



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 08:08 pm GMT

PDB ID : 7B8P
EMDB ID : EMD-12088
Title : Acinetobacter baumannii multidrug transporter AdeB in OOO state
Authors : Ornik-Cha, A.; Reitz, J.; Seybert, A.; Frangakis, A.; Pos, K.M.
Deposited on : 2020-12-13
Resolution : 3.54 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
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

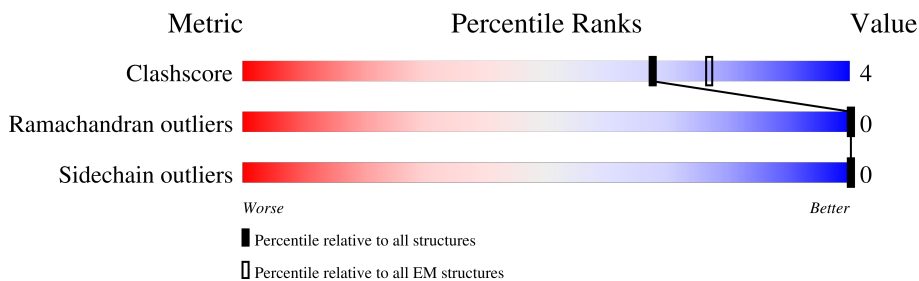
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.54 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 $\leq 5\%$. 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	1056	
1	B	1056	
1	C	1056	

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 23202 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1015	7734	5000	1258	1431	45	0	0
1	B	1015	7734	5000	1258	1431	45	0	0
1	C	1015	7734	5000	1258	1431	45	0	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP B0V4F5
A	0	SER	-	expression tag	UNP B0V4F5
A	1036	ALA	-	expression tag	UNP B0V4F5
A	1037	LEU	-	expression tag	UNP B0V4F5
A	1038	GLU	-	expression tag	UNP B0V4F5
A	1039	VAL	-	expression tag	UNP B0V4F5
A	1040	LEU	-	expression tag	UNP B0V4F5
A	1041	PHE	-	expression tag	UNP B0V4F5
A	1042	GLN	-	expression tag	UNP B0V4F5
A	1043	GLY	-	expression tag	UNP B0V4F5
A	1044	PRO	-	expression tag	UNP B0V4F5
A	1045	HIS	-	expression tag	UNP B0V4F5
A	1046	HIS	-	expression tag	UNP B0V4F5
A	1047	HIS	-	expression tag	UNP B0V4F5
A	1048	HIS	-	expression tag	UNP B0V4F5
A	1049	HIS	-	expression tag	UNP B0V4F5
A	1050	HIS	-	expression tag	UNP B0V4F5
A	1051	HIS	-	expression tag	UNP B0V4F5
A	1052	HIS	-	expression tag	UNP B0V4F5
A	1053	HIS	-	expression tag	UNP B0V4F5
A	1054	HIS	-	expression tag	UNP B0V4F5
B	-1	MET	-	initiating methionine	UNP B0V4F5
B	0	SER	-	expression tag	UNP B0V4F5
B	1036	ALA	-	expression tag	UNP B0V4F5

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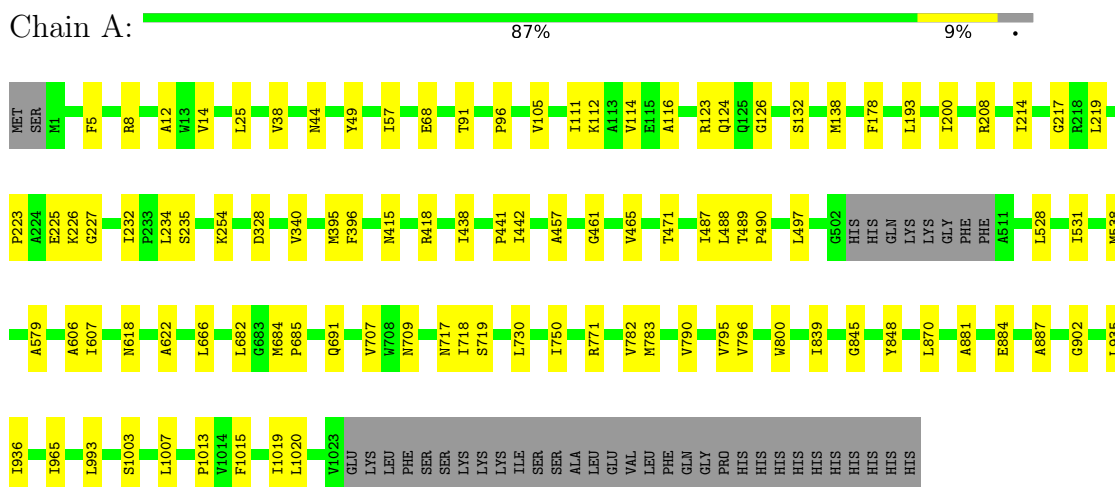
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1037	LEU	-	expression tag	UNP B0V4F5
B	1038	GLU	-	expression tag	UNP B0V4F5
B	1039	VAL	-	expression tag	UNP B0V4F5
B	1040	LEU	-	expression tag	UNP B0V4F5
B	1041	PHE	-	expression tag	UNP B0V4F5
B	1042	GLN	-	expression tag	UNP B0V4F5
B	1043	GLY	-	expression tag	UNP B0V4F5
B	1044	PRO	-	expression tag	UNP B0V4F5
B	1045	HIS	-	expression tag	UNP B0V4F5
B	1046	HIS	-	expression tag	UNP B0V4F5
B	1047	HIS	-	expression tag	UNP B0V4F5
B	1048	HIS	-	expression tag	UNP B0V4F5
B	1049	HIS	-	expression tag	UNP B0V4F5
B	1050	HIS	-	expression tag	UNP B0V4F5
B	1051	HIS	-	expression tag	UNP B0V4F5
B	1052	HIS	-	expression tag	UNP B0V4F5
B	1053	HIS	-	expression tag	UNP B0V4F5
B	1054	HIS	-	expression tag	UNP B0V4F5
C	-1	MET	-	initiating methionine	UNP B0V4F5
C	0	SER	-	expression tag	UNP B0V4F5
C	1036	ALA	-	expression tag	UNP B0V4F5
C	1037	LEU	-	expression tag	UNP B0V4F5
C	1038	GLU	-	expression tag	UNP B0V4F5
C	1039	VAL	-	expression tag	UNP B0V4F5
C	1040	LEU	-	expression tag	UNP B0V4F5
C	1041	PHE	-	expression tag	UNP B0V4F5
C	1042	GLN	-	expression tag	UNP B0V4F5
C	1043	GLY	-	expression tag	UNP B0V4F5
C	1044	PRO	-	expression tag	UNP B0V4F5
C	1045	HIS	-	expression tag	UNP B0V4F5
C	1046	HIS	-	expression tag	UNP B0V4F5
C	1047	HIS	-	expression tag	UNP B0V4F5
C	1048	HIS	-	expression tag	UNP B0V4F5
C	1049	HIS	-	expression tag	UNP B0V4F5
C	1050	HIS	-	expression tag	UNP B0V4F5
C	1051	HIS	-	expression tag	UNP B0V4F5
C	1052	HIS	-	expression tag	UNP B0V4F5
C	1053	HIS	-	expression tag	UNP B0V4F5
C	1054	HIS	-	expression tag	UNP B0V4F5

