



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:11 PM UTC

PDB ID : 7FJM / pdb_00007fjm
EMDB ID : EMD-31623
Title : Cryo EM structure of lysosomal ATPase
Authors : Zhang, S.S.
Deposited on : 2021-08-04
Resolution : 3.30 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

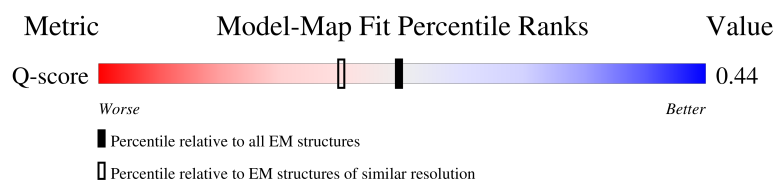
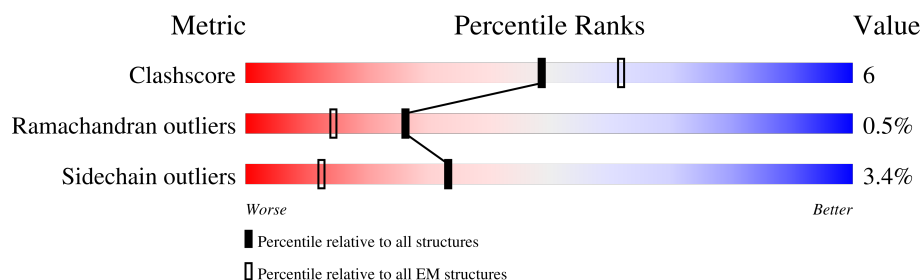
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	1149	

2 Entry composition

There is only 1 type of molecule 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
1	A	973	Total	C	N	O	S	0	0
			7086	4566	1206	1270	44		

There are 31 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
A	?	-	HIS	deletion	UNP Q9NQ11

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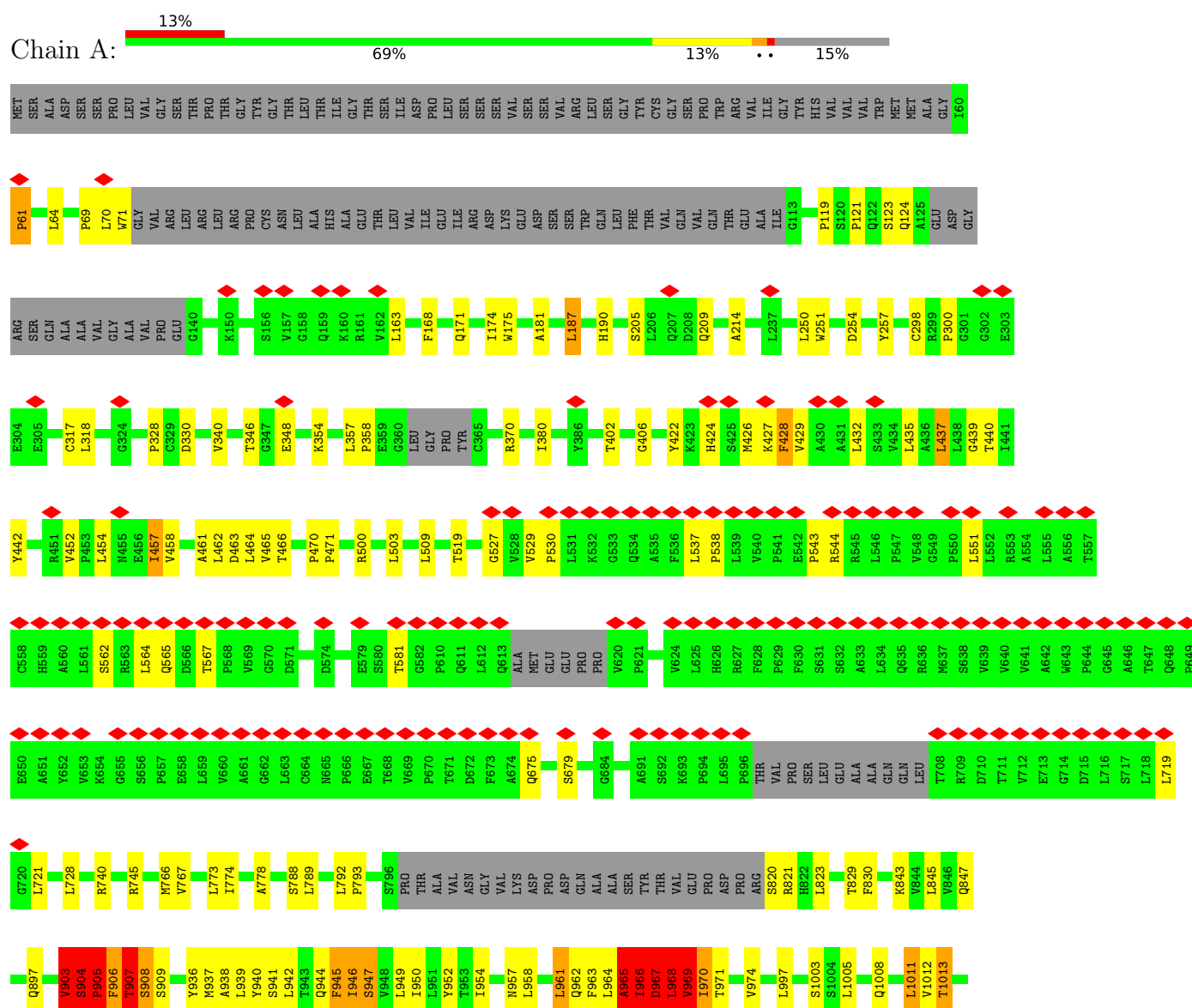
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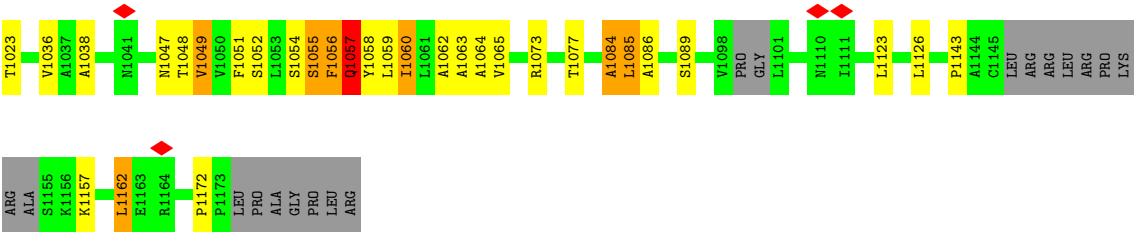
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP Q9NQ11
A	?	-	GLU	deletion	UNP Q9NQ11
A	?	-	ARG	deletion	UNP Q9NQ11

