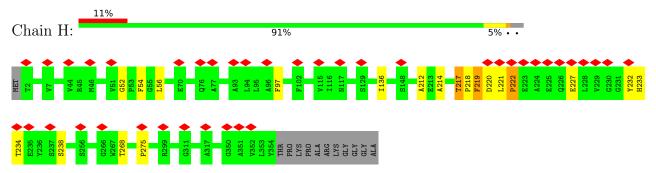




• Molecule 14: NADH-quinone oxidoreductase subunit 14



• Molecule 15: NADH-quinone oxidoreductase subunit 8





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	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	0.606	Depositor
Minimum map value	-0.190	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.143	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: FES, SF4

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	В	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	1	1.08	0/2135	1.16	0/2958
2	2	1.06	0/874	1.15	0/1213
3	3	1.06	0/3711	1.22	5/5157 (0.1%)
4	4	1.11	0/1889	1.15	0/2625
5	5	1.08	0/960	1.22	1/1331 (0.1%)
6	6	1.11	0/817	1.27	3/1135 (0.3%)
7	9	1.14	0/884	1.31	4/1227 (0.3%)
8	7	1.11	0/627	1.25	0/872
9	A	1.00	0/569	1.07	0/786
10	J	1.11	0/782	1.04	2/1083 (0.2%)
11	K	1.06	0/466	1.02	0/646
12	L	0.98	0/2954	1.07	0/4092
13	M	1.06	0/2275	1.07	0/3148
14	N	1.07	0/2091	1.04	0/2900
15	Н	1.08	0/1740	1.14	2/2420 (0.1%)
All	All	1.07	0/22774	1.14	17/31593 (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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2
3	3	0	4
6	6	0	3
7	9	0	3
10	J	0	2
11	K	0	1
12	L	0	2
13	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	1
15	Н	0	6
All	All	0	25

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
15	Н	220	ASP	N-CA-C	-6.18	94.30	111.00
3	3	259	CYS	N-CA-CB	5.87	121.17	110.60
7	9	100	PHE	CA-C-N	-5.86	104.32	117.20
3	3	291	CYS	N-CA-CB	5.85	121.13	110.60
10	J	36	PHE	CB-CA-C	-5.82	98.75	110.40
7	9	122	ALA	N-CA-CB	5.77	118.17	110.10
6	6	46	CYS	CB-CA-C	-5.54	99.32	110.40
7	9	36	ARG	N-CA-C	-5.53	96.07	111.00
15	Н	219	PHE	N-CA-CB	5.53	120.55	110.60
3	3	150	GLU	N-CA-CB	5.45	120.41	110.60
6	6	45	CYS	CB-CA-C	5.42	121.23	110.40
5	5	144	HIS	N-CA-C	-5.37	96.50	111.00
3	3	259	CYS	N-CA-C	-5.37	96.51	111.00
3	3	692	PHE	N-CA-C	-5.25	96.84	111.00
10	J	5	GLU	N-CA-CB	-5.15	101.33	110.60
6	6	178	ARG	N-CA-C	-5.04	97.39	111.00
7	9	178	GLU	N-CA-C	-5.02	97.46	111.00

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	203	PRO	Peptide
1	1	396	GLY	Peptide
3	3	183	HIS	Mainchain
3	3	185	LYS	Mainchain
3	3	258	LEU	Mainchain, Peptide
6	6	100	PRO	Peptide
6	6	175	ALA	Peptide
6	6	55	ASP	Peptide
7	9	100	PHE	Mainchain, Peptide
7	9	177	THR	Peptide
15	Н	217	THR	Mainchain, Peptide