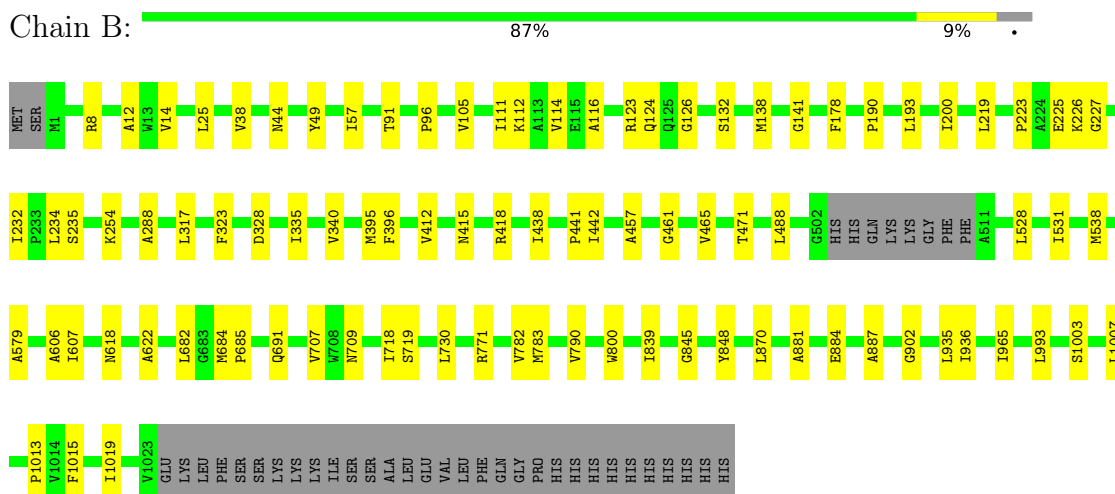
3 Residue-property plots

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: Efflux pump membrane transporter



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MET	SER	M1	R8	A12	W13	V14	L25	V38	N44	R67	E68	T91	P96	V105	I111	K112	A113	V114	E115	A116	R117	R123	Q124	Q125	G126	S132	G141	L166	F178	L193	I200	L219	P223	E225	K226	G227	I232	P233
L234	S235	K254	A268	N298	K301	L317	F323	V340	M395	F396	V412	N415	R418	I438	P441	I442	A457	G461	V465	T471	L488	G502	HIS	HIS	GLN	GLN	LYS	LYS	GLY	PHE	PHE	A511	L529	K530	A224	I531	M538	A579
A606	I607	N618	A622	L666	L682	G683	M684	P685	Q691	V707	W708	N709	I718	S719	L730	S738	M745	R771	V782	M783	V790	V795	V796	W800	I839	G845	Y848	L870	A881	E884	A887	G902	L935	I936				
I965	L993	S1003	L1007	F1015	I1019	V1023	GLU	LYS	LEU	PHE	SER	SER	LYS	LYS	LYS	ILE	SER	SER	ALA	LEU	GLU	VAL	LEU	PHE	GLN	GLY	PHO	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	132346	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 ($e^-/\text{\AA}^2$)	60	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	0.156	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.31	0/7873	0.50	4/10679 (0.0%)
1	B	0.31	0/7873	0.50	4/10679 (0.0%)
1	C	0.31	0/7873	0.50	4/10679 (0.0%)
All	All	0.31	0/23619	0.50	12/32037 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	LYS	CB-CA-C	-6.21	97.99	110.40
1	A	254	LYS	CB-CA-C	-6.19	98.01	110.40
1	B	254	LYS	CB-CA-C	-6.19	98.02	110.40
1	B	254	LYS	N-CA-C	6.10	127.46	111.00
1	C	254	LYS	N-CA-C	6.09	127.45	111.00
1	A	254	LYS	N-CA-C	6.08	127.42	111.00
1	A	707	VAL	N-CA-C	-5.16	97.06	111.00
1	B	707	VAL	N-CA-C	-5.16	97.07	111.00
1	C	707	VAL	N-CA-C	-5.16	97.08	111.00
1	B	227	GLY	N-CA-C	5.13	125.91	113.10
1	C	227	GLY	N-CA-C	5.13	125.92	113.10
1	A	227	GLY	N-CA-C	5.12	125.91	113.10

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	7734	0	8021	77	0
1	B	7734	0	8021	68	0
1	C	7734	0	8021	75	0
All	All	23202	0	24063	183	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 4.

