



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 12:33 AM UTC

PDB ID : 11SZ / pdb\_000011sz  
EMDB ID : EMD-76027  
Title : Antibody (1B2) Bound Rifamycin Synthetase Module 2  
Authors : Cogan, D.P.  
Deposited on : 2026-03-11  
Resolution : 2.94 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

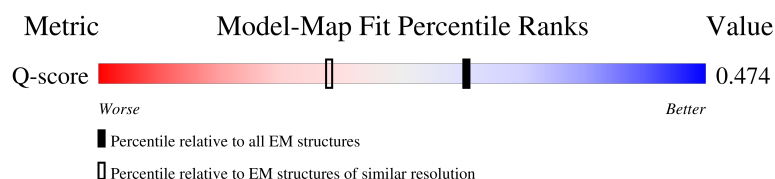
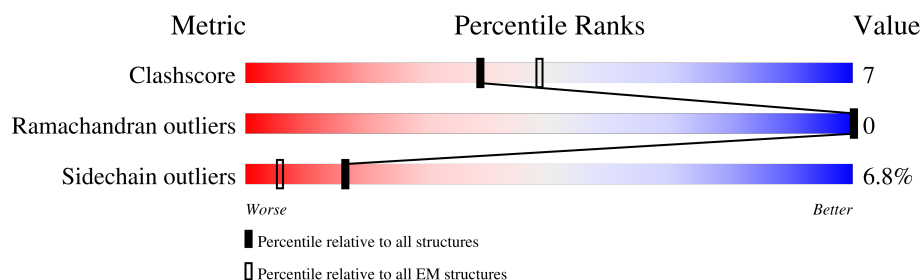
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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*



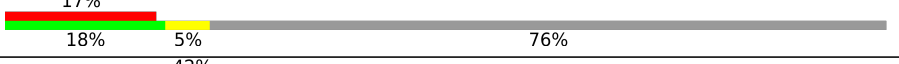

The reported resolution of this entry is 2.94 Å.

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	13068 ( 2.44 - 3.44 )

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  $\geq 3$ , 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	1094	
1	B	1094	
2	C	249	
2	H	249	

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Mol	Chain	Length	Quality of chain
3	D	236	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>41%28%18%52%</div></div>
3	L	236	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>18%12%6%81%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15743 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 6-deoxyerythronolide-B synthase, Erythronolide synthase EryA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	890	Total	C	N	O	S	0	0
			6580	4109	1182	1263	26		
1	B	892	Total	C	N	O	S	0	0
			6595	4117	1184	1268	26		

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O54666
A	2	ALA	-	expression tag	UNP O54666
A	3	SER	-	expression tag	UNP O54666
A	4	THR	-	expression tag	UNP O54666
A	5	ASP	-	expression tag	UNP O54666
A	6	SER	-	expression tag	UNP O54666
A	7	GLU	-	expression tag	UNP O54666
A	8	LYS	-	expression tag	UNP O54666
A	9	VAL	-	expression tag	UNP O54666
A	10	ALA	-	expression tag	UNP O54666
A	11	GLU	-	expression tag	UNP O54666
A	12	TYR	-	expression tag	UNP O54666
A	13	LEU	-	expression tag	UNP O54666
A	14	ARG	-	expression tag	UNP O54666
A	15	ARG	-	expression tag	UNP O54666
A	16	ALA	-	expression tag	UNP O54666
A	17	THR	-	expression tag	UNP O54666
A	18	LEU	-	expression tag	UNP O54666
A	19	ASP	-	expression tag	UNP O54666
A	20	LEU	-	expression tag	UNP O54666
A	21	ARG	-	expression tag	UNP O54666
A	22	ALA	-	expression tag	UNP O54666
A	23	ALA	-	expression tag	UNP O54666
A	24	ARG	-	expression tag	UNP O54666
A	25	GLN	-	expression tag	UNP O54666

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ARG	-	expression tag	UNP O54666
A	27	ILE	-	expression tag	UNP O54666
A	28	ARG	-	expression tag	UNP O54666
A	29	GLU	-	expression tag	UNP O54666
A	30	LEU	-	expression tag	UNP O54666
A	31	GLU	-	expression tag	UNP O54666
A	1075	GLY	-	expression tag	UNP Q03132
A	1076	ASN	-	expression tag	UNP Q03132
A	1077	SER	-	expression tag	UNP Q03132
A	1078	SER	-	expression tag	UNP Q03132
A	1079	SER	-	expression tag	UNP Q03132
A	1080	VAL	-	expression tag	UNP Q03132
A	1081	ASP	-	expression tag	UNP Q03132
A	1082	LYS	-	expression tag	UNP Q03132
A	1083	LEU	-	expression tag	UNP Q03132
A	1084	ALA	-	expression tag	UNP Q03132
A	1085	ALA	-	expression tag	UNP Q03132
A	1086	ALA	-	expression tag	UNP Q03132
A	1087	LEU	-	expression tag	UNP Q03132
A	1088	GLU	-	expression tag	UNP Q03132
A	1089	HIS	-	expression tag	UNP Q03132
A	1090	HIS	-	expression tag	UNP Q03132
A	1091	HIS	-	expression tag	UNP Q03132
A	1092	HIS	-	expression tag	UNP Q03132
A	1093	HIS	-	expression tag	UNP Q03132
A	1094	HIS	-	expression tag	UNP Q03132
B	1	MET	-	expression tag	UNP O54666
B	2	ALA	-	expression tag	UNP O54666
B	3	SER	-	expression tag	UNP O54666
B	4	THR	-	expression tag	UNP O54666
B	5	ASP	-	expression tag	UNP O54666
B	6	SER	-	expression tag	UNP O54666
B	7	GLU	-	expression tag	UNP O54666
B	8	LYS	-	expression tag	UNP O54666
B	9	VAL	-	expression tag	UNP O54666
B	10	ALA	-	expression tag	UNP O54666
B	11	GLU	-	expression tag	UNP O54666
B	12	TYR	-	expression tag	UNP O54666
B	13	LEU	-	expression tag	UNP O54666
B	14	ARG	-	expression tag	UNP O54666
B	15	ARG	-	expression tag	UNP O54666
B	16	ALA	-	expression tag	UNP O54666

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Chain	Residue	Modelled	Actual	Comment	Reference
B	17	THR	-	expression tag	UNP O54666
B	18	LEU	-	expression tag	UNP O54666
B	19	ASP	-	expression tag	UNP O54666
B	20	LEU	-	expression tag	UNP O54666
B	21	ARG	-	expression tag	UNP O54666
B	22	ALA	-	expression tag	UNP O54666
B	23	ALA	-	expression tag	UNP O54666
B	24	ARG	-	expression tag	UNP O54666
B	25	GLN	-	expression tag	UNP O54666
B	26	ARG	-	expression tag	UNP O54666
B	27	ILE	-	expression tag	UNP O54666
B	28	ARG	-	expression tag	UNP O54666
B	29	GLU	-	expression tag	UNP O54666
B	30	LEU	-	expression tag	UNP O54666
B	31	GLU	-	expression tag	UNP O54666
B	1075	GLY	-	expression tag	UNP Q03132
B	1076	ASN	-	expression tag	UNP Q03132
B	1077	SER	-	expression tag	UNP Q03132
B	1078	SER	-	expression tag	UNP Q03132
B	1079	SER	-	expression tag	UNP Q03132
B	1080	VAL	-	expression tag	UNP Q03132
B	1081	ASP	-	expression tag	UNP Q03132
B	1082	LYS	-	expression tag	UNP Q03132
B	1083	LEU	-	expression tag	UNP Q03132
B	1084	ALA	-	expression tag	UNP Q03132
B	1085	ALA	-	expression tag	UNP Q03132
B	1086	ALA	-	expression tag	UNP Q03132
B	1087	LEU	-	expression tag	UNP Q03132
B	1088	GLU	-	expression tag	UNP Q03132
B	1089	HIS	-	expression tag	UNP Q03132
B	1090	HIS	-	expression tag	UNP Q03132
B	1091	HIS	-	expression tag	UNP Q03132
B	1092	HIS	-	expression tag	UNP Q03132
B	1093	HIS	-	expression tag	UNP Q03132
B	1094	HIS	-	expression tag	UNP Q03132

- Molecule 2 is a protein called 1B2 Antibody Fragment (Fab) Heavy Chain.

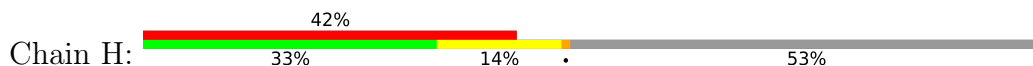
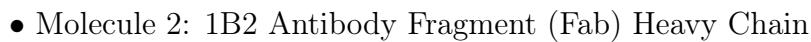
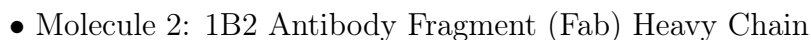
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	59	Total	C	N	O	S	0	0
			461	290	75	94	2		
2	H	117	Total	C	N	O	S	0	0
			888	560	153	171	4		