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Mol	Chain	Res	Type	Group
15	Н	219	PHE	Peptide
15	Н	221	LEU	Peptide
15	Н	222	PRO	Peptide
15	Н	227	GLU	Peptide
10	J	74	LEU	Mainchain
10	J	83	PHE	Peptide
11	K	50	GLY	Peptide
12	L	27	PRO	Peptide
12	L	462	PRO	Peptide
13	M	414	PHE	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	990	3	0
2	2	875	0	398	1	0
3	3	3714	0	1784	8	0
4	4	1890	0	833	1	0
5	5	961	0	427	1	0
6	6	818	0	388	4	0
7	9	885	0	408	4	0
8	7	628	0	300	1	0
9	A	570	0	280	0	0
10	J	783	0	409	1	0
11	K	467	0	248	0	0
12	L	2955	0	1499	1	0
13	M	2276	0	1200	2	0
14	N	2092	0	1120	2	0
15	Н	1741	0	818	3	0
16	1	8	0	0	1	0
16	3	24	0	0	2	0
16	6	8	0	0	3	0
16	9	16	0	0	0	0
17	2	4	0	0	0	0
17	3	4	0	0	0	0
All	All	22855	0	11102	31	0



The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 1.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
10:J:49:ARG:H	10:J:122:GLY:HA3	1.64	0.63
6:6:46:CYS:HA	16:6:201:SF4:S1	2.44	0.57
3:3:609:GLU:HA	3:3:627:ALA:H	1.70	0.56
15:H:52:GLY:HA2	15:H:56:LEU:H	1.72	0.54
1:1:400:CYS:CB	16:1:501:SF4:S2	2.95	0.54
6:6:109:GLY:HA3	16:6:201:SF4:S3	2.48	0.54
3:3:166:LYS:HA	3:3:177:ASP:HA	1.95	0.48
1:1:60:SER:HA	1:1:235:ALA:HB1	1.96	0.48
7:9:45:ARG:HA	7:9:52:LYS:H	1.78	0.48
2:2:41:ILE:H	2:2:72:PHE:HA	1.80	0.47
13:M:307:GLY:HA2	13:M:380:THR:HA	1.96	0.46
1:1:249:MET:HA	1:1:267:PRO:HA	1.97	0.46
4:4:173:ILE:HA	4:4:178:VAL:HA	1.97	0.46
6:6:57:ARG:HA	7:9:23:THR:HA	1.98	0.46
8:7:60:SER:HA	8:7:66:PRO:HA	1.98	0.46
5:5:28:VAL:HA	5:5:91:ARG:O	2.16	0.45
3:3:368:HIS:HA	3:3:552:GLY:H	1.81	0.45
3:3:184:CYS:O	16:3:802:SF4:S4	2.75	0.44
3:3:187:CYS:CB	16:3:802:SF4:S2	3.05	0.44
13:M:46:GLY:HA2	13:M:68:ASP:HA	2.00	0.44
15:H:52:GLY:CA	15:H:56:LEU:H	2.30	0.44
3:3:306:LEU:H	3:3:588:SER:C	2.22	0.43
3:3:762:ALA:HB3	3:3:767:ALA:CB	2.50	0.41
6:6:141:PRO:HA	16:6:201:SF4:S1	2.60	0.41
7:9:46:HIS:H	7:9:51:GLU:HA	1.86	0.41
15:H:212:ALA:C	15:H:214:ALA:H	2.24	0.41
14:N:49:ALA:HA	14:N:54:ALA:HA	2.03	0.40
12:L:353:GLY:HA3	12:L:427:GLY:C	2.42	0.40
3:3:49:LEU:HA	3:3:80:ALA:O	2.22	0.40
7:9:94:ASN:HA	7:9:130:VAL:HA	2.02	0.40
14:N:337:PRO:HA	14:N:339:LEU:H	1.86	0.40