All (183) 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:718:ILE:HG22	1:A:718:ILE:O	2.04	0.58
1:B:718:ILE:HG22	1:B:718:ILE:O	2.04	0.58
1:A:225:GLU:O	1:A:226:LYS:C	2.42	0.57
1:B:225:GLU:O	1:B:226:LYS:C	2.42	0.57
1:C:225:GLU:O	1:C:226:LYS:C	2.43	0.56
1:A:457:ALA:HB2	1:A:471:THR:HG21	1.88	0.56
1:C:457:ALA:HB2	1:C:471:THR:HG21	1.88	0.56
1:C:234:LEU:HG	1:C:235:SER:H	1.70	0.56
1:C:718:ILE:HG22	1:C:718:ILE:O	2.04	0.56
1:B:457:ALA:HB2	1:B:471:THR:HG21	1.88	0.55
1:B:881:ALA:HB2	1:C:14:VAL:HG11	1.88	0.55
1:A:1003:SER:O	1:A:1007:LEU:HB2	2.07	0.54
1:C:1003:SER:O	1:C:1007:LEU:HB2	2.08	0.54
1:A:881:ALA:HB2	1:B:14:VAL:HG11	1.88	0.54
1:A:14:VAL:HG11	1:C:881:ALA:HB2	1.89	0.53
1:B:1003:SER:O	1:B:1007:LEU:HB2	2.08	0.53
1:A:116:ALA:HB2	1:B:126:GLY:HA3	1.94	0.49
1:A:719:SER:HA	1:B:235:SER:HB2	1.94	0.49
1:B:691:GLN:HE22	1:B:709:ASN:ND2	2.10	0.49
1:C:691:GLN:HE22	1:C:709:ASN:ND2	2.11	0.49
1:A:935:LEU:HD13	1:A:965:ILE:HG13	1.95	0.49
1:A:691:GLN:HE22	1:A:709:ASN:ND2	2.10	0.49
1:B:12:ALA:HB1	1:B:488:LEU:HA	1.95	0.48
1:A:235:SER:HB2	1:C:719:SER:HA	1.96	0.48
1:B:935:LEU:HD13	1:B:965:ILE:HG13	1.95	0.48
1:A:887:ALA:HB1	1:A:1019:ILE:HG22	1.95	0.48
1:C:12:ALA:HB1	1:C:488:LEU:HA	1.95	0.48
1:A:126:GLY:HA3	1:C:116:ALA:HB2	1.95	0.48
1:A:771:ARG:O	1:B:219:LEU:HD23	2.13	0.48
1:A:219:LEU:HD23	1:C:771:ARG:O	2.14	0.48
1:B:116:ALA:HB2	1:C:126:GLY:HA3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:HB1	1:A:488:LEU:HA	1.96	0.47
1:B:887:ALA:HB1	1:B:1019:ILE:HG22	1.95	0.47
1:C:800:TRP:CD1	1:C:800:TRP:N	2.83	0.47
1:C:935:LEU:HD13	1:C:965:ILE:HG13	1.95	0.47
1:C:887:ALA:HB1	1:C:1019:ILE:HG22	1.95	0.47
1:B:234:LEU:HG	1:B:235:SER:H	1.79	0.47
1:A:415:ASN:HD22	1:A:418:ARG:HH21	1.63	0.47
1:B:38:VAL:HA	1:B:465:VAL:HG11	1.97	0.47
1:B:415:ASN:HD22	1:B:418:ARG:HH21	1.63	0.47
1:C:38:VAL:HA	1:C:465:VAL:HG11	1.97	0.47
1:C:438:ILE:HD12	1:C:442:ILE:HG12	1.97	0.47
1:A:340:VAL:CG1	1:A:395:MET:HB3	2.45	0.47
1:B:340:VAL:CG1	1:B:395:MET:HB3	2.45	0.46
1:C:96:PRO:HG2	1:C:461:GLY:HA2	1.97	0.46
1:B:800:TRP:N	1:B:800:TRP:CD1	2.83	0.46
1:B:870:LEU:HD11	1:C:25:LEU:HD11	1.97	0.46
1:A:96:PRO:HG2	1:A:461:GLY:HA2	1.97	0.46
1:A:800:TRP:N	1:A:800:TRP:CD1	2.83	0.46
1:A:870:LEU:HD11	1:B:25:LEU:HD11	1.96	0.46
1:B:719:SER:HA	1:C:235:SER:HB2	1.97	0.46
1:B:105:VAL:HG11	1:C:105:VAL:CG2	2.46	0.46
1:B:438:ILE:HD12	1:B:442:ILE:HG12	1.97	0.46
1:C:44:ASN:HB2	1:C:132:SER:HB3	1.98	0.46
1:C:234:LEU:HG	1:C:235:SER:N	2.31	0.46
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.45	0.46
1:A:44:ASN:HB2	1:A:132:SER:HB3	1.98	0.46
1:C:415:ASN:HD22	1:C:418:ARG:HH21	1.63	0.46
1:B:438:ILE:HD12	1:B:438:ILE:O	2.16	0.46
1:A:902:GLY:HA3	1:A:1003:SER:HB2	1.98	0.45
1:B:44:ASN:HB2	1:B:132:SER:HB3	1.98	0.45
1:B:606:ALA:HA	1:B:622:ALA:HA	1.99	0.45
1:A:105:VAL:HG11	1:B:105:VAL:CG2	2.46	0.45
1:A:438:ILE:HD12	1:A:438:ILE:O	2.16	0.45
1:A:438:ILE:HD12	1:A:442:ILE:HG12	1.97	0.45
1:A:606:ALA:HA	1:A:622:ALA:HA	1.99	0.45
1:B:96:PRO:HG2	1:B:461:GLY:HA2	1.97	0.45
1:B:839:ILE:HG21	1:B:848:TYR:HB3	1.99	0.45
1:A:25:LEU:HD11	1:C:870:LEU:HD11	1.98	0.45
1:C:438:ILE:HD12	1:C:438:ILE:O	2.16	0.45
1:A:38:VAL:HA	1:A:465:VAL:HG11	1.97	0.45
1:A:105:VAL:CG2	1:C:105:VAL:HG11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:902:GLY:HA3	1:C:1003:SER:HB2	1.98	0.45
1:C:606:ALA:HA	1:C:622:ALA:HA	1.99	0.45
1:C:396:PHE:HB3	1:C:993:LEU:CD2	2.47	0.44
1:A:193:LEU:CD2	1:A:200:ILE:HG12	2.48	0.44
1:B:936:ILE:HG13	1:B:965:ILE:HD11	1.99	0.44
1:C:67:ARG:HH21	1:C:117:ARG:HH22	1.66	0.44
1:B:902:GLY:HA3	1:B:1003:SER:HB2	1.98	0.44
1:A:232:ILE:HG21	1:C:718:ILE:HG13	1.99	0.44
1:A:839:ILE:HG21	1:A:848:TYR:HB3	1.99	0.44
1:A:936:ILE:HG13	1:A:965:ILE:HD11	1.99	0.44
1:B:396:PHE:HB3	1:B:993:LEU:CD2	2.47	0.44
1:B:718:ILE:HG13	1:C:232:ILE:HG21	2.00	0.44
1:C:1015:PHE:O	1:C:1019:ILE:HG12	2.18	0.44
1:B:684:MET:HB2	1:B:685:PRO:HD3	2.00	0.43
1:C:219:LEU:HD11	1:C:234:LEU:HD13	2.00	0.43
1:A:396:PHE:HB3	1:A:993:LEU:CD2	2.47	0.43
1:B:1015:PHE:O	1:B:1019:ILE:HG12	2.18	0.43
1:A:123:ARG:NH2	1:B:124:GLN:HA	2.33	0.43
1:C:193:LEU:CD2	1:C:200:ILE:CG1	2.97	0.43
1:C:839:ILE:HG21	1:C:848:TYR:HB3	1.99	0.43
1:A:234:LEU:HG	1:A:235:SER:H	1.84	0.43
1:A:718:ILE:HG13	1:B:232:ILE:HG21	2.01	0.43
1:B:193:LEU:CD2	1:B:200:ILE:HG12	2.48	0.43
1:C:936:ILE:HG13	1:C:965:ILE:HD11	1.99	0.43
1:A:684:MET:HB2	1:A:685:PRO:HD3	2.00	0.43
1:A:1015:PHE:O	1:A:1019:ILE:HG12	2.18	0.43
