



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:25 AM UTC

PDB ID : 5LJO / pdb_00005ljo
EMDB ID : EMD-4061
Title : E. coli BAM complex (BamABCDE) by cryoEM
Authors : Iadanza, M.G.; Ranson, N.A.; Radford, S.E.; Higgins, A.J.; Schffrin, B.; Calabrese, A.N.; Ashcroft, A.E.; Brockwell, D.J.
Deposited on : 2016-07-19
Resolution : 4.90 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:

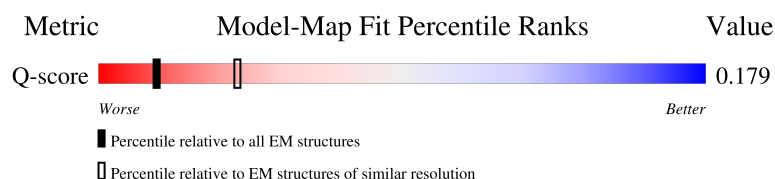
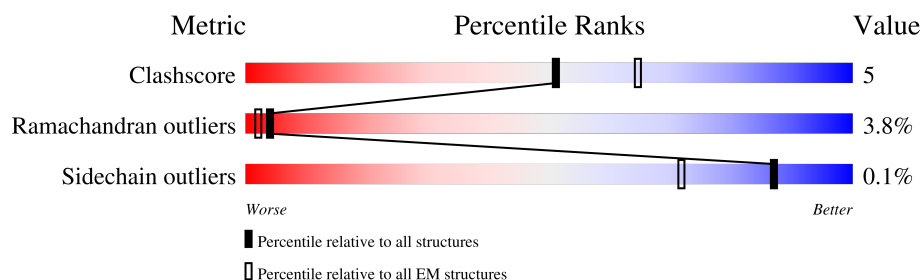
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.90 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	1274 (4.40 - 5.40)

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	B	371	15% 83% 14% ..
2	C	165	70% 86% 12% .
3	D	218	. 89% 9% .
4	E	87	83% 13% 5%

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Mol	Chain	Length	Quality of chain
5	A	783	13% 84% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24947 atoms, of which 12255 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 Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	371	Total	C	H	N	O	S	0	0
			5534	1754	2739	478	557	6		

- Molecule 2 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	165	Total	C	H	N	O	S	0	0
			2498	784	1241	223	248	2		

- Molecule 3 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	218	Total	C	H	N	O	S	0	0
			3461	1109	1700	309	336	7		

- Molecule 4 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	87	Total	C	H	N	O	S	0	0
			1352	432	667	119	132	2		

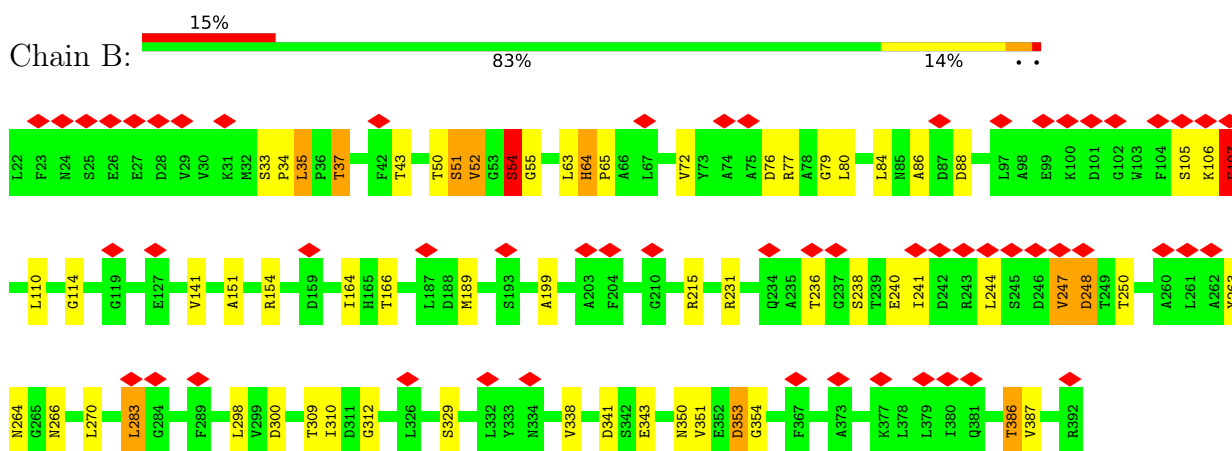
- Molecule 5 is a protein called Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	783	Total	C	H	N	O	S	0	0
			12102	3907	5908	1043	1228	16		

