Full wwPDB EM Validation Report ⓘ

Mar 1, 2023 – 10:13 AM JST

PDB ID	:	7FJQ
EMDB ID	:	EMD-31627
Title	:	Cryo EM structure of lysosomal ATPase
Authors	:	Zhang, S.S.
Deposited on	:	2021-08-04
Resolution	:	3.60 Å(reported)

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:

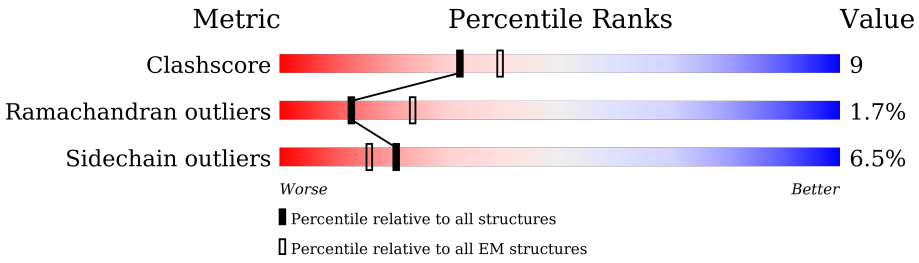
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1153	21% 62% 18% · 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7086 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.

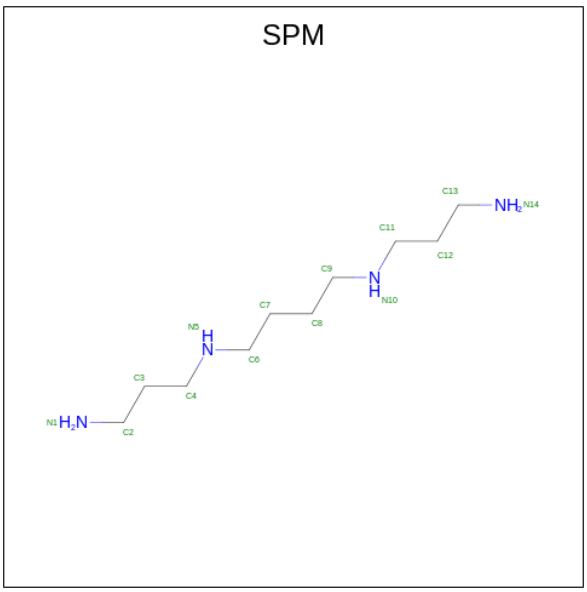
- Molecule 1 is a protein called Polyamine-transporting ATPase 13A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	973	7072	4560	1199	1269	44	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TRP	deletion	UNP Q9NQ11
A	?	-	VAL	deletion	UNP Q9NQ11
A	?	-	LEU	deletion	UNP Q9NQ11
A	?	-	GLU	deletion	UNP Q9NQ11
A	?	-	GLU	deletion	UNP Q9NQ11
A	?	-	GLU	deletion	UNP Q9NQ11
A	?	-	PRO	deletion	UNP Q9NQ11
A	?	-	ALA	deletion	UNP Q9NQ11
A	?	-	ALA	deletion	UNP Q9NQ11
A	?	-	ASP	deletion	UNP Q9NQ11
A	?	-	SER	deletion	UNP Q9NQ11
A	?	-	ALA	deletion	UNP Q9NQ11
A	?	-	PHE	deletion	UNP Q9NQ11
A	?	-	GLY	deletion	UNP Q9NQ11
A	?	-	THR	deletion	UNP Q9NQ11
A	?	-	GLN	deletion	UNP Q9NQ11
A	?	-	VAL	deletion	UNP Q9NQ11
A	?	-	LEU	deletion	UNP Q9NQ11
A	?	-	ALA	deletion	UNP Q9NQ11
A	?	-	VAL	deletion	UNP Q9NQ11
A	?	-	MET	deletion	UNP Q9NQ11
A	?	-	ARG	deletion	UNP Q9NQ11
A	?	-	PRO	deletion	UNP Q9NQ11
A	?	-	PRO	deletion	UNP Q9NQ11
A	?	-	LEU	deletion	UNP Q9NQ11
A	?	-	TRP	deletion	UNP Q9NQ11
A	?	-	GLU	deletion	UNP Q9NQ11

- Molecule 2 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



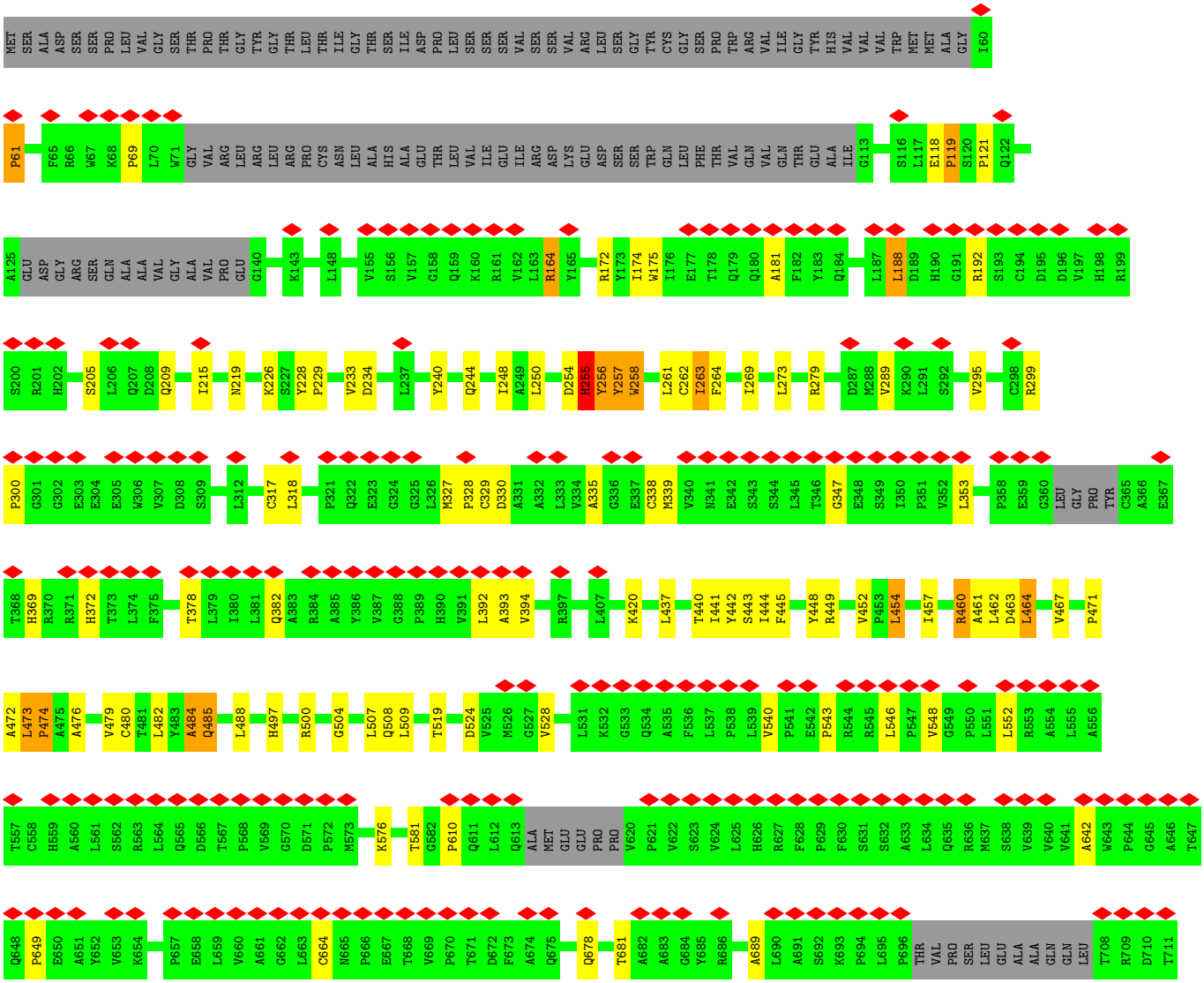
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
2	A	1	14	10	4	0