1:B:193:LEU:CD2	1:B:200:ILE:CG1	2.97	0.43
1:C:730:LEU:HD12	1:C:790:VAL:HG21	2.01	0.43
1:A:8:ARG:HG2	1:C:884:GLU:HG2	2.00	0.43
1:A:193:LEU:CD2	1:A:200:ILE:CG1	2.97	0.43
1:A:531:ILE:HG23	1:A:538:MET:HG3	2.01	0.43
1:B:682:LEU:HD11	1:B:845:GLY:HA3	2.01	0.43
1:C:682:LEU:HD11	1:C:845:GLY:HA3	2.01	0.43
1:A:730:LEU:HD12	1:A:790:VAL:HG21	2.01	0.43
1:B:531:ILE:HG23	1:B:538:MET:HG3	2.01	0.43
1:A:178:PHE:CE2	1:A:607:ILE:HD13	2.54	0.42
1:C:178:PHE:CE2	1:C:607:ILE:HD13	2.54	0.42
1:C:666:LEU:HD23	1:C:666:LEU:HA	1.88	0.42
1:B:178:PHE:CE2	1:B:607:ILE:HD13	2.54	0.42
1:C:91:THR:HG23	1:C:91:THR:O	2.20	0.42
1:B:91:THR:HG23	1:B:91:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:GLU:HG2	1:B:8:ARG:HG2	2.00	0.42
1:B:112:LYS:NZ	1:C:111:ILE:HD11	2.35	0.42
1:A:112:LYS:NZ	1:B:111:ILE:HD11	2.34	0.42
1:A:666:LEU:HD23	1:A:666:LEU:HA	1.88	0.42
1:B:123:ARG:NH2	1:C:124:GLN:HA	2.34	0.42
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.90	0.42
1:A:438:ILE:HA	1:A:441:PRO:HG2	2.02	0.42
1:B:730:LEU:HD12	1:B:790:VAL:HG21	2.01	0.42
1:B:884:GLU:HG2	1:C:8:ARG:HG2	2.00	0.42
1:C:684:MET:HB2	1:C:685:PRO:HD3	2.00	0.42
1:A:497:LEU:HD23	1:A:497:LEU:HA	1.93	0.42
1:B:412:VAL:HG22	1:B:438:ILE:HD11	2.02	0.42
1:C:531:ILE:HG23	1:C:538:MET:HG3	2.01	0.42
1:A:579:ALA:HB3	1:A:618:ASN:HB3	2.02	0.42
1:A:223:PRO:HD2	1:C:771:ARG:NH2	2.35	0.42
1:C:438:ILE:HA	1:C:441:PRO:HG2	2.02	0.42
1:C:457:ALA:HB2	1:C:471:THR:CB	2.50	0.42
1:A:123:ARG:HH2	1:B:124:GLN:HA	1.85	0.42
1:A:111:ILE:HD11	1:C:112:LYS:NZ	2.35	0.41
1:A:1020:LEU:HD23	1:A:1020:LEU:HA	1.87	0.41
1:B:335:ILE:HD12	1:B:335:ILE:HA	1.87	0.41
1:A:438:ILE:CD1	1:A:442:ILE:HG12	2.51	0.41
1:C:529:LEU:HD23	1:C:529:LEU:HA	1.93	0.41
1:C:782:VAL:HG22	1:C:783:MET:N	2.36	0.41
1:A:682:LEU:HD11	1:A:845:GLY:HA3	2.01	0.41
1:A:717:ASN:O	1:A:800:TRP:HA	2.20	0.41
1:B:771:ARG:NH2	1:C:223:PRO:HD2	2.35	0.41
1:A:91:THR:O	1:A:91:THR:HG23	2.20	0.41
1:A:124:GLN:HA	1:C:123:ARG:NH2	2.35	0.41
1:A:795:VAL:HG23	1:A:796:VAL:HG13	2.02	0.41
1:A:214:ILE:HG12	1:C:738:SER:HB2	2.02	0.41
1:A:771:ARG:NH2	1:B:223:PRO:HD2	2.36	0.41
1:A:782:VAL:HG22	1:A:783:MET:N	2.36	0.41
1:B:141:GLY:HA2	1:B:288:ALA:HA	2.03	0.41
1:C:579:ALA:HB3	1:C:618:ASN:HB3	2.02	0.41
1:A:217:GLY:HA3	1:C:745:MET:HB3	2.03	0.41
1:A:457:ALA:HB2	1:A:471:THR:CB	2.50	0.41
1:A:457:ALA:CB	1:A:471:THR:HG21	2.51	0.41
1:C:438:ILE:CD1	1:C:442:ILE:HG12	2.51	0.41
1:A:5:PHE:CE1	1:A:487:ILE:HG23	2.56	0.41
1:A:528:LEU:HD21	1:A:1013:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:HH22	1:C:124:GLN:HA	1.86	0.41
1:B:190:PRO:HA	1:B:193:LEU:HB2	2.03	0.41
1:B:528:LEU:HD21	1:B:1013:PRO:HG2	2.03	0.41
1:B:579:ALA:HB3	1:B:618:ASN:HB3	2.02	0.41
1:B:782:VAL:HG22	1:B:783:MET:N	2.36	0.41
1:C:68:GLU:HG3	1:C:114:VAL:HG13	2.03	0.41
1:C:795:VAL:HG23	1:C:796:VAL:HG13	2.02	0.41
1:A:138:MET:HE2	1:A:328:ASP:OD1	2.20	0.40
1:A:208:ARG:HG3	1:A:750:ILE:HG23	2.04	0.40
1:A:489:THR:OG1	1:A:490:PRO:HD3	2.22	0.40
1:B:49:TYR:HB3	1:B:57:ILE:HD12	2.03	0.40
1:B:438:ILE:CD1	1:B:442:ILE:HG12	2.51	0.40
1:B:457:ALA:HB2	1:B:471:THR:CB	2.50	0.40
1:C:141:GLY:HA2	1:C:288:ALA:HA	2.03	0.40
1:C:298:ASN:HB3	1:C:301:LYS:HB3	2.03	0.40
1:A:68:GLU:HG3	1:A:114:VAL:HG13	2.03	0.40
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.93	0.40
1:C:193:LEU:CD2	1:C:200:ILE:HG12	2.51	0.40
1:B:438:ILE:HA	1:B:441:PRO:HG2	2.02	0.40
1:C:317:LEU:HD11	1:C:323:PHE:CD1	2.56	0.40
1:C:412:VAL:HG22	1:C:438:ILE:HD11	2.02	0.40
1:A:49:TYR:HB3	1:A:57:ILE:HD12	2.03	0.40
1:A:839:ILE:HG21	1:A:848:TYR:CD2	2.57	0.40
1:B:138:MET:HE2	1:B:328:ASP:OD1	2.21	0.40
1:A:124:GLN:HA	1:C:123:ARG:HH22	1.87	0.40
1:A:219:LEU:HD11	1:A:234:LEU:HD13	2.03	0.40
1:B:111:ILE:HA	1:B:114:VAL:HG22	2.04	0.40
1:B:317:LEU:HD11	1:B:323:PHE:CD1	2.56	0.40
1:C:839:ILE:HG21	1:C:848:TYR:CD2	2.57	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	1011/1056 (96%)	965 (96%)	46 (4%)	0	100	100
1	B	1011/1056 (96%)	965 (96%)	46 (4%)	0	100	100
1	C	1011/1056 (96%)	965 (96%)	46 (4%)	0	100	100
All	All	3033/3168 (96%)	2895 (96%)	138 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	850/888 (96%)	850 (100%)	0	100	100
1	B	850/888 (96%)	850 (100%)	0	100	100
1	C	850/888 (96%)	850 (100%)	0	100	100
All	All	2550/2664 (96%)	2550 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	239	GLN
1	A	415	ASN
1	A	574	GLN
1	A	677	GLN
1	A	691	GLN
1	A	701	ASN
1	A	863	GLN
1	B	239	GLN
1	B	415	ASN
1	B	574	GLN
1	B	677	GLN
1	B	691	GLN