3 Residue-property plots

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

• Molecule 1: Polyamine-transporting ATPase 13A2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153193	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	3.746	Depositor
Minimum map value	-1.925	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.084	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 i

5.1 Standard geometry i

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	1.03	81/7225 (1.1%)	1.02	52/9876 (0.5%)

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	6

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	965	ALA	CA-C	-15.21	1.33	1.52
1	A	966	ILE	CA-C	-11.81	1.39	1.52
1	A	961	LEU	C-O	-10.64	1.10	1.24
1	A	1052	SER	C-O	10.45	1.36	1.24
1	A	904	SER	CA-C	-10.27	1.39	1.52
1	A	941	SER	CA-C	-9.82	1.40	1.52
1	A	941	SER	CA-CB	-9.28	1.38	1.53
1	A	1062	ALA	CA-C	-8.53	1.42	1.52
1	A	1064	ALA	CA-C	-8.32	1.42	1.52
1	A	908	SER	CA-C	-8.26	1.41	1.52
1	A	971	THR	CA-C	-8.24	1.41	1.52
1	A	1084	ALA	CA-C	-8.24	1.42	1.52
1	A	965	ALA	C-O	-8.16	1.14	1.24
1	A	907	THR	C-O	-8.14	1.14	1.23
1	A	964	LEU	CA-C	-8.02	1.42	1.52
1	A	903	VAL	CA-C	-7.51	1.43	1.52
1	A	907	THR	CA-C	-7.51	1.43	1.52
1	A	1056	PHE	N-CA	-7.20	1.37	1.46
1	A	945	PHE	CA-C	-7.19	1.43	1.52
1	A	964	LEU	C-O	-7.12	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1054	SER	CA-CB	-7.10	1.42	1.53
1	A	962	GLN	C-O	-7.01	1.15	1.24
1	A	907	THR	N-CA	-6.94	1.37	1.46
1	A	1047	ASN	C-O	-6.93	1.14	1.23
1	A	970	ILE	CA-C	-6.89	1.43	1.52
1	A	947	SER	CA-CB	-6.88	1.42	1.53
1	A	967	ASP	CA-C	-6.80	1.44	1.52
1	A	963	PHE	CA-C	-6.76	1.44	1.52
1	A	965	ALA	N-CA	-6.71	1.38	1.46
1	A	941	SER	N-CA	-6.58	1.38	1.46
1	A	1084	ALA	C-O	-6.55	1.16	1.24
1	A	938	ALA	CA-CB	-6.52	1.43	1.53
1	A	1049	VAL	CA-CB	-6.49	1.46	1.54
1	A	1057	GLN	CA-C	-6.41	1.44	1.52
1	A	963	PHE	CA-CB	-6.37	1.43	1.53
1	A	905	PRO	N-CA	-6.31	1.39	1.47
1	A	1056	PHE	CA-C	-6.21	1.44	1.52
1	A	905	PRO	CA-C	-6.21	1.43	1.52
1	A	906	PHE	N-CA	-6.16	1.38	1.46
1	A	908	SER	N-CA	-6.16	1.38	1.46
1	A	1048	THR	N-CA	-6.12	1.39	1.46
1	A	938	ALA	N-CA	-6.06	1.39	1.46
1	A	1055	SER	C-O	6.02	1.31	1.24
1	A	1056	PHE	CA-CB	-6.01	1.43	1.53
1	A	428	PHE	C-O	-5.97	1.17	1.24
1	A	1038	ALA	C-N	5.96	1.38	1.33
1	A	1060	ILE	CA-C	-5.93	1.45	1.52
1	A	1063	ALA	CA-CB	-5.86	1.43	1.53
1	A	968	LEU	N-CA	-5.83	1.39	1.46
1	A	1051	PHE	CA-CB	-5.77	1.44	1.53
1	A	961	LEU	N-CA	-5.74	1.38	1.46
1	A	1062	ALA	CA-CB	-5.73	1.44	1.53
1	A	962	GLN	CA-C	-5.72	1.45	1.52
1	A	1052	SER	CA-CB	-5.71	1.44	1.53
1	A	1086	ALA	CA-CB	-5.54	1.44	1.53
1	A	971	THR	CA-CB	-5.52	1.45	1.53
1	A	1084	ALA	CA-CB	-5.52	1.44	1.53
1	A	908	SER	CA-CB	-5.47	1.44	1.53
1	A	965	ALA	CA-CB	-5.41	1.45	1.53
1	A	1005	LEU	CA-C	-5.40	1.46	1.52
1	A	1089	SER	CA-CB	-5.38	1.44	1.53
1	A	1056	PHE	C-O	-5.34	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1063	ALA	C-O	-5.32	1.17	1.24