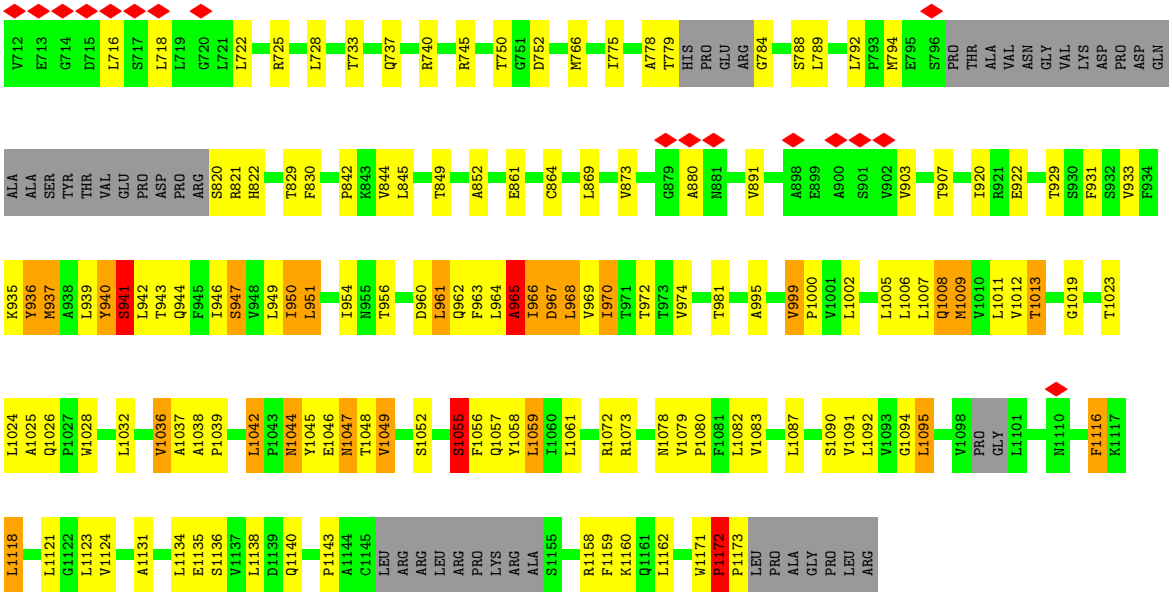
3 Residue-property plots (i)

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: Polyamine-transporting ATPase 13A2

Chain A:




V712 E713 G714 D715 L716 S717 L718 L719 G720 L721 L722 R725 L728 T733 Q737 R740 R745 T750 G751 D752 M766 I775 A778 T779 HIS PRO GLU ARG G784 S788 L789 L792 P793 M794 E795 S796 PRO THR ALA VAL ASN GLY VAL LYS ASP PRO ASP GLN
ALA ALA SER TYR THR VAL GLU PRO ASP PRO ARG S820 R821 H822 T829 F830 P842 K843 V844 L845 T849 A852 E861 C864 L869 V873 G879 A880 N881 V891 A898 E899 A900 S901 V902 V903 T907 I920 R921 E922 T929 S930 F931 S932 V933 F934
K935 Y936 M937 A938 L939 Y940 S941 L942 T943 Q944 F945 I946 S947 V948 L949 I950 L951 I954 N955 T956 D960 L961 Q962 F963 L964 A965 I966 D967 L968 V969 I970 T971 T972 T973 V974 T981 A995 V999 P1000 V1001 L1002 L1005 L1006 L1007 Q1008 M1009 V1010 L1011 V1012 T1013 G1019 T1023
L1024 A1025 Q1026 P1027 W1028 L1032 V1036 A1037 A1038 P1039 L1042 P1043 N1044 Y1045 E1046 N1047 T1048 V1049 S1052 S1055 F1056 Q1057 Y1058 L1059 I1060 L1061 R1072 R1073 N1078 V1079 P1080 F1081 L1082 V1083 L1087 S1090 V1091 L1092 V1093 G1094 L1095 V1098 PRO GLY L1101 N1110 F1116 K1117
L1118 L1121 G1122 L1123 V1124 A1131 L1134 E1135 S1136 V1137 L1138 D1139 Q1140 P1143 A1144 C1145 LEU ARG ARG LEU ARG PRO LYS ARG ALA S1155 R1158 F1159 K1160 Q1161 L1162 W1171 P1172 P1173 LEU PRO ALA GLY PRO LEU ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	256000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.722	Depositor
Minimum map value	-2.106	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	263.496, 263.496, 263.496	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.91	18/7210 (0.2%)	1.00	31/9858 (0.3%)