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Mol	Chain	Res	Type
1	B	701	ASN
1	B	863	GLN
1	C	211	ASN
1	C	239	GLN
1	C	415	ASN
1	C	574	GLN
1	C	677	GLN
1	C	691	GLN
1	C	701	ASN
1	C	863	GLN

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](#)

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.

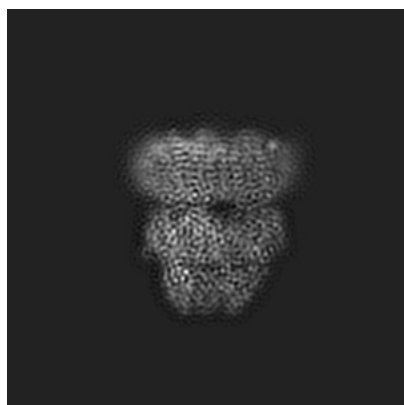
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12088. 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](#)

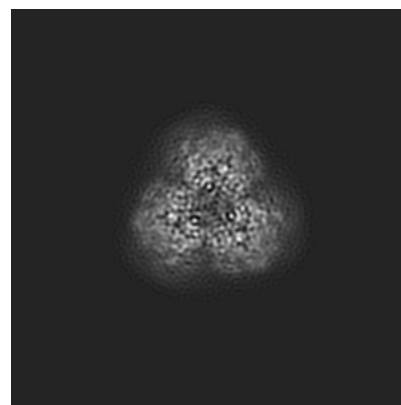
6.1.1 Primary map



X



Y

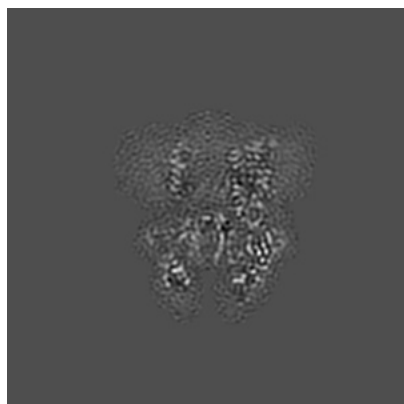


Z

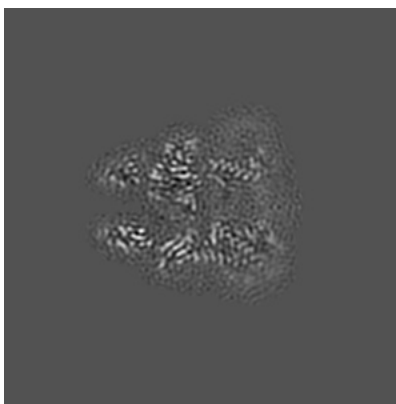
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

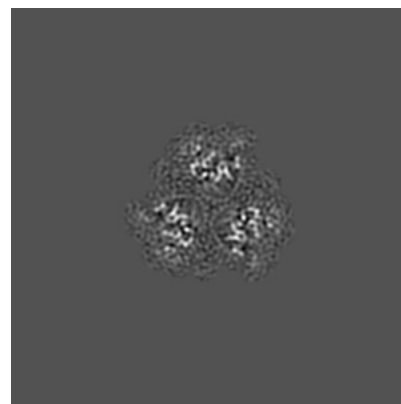
6.2.1 Primary map



X Index: 128



Y Index: 128

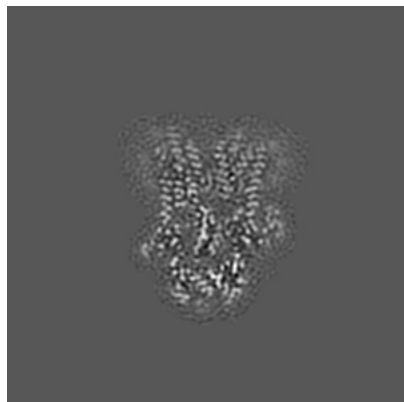


Z Index: 128

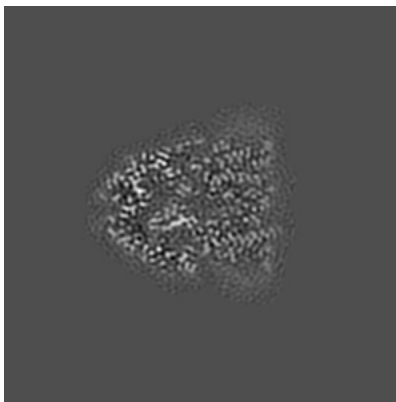
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

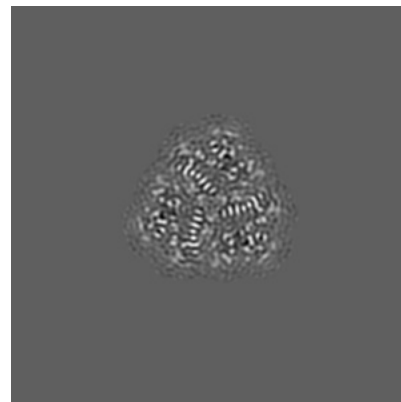
6.3.1 Primary map



X Index: 144



Y Index: 111



Z Index: 108

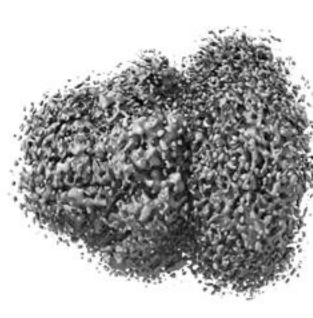
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

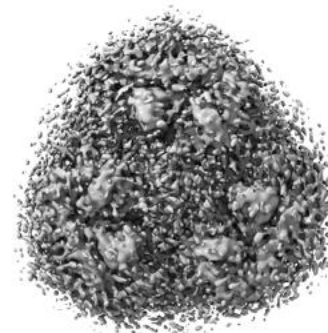
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