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	Perce	entiles
1	1	435/438 (99%)	384 (88%)	41 (9%)	10 (2%)	6	34
2	2	176/181 (97%)	155 (88%)	18 (10%)	3 (2%)	9	42
3	3	748/783 (96%)	655 (88%)	71 (10%)	22 (3%)	4	29
4	4	382/409 (93%)	339 (89%)	31 (8%)	12 (3%)	4	27
5	5	194/207 (94%)	172 (89%)	18 (9%)	4 (2%)	7	36
6	6	164/181 (91%)	137 (84%)	25 (15%)	2 (1%)	13	50
7	9	178/182 (98%)	157 (88%)	15 (8%)	6 (3%)	3	26
8	7	125/129 (97%)	111 (89%)	8 (6%)	6 (5%)	2	20
9	A	115/119 (97%)	105 (91%)	7 (6%)	3 (3%)	5	31
10	J	158/176 (90%)	141 (89%)	16 (10%)	1 (1%)	25	66
11	K	93/95 (98%)	83 (89%)	9 (10%)	1 (1%)	14	52
12	L	603/606 (100%)	539 (89%)	49 (8%)	15 (2%)	5	32
13	M	465/469 (99%)	410 (88%)	41 (9%)	14 (3%)	4	28
14	N	425/427 (100%)	382 (90%)	36 (8%)	7 (2%)	9	43
15	Н	351/365 (96%)	301 (86%)	38 (11%)	12 (3%)	3	26
All	All	4612/4767 (97%)	4071 (88%)	423 (9%)	118 (3%)	8	31

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	179	ALA
1	1	334	ARG
3	3	288	ILE
4	4	211	SER
6	6	128	ASP
7	9	21	PRO
7	9	36	ARG
7	9	122	ALA

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Mol	Chain	Res	Type				
9	A	46	SER				
12	L	121	ALA				
12	L	436	HIS				
13	M	72	ALA ALA				
13	M	351	ALA				
15	Н	217	THR				
1	1	5	ILE				
1	1	294	GLY				
2	2	86	LEU				
3	3	165	ASP				
3	3	204	GLU				
3	3	530	ALA				
3	3	616	ASN				
3	3	729	PRO				
4	4	37	THR				
4	4	41	LEU				
5	5	58	LEU				
5	5	182	THR				
6	6	56	ALA				
7	9	22	VAL				
8	7	43	ARG				
8	7	90	HIS				
10	J	117	GLN				
12	L	397	PHE				
15	Н	233	HIS				
15	Н	234	THR				
1	1	101	PHE				
1	1	322	MET				
2	2	140	PRO				
3	3	425	ARG				
3	3	631	ASN				
3	3	679	ARG				
4	4	170	HIS				
4	4	172	TYR				
8	7	49	ASP				
8	7	89	ALA				
11	K	94	ARG				
12	L	223	MET				
12	L	346	GLU				
12	L	399	GLY				
12	L	435	PRO				
12	L	519	ALA				
14			ext page				
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Mol	Chain	Res	Type				
13	M	89	ALA				
13	M	90	ARG				
14	N	166	PRO				
14	N	390	PRO				
14	N	424	ALA				
15	Н	54	PHE				
15	Н	232	TYR				
15	Н	238	SER				
15	Н	275	PRO				
1	1	137	GLU				
2	2	144	CYS				
3	3	407	PRO				
3	3	556	ALA				
4	4	299	PRO				
4	4	401	ASP				
8	7	45	GLU				
9	A	38	ARG				
9	A	39	ALA				
12	L	102	SER				
12	L	437	GLU				
12	L	484	HIS				
13	M	44	PRO				
13	M	387	ALA				
13	M	404	ALA				
14	N	397	TRP				
14	N	417	GLY				
15	Н	97	PHE				
1	1	68	ALA				
1	1	418	LYS				
3	3	97	SER				
3	3	231	PRO				
3	3	442	PRO				
3	3	445	THR				
3	3	540	ASN				
4	4	175	ILE				
4	4	258	GLU				
4	4	318	GLU				
4	4	402	PRO				
13	M	222	HIS				
13	M	223	PRO				
13	M	452	ARG				
15	Н	218	PRO				

Continued on next page...