1	A	1085	LEU	C-O	-5.30	1.18	1.24
1	A	937	MET	CA-C	-5.28	1.46	1.52
1	A	1062	ALA	C-O	-5.28	1.18	1.24
1	A	969	VAL	C-N	-5.25	1.27	1.34
1	A	967	ASP	C-N	-5.24	1.27	1.33
1	A	1059	LEU	CA-C	5.17	1.59	1.52
1	A	1064	ALA	CA-CB	-5.16	1.45	1.53
1	A	937	MET	N-CA	-5.16	1.40	1.46
1	A	1064	ALA	C-O	-5.14	1.18	1.24
1	A	945	PHE	C-O	-5.14	1.18	1.24
1	A	903	VAL	CA-CB	-5.13	1.47	1.54
1	A	966	ILE	N-CA	-5.09	1.40	1.46
1	A	970	ILE	N-CA	-5.08	1.39	1.46
1	A	1011	LEU	C-O	-5.06	1.18	1.24
1	A	1065	VAL	C-O	-5.06	1.17	1.24
1	A	1057	GLN	CA-CB	-5.06	1.45	1.53
1	A	963	PHE	N-CA	-5.01	1.40	1.46
1	A	1063	ALA	CA-C	-5.01	1.45	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	904	SER	CA-C-N	-13.95	102.41	119.84
1	A	904	SER	C-N-CA	-13.95	102.41	119.84
1	A	904	SER	N-CA-C	-11.04	85.40	109.81
1	A	432	LEU	N-CA-C	-9.05	101.41	111.28
1	A	64	LEU	N-CA-C	-8.80	102.25	113.16
1	A	426	MET	N-CA-C	-8.79	103.67	114.75
1	A	1054	SER	N-CA-C	8.51	120.56	111.28
1	A	945	PHE	N-CA-C	-8.34	102.14	111.07
1	A	936	TYR	N-CA-C	-8.32	102.94	113.43
1	A	61	PRO	N-CA-CB	7.99	111.64	103.25
1	A	968	LEU	CA-C-N	-7.63	110.80	120.56
1	A	968	LEU	C-N-CA	-7.63	110.80	120.56
1	A	1143	PRO	N-CA-CB	7.35	110.96	103.25
1	A	124	GLN	N-CA-C	7.25	118.16	108.38
1	A	970	ILE	CA-C-N	-7.11	111.20	122.29
1	A	970	ILE	C-N-CA	-7.11	111.20	122.29
1	A	906	PHE	N-CA-C	7.10	122.03	111.81
1	A	966	ILE	CB-CA-C	-7.02	103.03	111.81
1	A	123	SER	N-CA-C	6.87	118.77	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	PRO	N-CA-CB	6.83	110.84	103.33
1	A	965	ALA	CA-C-O	-6.62	113.86	120.82
1	A	965	ALA	N-CA-C	-6.62	103.99	111.07
1	A	967	ASP	CA-C-N	-6.34	112.20	120.44
1	A	967	ASP	C-N-CA	-6.34	112.20	120.44
1	A	1055	SER	CA-C-O	6.23	127.15	120.55
1	A	300	PRO	N-CA-CB	6.18	110.08	103.52
1	A	1058	TYR	N-CA-C	6.17	117.67	111.07
1	A	903	VAL	N-CA-C	-6.16	96.53	109.34
1	A	121	PRO	N-CA-CB	6.08	110.02	103.33
1	A	461	ALA	N-CA-C	5.96	117.77	111.28
1	A	1047	ASN	N-CA-CB	5.91	118.45	110.59
1	A	966	ILE	CA-C-N	-5.81	112.98	120.65
1	A	966	ILE	C-N-CA	-5.81	112.98	120.65
1	A	428	PHE	N-CA-C	-5.75	105.01	111.28
1	A	944	GLN	N-CA-C	5.72	117.60	111.36
1	A	1060	ILE	CB-CA-C	-5.70	104.44	112.14
1	A	966	ILE	N-CA-CB	5.69	116.82	110.62
1	A	1058	TYR	CA-C-N	-5.55	112.84	120.28
1	A	1058	TYR	C-N-CA	-5.55	112.84	120.28
1	A	119	PRO	N-CA-CB	5.55	109.43	103.33
1	A	1084	ALA	N-CA-C	-5.52	105.18	111.14
1	A	1055	SER	N-CA-CB	-5.44	102.12	110.12
1	A	967	ASP	N-CA-C	5.43	116.89	110.97
1	A	1062	ALA	CA-C-N	-5.38	112.53	120.28
1	A	1062	ALA	C-N-CA	-5.38	112.53	120.28
1	A	1064	ALA	N-CA-C	5.30	117.06	111.28
1	A	1063	ALA	N-CA-C	5.29	117.80	111.71
1	A	1003	SER	N-CA-C	5.27	117.02	111.28
1	A	942	LEU	N-CA-C	5.22	116.97	111.28
1	A	1055	SER	O-C-N	-5.08	116.73	122.12
1	A	187	LEU	CA-CB-CG	5.08	134.08	116.30
1	A	962	GLN	N-CA-C	5.08	116.89	111.36