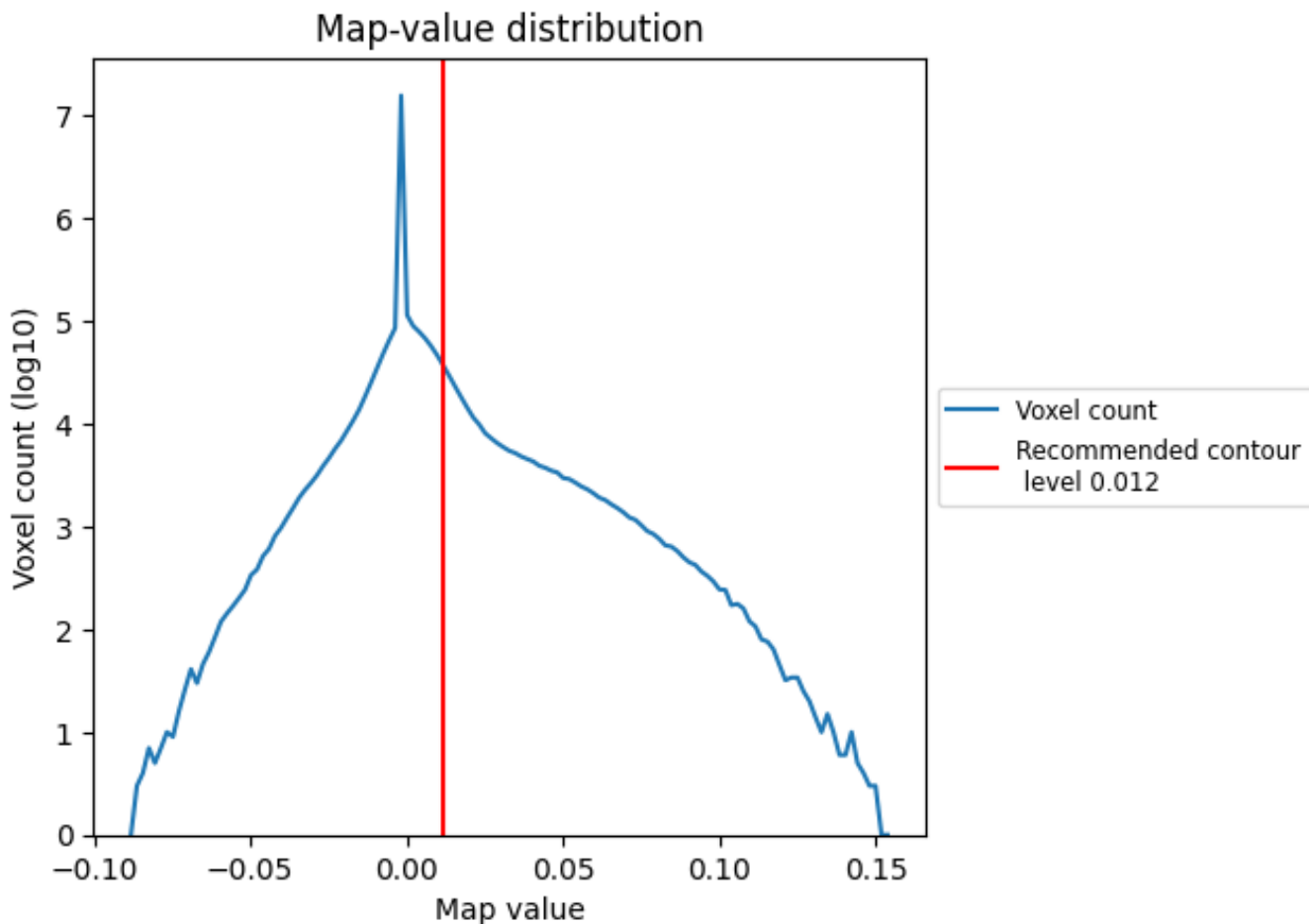
6.5 Mask visualisation

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

7 Map analysis [i](#)

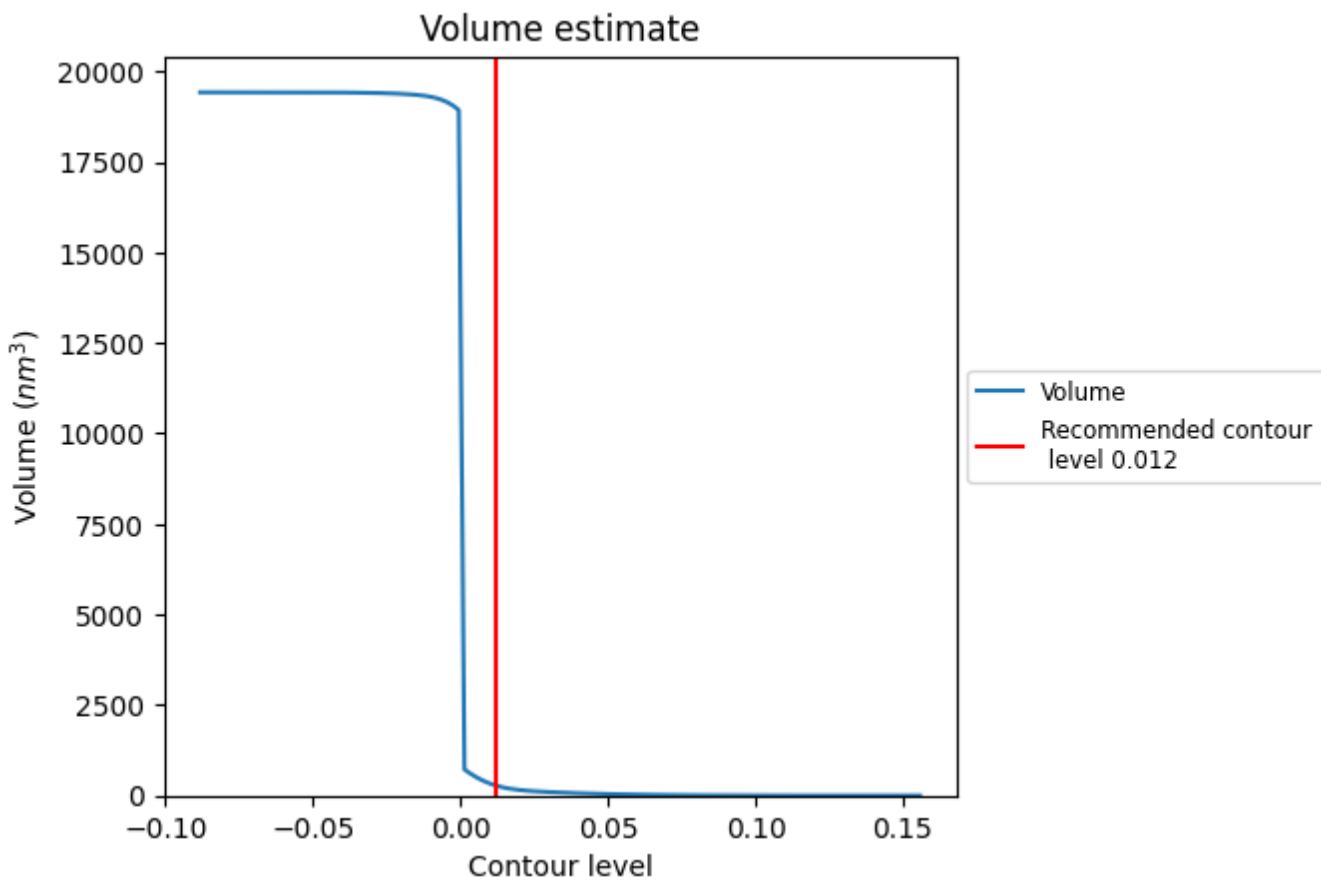
This section contains the results of statistical analysis of the map.

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.

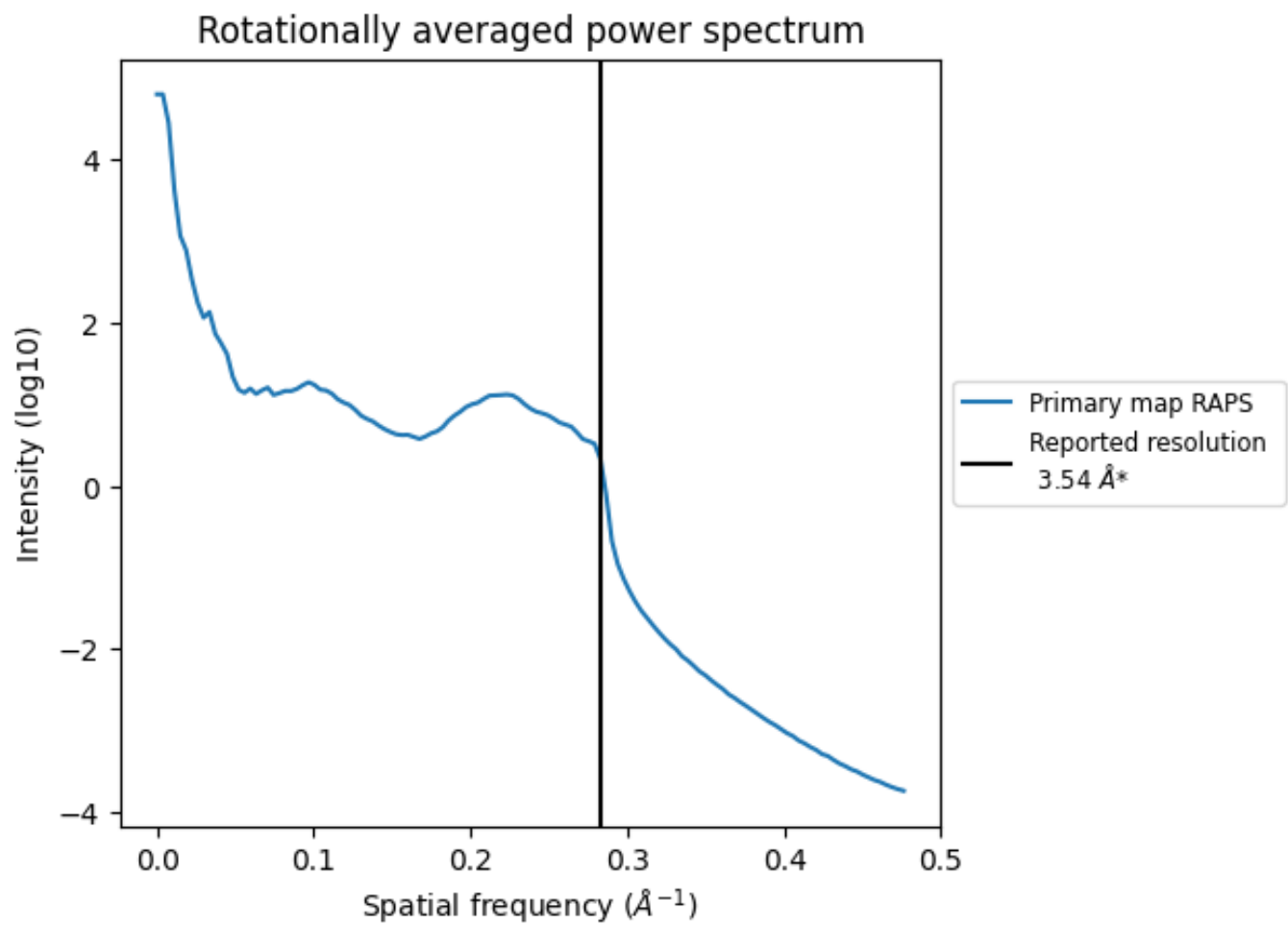
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 280 nm³; this corresponds to an approximate mass of 253 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](#)