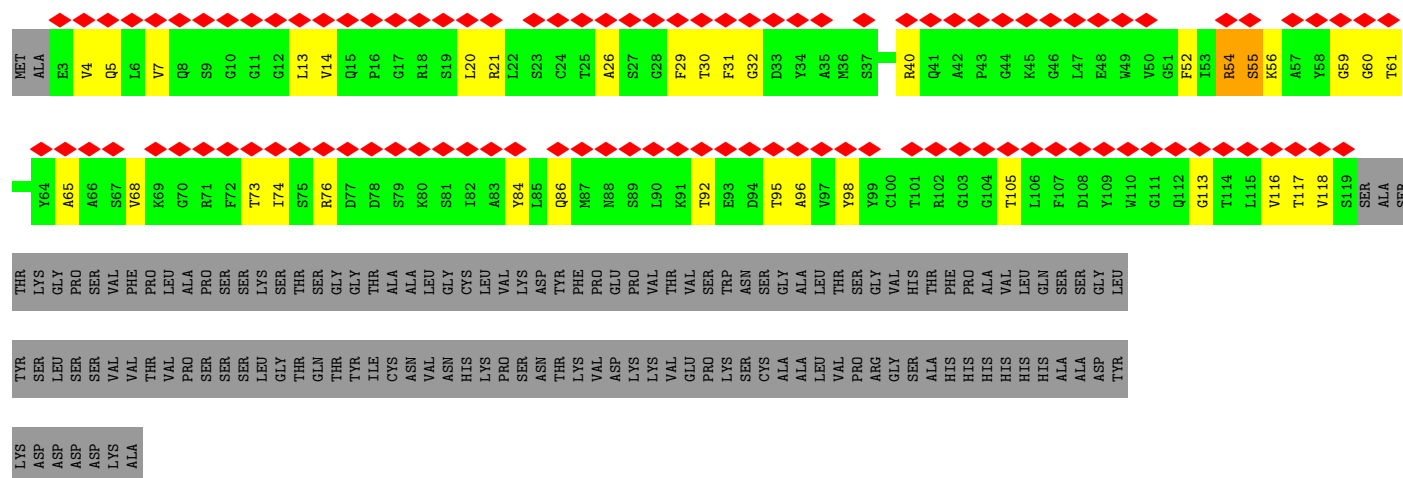
- Molecule 3 is a protein called 1B2 Antibody Fragment (Fab) Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	113	Total	C	N	O	S	0	0
			861	542	145	170	4		
3	L	44	Total	C	N	O	S	0	0
			358	231	61	64	2		

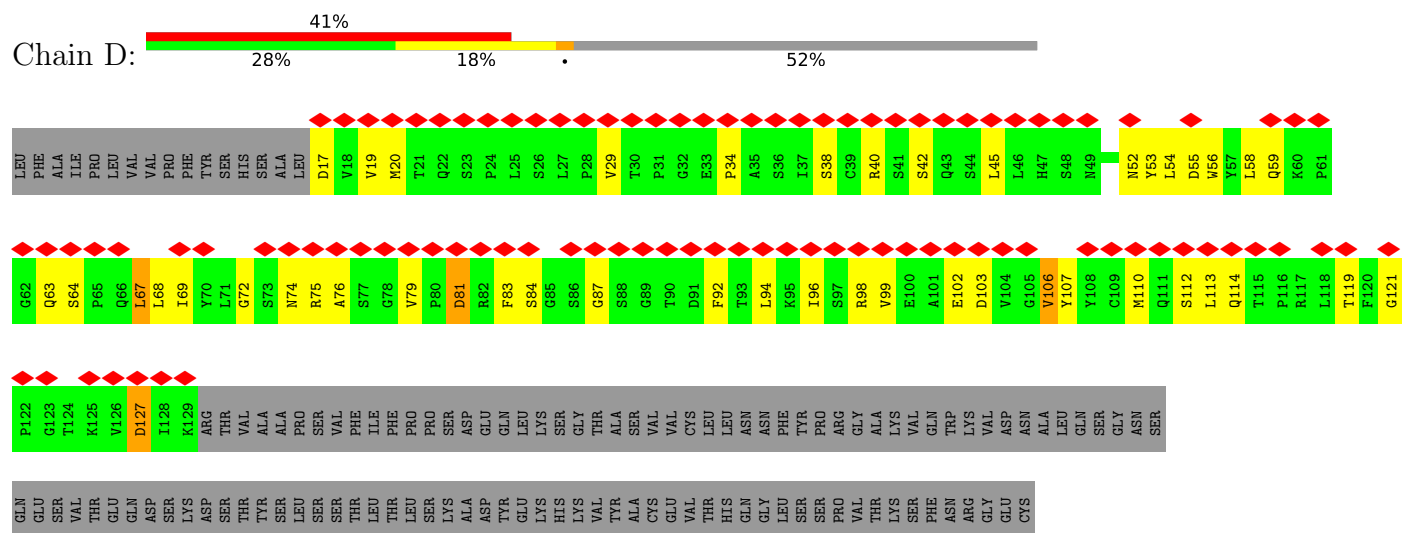




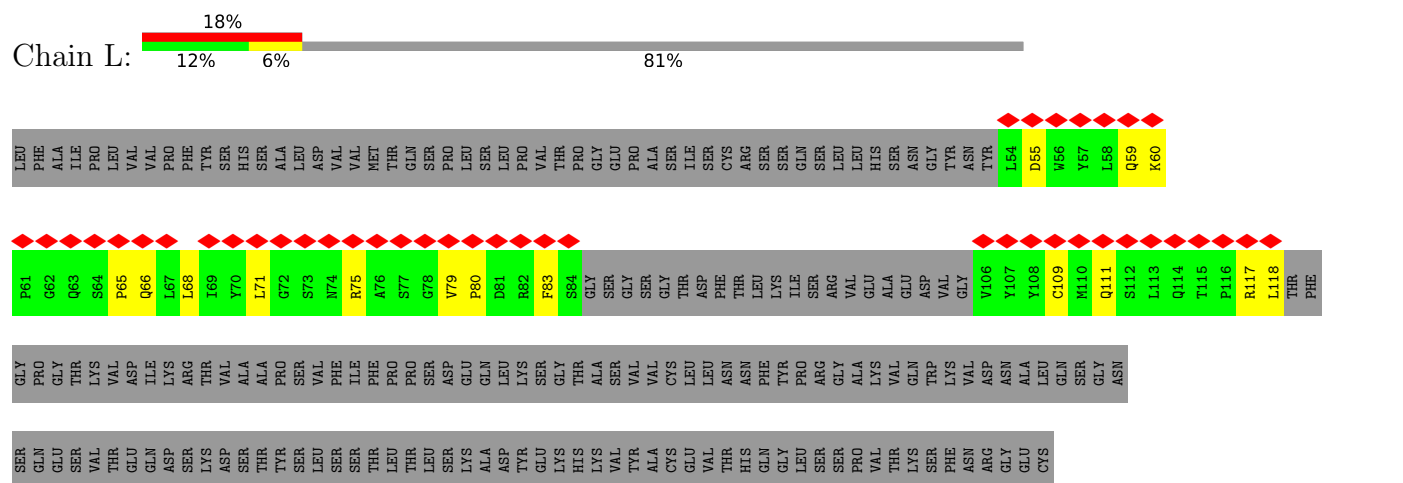




### • Molecule 3: 1B2 Antibody Fragment (Fab) Light Chain



### • Molecule 3: 1B2 Antibody Fragment (Fab) Light Chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	852885	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1188	Depositor
Maximum defocus (nm)	3988	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.955	Depositor
Minimum map value	-0.275	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.235	Depositor
Map size ( $\text{\AA}$ )	492.80002, 492.80002, 492.80002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	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	0.13	0/6708	0.30	0/9139
1	B	0.12	0/6723	0.29	0/9159
2	C	0.13	0/469	0.39	0/635
2	H	0.11	0/906	0.30	0/1224
3	D	0.10	0/881	0.32	0/1198
3	L	0.10	0/367	0.26	0/497
All	All	0.12	0/16054	0.30	0/21852