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Mol	Chain	Res	Type
3	3	194	VAL
3	3	572	PRO
3	3	673	MET
3	3	685	PRO
4	4	59	ILE
12	L	347	GLN
12	L	440	PRO
12	L	518	PRO
13	M	236	VAL
13	M	249	ALA
14	N	302	ILE
15	Н	268	THR
12	L	480	VAL
13	M	57	PRO
13	M	360	ILE
14	N	304	PRO
15	Н	222	PRO
1	1	257	PRO
3	3	218	LEU
3	3	172	PRO
7	9	54	ILE
8	7	46	ARG
5	5	99	PRO
5	5	179	PRO
15	Н	136	ILE
7	9	27	PRO

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	В	ond leng	$_{ m gths}$	В	ond angles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	$\mid \text{RMSZ} \mid \# Z > 2$
16	SF4	1	501	-	0,12,12	-	-	-	
17	FES	2	201	-	0,4,4	-	-	-	
16	SF4	3	802	_	0,12,12	-	-	-	
17	FES	3	804	-	0,4,4	-	-	-	
16	SF4	9	202	7	0,12,12	-	-	-	
16	SF4	3	801	-	0,12,12	-	-	-	
16	SF4	3	803	-	0,12,12	-	-	-	
16	SF4	6	201	6	0,12,12	-	-	-	
16	SF4	9	201	-	0,12,12	-	-	-	

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

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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	501	SF4	1	0
16	3	802	SF4	2	0
16	6	201	SF4	3	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.



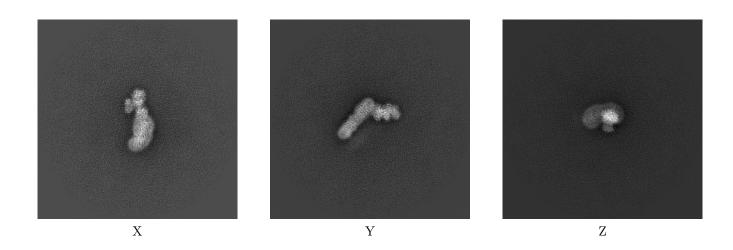
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11237. 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)

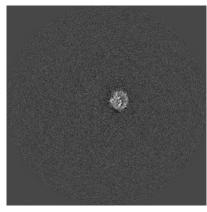
6.2.1 Primary map







Y Index: 256



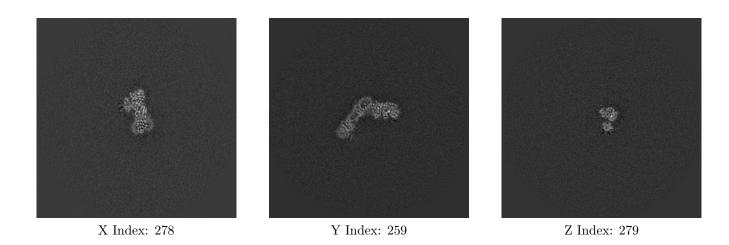
Z Index: 256



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

6.3 Largest variance slices (i)

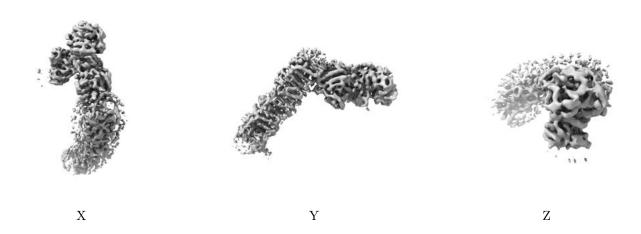
6.3.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.143. 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)

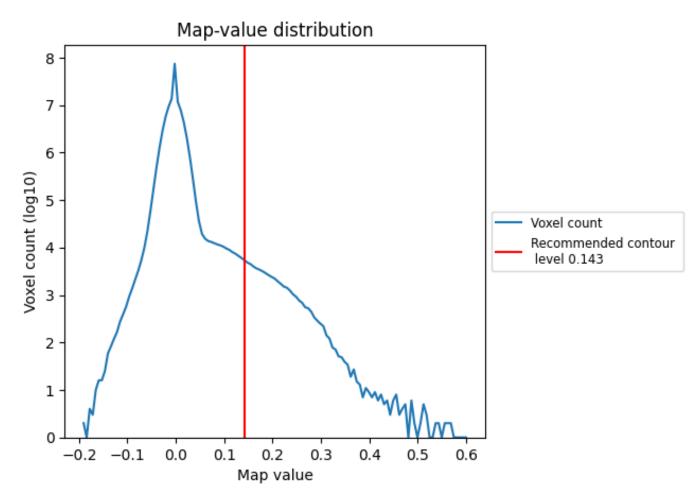
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