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	ASP	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

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	7086	0	7016	82	0
All	All	7086	0	7016	82	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 6.

All (82) 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:904:SER:HB3	1:A:905:PRO:HD3	1.65	0.76
1:A:903:VAL:HG11	1:A:907:THR:HG22	1.72	0.72
1:A:1023:THR:HG21	1:A:1049:VAL:HG11	1.76	0.67
1:A:437:LEU:HA	1:A:440:THR:HG22	1.77	0.66
1:A:439:GLY:HA3	1:A:945:PHE:HZ	1.63	0.64
1:A:904:SER:HB3	1:A:905:PRO:CD	2.29	0.63
1:A:1073:ARG:HE	1:A:1077:THR:HG21	1.65	0.62
1:A:967:ASP:O	1:A:968:LEU:C	2.39	0.61
1:A:905:PRO:HD2	1:A:906:PHE:CD1	2.38	0.59
1:A:424:HIS:HB3	1:A:427:LYS:HG2	1.85	0.59
1:A:897:GLN:HE21	1:A:907:THR:HB	1.68	0.58
1:A:340:VAL:HG12	1:A:380:ILE:HG22	1.84	0.58
1:A:551:LEU:HD12	1:A:719:LEU:HB3	1.86	0.58
1:A:904:SER:CB	1:A:905:PRO:HD3	2.34	0.58
1:A:946:ILE:HD12	1:A:1013:THR:HG23	1.85	0.57
1:A:970:ILE:O	1:A:974:VAL:HG22	2.05	0.56
1:A:565:GLN:NE2	1:A:567:THR:OG1	2.39	0.55
1:A:767:VAL:HG21	1:A:773:LEU:HD13	1.88	0.55
1:A:346:THR:HG23	1:A:348:GLU:H	1.72	0.55
1:A:509:LEU:HD23	1:A:745:ARG:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:VAL:HG22	1:A:904:SER:H	1.72	0.54
1:A:906:PHE:O	1:A:907:THR:C	2.48	0.54
1:A:965:ALA:O	1:A:966:ILE:C	2.51	0.53
1:A:500:ARG:HA	1:A:503:LEU:HD23	1.91	0.52
1:A:402:THR:O	1:A:406:GLY:N	2.42	0.52
1:A:454:LEU:HA	1:A:457:ILE:HG12	1.90	0.52
1:A:464:LEU:HG	1:A:952:TYR:CE2	2.45	0.52
1:A:966:ILE:O	1:A:967:ASP:C	2.50	0.51
1:A:527:GLY:HA2	1:A:543:PRO:HG3	1.93	0.51
1:A:968:LEU:O	1:A:969:VAL:C	2.53	0.50
1:A:903:VAL:HG13	1:A:904:SER:O	2.11	0.50
1:A:843:LYS:HD3	1:A:1162:LEU:HD21	1.93	0.49
1:A:1056:PHE:O	1:A:1060:ILE:HG12	2.12	0.49
1:A:740:ARG:NH1	1:A:766:MET:O	2.46	0.48
1:A:318:LEU:HD11	1:A:328:PRO:HG2	1.96	0.48
1:A:830:PHE:HE1	1:A:845:LEU:HD11	1.78	0.47
1:A:250:LEU:HD21	1:A:462:LEU:HB3	1.97	0.47
1:A:70:LEU:O	1:A:71:TRP:C	2.57	0.47
1:A:519:THR:HG22	1:A:728:LEU:HD23	1.96	0.47
1:A:908:SER:OG	1:A:909:SER:N	2.48	0.46
1:A:251:TRP:CH2	1:A:463:ASP:HB3	2.49	0.46
1:A:464:LEU:HG	1:A:952:TYR:HE2	1.81	0.46
1:A:823:LEU:HD13	1:A:847:GLN:HG3	1.98	0.46
1:A:903:VAL:HG22	1:A:904:SER:N	2.31	0.45
1:A:904:SER:CB	1:A:905:PRO:CD	2.94	0.45
1:A:1123:LEU:HA	1:A:1126:LEU:HG	2.00	0.44
1:A:427:LYS:HA	1:A:427:LYS:HD3	1.78	0.44
1:A:965:ALA:O	1:A:966:ILE:O	2.35	0.44
1:A:675:GLN:NE2	1:A:679:SER:OG	2.50	0.44
1:A:530:PRO:HB2	1:A:537:LEU:HD21	1.99	0.44
1:A:205:SER:O	1:A:209:GLN:N	2.51	0.43
1:A:537:LEU:HA	1:A:538:PRO:HD3	1.87	0.43
1:A:452:VAL:HG21	1:A:457:ILE:HG23	2.01	0.43
1:A:354:LYS:NZ	1:A:370:ARG:O	2.49	0.43
1:A:966:ILE:O	1:A:967:ASP:O	2.37	0.43
1:A:464:LEU:HD11	1:A:949:LEU:HD13	2.01	0.43
1:A:470:PRO:HA	1:A:471:PRO:HD3	1.87	0.42
1:A:947:SER:HA	1:A:950:ILE:HG22	2.00	0.42
1:A:957:ASN:HD22	1:A:958:LEU:H	1.66	0.42
1:A:298:CYS:N	1:A:317:CYS:SG	2.89	0.42
1:A:464:LEU:HD23	1:A:464:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ILE:HG22	1:A:793:PRO:HA	2.00	0.42
1:A:330:ASP:OD1	1:A:330:ASP:N	2.52	0.42
1:A:1084:ALA:O	1:A:1085:LEU:C	2.58	0.42
1:A:1012:VAL:HG13	1:A:1057:GLN:OE1	2.19	0.42
1:A:847:GLN:HE22	1:A:1172:PRO:HD3	1.85	0.42
1:A:168:PHE:HE1	1:A:171:GLN:HB2	1.84	0.41
1:A:778:ALA:H	1:A:829:THR:HG23	1.85	0.41
1:A:163:LEU:HD11	1:A:214:ALA:HB1	2.02	0.41
1:A:357:LEU:HD22	1:A:358:PRO:HD2	2.03	0.41
1:A:788:SER:OG	1:A:789:LEU:N	2.52	0.41
1:A:952:TYR:HD1	1:A:952:TYR:HA	1.77	0.41
1:A:187:LEU:HB2	1:A:190:HIS:HB2	2.02	0.41
1:A:175:TRP:HA	1:A:181:ALA:HB1	2.03	0.40
1:A:428:PHE:HB2	1:A:997:LEU:HD11	2.02	0.40
1:A:422:TYR:OH	1:A:428:PHE:HB3	2.22	0.40
1:A:529:VAL:HB	1:A:721:LEU:HB2	2.03	0.40
1:A:442:TYR:HD2	1:A:949:LEU:HD11	1.87	0.40
1:A:544:ARG:HG2	1:A:581:THR:HA	2.02	0.40
1:A:562:SER:HB2	1:A:564:LEU:HD23	2.03	0.40
1:A:820:SER:OG	1:A:821:ARG:N	2.52	0.40
1:A:967:ASP:O	1:A:968:LEU:O	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	955/1149 (83%)	862 (90%)	88 (9%)	5 (0%)	24 55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PRO
1	A	905	PRO
1	A	904	SER
1	A	954	ILE
1	A	903	VAL

5.3.2 Protein sidechains ⓘ

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	727/976 (74%)	702 (97%)	25 (3%)	32 59

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	ILE
1	A	257	TYR
1	A	429	VAL
1	A	435	LEU
1	A	437	LEU
1	A	457	ILE
1	A	458	VAL
1	A	465	VAL
1	A	466	THR
1	A	792	LEU
1	A	907	THR
1	A	939	LEU
1	A	940	TYR
1	A	946	ILE
1	A	961	LEU
1	A	968	LEU
1	A	969	VAL
1	A	1008	GLN
1	A	1011	LEU
1	A	1013	THR
1	A	1036	VAL
1	A	1055	SER

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Mol	Chain	Res	Type
1	A	1057	GLN
1	A	1157	LYS
1	A	1162	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	209	GLN
1	A	424	HIS
1	A	565	GLN
1	A	675	GLN
1	A	897	GLN
1	A	957	ASN
1	A	1016	GLN
1	A	1127	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

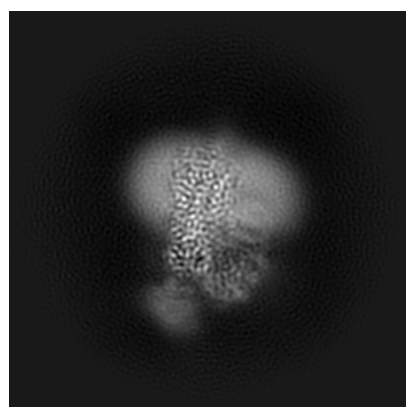
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31623. These allow visual inspection of the internal detail of the map and identification of artifacts.