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	6580	0	6451	92	0
1	B	6595	0	6462	76	0
2	C	461	0	444	6	0
2	H	888	0	864	25	0
3	D	861	0	844	29	0
3	L	358	0	353	11	0
All	All	15743	0	15418	227	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 7.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:PRO:HA	3:D:96:ILE:O	1.74	0.85
1:B:612:MET:SD	1:B:612:MET:N	2.60	0.75
2:H:21:ARG:HD2	2:H:84:TYR:HB3	1.67	0.73
2:H:54:ARG:HB2	2:H:61:THR:H	1.57	0.69
3:L:75:ARG:NH2	3:L:80:PRO:O	2.25	0.68
1:A:612:MET:SD	1:A:612:MET:N	2.61	0.68
1:A:171:GLU:HB3	1:B:245:ARG:HH12	1.59	0.68
1:A:671:LEU:HB3	1:A:750:MET:HG3	1.77	0.67
1:A:750:MET:N	1:A:750:MET:HE2	2.10	0.66
1:B:99:ASP:OD1	1:B:99:ASP:N	2.28	0.66
3:D:17:ASP:O	3:D:114:GLN:NE2	2.27	0.66
2:H:40:ARG:HH11	2:H:96:ALA:HB3	1.60	0.65
2:H:54:ARG:O	2:H:76:ARG:NH1	2.30	0.65
1:A:751:LEU:HD12	1:A:788:VAL:HG13	1.79	0.65
1:A:164:MET:HE1	1:A:893:VAL:HG21	1.78	0.64
1:A:10:ALA:HB3	2:H:54:ARG:HH22	1.62	0.64
1:B:732:LYS:HE2	1:B:732:LYS:H	1.63	0.63
3:D:102:GLU:N	3:D:102:GLU:OE1	2.31	0.63
3:D:52:ASN:HB2	3:D:72:GLY:HA3	1.81	0.63
1:A:792:ARG:NH1	1:A:792:ARG:O	2.32	0.61
1:B:182:VAL:HG12	1:B:186:ARG:HG2	1.83	0.60
2:H:21:ARG:HH21	2:H:86:GLN:HB2	1.67	0.59
3:D:75:ARG:NH1	3:D:83:PHE:O	2.35	0.59
2:H:54:ARG:HB3	2:H:60:GLY:H	1.68	0.59
1:A:162:MET:HE1	1:B:165:HIS:HD1	1.67	0.59
1:B:872:GLU:HG3	1:B:873:PRO:HD2	1.85	0.59
1:A:260:ASP:OD2	1:A:407:ARG:NH2	2.37	0.58
1:B:792:ARG:O	1:B:792:ARG:NH1	2.36	0.58
3:D:45:LEU:HB3	3:D:54:LEU:HD21	1.84	0.58
1:B:96:ALA:HB3	1:B:268:SER:HB2	1.85	0.58
3:D:38:SER:OG	3:D:40:ARG:NH1	2.36	0.58
2:H:98:TYR:O	2:H:113:GLY:HA2	2.04	0.58
3:L:75:ARG:NH1	3:L:83:PHE:O	2.38	0.57
1:A:62:ALA:O	1:A:374:ASN:ND2	2.37	0.56
1:A:24:ARG:HH22	1:B:23:ALA:HB1	1.69	0.56
1:A:13:LEU:HB2	1:B:13:LEU:HD21	1.87	0.56
1:A:683:ALA:N	1:A:734:ARG:O	2.36	0.56
1:A:750:MET:HE2	1:A:750:MET:H	1.69	0.56
1:A:638:LEU:HG	1:A:769:PRO:HB2	1.87	0.56
1:B:563:TRP:CG	1:B:842:LYS:HZ1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:55:ASP:HB2	3:D:110:MET:SD	2.46	0.55
1:A:701:VAL:HA	1:A:712:LEU:HD23	1.87	0.55
1:A:557:THR:HA	1:A:821:LEU:HD22	1.88	0.55
1:A:732:LYS:HE3	1:A:732:LYS:HA	1.87	0.55
1:A:28:ARG:NH1	1:B:27:ILE:HD11	2.22	0.55
1:B:268:SER:OG	1:B:269:GLU:N	2.37	0.55
1:A:752:ASP:OD1	1:A:752:ASP:N	2.36	0.55
1:B:180:ALA:O	1:B:183:LEU:HB2	2.07	0.55
1:B:751:LEU:HD12	1:B:788:VAL:HG13	1.88	0.55
2:H:30:THR:HG22	2:H:32:GLY:H	1.71	0.55
1:A:121:PRO:HA	1:A:124:ARG:HG3	1.89	0.55
1:B:28:ARG:HA	1:B:31:GLU:HB2	1.88	0.55
2:H:105:THR:O	3:L:117:ARG:NH1	2.39	0.55
1:A:165:HIS:CD2	1:A:166:ARG:HG3	2.42	0.54
1:A:263:ASP:N	1:A:263:ASP:OD1	2.39	0.54
1:B:165:HIS:CD2	1:B:166:ARG:HG3	2.43	0.54
1:B:563:TRP:CD1	1:B:842:LYS:HZ1	2.27	0.53
1:A:682:VAL:HG12	1:A:712:LEU:HB2	1.90	0.53
3:D:53:TYR:HB3	3:D:112:SER:HB2	1.89	0.53
1:A:91:TYR:HB2	1:A:247:ARG:HH12	1.74	0.53
1:A:643:SER:OG	1:A:644:ILE:N	2.40	0.53
2:H:65:ALA:HB3	2:H:68:VAL:HG22	1.91	0.53
3:L:68:LEU:HA	3:L:79:VAL:HG11	1.91	0.53
3:D:99:VAL:HG13	3:D:103:ASP:OD2	2.08	0.53
1:B:673:GLN:O	1:B:673:GLN:NE2	2.41	0.52
1:B:752:ASP:N	1:B:752:ASP:OD1	2.40	0.52
1:B:894:ASP:OD1	1:B:894:ASP:N	2.43	0.52
1:A:126:LEU:O	1:A:130:SER:OG	2.24	0.52
1:A:702:ALA:HB2	1:A:713:SER:HB3	1.91	0.52
1:A:896:ASP:N	1:A:896:ASP:OD1	2.42	0.52
1:B:587:ALA:O	1:B:590:THR:OG1	2.28	0.52
3:D:127:ASP:N	3:D:127:ASP:OD1	2.43	0.52
1:A:317:ARG:NH2	1:B:194:GLU:OE1	2.41	0.52
1:B:589:ASP:O	1:B:593:ARG:NH2	2.42	0.52
1:B:249:LEU:HD21	1:B:267:TRP:HE1	1.75	0.52
1:A:813:LEU:HD22	1:A:857:LEU:HD11	1.92	0.51
1:A:29:GLU:HB3	1:A:33:GLU:HB2	1.93	0.51
1:B:104:PHE:CD1	1:B:124:ARG:HB3	2.46	0.51
3:D:29:VAL:HG21	3:D:99:VAL:HG21	1.92	0.51
3:L:118:LEU:H	3:L:118:LEU:HD23	1.75	0.51
1:B:23:ALA:HA	1:B:26:ARG:CZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:VAL:HG12	1:B:740:HIS:H	1.75	0.51
2:H:5:GLN:HE21	2:H:7:VAL:HG23	1.74	0.51
3:D:38:SER:O	3:D:40:ARG:NH1	2.44	0.51
1:A:164:MET:HE2	1:A:164:MET:HA	1.94	0.50
1:A:833:GLU:CD	1:A:833:GLU:H	2.17	0.50
1:A:608:LEU:O	1:A:614:THR:OG1	2.28	0.50
1:A:194:GLU:OE1	1:B:317:ARG:NH2	2.42	0.50
2:C:65:ALA:HB3	2:C:68:VAL:HG22	1.94	0.50
2:H:56:LYS:HD2	2:H:56:LYS:C	2.37	0.50
3:D:59:GLN:HB3	3:D:106:VAL:HG23	1.93	0.50
1:A:604:ASP:OD1	1:A:605:SER:N	2.45	0.50
1:B:252:ASP:OD1	1:B:252:ASP:N	2.41	0.50
1:A:249:LEU:HD21	1:A:267:TRP:HE1	1.77	0.50
1:A:571:ALA:HB1	1:A:578:ARG:HG3	1.93	0.50
1:B:338:ALA:HB2	1:B:368:LEU:HD11	1.94	0.50
1:A:436:ARG:NE	1:A:454:GLU:OE1	2.41	0.49
1:B:334:ASP:N	1:B:334:ASP:OD1	2.44	0.49
1:A:247:ARG:HA	1:A:247:ARG:NE	2.27	0.49
1:B:566:MET:HE3	1:B:621:VAL:HG21	1.94	0.49
1:B:842:LYS:HD3	1:B:843:ASN:H	1.77	0.49
1:A:668:ARG:O	1:A:672:MET:HG3	2.12	0.49
1:A:673:GLN:O	1:A:673:GLN:NE2	2.45	0.49
1:B:24:ARG:NE	1:B:29:GLU:OE2	2.43	0.49
1:A:216:GLN:NE2	1:B:222:GLU:OE2	2.46	0.48
1:B:757:VAL:HA	1:B:760:ARG:HD3	1.95	0.48
1:B:595:ARG:HE	1:B:596:PRO:HD2	1.78	0.48
3:D:20:MET:HE2	3:D:20:MET:H	1.78	0.48
3:D:45:LEU:HD22	3:D:54:LEU:HD11	1.95	0.48
2:C:66:ALA:HA	2:C:69:LYS:HE2	1.95	0.48
2:C:90:LEU:HD12	2:C:90:LEU:H	1.78	0.48
1:A:310:PRO:HD2	1:A:349:ILE:HD12	1.96	0.48
1:A:585:CYS:O	1:A:589:ASP:HB2	2.13	0.48
3:D:63:GLN:NE2	3:D:64:SER:O	2.47	0.48
1:B:202:THR:HG22	1:B:202:THR:O	2.14	0.48
1:A:749:PRO:HD2	1:A:750:MET:HE1	1.96	0.47
1:B:478:ALA:HA	1:B:517:LEU:HD12	1.96	0.47
1:A:159:ASP:OD1	1:A:159:ASP:N	2.35	0.47
1:A:595:ARG:HH11	1:A:596:PRO:HD2	1.79	0.47
2:H:95:THR:HG1	2:H:118:VAL:H	1.59	0.47
1:B:27:ILE:HG22	1:B:28:ARG:H	1.79	0.47
1:A:687:THR:HG23	1:A:690:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASP:OD1	1:B:60:ASP:N	2.47	0.47
1:B:896:ASP:OD1	1:B:896:ASP:N	2.46	0.47
1:A:738:VAL:HG12	1:A:740:HIS:H	1.79	0.47
1:A:682:VAL:HG21	1:A:723:ALA:HB2	1.95	0.47
1:A:389:LYS:HE2	1:A:400:PRO:HG2	1.97	0.47
1:A:749:PRO:HD2	1:A:750:MET:CE	2.46	0.47
1:A:556:PHE:HE2	1:A:639:LEU:HD23	1.80	0.46
3:D:58:LEU:HD13	3:D:107:TYR:CZ	2.50	0.46
2:H:55:SER:O	2:H:59:GLY:N	2.44	0.46
2:H:95:THR:HG23	2:H:117:THR:HA	1.96	0.46
1:A:293:VAL:HG22	1:A:453:LEU:HD23	1.97	0.46
1:B:176:THR:HA	1:B:182:VAL:HG21	1.97	0.46
1:A:268:SER:OG	1:A:269:GLU:N	2.44	0.46
1:A:590:THR:HG23	1:A:591:HIS:ND1	2.31	0.46
1:B:66:THR:OG1	1:B:67:GLU:N	2.49	0.46
1:A:875:THR:OG1	1:A:877:VAL:O	2.30	0.45
2:H:4:VAL:HG22	2:H:29:PHE:HB3	1.97	0.45
1:A:657:ASP:OD2	1:A:764:ARG:NH2	2.49	0.45
1:A:8:LYS:HG3	1:A:9:VAL:H	1.81	0.45
1:B:840:LEU:HD12	1:B:840:LEU:HA	1.85	0.45
1:A:119:MET:HE2	1:A:123:GLN:HG2	1.97	0.45
1:A:621:VAL:HG23	1:A:622:GLU:OE2	2.16	0.45
1:B:363:GLU:N	1:B:363:GLU:OE1	2.50	0.45
1:B:525:ALA:HB2	1:B:531:LEU:HD13	1.99	0.45
1:B:704:VAL:HG12	1:B:710:VAL:HG23	1.99	0.45
3:D:103:ASP:HB2	3:D:107:TYR:OH	2.17	0.45
1:A:785:ASP:OD1	1:A:785:ASP:N	2.36	0.45
1:B:119:MET:HE3	1:B:124:ARG:HG2	1.99	0.45
1:B:750:MET:N	1:B:750:MET:HE3	2.32	0.45
2:H:31:PHE:O	2:H:76:ARG:NH2	2.50	0.45
1:A:91:TYR:CB	1:A:247:ARG:HH12	2.30	0.45
1:A:179:SER:HB2	1:A:182:VAL:HG23	1.99	0.45
1:A:476:VAL:HG23	1:A:521:ALA:HB3	1.99	0.45
3:L:55:ASP:OD2	3:L:117:ARG:NH2	2.51	0.45
3:L:60:LYS:NZ	3:L:66:GLN:OE1	2.39	0.45
1:A:600:VAL:HG23	1:A:604:ASP:HB3	1.99	0.44
1:B:165:HIS:CD2	1:B:165:HIS:C	2.95	0.44
3:L:59:GLN:HA	3:L:65:PRO:HA	1.99	0.44
1:B:597:LEU:HD23	1:B:597:LEU:HA	1.80	0.44
1:A:681:MET:SD	1:A:713:SER:HB2	2.58	0.44
1:A:781:LEU:HD22	1:A:786:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ARG:NE	1:B:454:GLU:OE1	2.39	0.44
1:A:104:PHE:CD1	1:A:124:ARG:HB3	2.53	0.44
1:A:799:ASP:OD1	1:A:799:ASP:N	2.50	0.44
3:D:19:VAL:HG13	3:D:42:SER:H	1.82	0.44
1:B:22:ALA:HA	1:B:25:GLN:HB2	1.99	0.44
1:A:655:VAL:HG13	1:A:656:LEU:HG	2.00	0.43
3:D:68:LEU:HA	3:D:79:VAL:HG11	1.99	0.43
2:H:26:ALA:HB3	2:H:31:PHE:CZ	2.54	0.43
1:B:181:SER:HA	1:B:199:THR:HG21	2.00	0.43
1:B:604:ASP:OD1	1:B:605:SER:N	2.52	0.43
2:C:80:LYS:NZ	2:C:82:ILE:HB	2.33	0.43
2:C:87:MET:HE1	2:C:90:LEU:HA	2.01	0.43
3:D:67:LEU:HD11	3:D:76:ALA:HB3	2.00	0.43
2:H:20:LEU:HD23	2:H:20:LEU:HA	1.80	0.43
1:A:444:ILE:HD13	1:A:444:ILE:HA	1.81	0.43
1:B:23:ALA:HA	1:B:26:ARG:NH2	2.34	0.43
1:B:500:ASP:OD1	1:B:500:ASP:N	2.47	0.43
1:B:682:VAL:HG21	1:B:723:ALA:HB2	2.00	0.43
3:L:111:GLN:OE1	3:L:111:GLN:N	2.52	0.43
1:A:13:LEU:HD21	2:H:52:PHE:HZ	1.84	0.43
1:B:696:ASP:OD1	1:B:696:ASP:N	2.52	0.43
3:D:56:TRP:CE2	3:D:94:LEU:HB2	2.54	0.43
1:A:182:VAL:HG12	1:A:186:ARG:HG2	2.01	0.43
1:B:27:ILE:HG22	1:B:28:ARG:N	2.33	0.43
1:A:244:SER:O	1:A:247:ARG:HD2	2.19	0.43
1:A:734:ARG:HA	1:A:734:ARG:NE	2.33	0.43
1:A:750:MET:O	1:A:754:PHE:HB2	2.19	0.43
1:A:840:LEU:HD12	1:A:840:LEU:HA	1.85	0.42
1:B:23:ALA:HA	1:B:26:ARG:NE	2.35	0.42
1:A:202:THR:OG1	1:A:206:SER:HA	2.20	0.42
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.84	0.42
1:B:27:ILE:CG2	1:B:28:ARG:H	2.31	0.42
1:B:226:ALA:HB3	1:B:276:VAL:HG23	2.02	0.42
3:D:81:ASP:OD1	3:D:98:ARG:NH2	2.40	0.42
1:A:855:ALA:O	1:A:859:VAL:HG13	2.20	0.42
3:D:81:ASP:OD1	3:D:81:ASP:N	2.43	0.42
1:A:831:GLY:HA3	1:A:834:GLN:HE22	1.84	0.42
2:C:76:ARG:NE	2:C:78:ASP:OD1	2.43	0.42
2:H:31:PHE:HD2	2:H:76:ARG:HE	1.68	0.42
1:A:136:ARG:HA	1:A:136:ARG:HD2	1.69	0.41
1:A:222:GLU:H	1:A:222:GLU:HG2	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:HA	1:A:485:ARG:HD2	1.79	0.41
3:D:87:GLY:HA3	3:D:92:PHE:HA	2.02	0.41
1:A:72:ARG:NH1	1:A:234:MET:O	2.54	0.41
3:L:75:ARG:HH12	3:L:83:PHE:HB2	1.85	0.41
1:A:690:GLU:HG2	1:A:731:ARG:HH12	1.85	0.41
1:B:281:GLU:OE1	1:B:284:ARG:NH2	2.53	0.41
2:H:13:LEU:HD12	2:H:14:VAL:H	1.86	0.41
1:B:592:LEU:HD12	1:B:592:LEU:HA	1.81	0.41
3:D:69:ILE:HD11	3:D:84:SER:HA	2.02	0.41
1:B:40:MET:HE3	1:B:388:ILE:HG12	2.03	0.41
2:H:55:SER:OG	2:H:56:LYS:N	2.53	0.41
1:B:521:ALA:HA	1:B:543:VAL:O	2.20	0.41
1:B:832:PRO:O	1:B:833:GLU:C	2.63	0.41
3:D:119:THR:HG23	3:D:121:GLY:H	1.85	0.41
1:A:24:ARG:HH12	1:B:23:ALA:HB3	1.86	0.41
1:B:323:LEU:HD23	1:B:323:LEU:HA	1.91	0.41
1:A:252:ASP:OD1	1:A:252:ASP:N	2.44	0.40
3:D:20:MET:HE2	3:D:20:MET:N	2.36	0.40
2:H:95:THR:HA	2:H:116:VAL:O	2.21	0.40
1:B:28:ARG:HB3	1:B:32:GLU:HG2	2.04	0.40
1:B:681:MET:HB3	1:B:736:LEU:HD23	2.02	0.40
3:L:71:LEU:HD23	3:L:71:LEU:HA	1.86	0.40
1:B:855:ALA:O	1:B:859:VAL:HG13	2.22	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	888/1094 (81%)	864 (97%)	24 (3%)	0	100	100
1	B	890/1094 (81%)	868 (98%)	22 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	57/249 (23%)	53 (93%)	4 (7%)	0	100	100
2	H	115/249 (46%)	112 (97%)	3 (3%)	0	100	100
3	D	111/236 (47%)	109 (98%)	2 (2%)	0	100	100
3	L	40/236 (17%)	39 (98%)	1 (2%)	0	100	100
All	All	2101/3158 (66%)	2045 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	661/830 (80%)	608 (92%)	53 (8%)	11	27
1	B	663/830 (80%)	622 (94%)	41 (6%)	16	37
2	C	50/203 (25%)	47 (94%)	3 (6%)	17	38
2	H	92/203 (45%)	87 (95%)	5 (5%)	20	42
3	D	99/208 (48%)	93 (94%)	6 (6%)	17	38
3	L	40/208 (19%)	39 (98%)	1 (2%)	42	66
All	All	1605/2482 (65%)	1496 (93%)	109 (7%)	16	33