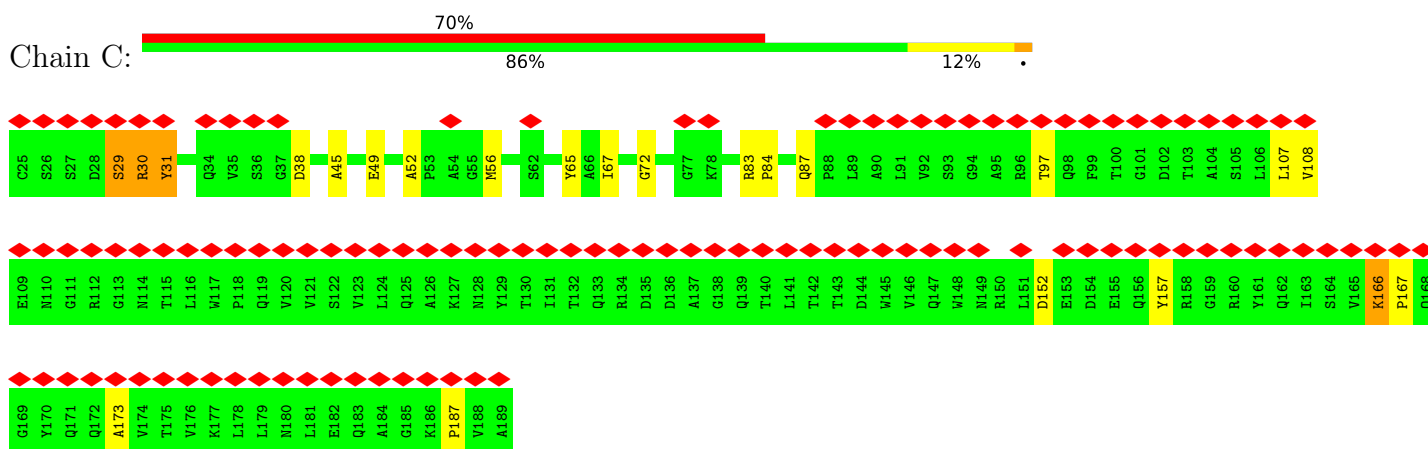
3 Residue-property plots

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.

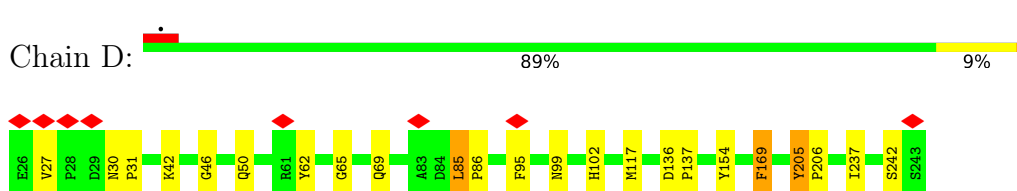
- Molecule 1: Outer membrane protein assembly factor BamB