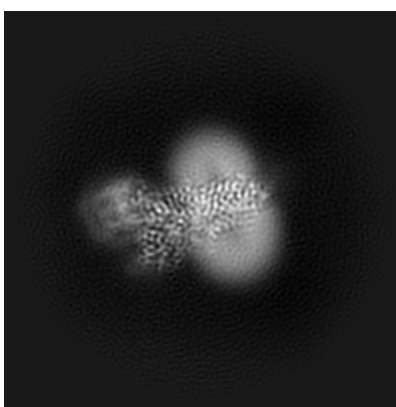
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

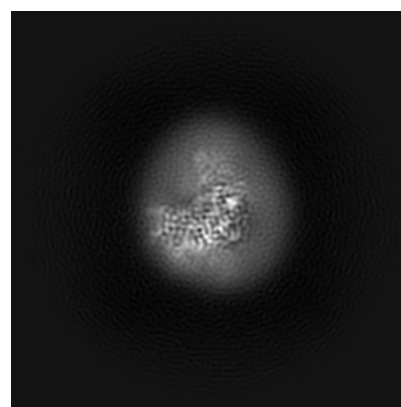
6.1.1 Primary map



X



Y

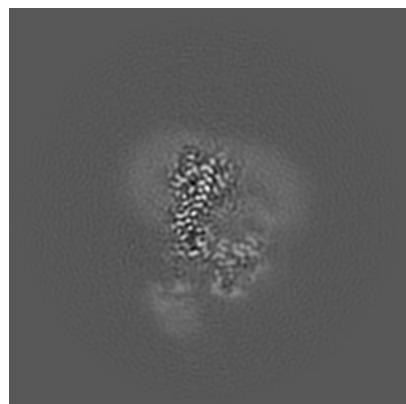


Z

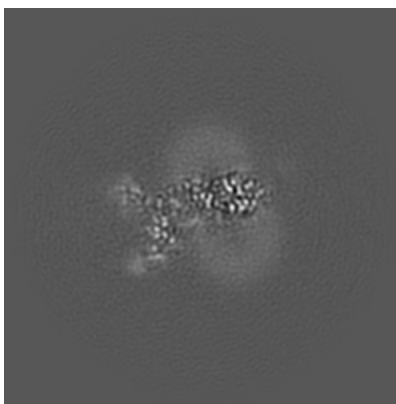
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

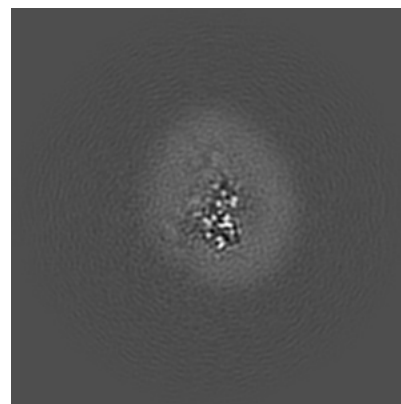
6.2.1 Primary map



X Index: 120



Y Index: 120

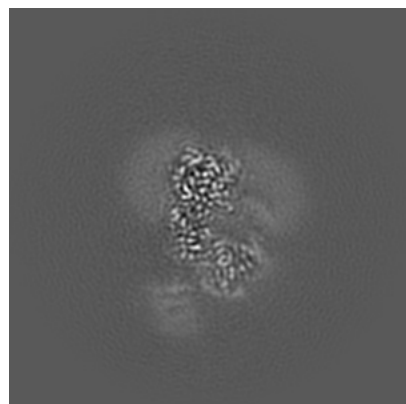


Z Index: 120

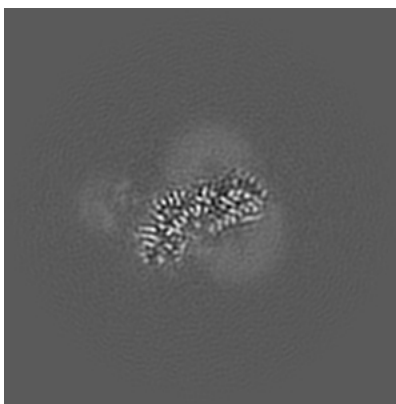
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

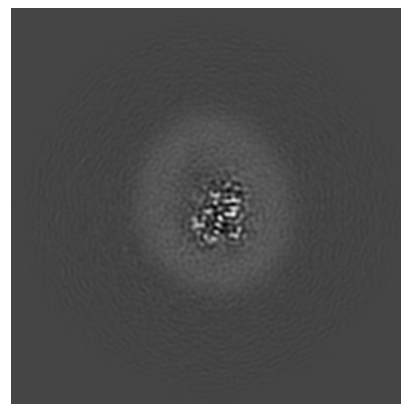
6.3.1 Primary map



X Index: 122



Y Index: 110

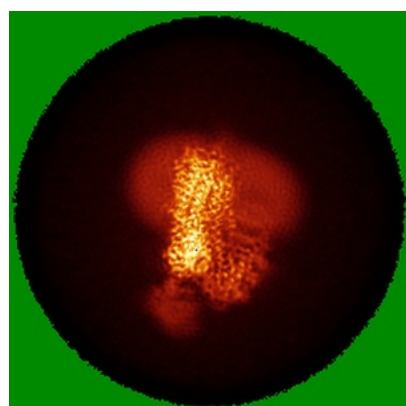


Z Index: 133

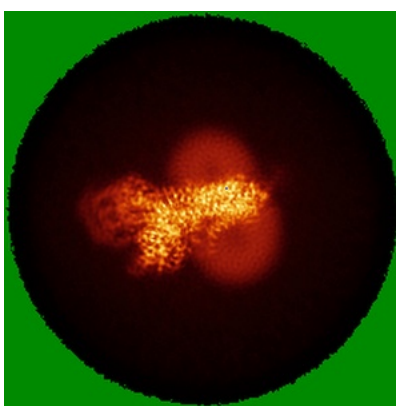
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