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	76	THR
1	A	124	ARG
1	A	133	LEU
1	A	157	SER
1	A	165	HIS
1	A	175	LEU
1	A	182	VAL
1	A	184	SER

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Mol	Chain	Res	Type
1	A	199	THR
1	A	200	VAL
1	A	202	THR
1	A	205	SER
1	A	224	SER
1	A	256	LYS
1	A	274	LEU
1	A	292	VAL
1	A	301	ASP
1	A	341	THR
1	A	366	LEU
1	A	378	THR
1	A	412	VAL
1	A	444	ILE
1	A	453	LEU
1	A	513	THR
1	A	542	VAL
1	A	544	THR
1	A	554	VAL
1	A	555	LEU
1	A	631	SER
1	A	634	VAL
1	A	643	SER
1	A	647	LEU
1	A	655	VAL
1	A	664	LEU
1	A	681	MET
1	A	682	VAL
1	A	701	VAL
1	A	713	SER
1	A	753	ASP
1	A	775	THR
1	A	783	SER
1	A	785	ASP
1	A	811	THR
1	A	826	LEU
1	A	834	GLN
1	A	835	SER
1	A	836	CYS
1	A	840	LEU
1	A	847	VAL
1	A	877	VAL

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Mol	Chain	Res	Type
1	A	883	THR
1	A	895	VAL
1	B	38	VAL
1	B	60	ASP
1	B	76	THR
1	B	99	ASP
1	B	133	LEU
1	B	144	LEU
1	B	161	SER
1	B	170	VAL
1	B	182	VAL
1	B	183	LEU
1	B	199	THR
1	B	200	VAL
1	B	207	SER
1	B	239	THR
1	B	256	LYS
1	B	265	THR
1	B	268	SER
1	B	274	LEU
1	B	292	VAL
1	B	314	SER
1	B	333	VAL
1	B	334	ASP
1	B	364	THR
1	B	412	VAL
1	B	460	ILE
1	B	513	THR
1	B	542	VAL
1	B	548	VAL
1	B	554	VAL
1	B	615	GLN
1	B	639	LEU
1	B	687	THR
1	B	767	SER
1	B	783	SER
1	B	785	ASP
1	B	826	LEU
1	B	835	SER
1	B	836	CYS
1	B	837	VAL
1	B	840	LEU

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Mol	Chain	Res	Type
1	B	880	VAL
2	C	64	TYR
2	C	101	THR
2	C	107	PHE
3	D	67	LEU
3	D	74	ASN
3	D	81	ASP
3	D	106	VAL
3	D	113	LEU
3	D	127	ASP
2	H	54	ARG
2	H	55	SER
2	H	73	THR
2	H	74	ILE
2	H	92	THR
3	L	109	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	156	ASN
1	A	165	HIS
1	A	834	GLN
1	A	858	HIS
1	A	888	HIS
1	B	122	GLN
1	B	156	ASN
1	B	165	HIS
1	B	299	ASN
1	B	305	ASN
1	B	404	HIS
1	B	448	ASN
1	B	615	GLN
1	B	843	ASN
1	B	858	HIS
3	D	52	ASN
3	D	74	ASN
2	H	88	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 [i](#)

There are no chain breaks in this entry.

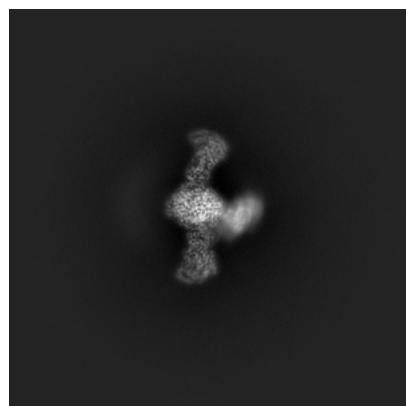
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-76027. These allow visual inspection of the internal detail of the map and identification of artifacts.