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	A	0	7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1055	SER	CA-CB	-10.10	1.37	1.52
1	A	941	SER	CA-CB	-9.56	1.38	1.52
1	A	256	TYR	CA-C	-8.33	1.31	1.52
1	A	947	SER	CA-CB	-7.24	1.42	1.52
1	A	255	HIS	CA-C	-6.85	1.35	1.52
1	A	964	LEU	C-O	-6.49	1.11	1.23
1	A	257	TYR	N-CA	-6.34	1.33	1.46
1	A	965	ALA	CA-C	-6.22	1.36	1.52
1	A	443	SER	CA-CB	-6.14	1.43	1.52
1	A	963	PHE	CA-CB	-5.98	1.40	1.53
1	A	1055	SER	C-O	5.83	1.34	1.23
1	A	454	LEU	N-CA	5.70	1.57	1.46
1	A	476	ALA	CA-CB	-5.42	1.41	1.52
1	A	936	TYR	CA-C	-5.38	1.39	1.52
1	A	941	SER	CA-C	-5.34	1.39	1.52
1	A	454	LEU	C-O	5.29	1.33	1.23
1	A	1052	SER	C-O	5.25	1.33	1.23
1	A	961	LEU	C-O	-5.19	1.13	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1172	PRO	N-CA-C	-10.00	86.09	112.10
1	A	1042	LEU	N-CA-C	8.31	133.44	111.00
1	A	964	LEU	CA-CB-CG	8.12	133.97	115.30
1	A	255	HIS	CB-CA-C	-7.98	94.43	110.40
1	A	257	TYR	CB-CA-C	7.74	125.87	110.40
1	A	256	TYR	CB-CA-C	-7.67	95.06	110.40
1	A	951	LEU	CA-CB-CG	7.38	132.27	115.30
1	A	61	PRO	N-CA-CB	7.05	111.76	103.30
1	A	454	LEU	N-CA-C	6.89	129.61	111.00
1	A	1009	MET	CB-CG-SD	-6.87	91.80	112.40
1	A	464	LEU	CB-CG-CD2	-6.40	100.12	111.00
1	A	1143	PRO	N-CA-CB	6.29	110.85	103.30
1	A	944	GLN	N-CA-CB	6.04	121.48	110.60
1	A	960	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	A	1055	SER	N-CA-CB	-5.76	101.86	110.50
1	A	121	PRO	N-CA-CB	5.74	110.19	103.30
1	A	69	PRO	N-CA-CB	5.73	110.17	103.30
1	A	300	PRO	N-CA-CB	5.72	110.17	103.30
1	A	119	PRO	N-CA-CB	5.71	110.16	103.30
1	A	188	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	257	TYR	N-CA-C	-5.51	96.11	111.00
1	A	258	TRP	N-CA-CB	-5.50	100.69	110.60
1	A	1032	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	1082	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	A	999	VAL	C-N-CD	5.21	139.34	128.40
1	A	1091	VAL	CB-CA-C	-5.20	101.53	111.40
1	A	1095	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	255	HIS	N-CA-CB	5.19	119.95	110.60
1	A	963	PHE	CB-CA-C	-5.17	100.05	110.40
1	A	261	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	943	THR	N-CA-CB	5.03	119.86	110.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1044	ASN	Mainchain
1	A	289	VAL	Peptide
1	A	965	ALA	Mainchain
1	A	966	ILE	Mainchain
1	A	967	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	A	968	LEU	Mainchain
1	A	969	VAL	Mainchain