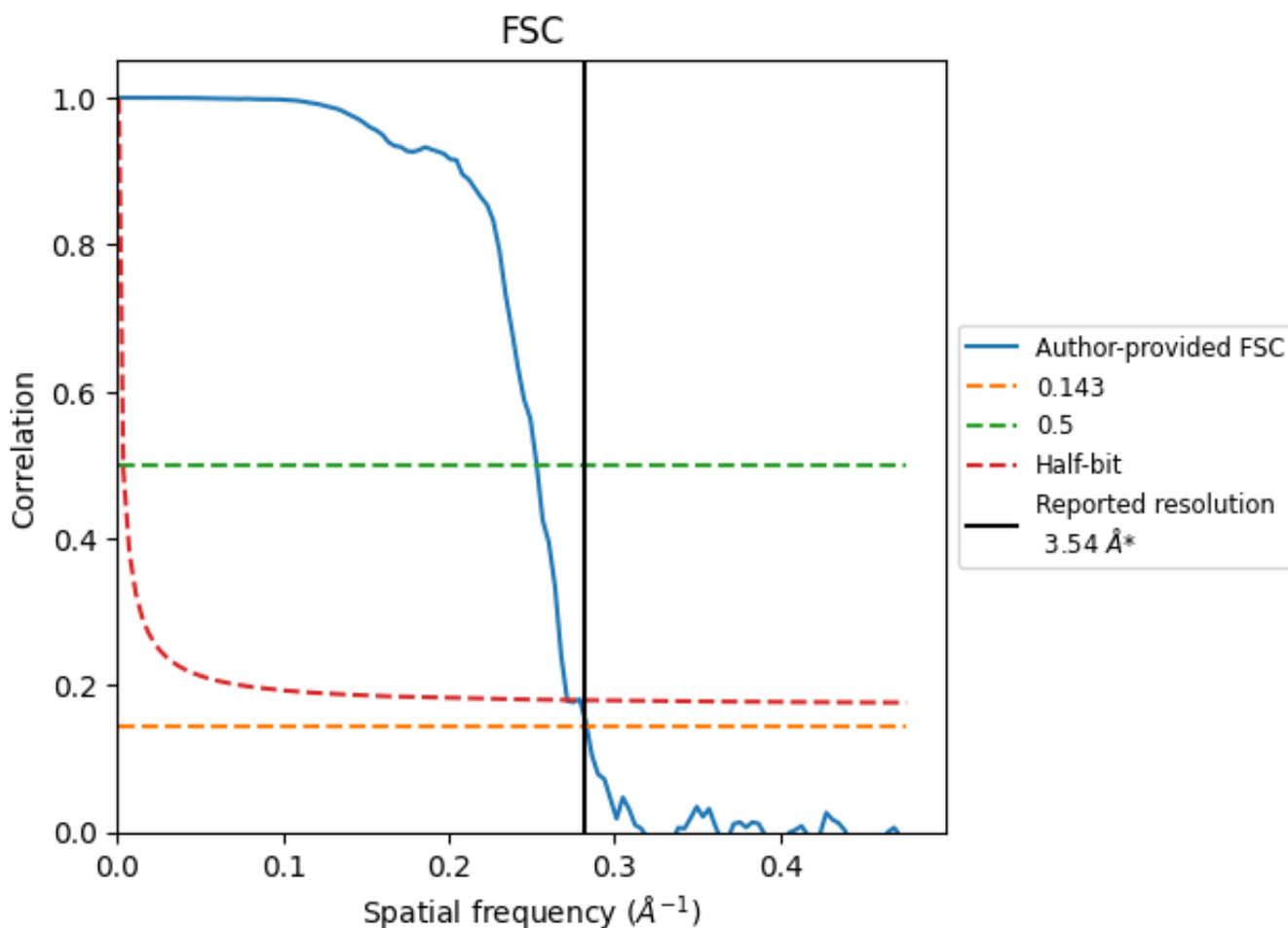


*Reported resolution corresponds to spatial frequency of 0.282\AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

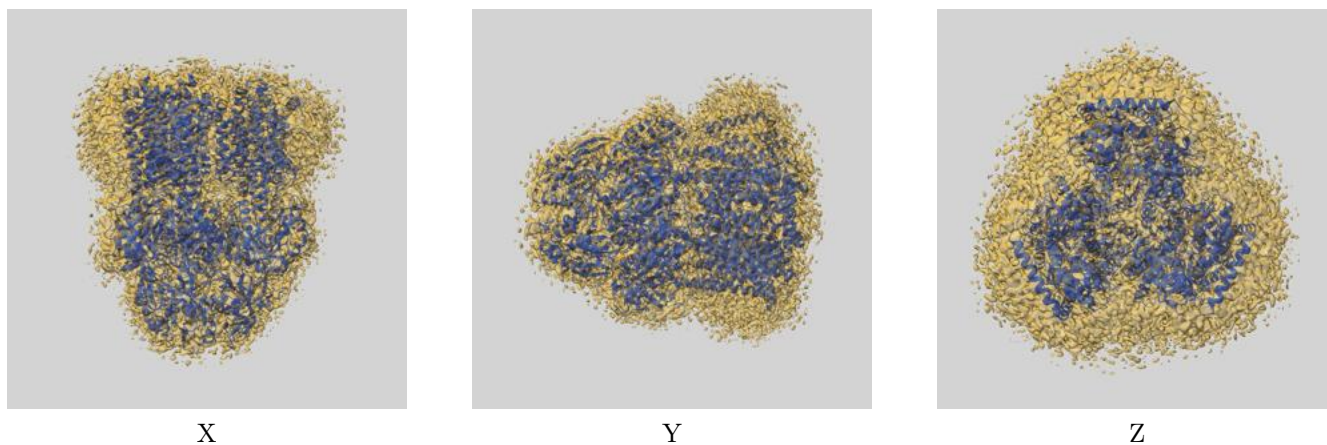
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.53	3.95	3.68
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