- Molecule 2: Outer membrane protein assembly factor BamC

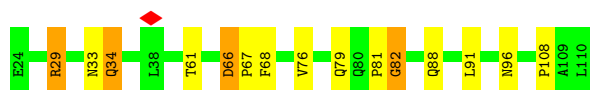


- Molecule 3: Outer membrane protein assembly factor BamD



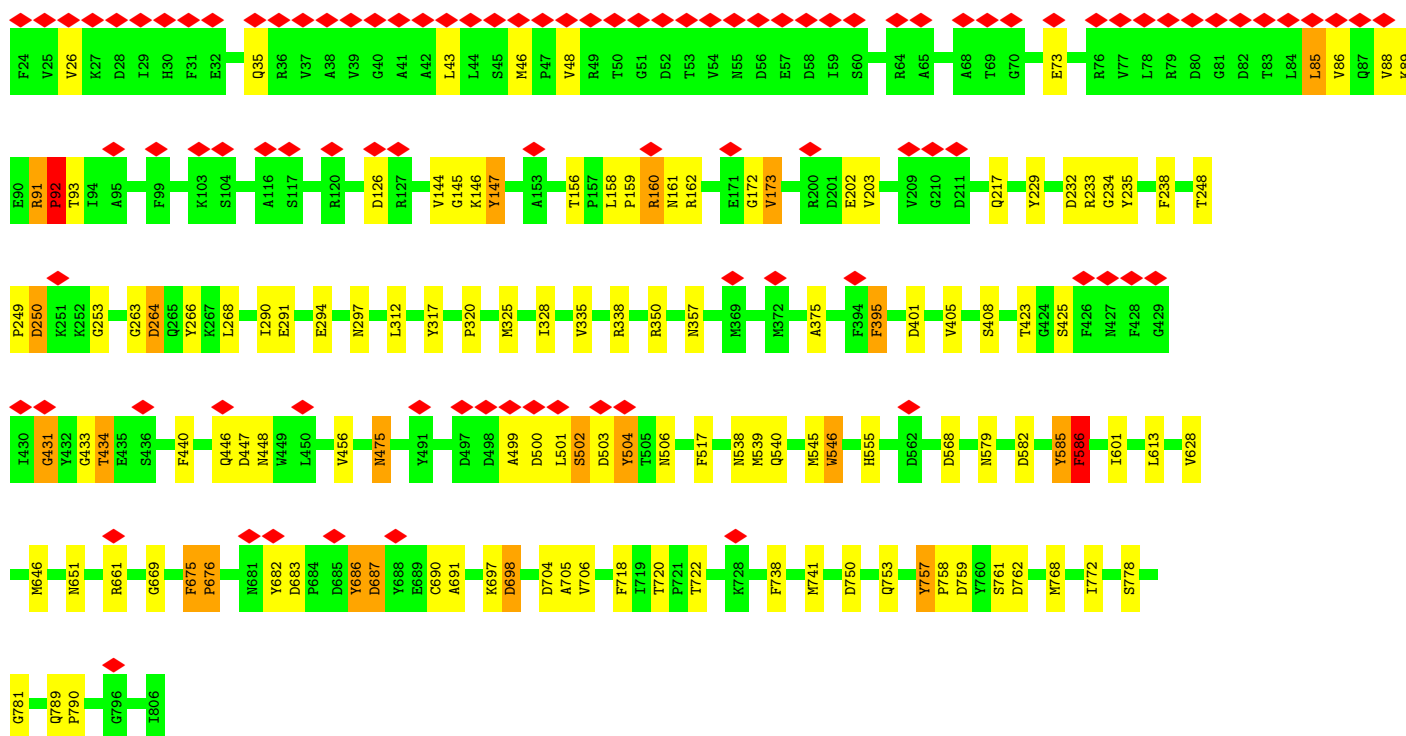
• Molecule 4: Outer membrane protein assembly factor BamE

Chain E:  83% 13% 5%



• Molecule 5: Outer membrane protein assembly factor BamA

Chain A:  13% 84% 14%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95878	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.375	Depositor
Minimum map value	-0.280	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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	B	0.90	0/2846	1.24	28/3881 (0.7%)
2	C	0.75	0/1281	1.23	15/1748 (0.9%)
3	D	0.93	0/1801	1.23	25/2447 (1.0%)
4	E	0.89	0/700	1.21	8/955 (0.8%)
5	A	0.89	0/6337	1.24	66/8598 (0.8%)
All	All	0.89	0/12965	1.24	142/17629 (0.8%)

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	B	0	4
2	C	0	2
5	A	0	4
All	All	0	10

There are no bond length outliers.