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	A	7072	0	6988	132	0
2	A	14	0	26	1	0
All	All	7086	0	7014	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (132) 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)
1:A:844:VAL:HG22	1:A:1171:TRP:HZ3	1.26	0.98
1:A:1023:THR:HG21	1:A:1049:VAL:HG11	1.52	0.92
1:A:448:TYR:HB2	1:A:457:ILE:HD11	1.57	0.87
1:A:844:VAL:HG22	1:A:1171:TRP:CZ3	2.12	0.84
1:A:949:LEU:C	1:A:951:LEU:H	1.79	0.82
1:A:256:TYR:O	1:A:258:TRP:N	2.20	0.74
1:A:250:LEU:HD11	1:A:462:LEU:CB	2.21	0.70
1:A:256:TYR:O	1:A:257:TYR:C	2.29	0.68
1:A:452:VAL:HG21	1:A:457:ILE:HG13	1.77	0.66
1:A:844:VAL:CG2	1:A:1171:TRP:CZ3	2.79	0.66
1:A:250:LEU:HD11	1:A:462:LEU:HB3	1.79	0.64
1:A:1055:SER:HB2	1:A:1092:LEU:HD13	1.80	0.64
1:A:949:LEU:C	1:A:951:LEU:N	2.48	0.62
1:A:750:THR:HG22	1:A:752:ASP:H	1.65	0.61
1:A:250:LEU:HD11	1:A:462:LEU:HB2	1.84	0.60
1:A:970:ILE:O	1:A:974:VAL:HG22	2.00	0.60
1:A:240:TYR:CE2	1:A:474:PRO:HG2	2.37	0.59
1:A:317:CYS:HA	1:A:394:VAL:HA	1.85	0.59
1:A:464:LEU:HD21	1:A:949:LEU:HD11	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:CG2	1:A:457:ILE:HG13	2.33	0.58
1:A:524:ASP:HA	1:A:576:LYS:HG2	1.84	0.58
1:A:779:THR:HG1	1:A:784:GLY:N	2.01	0.58
1:A:733:THR:O	1:A:737:GLN:NE2	2.37	0.58
1:A:369:HIS:HB3	1:A:372:HIS:HB2	1.86	0.58
1:A:1008:GLN:HE21	1:A:1131:ALA:HB1	1.69	0.58
1:A:440:THR:OG1	1:A:461:ALA:HB1	2.04	0.57
1:A:581:THR:HG23	1:A:610:PRO:HD3	1.85	0.57
1:A:463:ASP:CG	2:A:1201:SPM:H91	2.25	0.57
1:A:1171:TRP:N	1:A:1172:PRO:HD3	2.18	0.56
1:A:543:PRO:HB2	1:A:581:THR:HB	1.87	0.56
1:A:821:ARG:NH1	1:A:1172:PRO:HG2	2.21	0.55
1:A:1007:LEU:HD12	1:A:1138:LEU:HD11	1.87	0.55
1:A:931:PHE:O	1:A:935:LYS:HG2	2.06	0.55
1:A:347:GLY:HA3	1:A:880:ALA:HA	1.88	0.54
1:A:1172:PRO:O	1:A:1173:PRO:C	2.46	0.54
1:A:339:MET:HG2	1:A:353:LEU:HA	1.88	0.53
1:A:750:THR:HB	1:A:852:ALA:HA	1.90	0.53
1:A:339:MET:SD	1:A:382:GLN:NE2	2.82	0.53
1:A:460:ARG:HH22	1:A:1038:ALA:HB3	1.72	0.53
1:A:263:ILE:HD11	1:A:472:ALA:HB2	1.91	0.53
1:A:903:VAL:HG21	1:A:907:THR:HB	1.89	0.53
1:A:822:HIS:ND1	1:A:849:THR:OG1	2.41	0.53
1:A:775:ILE:HB	1:A:792:LEU:HB2	1.90	0.52
1:A:740:ARG:NH1	1:A:766:MET:O	2.42	0.52
1:A:778:ALA:HB2	1:A:789:LEU:HD13	1.90	0.51
1:A:1007:LEU:HB3	1:A:1134:LEU:HD21	1.92	0.51
1:A:175:TRP:HA	1:A:181:ALA:HB1	1.91	0.51
1:A:258:TRP:N	1:A:258:TRP:CD1	2.79	0.51
1:A:642:ALA:HB2	1:A:649:PRO:HB3	1.91	0.51
1:A:228:TYR:O	1:A:229:PRO:C	2.43	0.51
1:A:1019:GLY:O	1:A:1023:THR:HG23	2.11	0.51
1:A:329:CYS:SG	1:A:330:ASP:N	2.85	0.50
1:A:244:GLN:NE2	1:A:471:PRO:O	2.41	0.48
1:A:1079:VAL:O	1:A:1080:PRO:C	2.50	0.48
1:A:473:LEU:H	1:A:474:PRO:CD	2.25	0.48
1:A:966:ILE:O	1:A:967:ASP:C	2.52	0.48
1:A:318:LEU:N	1:A:393:ALA:O	2.47	0.48
1:A:254:ASP:O	1:A:255:HIS:HB2	2.13	0.48
1:A:949:LEU:O	1:A:951:LEU:N	2.45	0.48
1:A:519:THR:HA	1:A:728:LEU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HB2	1:A:174:ILE:HG13	1.94	0.48
1:A:327:MET:SD	1:A:378:THR:OG1	2.70	0.48
1:A:295:VAL:HG21	1:A:328:PRO:HG3	1.96	0.47
1:A:488:LEU:HD21	1:A:922:GLU:HG3	1.96	0.47
1:A:1036:VAL:HB	1:A:1037:ALA:H	1.42	0.47
1:A:1159:PHE:CE2	1:A:1160:LYS:HG3	2.49	0.47
1:A:269:ILE:HG22	1:A:273:LEU:HD23	1.97	0.47
1:A:775:ILE:HD11	1:A:794:MET:HG3	1.95	0.47
1:A:1008:GLN:NE2	1:A:1131:ALA:HB1	2.30	0.47
1:A:473:LEU:H	1:A:474:PRO:HD2	1.80	0.47
1:A:448:TYR:HB2	1:A:457:ILE:CD1	2.38	0.47
1:A:1072:ARG:HG3	1:A:1073:ARG:H	1.80	0.47
1:A:448:TYR:O	1:A:449:ARG:C	2.48	0.46
1:A:335:ALA:HB3	1:A:392:LEU:HB2	1.96	0.46
1:A:1024:LEU:C	1:A:1026:GLN:H	2.19	0.46
1:A:967:ASP:O	1:A:968:LEU:C	2.51	0.46
1:A:820:SER:OG	1:A:821:ARG:N	2.46	0.46
1:A:172:ARG:NH1	1:A:215:ILE:O	2.49	0.46
1:A:929:THR:O	1:A:933:VAL:HG22	2.16	0.46
1:A:508:GLN:OE1	1:A:1159:PHE:CZ	2.69	0.45
1:A:1158:ARG:O	1:A:1159:PHE:C	2.54	0.45
1:A:678:GLN:HA	1:A:681:THR:HG22	1.98	0.45
1:A:788:SER:OG	1:A:789:LEU:N	2.49	0.45
1:A:1024:LEU:O	1:A:1026:GLN:N	2.49	0.45
1:A:1009:MET:O	1:A:1013:THR:HG23	2.16	0.45
1:A:1028:TRP:HZ3	1:A:1045:TYR:CZ	2.35	0.45
1:A:248:ILE:HD11	1:A:263:ILE:HG22	1.99	0.45
1:A:775:ILE:N	1:A:792:LEU:O	2.49	0.45
1:A:233:VAL:O	1:A:234:ASP:C	2.53	0.45
1:A:437:LEU:HA	1:A:440:THR:HG22	1.98	0.45
1:A:473:LEU:HB3	1:A:474:PRO:HD3	1.98	0.45
1:A:1045:TYR:O	1:A:1049:VAL:HG12	2.17	0.44
1:A:981:THR:HG22	1:A:1073:ARG:HB3	1.98	0.44
1:A:463:ASP:O	1:A:467:VAL:HG13	2.17	0.44
1:A:509:LEU:HD12	1:A:873:VAL:HG12	1.99	0.44
1:A:939:LEU:HG	1:A:1005:LEU:HD22	2.00	0.44
1:A:940:TYR:O	1:A:941:SER:C	2.51	0.44
1:A:965:ALA:O	1:A:966:ILE:O	2.36	0.44
1:A:937:MET:HE2	1:A:937:MET:HB2	1.82	0.43
1:A:504:GLY:HA2	1:A:891:VAL:HG21	1.99	0.43
1:A:507:LEU:HD12	1:A:920:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ALA:HB1	1:A:718:LEU:HD21	2.00	0.43
1:A:254:ASP:N	1:A:254:ASP:OD1	2.51	0.43
1:A:540:VAL:HG21	1:A:546:LEU:HD22	1.99	0.43
1:A:946:ILE:HD12	1:A:946:ILE:HG23	1.76	0.43
1:A:947:SER:HA	1:A:950:ILE:HG22	2.00	0.43
1:A:1055:SER:O	1:A:1056:PHE:C	2.53	0.43
1:A:444:ILE:O	1:A:445:PHE:C	2.54	0.43
1:A:497:HIS:HD2	1:A:500:ARG:HB2	1.83	0.43
1:A:1116:PHE:C	1:A:1118:LEU:N	2.70	0.43
1:A:956:THR:HG21	1:A:1044:ASN:HD21	1.83	0.42
1:A:255:HIS:CG	1:A:256:TYR:N	2.67	0.42
1:A:1094:GLY:O	1:A:1095:LEU:C	2.57	0.42
1:A:1047:ASN:O	1:A:1048:THR:C	2.56	0.42
1:A:842:PRO:HB3	1:A:869:LEU:HD21	2.00	0.42
1:A:1012:VAL:O	1:A:1013:THR:C	2.56	0.42
1:A:664:CYS:HA	1:A:716:LEU:H	1.85	0.42
1:A:548:VAL:HG23	1:A:552:LEU:HD11	2.02	0.41
1:A:226:LYS:O	1:A:279:ARG:NH2	2.52	0.41
1:A:240:TYR:OH	1:A:474:PRO:HD2	2.20	0.41
1:A:999:VAL:O	1:A:1000:PRO:C	2.53	0.41
1:A:441:ILE:HG13	1:A:442:TYR:N	2.35	0.41
1:A:1058:TYR:O	1:A:1059:LEU:C	2.56	0.41
1:A:830:PHE:HE1	1:A:845:LEU:HD11	1.86	0.41
1:A:528:VAL:HG22	1:A:722:LEU:HD23	2.03	0.41
1:A:420:LYS:HE2	1:A:995:ALA:HB2	2.03	0.41
1:A:778:ALA:H	1:A:829:THR:HG23	1.85	0.41
1:A:205:SER:O	1:A:209:GLN:N	2.49	0.41
1:A:484:ALA:O	1:A:485:GLN:C	2.59	0.40
1:A:861:GLU:HA	1:A:864:CYS:HB3	2.03	0.40
1:A:935:LYS:O	1:A:936:TYR:C	2.55	0.40
1:A:338:CYS:SG	1:A:339:MET:N	2.95	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	Percentiles
1	A	953/1153 (83%)	840 (88%)	97 (10%)	16 (2%)	9 45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PRO
1	A	255	HIS
1	A	454	LEU
1	A	1172	PRO
1	A	119	PRO
1	A	1025	ALA
1	A	484	ALA
1	A	954	ILE
1	A	1036	VAL
1	A	188	LEU
1	A	485	GLN
1	A	299	ARG
1	A	1039	PRO
1	A	118	GLU
1	A	1042	LEU
1	A	473	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	724/980 (74%)	677 (94%)	47 (6%)	17 51