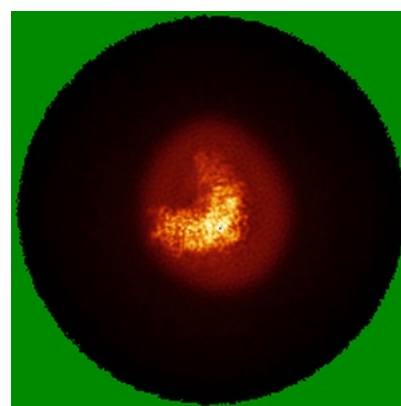
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

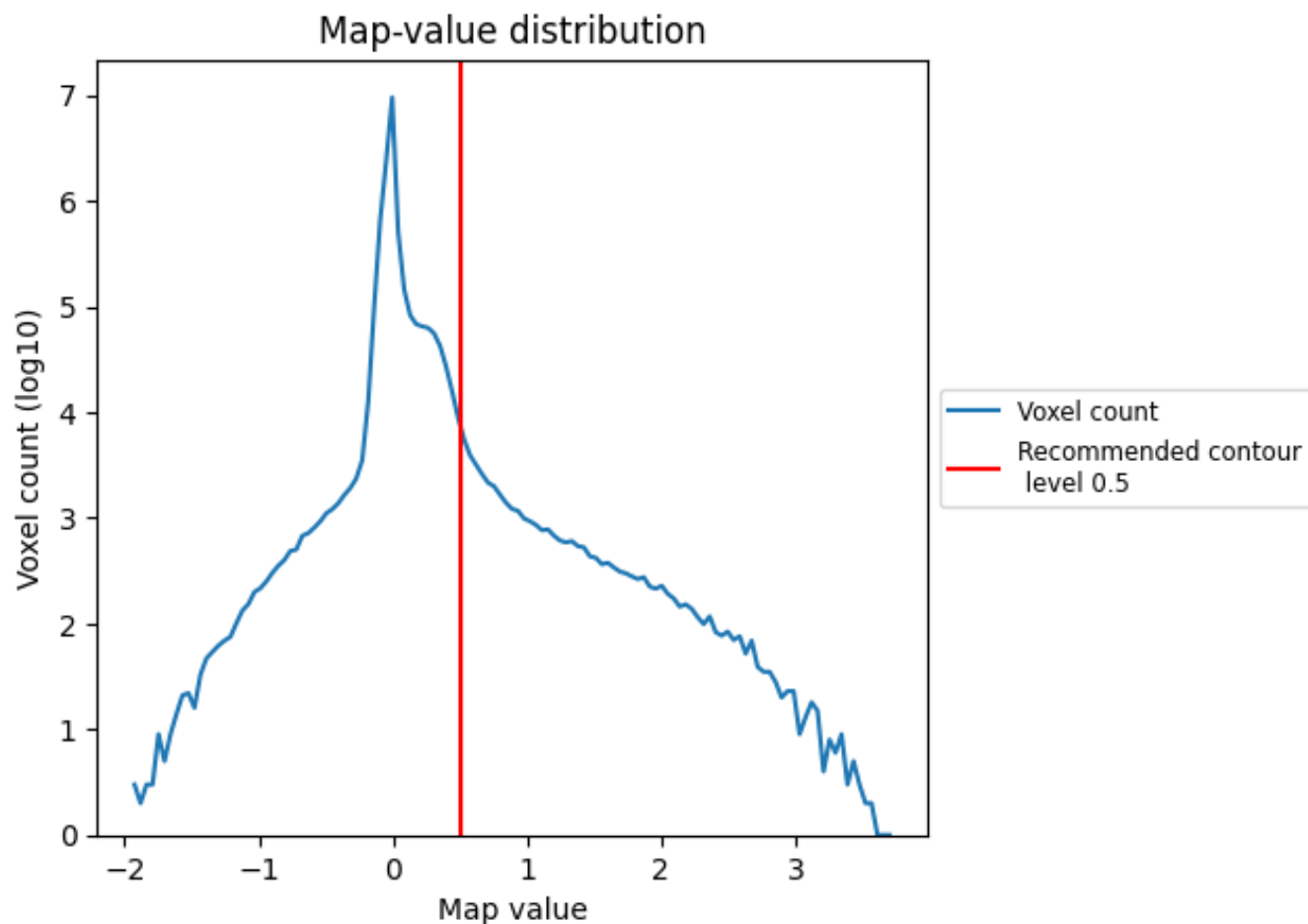
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