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	395	PHE	CA-CB-CG	-8.88	104.92	113.80
3	D	62	TYR	CA-C-N	8.75	128.48	119.56
3	D	62	TYR	C-N-CA	8.75	128.48	119.56
5	A	762	ASP	CA-C-N	8.64	128.29	119.82
5	A	762	ASP	C-N-CA	8.64	128.29	119.82
2	C	45	ALA	CA-C-N	8.57	128.51	120.03
2	C	45	ALA	C-N-CA	8.57	128.51	120.03
5	A	781	GLY	CA-C-N	8.52	129.87	119.98
5	A	781	GLY	C-N-CA	8.52	129.87	119.98
2	C	52	ALA	CA-C-N	8.35	128.29	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	52	ALA	C-N-CA	8.35	128.29	120.03
2	C	84	PRO	CA-C-N	8.18	128.24	119.89
2	C	84	PRO	C-N-CA	8.18	128.24	119.89
2	C	87	GLN	CA-C-N	8.07	127.95	120.21
2	C	87	GLN	C-N-CA	8.07	127.95	120.21
5	A	203	VAL	CA-C-N	7.83	127.85	119.78
5	A	203	VAL	C-N-CA	7.83	127.85	119.78
3	D	65	GLY	CA-C-N	7.83	128.55	119.47
3	D	65	GLY	C-N-CA	7.83	128.55	119.47
5	A	408	SER	CA-C-N	7.83	128.81	120.12
5	A	408	SER	C-N-CA	7.83	128.81	120.12
1	B	387	VAL	N-CA-C	7.83	119.17	108.84
1	B	43	THR	CA-C-N	7.69	127.62	119.85
1	B	43	THR	C-N-CA	7.69	127.62	119.85
1	B	35	LEU	CA-C-N	7.66	127.67	119.78
1	B	35	LEU	C-N-CA	7.66	127.67	119.78
5	A	586	PHE	CA-C-N	7.61	127.51	120.21
5	A	586	PHE	C-N-CA	7.61	127.51	120.21
5	A	669	GLY	CA-C-N	7.50	127.49	119.76
5	A	669	GLY	C-N-CA	7.50	127.49	119.76
3	D	99	ASN	CA-C-N	7.48	127.85	119.32
3	D	99	ASN	C-N-CA	7.48	127.85	119.32
5	A	720	THR	CA-C-N	7.46	128.05	120.14
5	A	720	THR	C-N-CA	7.46	128.05	120.14
3	D	169	PHE	CA-CB-CG	-7.35	106.45	113.80
5	A	46	MET	CA-C-N	7.34	126.98	119.56
5	A	46	MET	C-N-CA	7.34	126.98	119.56
1	B	250	THR	CA-C-N	7.32	127.24	119.85
1	B	250	THR	C-N-CA	7.32	127.24	119.85
5	A	555	HIS	CA-C-N	7.32	127.24	119.85
5	A	555	HIS	C-N-CA	7.32	127.24	119.85
2	C	84	PRO	N-CA-C	-7.26	101.85	110.70
1	B	64	HIS	CA-C-N	7.18	127.14	120.03
1	B	64	HIS	C-N-CA	7.18	127.14	120.03
5	A	757	TYR	CA-C-N	7.07	128.02	120.11
5	A	757	TYR	C-N-CA	7.07	128.02	120.11
2	C	67	ILE	CA-C-N	7.00	126.92	119.85
2	C	67	ILE	C-N-CA	7.00	126.92	119.85
3	D	27	VAL	CA-C-N	6.98	126.74	119.76
3	D	27	VAL	C-N-CA	6.98	126.74	119.76
5	A	162	ARG	N-CA-C	6.92	119.23	110.24