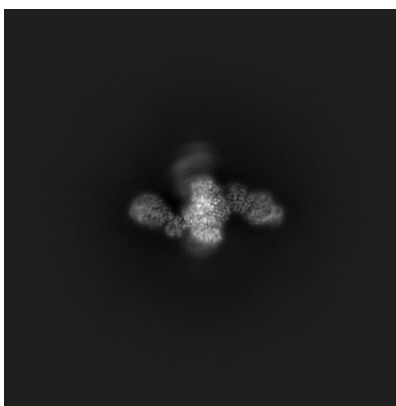
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

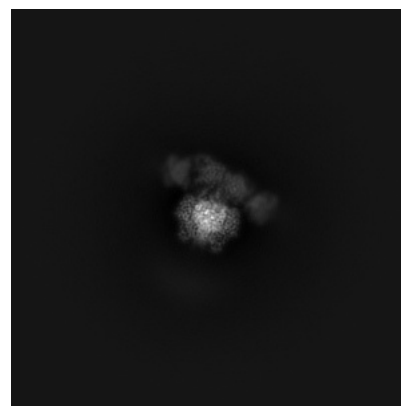
#### 6.1.1 Primary map



X

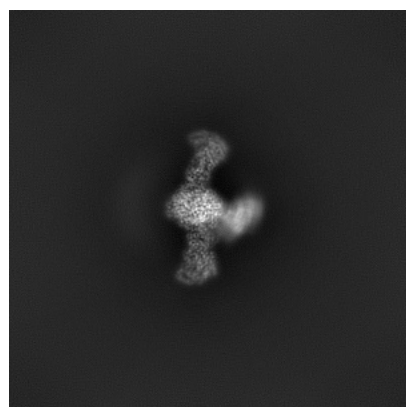


Y

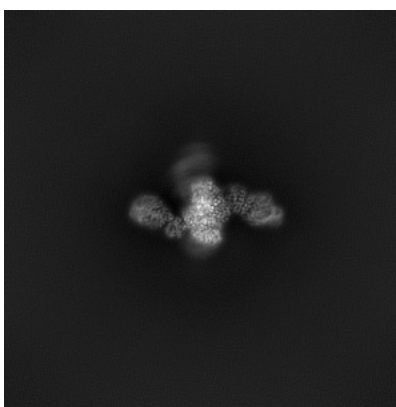


Z

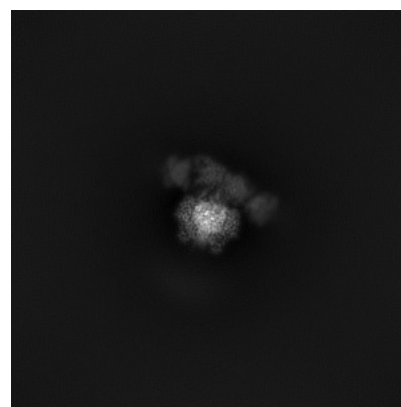
#### 6.1.2 Raw map



X



Y



Z

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



## 6.2 Central slices [i](#)

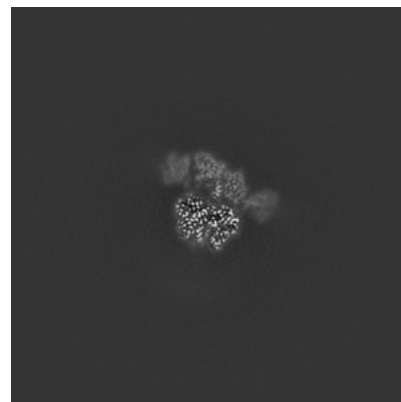
### 6.2.1 Primary map



X Index: 224

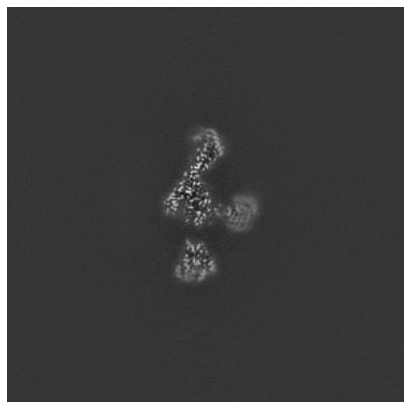


Y Index: 224

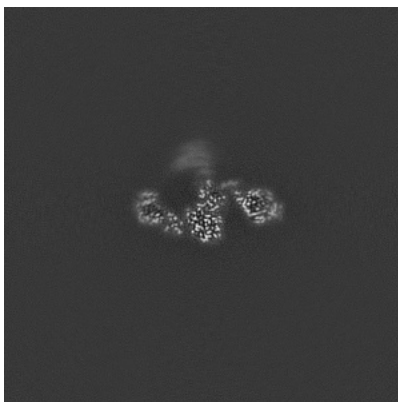


Z Index: 224

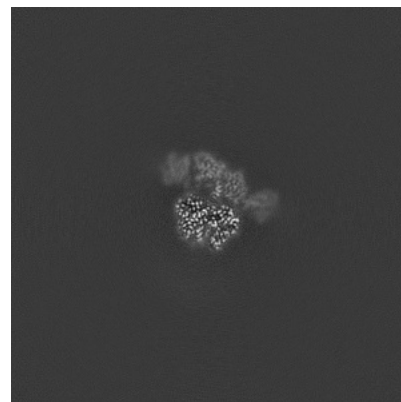
### 6.2.2 Raw map



X Index: 224



Y Index: 224

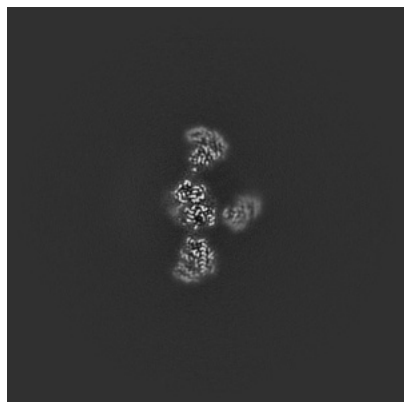


Z Index: 224

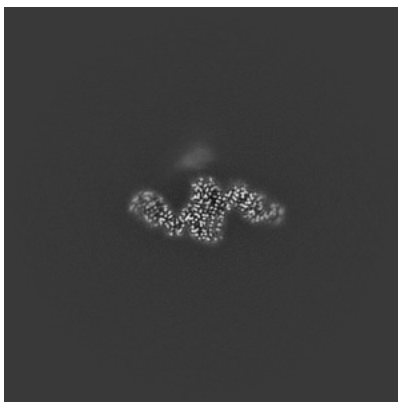
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

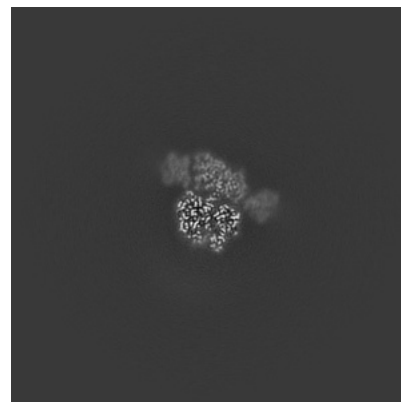
### 6.3.1 Primary map



X Index: 218

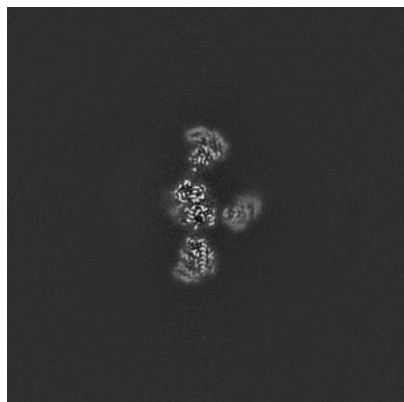


Y Index: 215

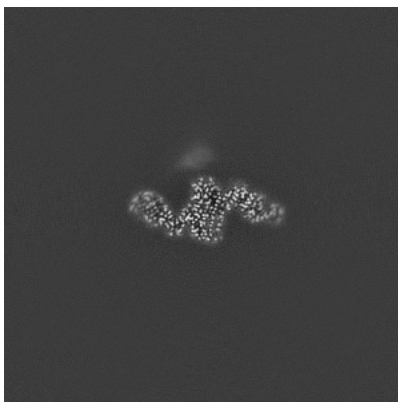


Z Index: 221

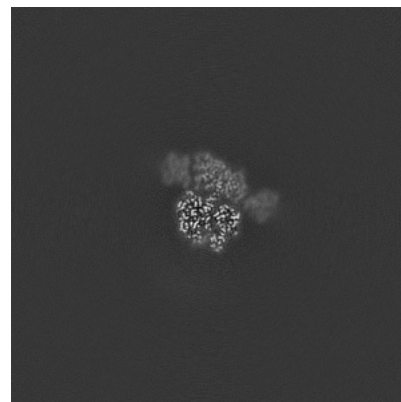
### 6.3.2 Raw map



X Index: 218



Y Index: 215

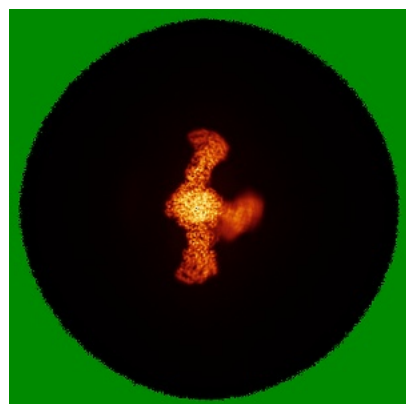


Z Index: 221

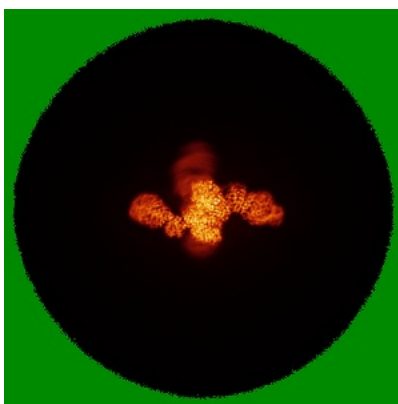
The images above show the largest variance slices of the map in three orthogonal directions.