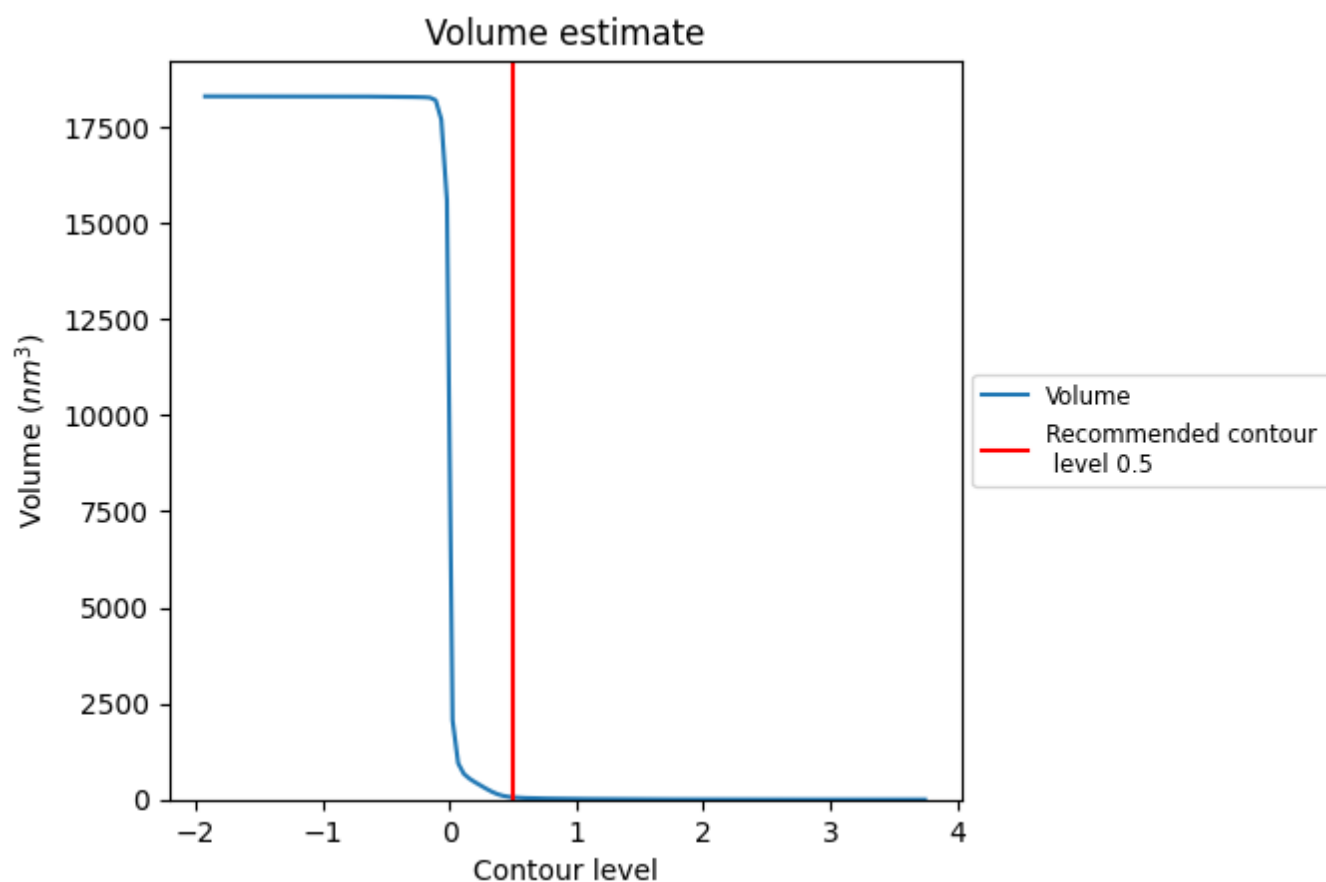
This section contains the results of statistical analysis of the map.

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.

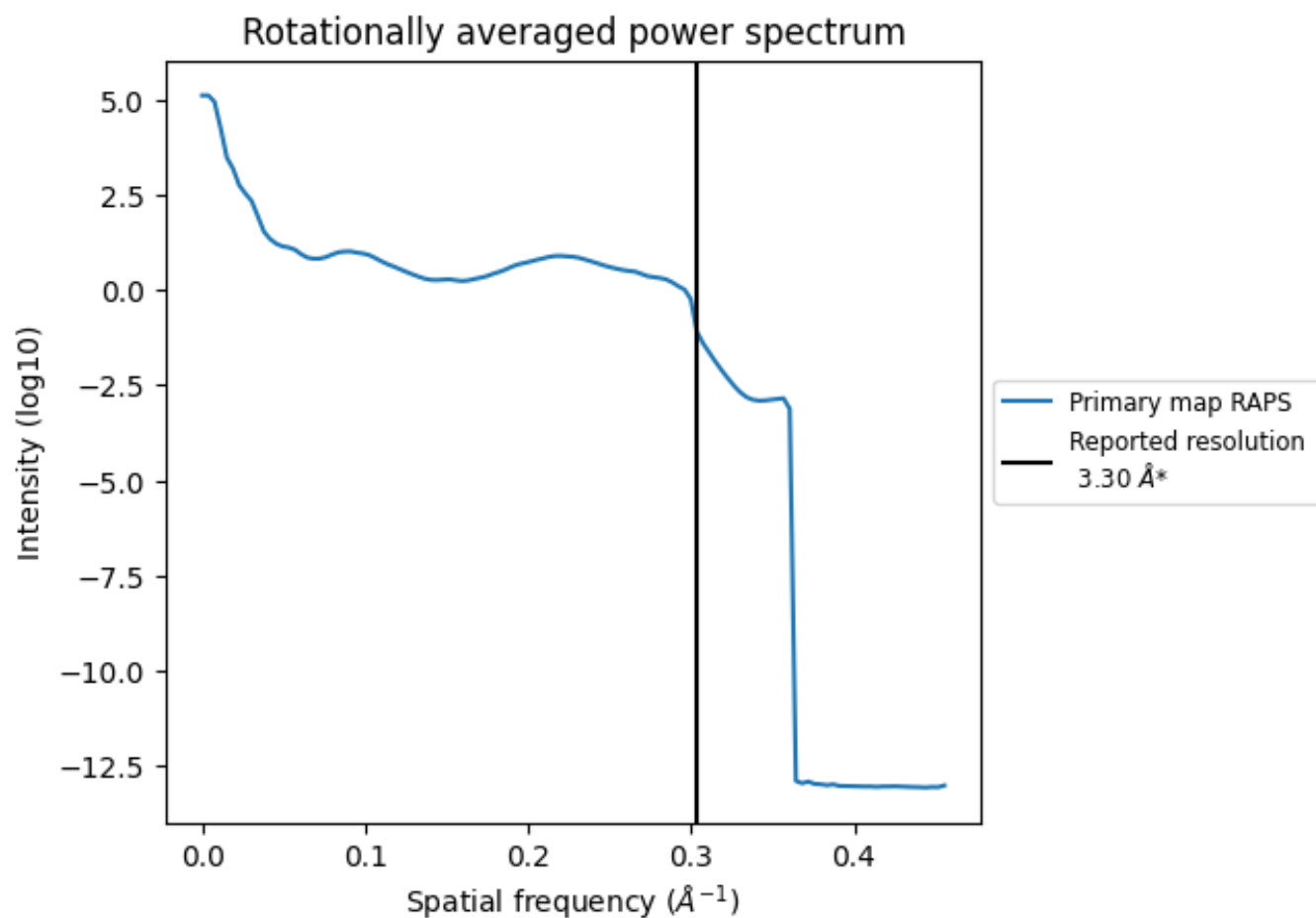
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm³; this corresponds to an approximate mass of 54 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