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	192	ARG
1	A	219	ASN

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Mol	Chain	Res	Type
1	A	262	CYS
1	A	263	ILE
1	A	264	PHE
1	A	460	ARG
1	A	474	PRO
1	A	479	VAL
1	A	480	CYS
1	A	482	LEU
1	A	725	ARG
1	A	745	ARG
1	A	937	MET
1	A	940	TYR
1	A	941	SER
1	A	942	LEU
1	A	950	ILE
1	A	961	LEU
1	A	962	GLN
1	A	970	ILE
1	A	972	THR
1	A	1002	LEU
1	A	1006	LEU
1	A	1008	GLN
1	A	1011	LEU
1	A	1013	THR
1	A	1046	GLU
1	A	1047	ASN
1	A	1049	VAL
1	A	1055	SER
1	A	1057	GLN
1	A	1059	LEU
1	A	1061	LEU
1	A	1078	ASN
1	A	1083	VAL
1	A	1087	LEU
1	A	1090	SER
1	A	1116	PHE
1	A	1118	LEU
1	A	1121	LEU
1	A	1123	LEU
1	A	1124	VAL
1	A	1135	GLU
1	A	1136	SER

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Mol	Chain	Res	Type
1	A	1140	GLN
1	A	1162	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	255	HIS
1	A	497	HIS
1	A	726	ASN
1	A	737	GLN
1	A	836	HIS
1	A	1078	ASN

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)

1 ligand is 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	$\#\|Z\|>2$
2	SPM	A	1201	-	13,13,13	0.28	0	12,12,12	1.58	3 (25%)

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
2	SPM	A	1201	-	-	3/11/11/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	SPM	C7-C6-N5	-3.07	103.87	112.14
2	A	1201	SPM	C11-N10-C9	-2.30	102.59	113.45
2	A	1201	SPM	C3-C4-N5	-2.10	106.47	112.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	SPM	C8-C9-N10-C11
2	A	1201	SPM	C3-C4-N5-C6
2	A	1201	SPM	C2-C3-C4-N5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	SPM	1	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.

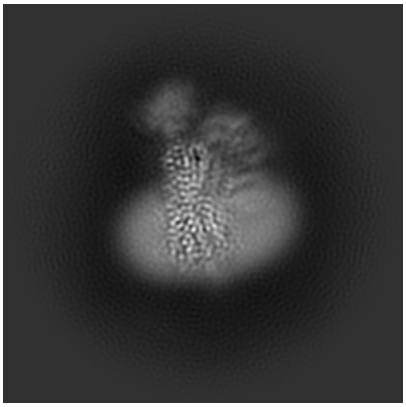
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31627. These allow visual inspection of the internal detail of the map and identification of artifacts.

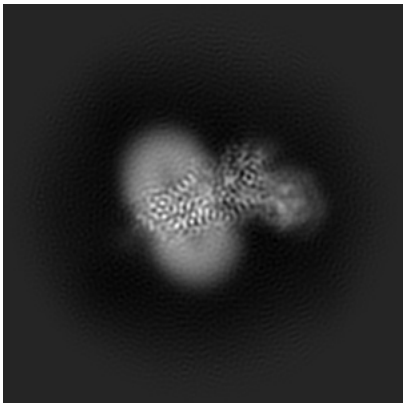
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

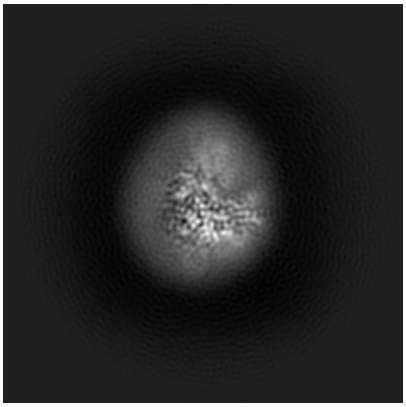
6.1.1 Primary map



X



Y

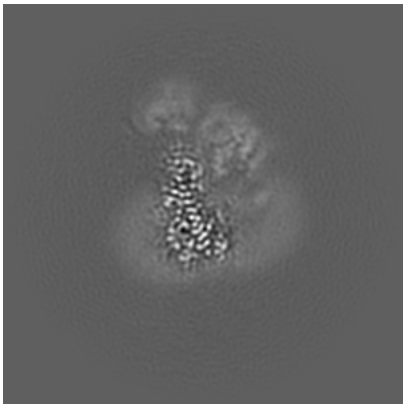


Z

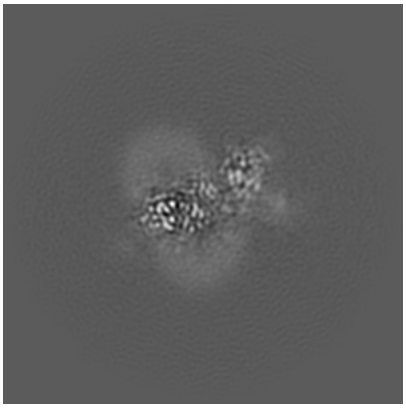
The images above show the map projected in three orthogonal directions.

6.2 Central slices

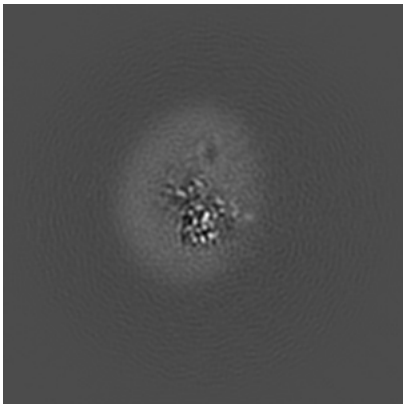
6.2.1 Primary map



X Index: 120



Y Index: 120

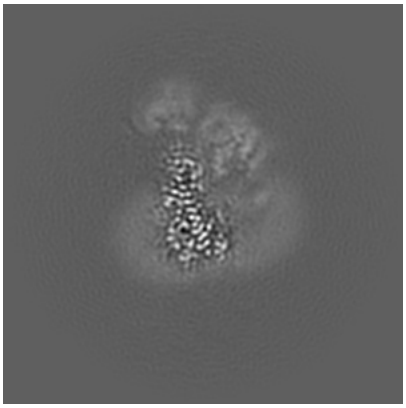


Z Index: 120

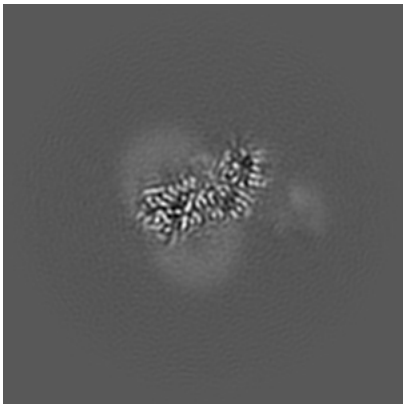
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