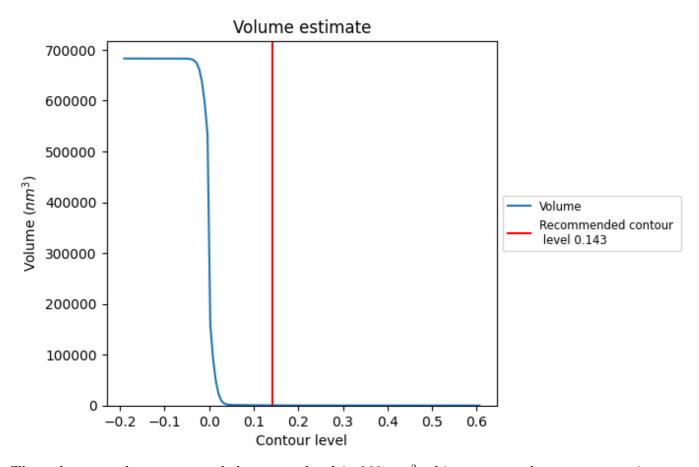
7.1 Map-value distribution (i)



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)

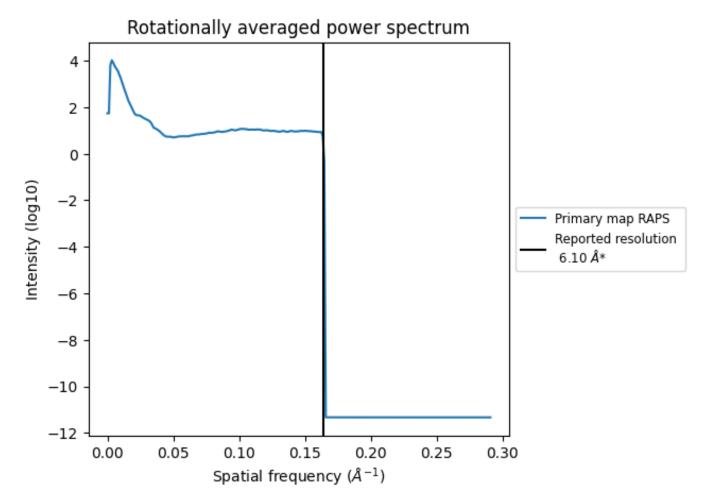


The volume at the recommended contour level is $268~\mathrm{nm^3}$; this corresponds to an approximate mass of $242~\mathrm{kDa}$.

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)



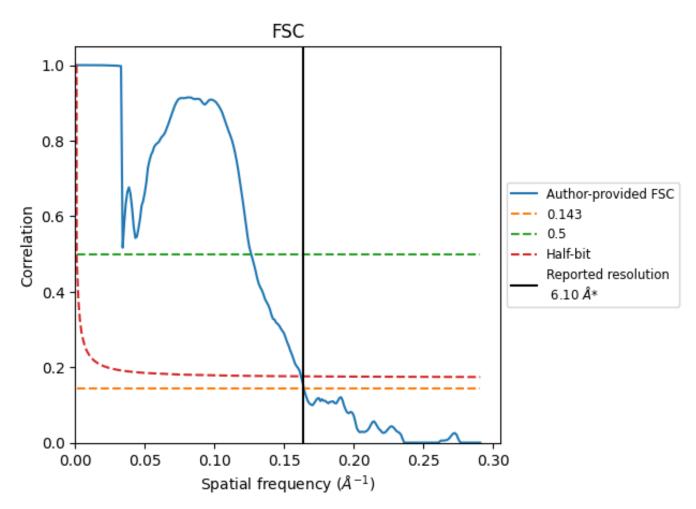
^{*}Reported resolution corresponds to spatial frequency of 0.164 $\rm \mathring{A}^{-1}$