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

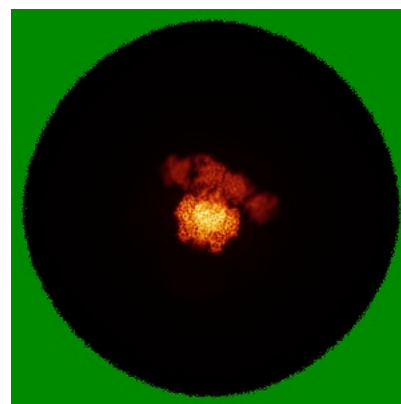
### 6.4.1 Primary map



X

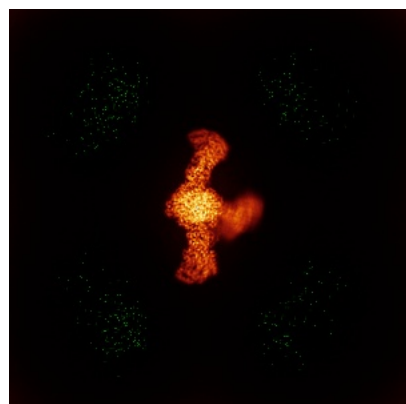


Y

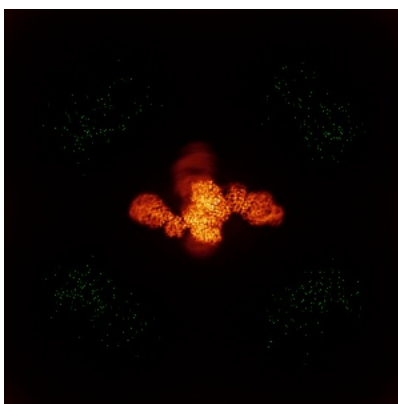


Z

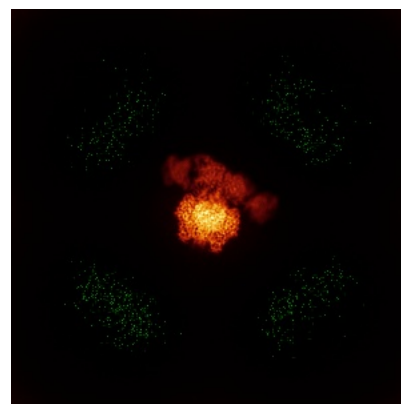
### 6.4.2 Raw map



X



Y

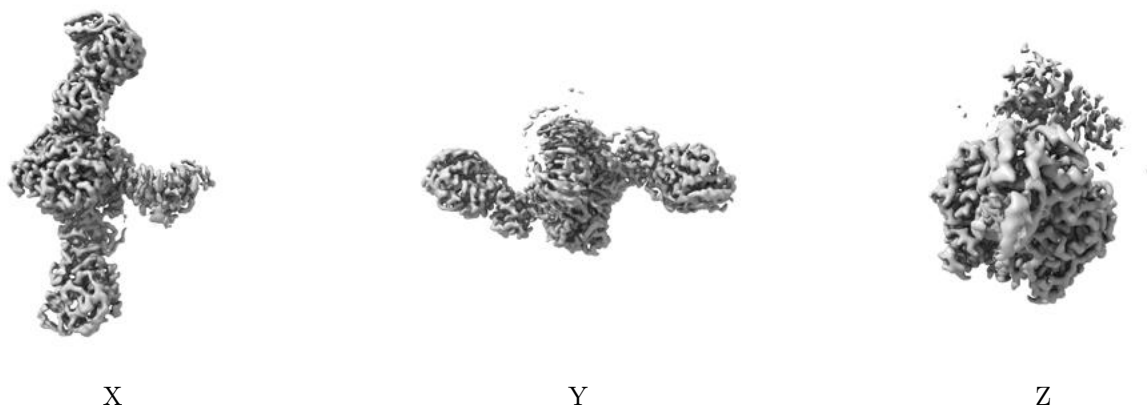


Z

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.

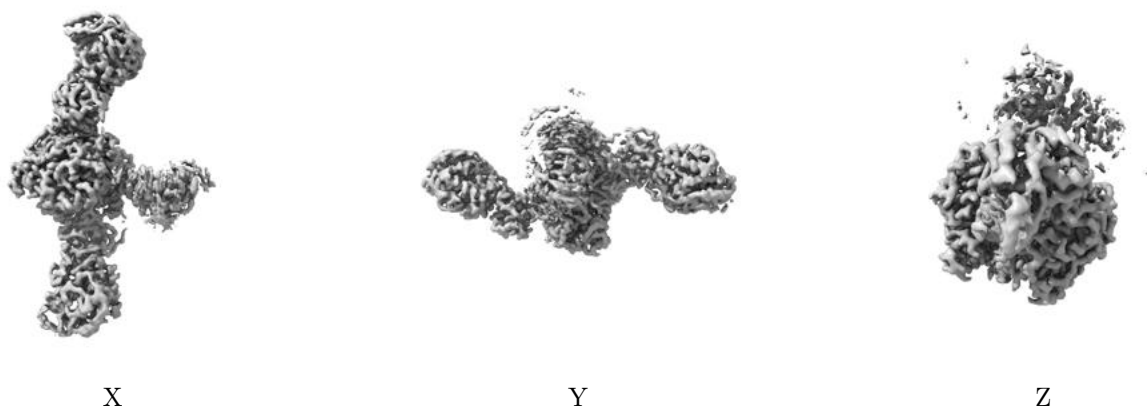
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.235. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

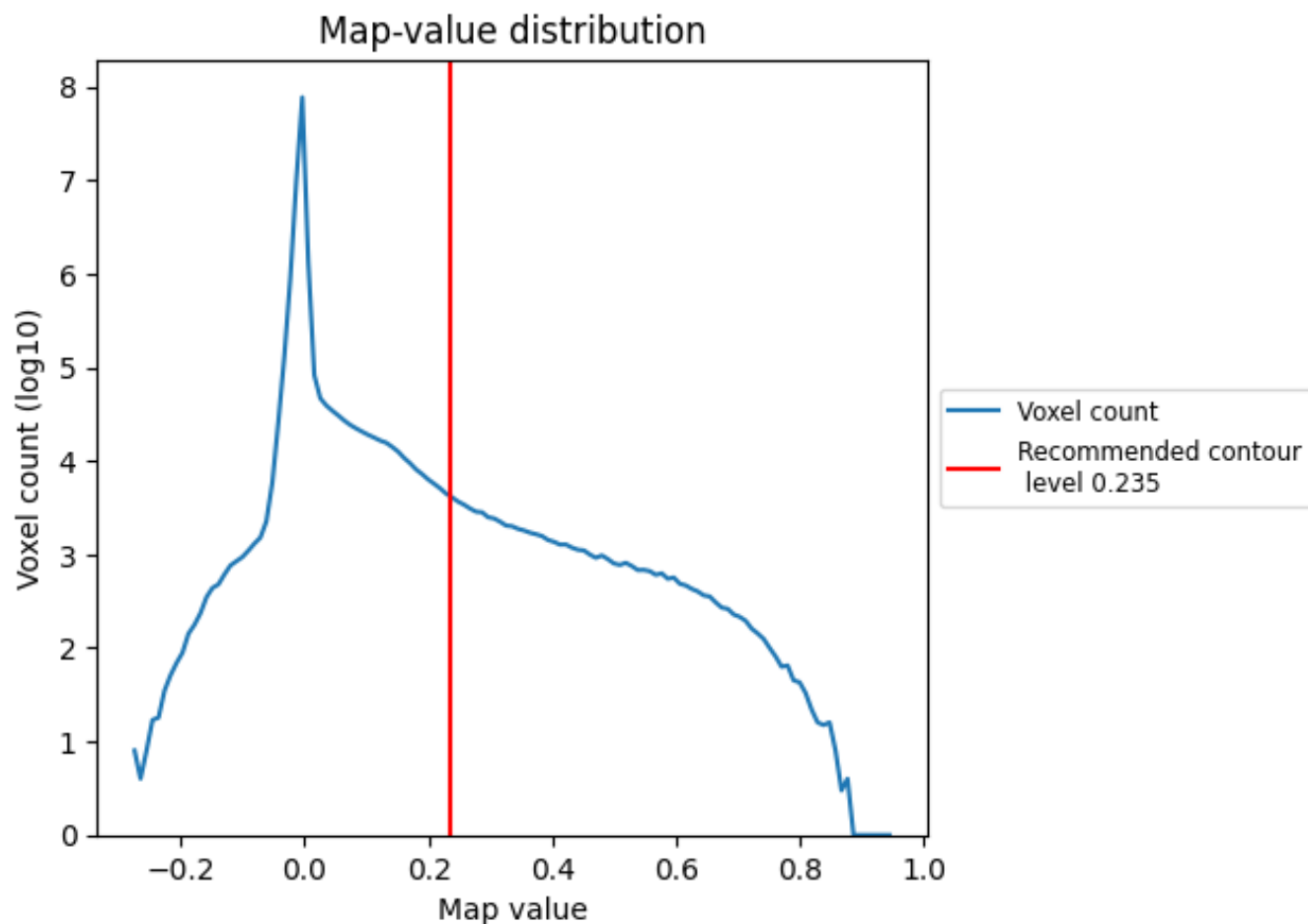
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