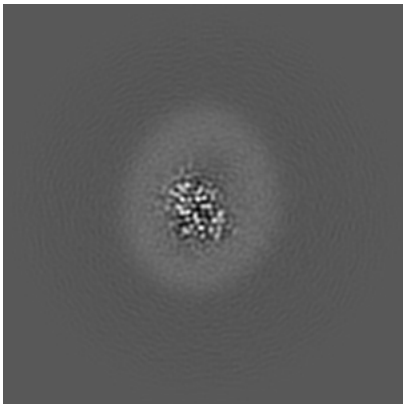
6.3.1 Primary map



X Index: 120



Y Index: 112



Z Index: 105

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

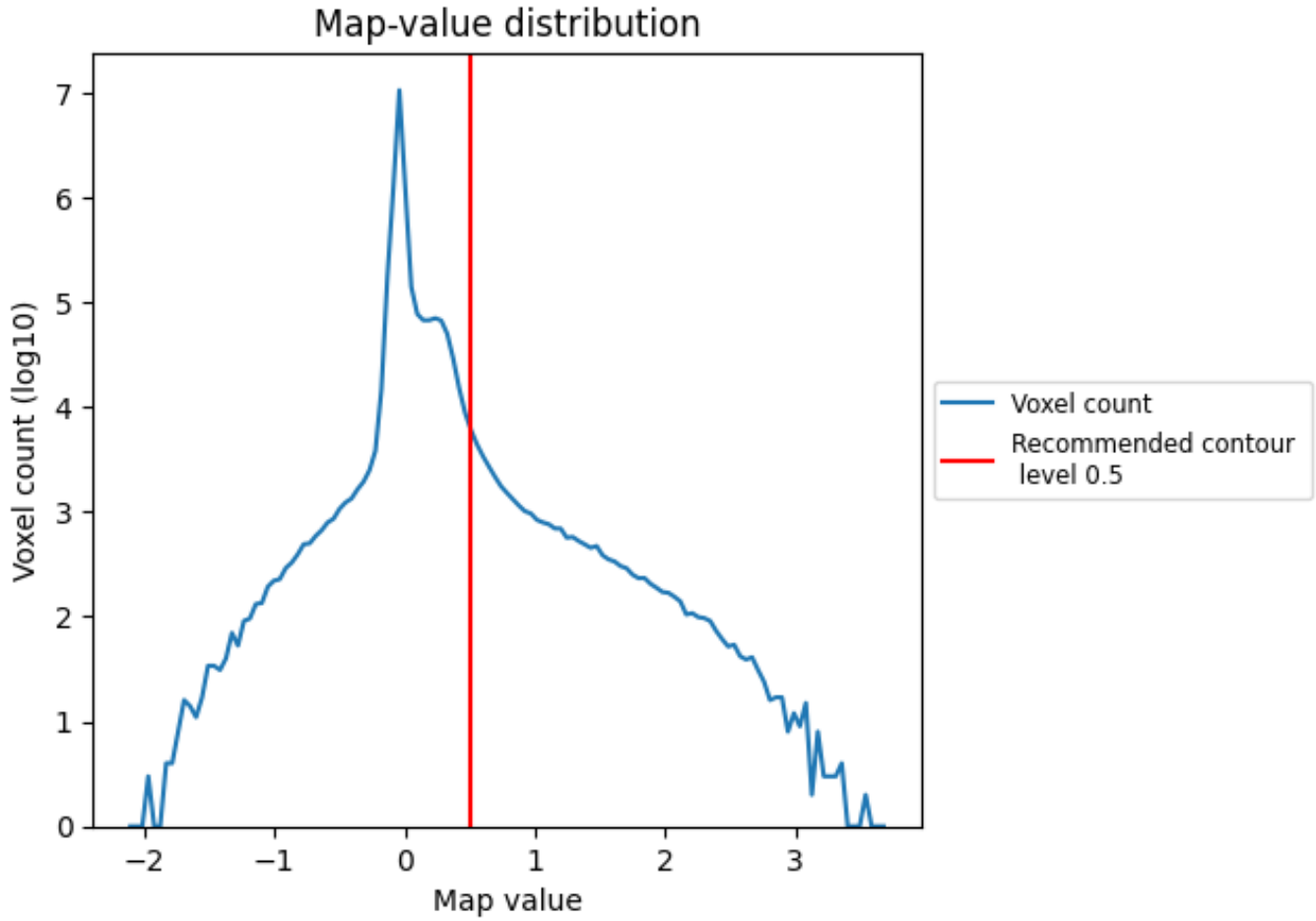
6.5 Mask visualisation (i)

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

7 Map analysis

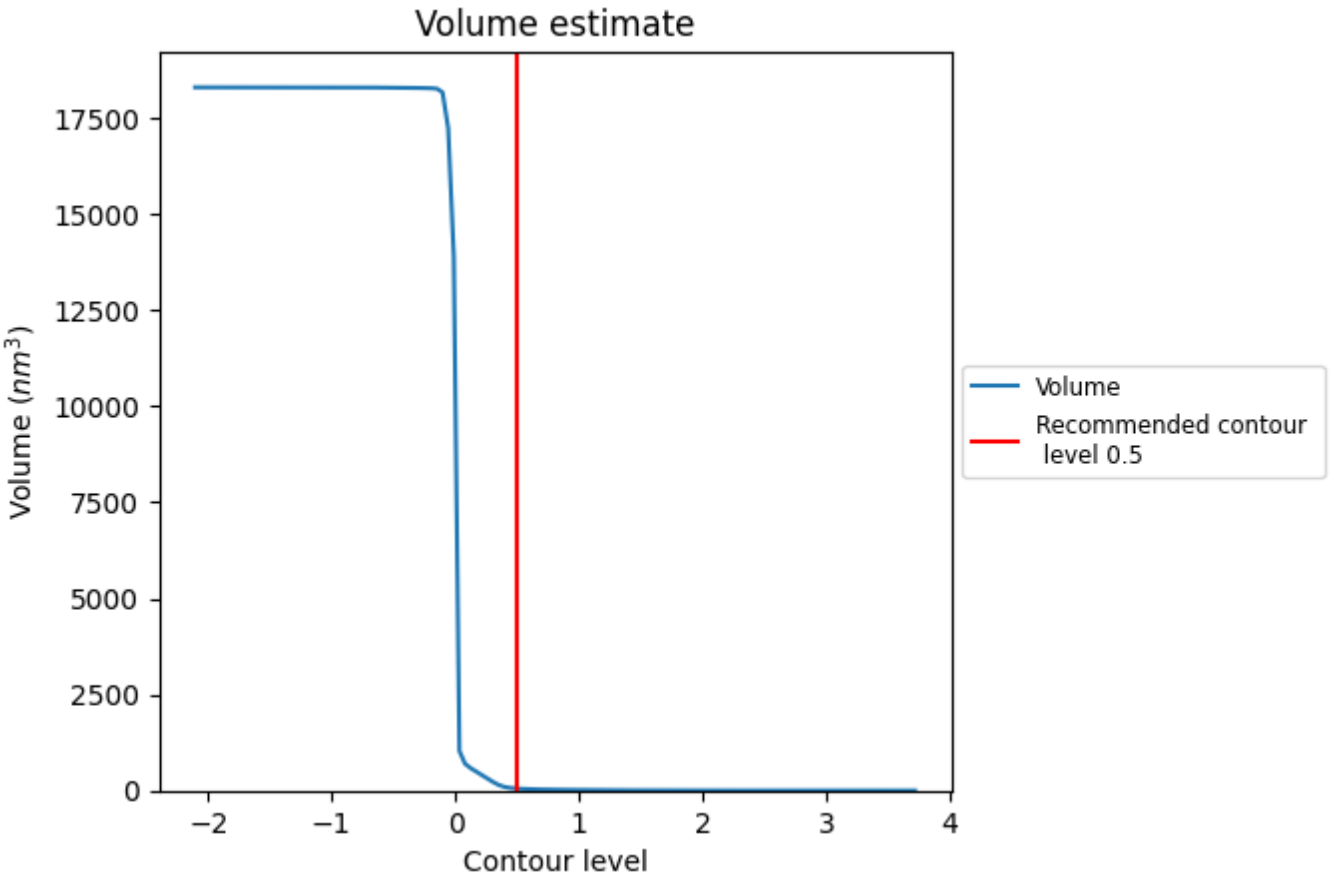
This section contains the results of statistical analysis of the map.