1	B	189	MET	CA-C-N	6.81	128.27	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	MET	C-N-CA	6.81	128.27	120.98
3	D	154	TYR	CA-C-N	6.81	128.35	119.84
3	D	154	TYR	C-N-CA	6.81	128.35	119.84
5	A	646	MET	CA-C-N	6.79	126.75	119.76
5	A	646	MET	C-N-CA	6.79	126.75	119.76
5	A	601	ILE	CA-C-N	6.76	126.80	119.90
5	A	601	ILE	C-N-CA	6.76	126.80	119.90
1	B	107	GLU	CA-C-N	6.73	128.25	119.84
1	B	107	GLU	C-N-CA	6.73	128.25	119.84
5	A	722	THR	CA-C-N	6.72	128.25	119.84
5	A	722	THR	C-N-CA	6.72	128.25	119.84
3	D	136	ASP	CA-C-N	6.68	128.20	119.84
3	D	136	ASP	C-N-CA	6.68	128.20	119.84
3	D	102	HIS	CA-C-N	6.67	127.21	119.47
3	D	102	HIS	C-N-CA	6.67	127.21	119.47
5	A	778	SER	CA-C-N	6.60	126.29	119.56
5	A	778	SER	C-N-CA	6.60	126.29	119.56
3	D	30	ASN	CA-C-N	6.60	124.48	119.66
3	D	30	ASN	C-N-CA	6.60	124.48	119.66
5	A	738	PHE	N-CA-C	6.53	118.99	109.07
5	A	683	ASP	CA-C-N	6.47	127.93	119.84
5	A	683	ASP	C-N-CA	6.47	127.93	119.84
5	A	540	GLN	CA-C-N	6.44	127.89	119.84
5	A	540	GLN	C-N-CA	6.44	127.89	119.84
5	A	158	LEU	CA-C-N	6.37	127.81	119.84
5	A	158	LEU	C-N-CA	6.37	127.81	119.84
1	B	199	ALA	CA-C-N	6.28	126.49	119.90
1	B	199	ALA	C-N-CA	6.28	126.49	119.90
1	B	266	ASN	CA-CB-CG	-6.27	106.33	112.60
3	D	31	PRO	CA-C-N	6.16	126.06	119.28
3	D	31	PRO	C-N-CA	6.16	126.06	119.28
5	A	156	THR	CA-C-N	6.12	126.60	119.99
5	A	156	THR	C-N-CA	6.12	126.60	119.99
5	A	517	PHE	CA-C-N	6.12	127.48	119.84
5	A	517	PHE	C-N-CA	6.12	127.48	119.84
5	A	675	PHE	CA-C-N	5.99	127.33	119.84
5	A	675	PHE	C-N-CA	5.99	127.33	119.84
4	E	88	GLN	N-CA-C	5.97	117.47	108.46
1	B	353	ASP	CA-C-O	-5.95	114.92	121.58
5	A	248	THR	CA-C-N	5.94	127.27	119.84
5	A	248	THR	C-N-CA	5.94	127.27	119.84
5	A	431	GLY	CA-C-O	-5.92	114.29	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	31	PRO	N-CA-C	-5.91	104.80	110.47
2	C	108	VAL	N-CA-C	5.91	116.62	108.12
5	A	540	GLN	N-CA-C	5.87	117.28	109.83
5	A	761	SER	N-CA-C	-5.82	106.01	113.23
4	E	66	ASP	CA-C-N	5.79	127.08	119.84
4	E	66	ASP	C-N-CA	5.79	127.08	119.84
5	A	475	ASN	CA-C-N	5.77	127.05	119.84