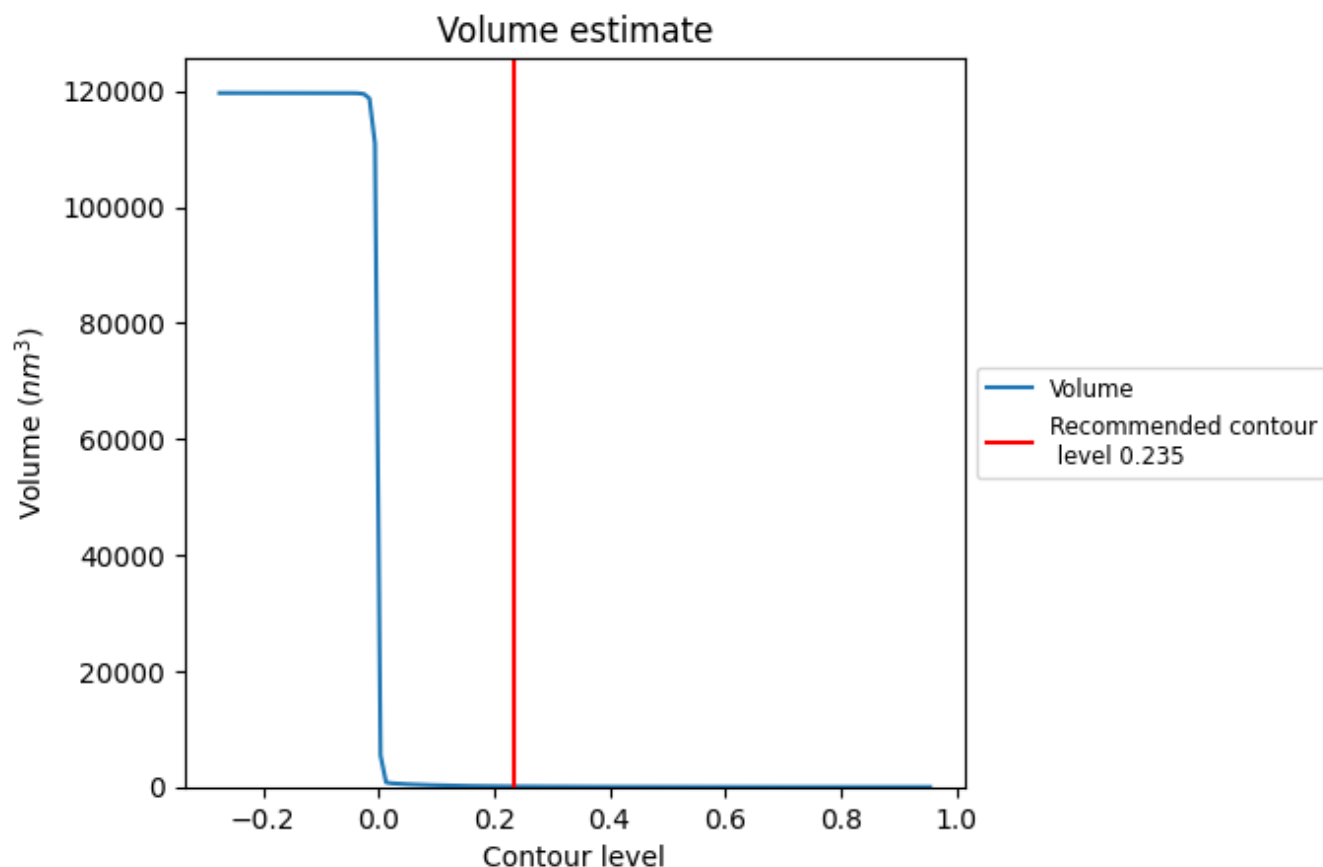
This section contains the results of statistical analysis of the map.

### 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.

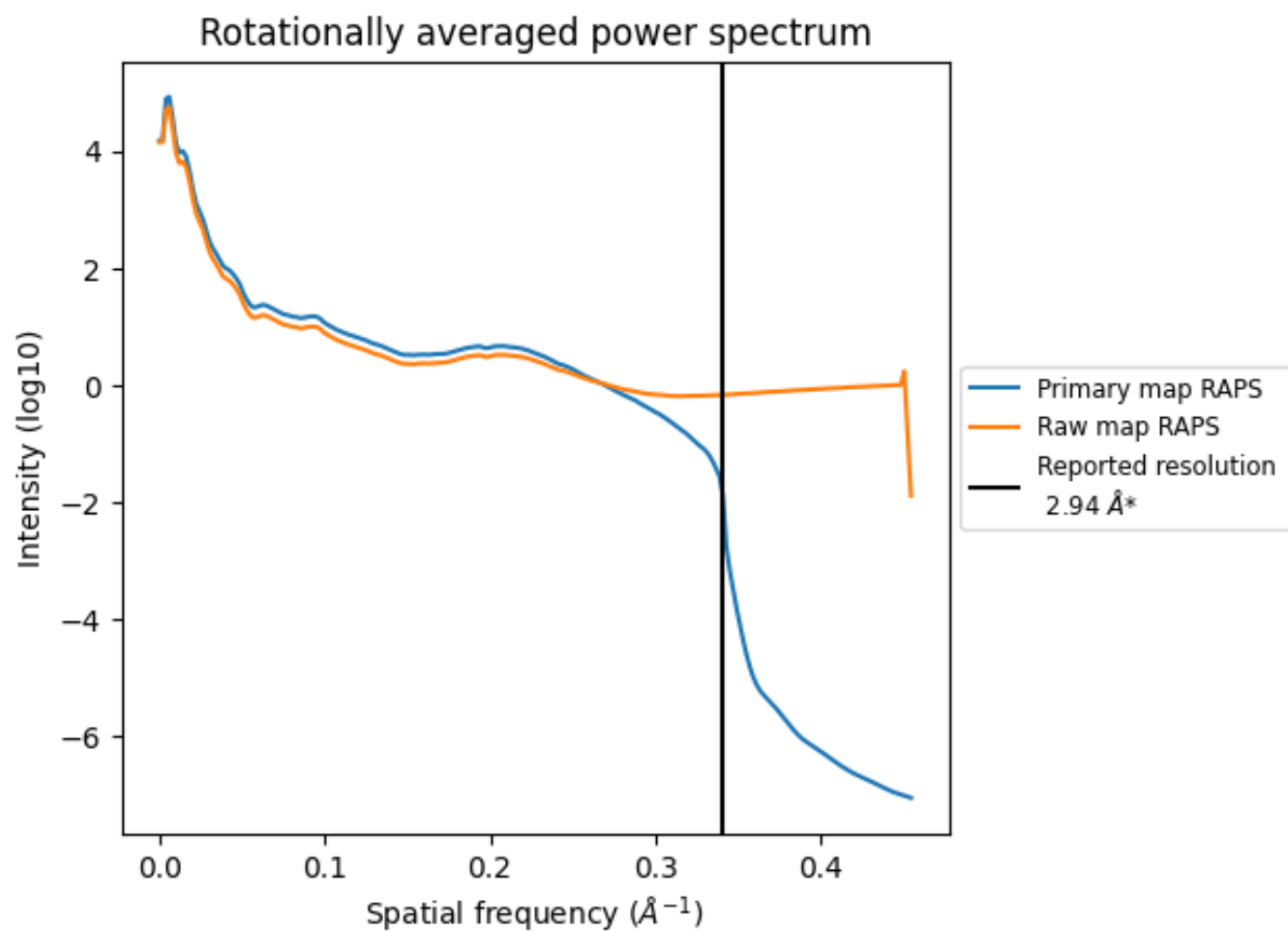
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88  $\text{nm}^3$ ; this corresponds to an approximate mass of 80 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 ⓘ