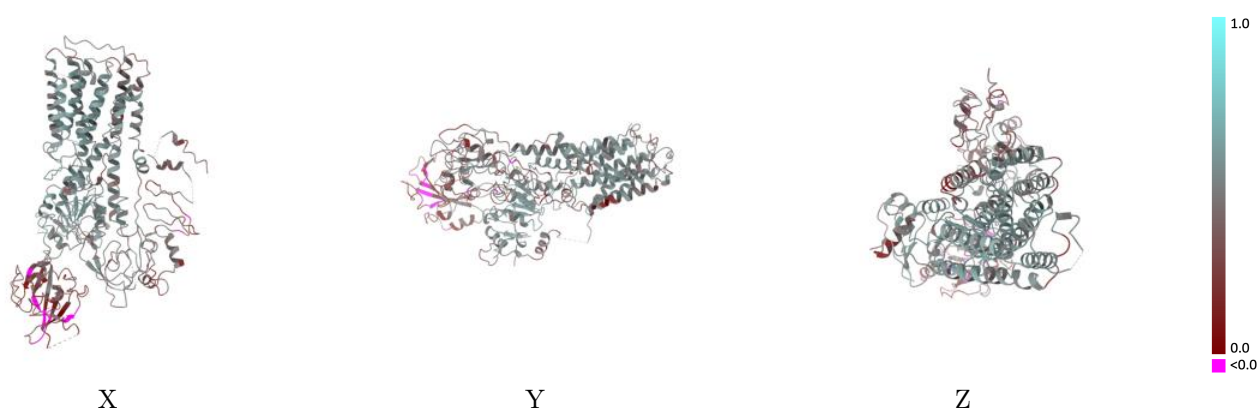
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31623 and PDB model 7FJM. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

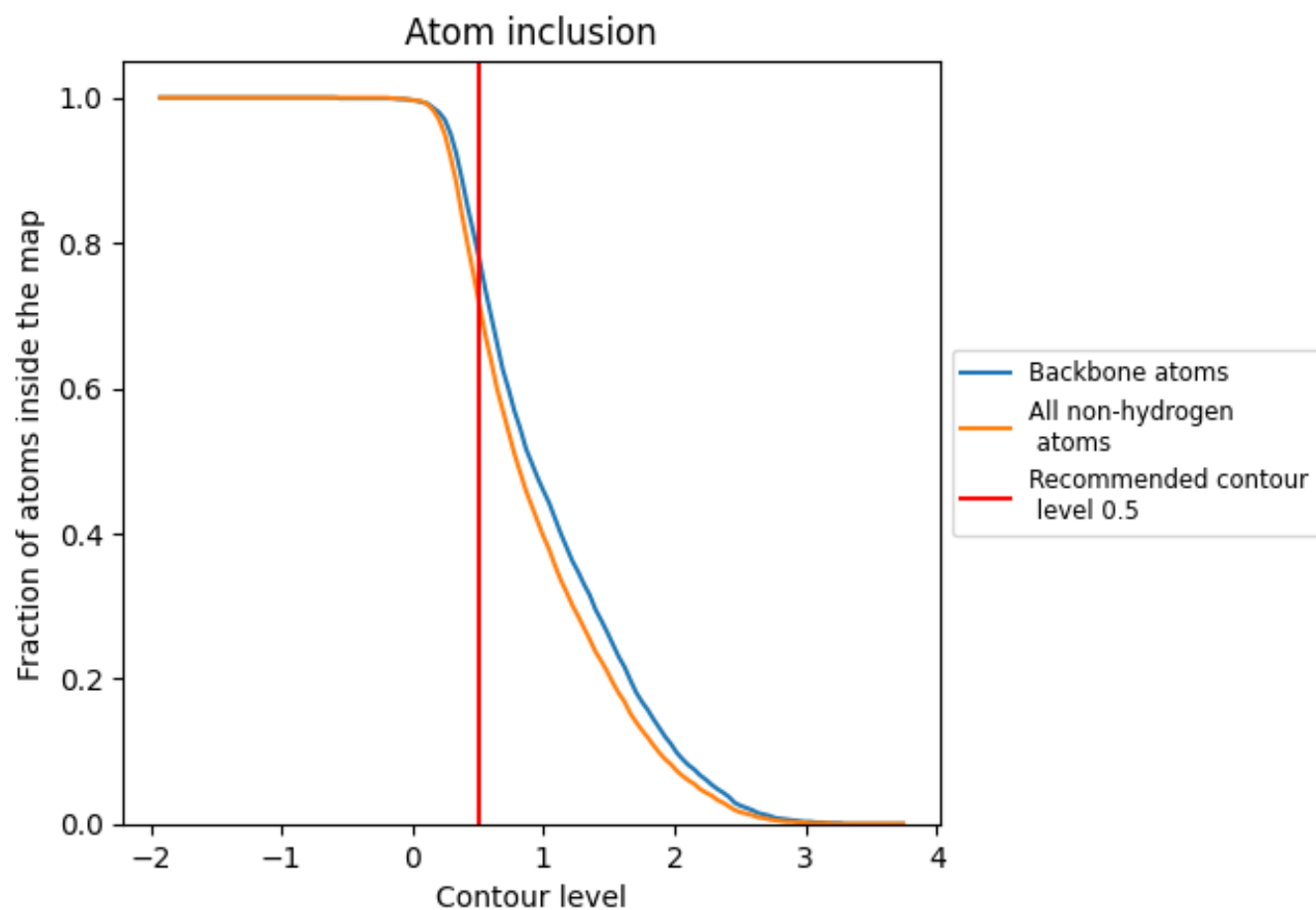


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.4400
A	0.7260	0.4400