5	A	475	ASN	C-N-CA	5.77	127.05	119.84
1	B	33	SER	N-CA-C	-5.76	102.13	110.08
4	E	29	ARG	CA-C-N	5.70	125.98	119.83
4	E	29	ARG	C-N-CA	5.70	125.98	119.83
2	C	157	TYR	N-CA-C	5.63	117.17	109.18
5	A	405	VAL	CA-C-N	5.62	125.38	119.76
5	A	405	VAL	C-N-CA	5.62	125.38	119.76
5	A	335	VAL	N-CA-C	5.61	115.75	108.35
5	A	85	LEU	CA-C-N	-5.60	115.38	123.11
5	A	85	LEU	C-N-CA	-5.60	115.38	123.11
5	A	789	GLN	CA-C-N	5.59	126.83	119.84
5	A	789	GLN	C-N-CA	5.59	126.83	119.84
1	B	80	LEU	N-CA-C	5.56	118.29	110.23
5	A	145	GLY	N-CA-C	-5.56	107.35	115.63
4	E	61	THR	CA-C-N	5.48	125.94	120.52
4	E	61	THR	C-N-CA	5.48	125.94	120.52
1	B	51	SER	N-CA-C	5.46	117.68	111.02
4	E	76	VAL	N-CA-C	5.43	115.78	108.17
1	B	164	ILE	N-CA-C	5.38	116.23	108.48
2	C	166	LYS	CA-C-N	5.35	126.53	119.84
2	C	166	LYS	C-N-CA	5.35	126.53	119.84
1	B	263	TYR	CA-CB-CG	-5.30	104.35	113.90
5	A	718	PHE	CA-CB-CG	-5.24	108.56	113.80
5	A	628	VAL	N-CA-C	5.23	115.81	108.17
5	A	753	GLN	N-CA-C	-5.22	107.08	113.50
5	A	772	ILE	N-CA-C	5.18	116.12	108.45
1	B	154	ARG	CA-C-N	5.18	124.94	119.76
1	B	154	ARG	C-N-CA	5.18	124.94	119.76
3	D	46	GLY	N-CA-C	-5.17	107.97	115.27
1	B	329	SER	CA-C-N	5.15	126.28	119.84
1	B	329	SER	C-N-CA	5.15	126.28	119.84
3	D	85	LEU	CA-C-N	5.12	124.91	119.28
3	D	85	LEU	C-N-CA	5.12	124.91	119.28
5	A	328	ILE	N-CA-C	5.11	115.69	109.30
5	A	291	GLU	CA-C-N	5.10	125.33	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	291	GLU	C-N-CA	5.10	125.33	119.83
1	B	54	SER	CA-C-O	-5.07	115.62	121.19
1	B	338	VAL	N-CA-C	5.07	115.26	108.17
5	A	375	ALA	N-CA-C	5.05	116.66	109.14
3	D	205	TYR	CA-C-N	5.01	126.10	119.84
3	D	205	TYR	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	431	GLY	Peptide,Mainchain
5	A	92	PRO	Peptide,Mainchain
1	B	353	ASP	Peptide,Mainchain
1	B	54	SER	Peptide,Mainchain
2	C	72	GLY	Peptide,Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2795	2739	2738	33	0
2	C	1257	1241	1240	14	0
3	D	1761	1700	1699	9	0
4	E	685	667	666	10	0
5	A	6194	5908	5907	72	0
All	All	12692	12255	12250	137	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 5.