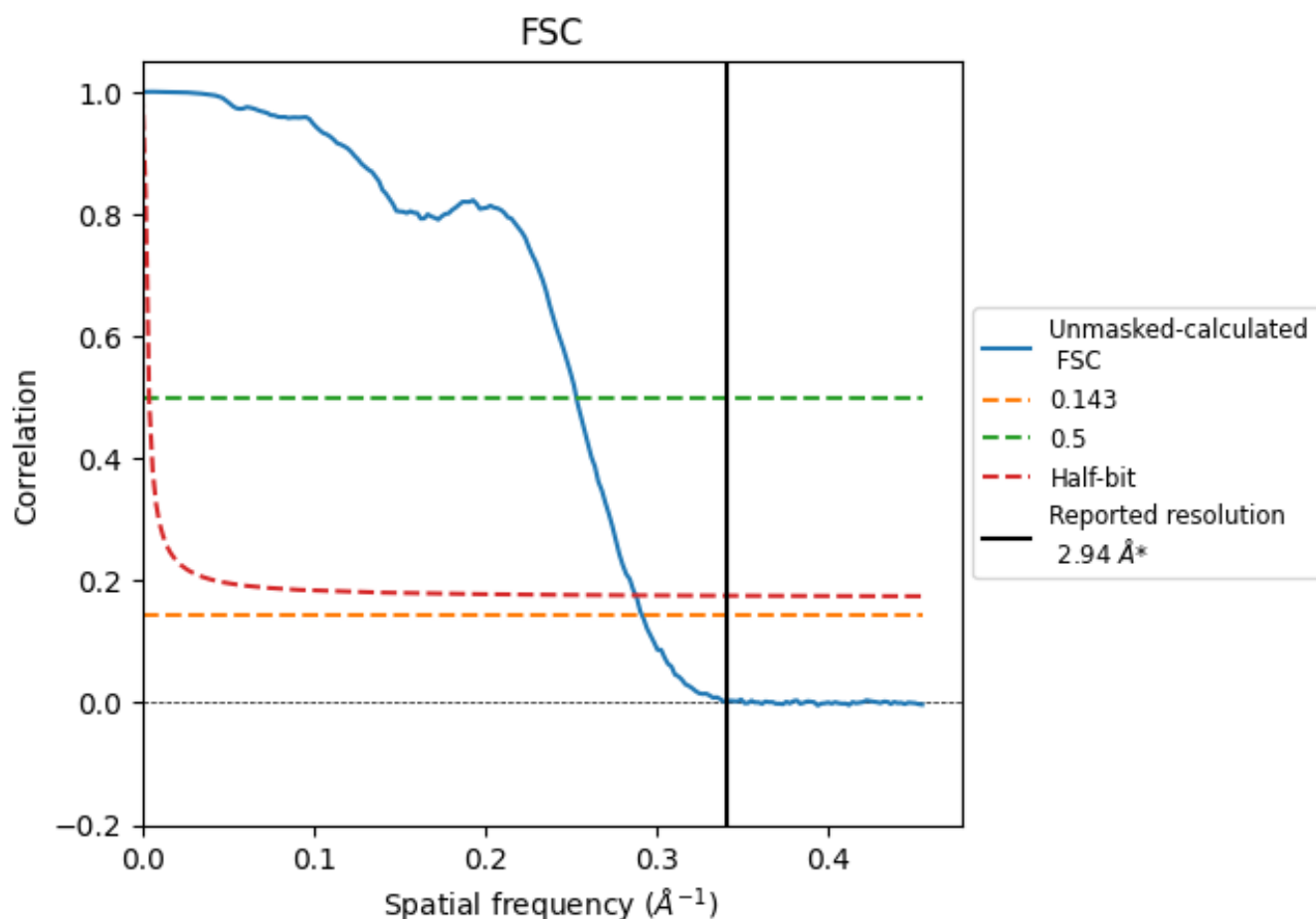


\*Reported resolution corresponds to spatial frequency of 0.340 Å<sup>-1</sup>

## 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 0.340  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

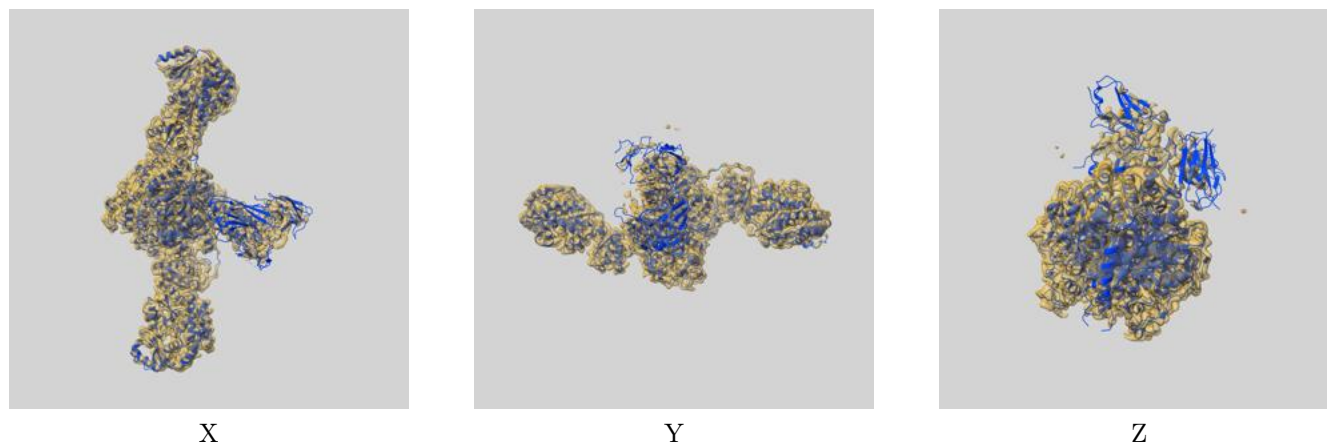
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.43	3.95	3.48

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.43 differs from the reported value 2.94 by more than 10 %

## 9 Map-model fit [i](#)

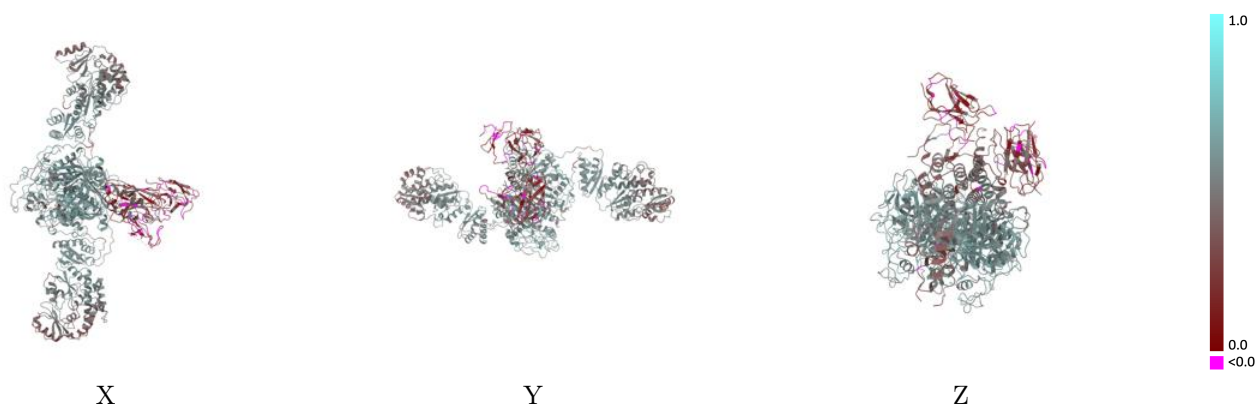
This section contains information regarding the fit between EMDB map EMD-76027 and PDB model 11SZ. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



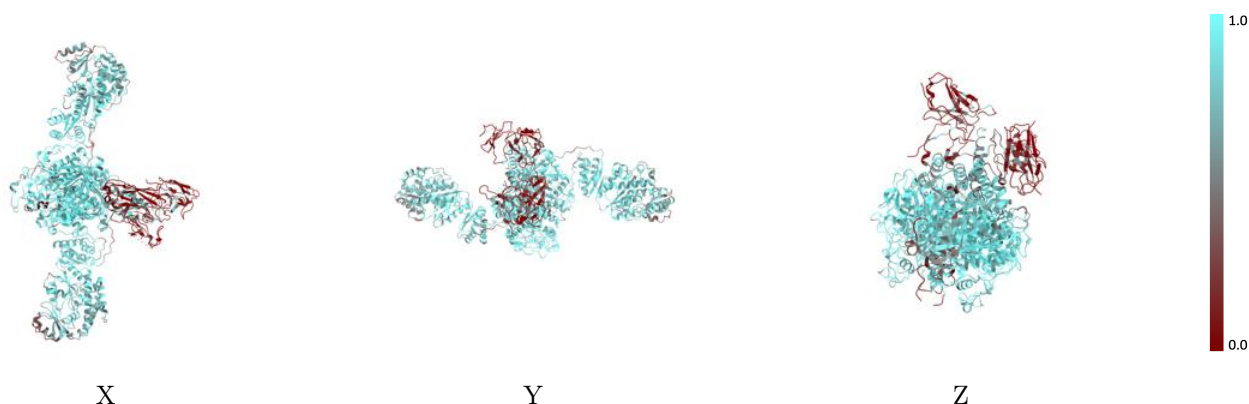
The images above show the 3D surface view of the map at the recommended contour level 0.235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



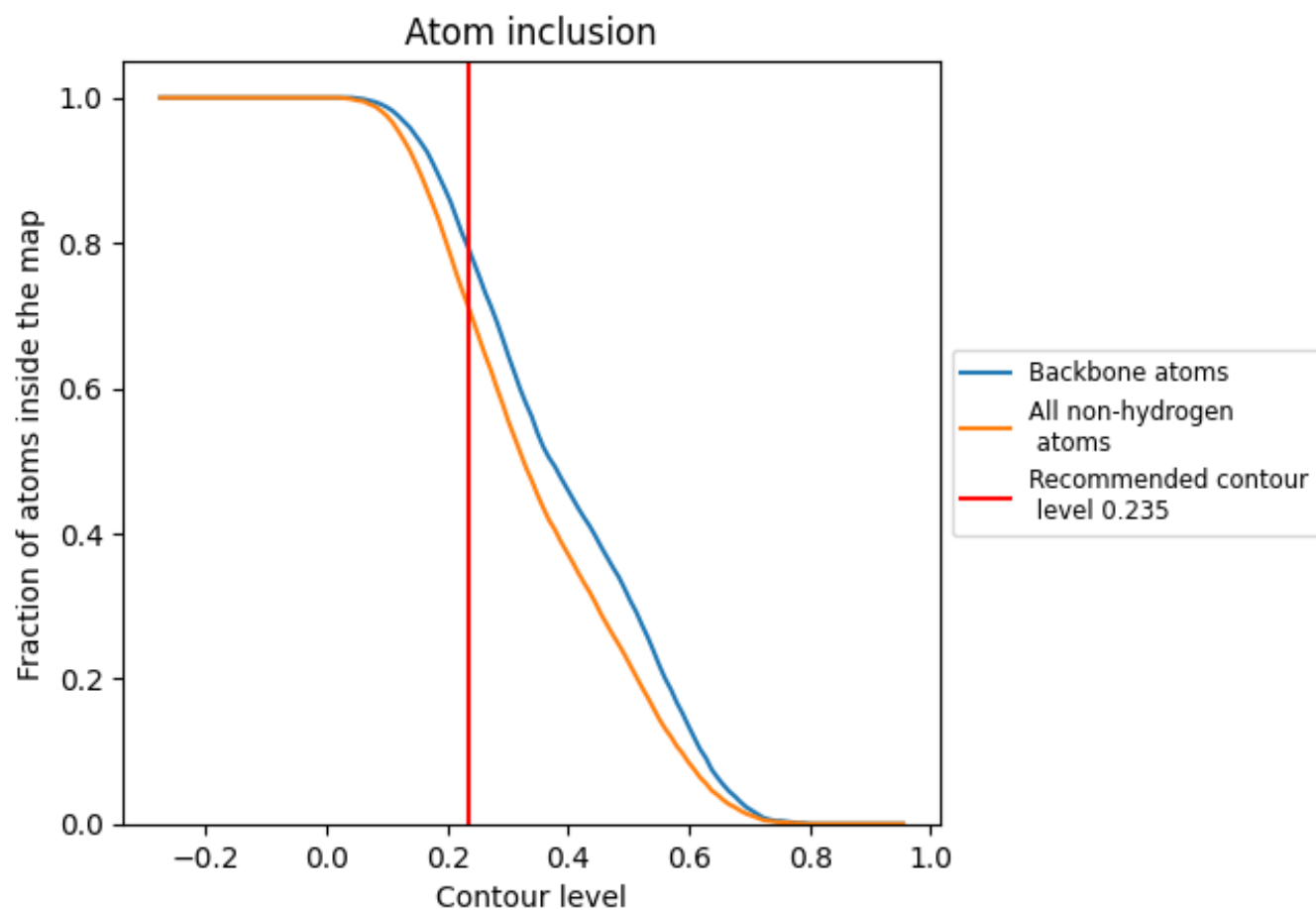
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.235).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7120</div>	<div><div></div>0.4740</div>
A	<div><div></div>0.8160</div>	<div><div></div>0.5270</div>
B	<div><div></div>0.8220</div>	<div><div></div>0.5260</div>
C	<div><div></div>0.2740</div>	<div><div></div>0.2800</div>
D	<div><div></div>0.1660</div>	<div><div></div>0.1870</div>
H	<div><div></div>0.1410</div>	<div><div></div>0.2290</div>
L	<div><div></div>0.0460</div>	<div><div></div>0.1100</div>

1.0

0.0

<0.0