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 0.164 $\rm \mathring{A}^{-1}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	6.10	-	-	
Author-provided FSC curve	6.09	7.92	6.17	
Unmasked-calculated*	-	-	-	

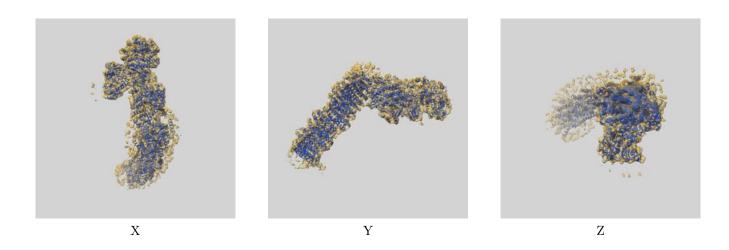
^{*}Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11237 and PDB model 6ZJN. Per-residue inclusion information can be found in section 3 on page 8.

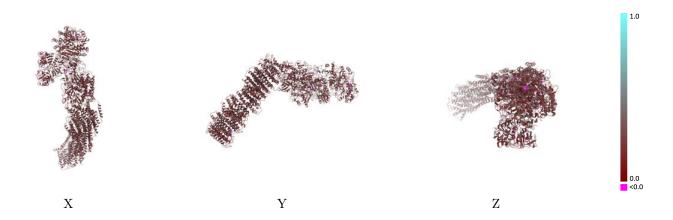
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.143 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.

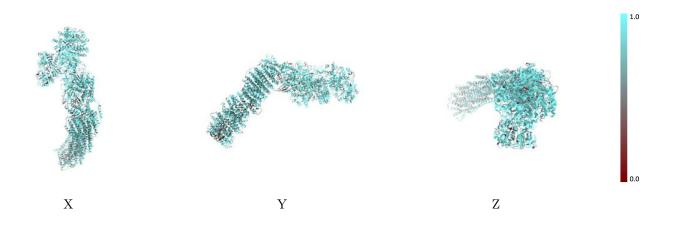


9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according 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.

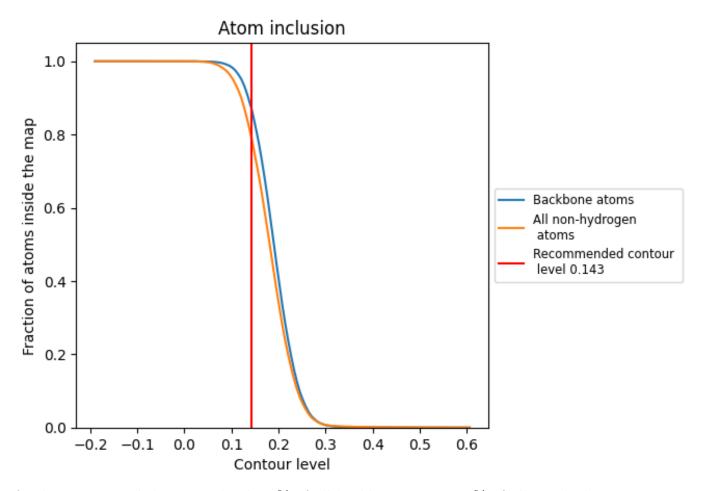
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.143).



9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.143) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7887	0.2760
1	0.8493	0.2630
2	0.8555	0.2820
3	0.8092	0.2760
4	0.7952	0.2830
5	0.8626	0.3090
6	0.7567	0.2630
7	0.8408	0.2970
9	0.8291	0.2760
A	0.6175	0.2580
Н	0.7794	0.2790
J	0.7727	0.2950
K	0.8158	0.2910
L	0.7208	0.2580
M	0.7707	0.2730
N	0.7715	0.2860