All (137) 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:B:50:THR:O	1:B:50:THR:HG23	1.56	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:169:PHE:CD1	3:D:169:PHE:O	2.33	0.81
1:B:50:THR:O	1:B:50:THR:CG2	2.31	0.77
5:A:586:PHE:CD2	5:A:586:PHE:O	2.37	0.77
5:A:586:PHE:CD2	5:A:586:PHE:C	2.64	0.73
1:B:76:ASP:OD1	1:B:76:ASP:C	2.30	0.72
1:B:343:GLU:N	1:B:343:GLU:OE2	2.26	0.67
5:A:586:PHE:C	5:A:586:PHE:HD2	2.03	0.66
3:D:69:GLN:N	3:D:69:GLN:OE1	2.29	0.66
4:E:79:GLN:OE1	4:E:79:GLN:O	2.15	0.64
4:E:68:PHE:CD1	4:E:68:PHE:C	2.75	0.64
3:D:169:PHE:CD1	3:D:169:PHE:C	2.70	0.62
1:B:270:LEU:C	1:B:270:LEU:HD12	2.25	0.62
5:A:217:GLN:N	5:A:217:GLN:OE1	2.31	0.61
2:C:83:ARG:HG3	2:C:83:ARG:O	2.00	0.60
1:B:51:SER:O	1:B:386:THR:OG1	2.20	0.60
1:B:35:LEU:HD23	1:B:35:LEU:O	2.02	0.59
1:B:37:THR:HG22	1:B:37:THR:O	2.02	0.58
5:A:506:ASN:OD1	5:A:506:ASN:C	2.45	0.58
1:B:247:VAL:HG12	1:B:248:ASP:H	1.69	0.57
5:A:661:ARG:HD2	5:A:661:ARG:H	1.70	0.56
4:E:68:PHE:O	4:E:68:PHE:HD1	1.89	0.56
1:B:310:ILE:HD12	1:B:310:ILE:C	2.31	0.55
1:B:298:LEU:HD12	1:B:298:LEU:C	2.32	0.55
1:B:244:LEU:C	1:B:244:LEU:HD23	2.32	0.55
1:B:35:LEU:HD23	1:B:35:LEU:C	2.31	0.55
4:E:91:LEU:C	4:E:91:LEU:HD23	2.32	0.54
1:B:76:ASP:OD1	1:B:76:ASP:O	2.26	0.54
1:B:309:THR:OG1	1:B:312:GLY:O	2.25	0.54
4:E:68:PHE:CD1	4:E:68:PHE:O	2.60	0.54
5:A:91:ARG:N	5:A:92:PRO:CD	2.71	0.54
2:C:38:ASP:OD1	2:C:38:ASP:C	2.53	0.51
5:A:290:ILE:C	5:A:290:ILE:HD12	2.36	0.51
5:A:229:TYR:C	5:A:229:TYR:CD2	2.89	0.51
5:A:232:ASP:OD1	5:A:232:ASP:C	2.54	0.51
5:A:579:ASN:OD1	5:A:579:ASN:C	2.53	0.50
1:B:270:LEU:HD12	1:B:270:LEU:O	2.11	0.50
5:A:503:ASP:O	5:A:504:TYR:HB3	2.12	0.49
5:A:395:PHE:CD2	5:A:395:PHE:N	2.78	0.49
1:B:264:ASN:OD1	1:B:264:ASN:C	2.57	0.48
5:A:86:VAL:HG12	5:A:88:VAL:HG23	1.96	0.48
5:A:92:PRO:HB3	5:A:93:THR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:VAL:HG12	1:B:248:ASP:N	2.28	0.48
1:B:64:HIS:HB2	1:B:65:PRO:HD2	1.97	0.47
3:D:117:MET:C	3:D:117:MET:SD	2.97	0.47
5:A:325:MET:N	5:A:338:ARG:O	2.47	0.47
5:A:704:ASP:O	5:A:706:VAL:N	2.47	0.47
1:B:350:ASN:HB3	1:B:354:GLY:H	1.79	0.47
1:B:244:LEU:HD23	1:B:244:LEU:O	2.14	0.47
3:D:205:TYR:O	3:D:205:TYR:CD2	2.68	0.47
1:B:341:ASP:OD1	1:B:341:ASP:C	2.57	0.47
4:E:66:ASP:C	4:E:66:ASP:OD1	2.56	0.47
5:A:546:TRP:HA	5:A:546:TRP:CE3	2.49	0.47
4:E:33:ASN:O	4:E:34:GLN:HB2	2.16	0.46
2:C:49:GLU:O	2:C:49:GLU:HG2	2.16	0.46
2:C:29:SER:O	2:C:30:ARG:HB2	2.15	0.46
4:E:79:GLN:CD	4:E:79:GLN:C	2.84	0.46