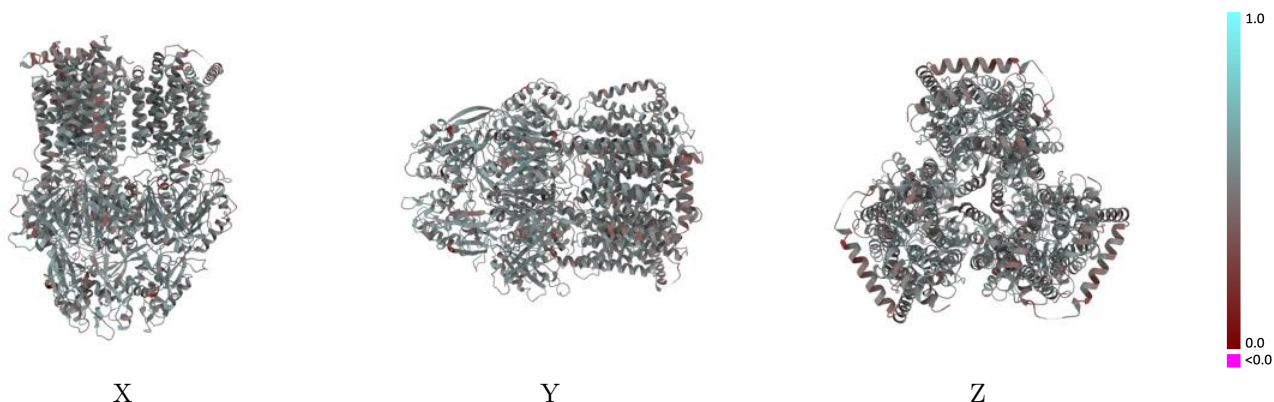
This section contains information regarding the fit between EMDB map EMD-12088 and PDB model 7B8P. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



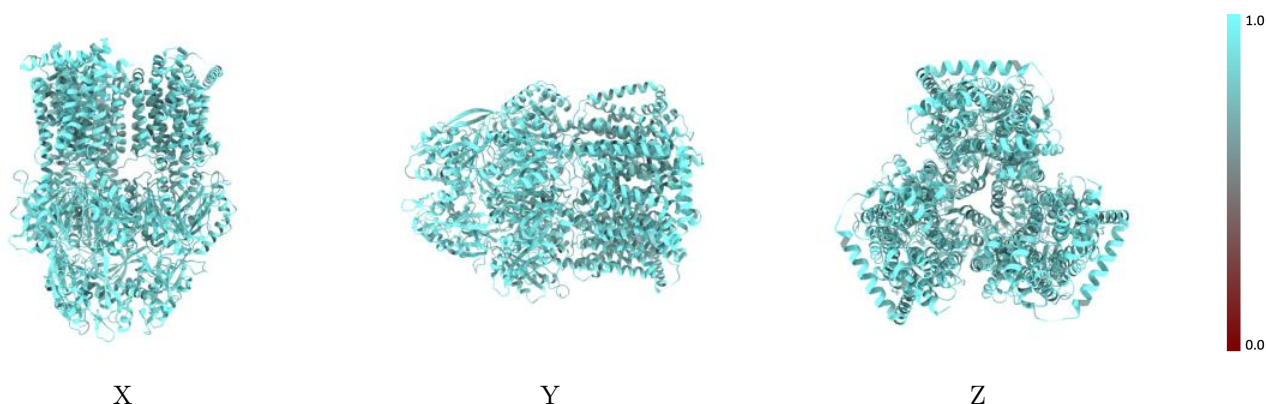
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



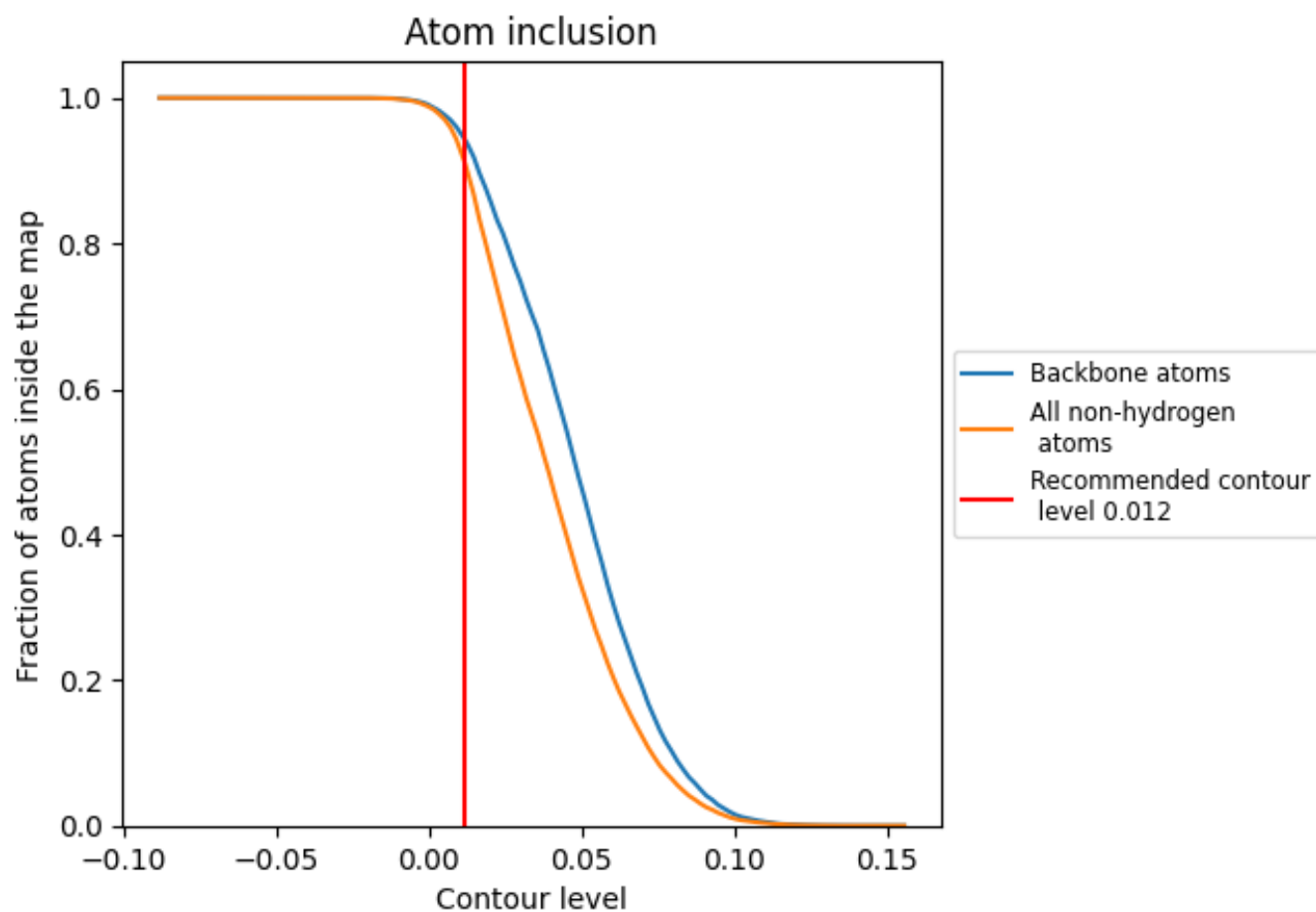
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).









9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9086	 0.4950
A	 0.9077	 0.4940
B	 0.9092	 0.4950
C	 0.9089	 0.4950