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.

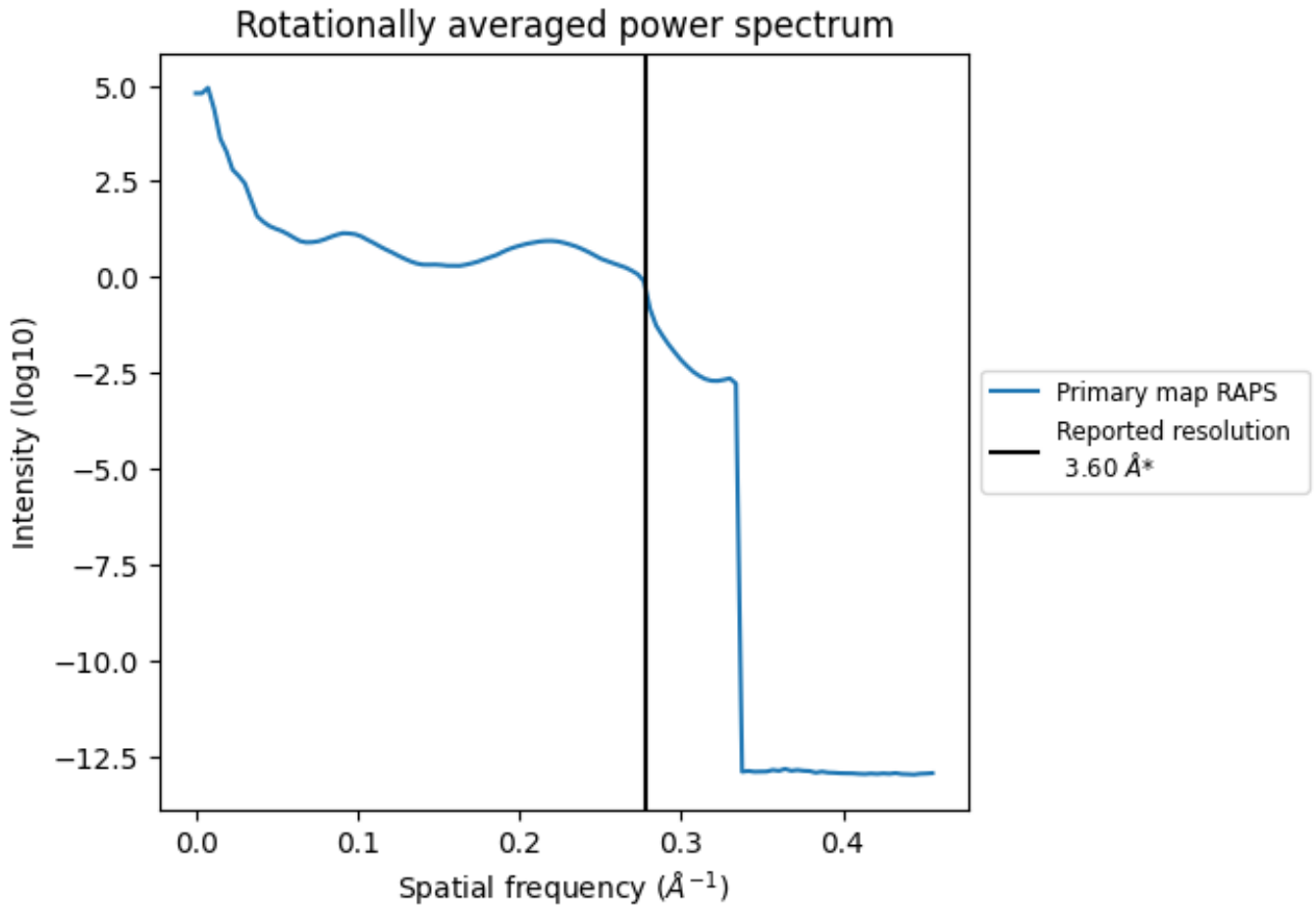
7.2 Volume estimate



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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 0.278 $Å^{-1}$

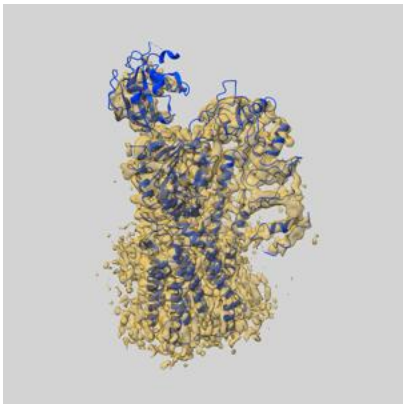
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

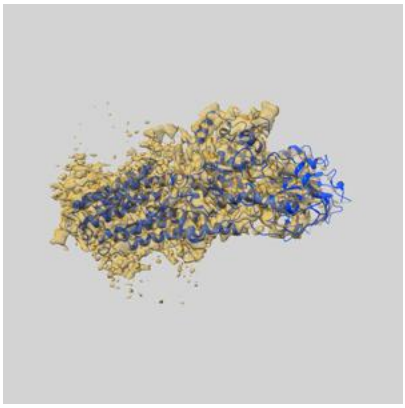
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31627 and PDB model 7FJQ. Per-residue inclusion information can be found in section 3 on page 5.

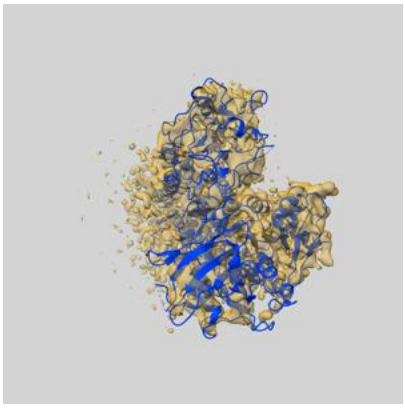
9.1 Map-model overlay



X



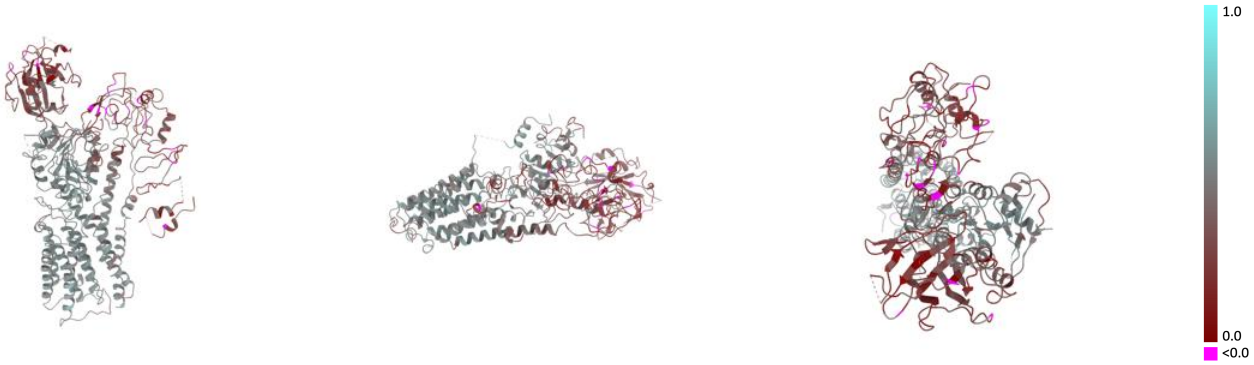
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

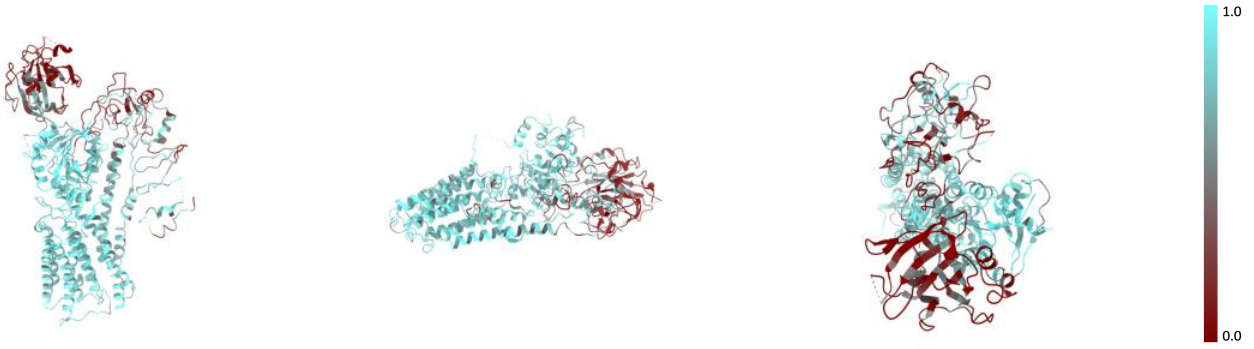
9.2 Q-score mapped to coordinate model



X Y Z

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

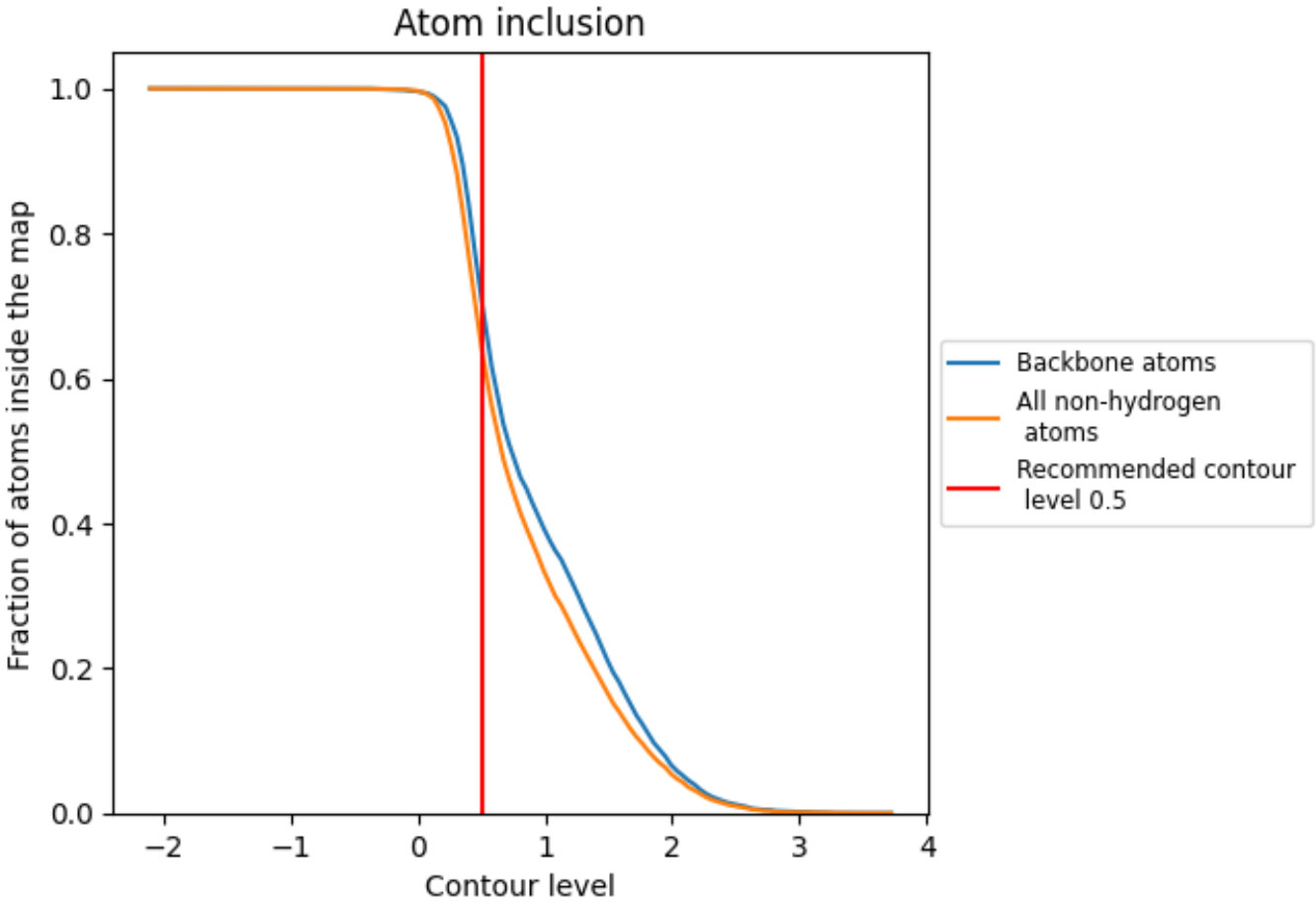
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 64% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6423	0.3990
A	0.6423	0.3990