5:A:446:GLN:HB2	5:A:456:VAL:HB	1.97	0.46
5:A:504:TYR:CD2	5:A:504:TYR:O	2.69	0.45
1:B:35:LEU:O	1:B:35:LEU:CD2	2.65	0.45
2:C:30:ARG:O	2:C:31:TYR:HB3	2.16	0.45
5:A:48:VAL:O	5:A:48:VAL:HG23	2.15	0.45
1:B:51:SER:O	1:B:52:VAL:HB	2.17	0.45
2:C:65:TYR:N	2:C:65:TYR:CD1	2.84	0.45
5:A:741:MET:SD	5:A:741:MET:N	2.89	0.45
5:A:585:TYR:C	5:A:585:TYR:CD1	2.94	0.45
2:C:30:ARG:O	2:C:31:TYR:CB	2.65	0.45
5:A:235:TYR:HB3	5:A:238:PHE:HB2	1.98	0.45
5:A:395:PHE:CD1	5:A:395:PHE:C	2.89	0.45
1:B:72:VAL:HB	1:B:84:LEU:HB2	1.98	0.45
5:A:433:GLY:O	5:A:434:THR:CB	2.65	0.45
5:A:43:LEU:C	5:A:43:LEU:HD23	2.41	0.44
2:C:83:ARG:O	2:C:83:ARG:CG	2.66	0.44
5:A:759:ASP:OD1	5:A:759:ASP:C	2.59	0.44
1:B:215:ARG:HG2	1:B:231:ARG:HA	1.99	0.44
5:A:144:VAL:O	5:A:144:VAL:HG12	2.17	0.44
5:A:263:GLY:O	5:A:264:ASP:CB	2.66	0.44
5:A:357:ASN:OD1	5:A:357:ASN:C	2.58	0.44
1:B:283:LEU:HD12	1:B:283:LEU:C	2.43	0.44
1:B:54:SER:HA	1:B:55:GLY:HA3	1.79	0.44
4:E:29:ARG:HB3	4:E:82:GLY:HA2	1.99	0.44
5:A:268:LEU:N	5:A:294:GLU:O	2.48	0.44
5:A:92:PRO:CB	5:A:93:THR:HA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:297:ASN:OD1	5:A:297:ASN:C	2.60	0.44
5:A:539:MET:HB3	5:A:545:MET:SD	2.58	0.43
5:A:229:TYR:O	5:A:233:ARG:HG2	2.18	0.43
5:A:586:PHE:O	5:A:586:PHE:CG	2.64	0.43
3:D:42:LYS:HD3	3:D:50:GLN:HB3	2.00	0.43
5:A:266:TYR:N	5:A:266:TYR:CD1	2.86	0.43
5:A:661:ARG:HD2	5:A:661:ARG:N	2.34	0.43
5:A:704:ASP:OD1	5:A:704:ASP:C	2.60	0.43
1:B:151:ALA:HA	1:B:166:THR:HA	2.01	0.43
5:A:423:THR:HB	5:A:447:ASP:HB2	2.00	0.43
1:B:236:THR:HA	1:B:240:GLU:HA	2.01	0.42
5:A:675:PHE:HB3	5:A:676:PRO:HD2	2.01	0.42
5:A:750:ASP:OD1	5:A:750:ASP:C	2.61	0.42
3:D:95:PHE:CD2	3:D:95:PHE:C	2.98	0.42
5:A:447:ASP:O	5:A:448:ASN:HB3	2.19	0.42
5:A:501:LEU:C	5:A:501:LEU:HD12	2.44	0.42
1:B:106:LYS:O	1:B:107:GLU:C	2.63	0.42
2:C:107:LEU:HD12	2:C:107:LEU:N	2.35	0.42
3:D:85:LEU:HB2	3:D:86:PRO:HD3	2.02	0.42
5:A:73:GLU:N	5:A:89:LYS:O	2.52	0.42
5:A:613:LEU:C	5:A:613:LEU:HD23	2.45	0.42
5:A:312:LEU:HB3	5:A:317:TYR:HB2	2.02	0.42
5:A:768:MET:C	5:A:768:MET:SD	3.03	0.42
5:A:144:VAL:O	5:A:144:VAL:CG1	2.68	0.42
5:A:546:TRP:HA	5:A:546:TRP:HE3	1.83	0.42
5:A:395:PHE:CD2	5:A:395:PHE:O	2.73	0.41
5:A:266:TYR:N	5:A:266:TYR:HD1	2.18	0.41
5:A:440:PHE:CD1	5:A:440:PHE:C	2.98	0.41
5:A:159:PRO:O	5:A:160:ARG:HB2	2.20	0.41
5:A:26:VAL:HG13	5:A:26:VAL:O	2.19	0.41
5:A:585:TYR:O	5:A:586:PHE:HB2	2.21	0.41
2:C:166:LYS:HB2	2:C:173:ALA:HB3	2.03	0.41
5:A:697:LYS:O	5:A:698:ASP:HB2	2.19	0.41
5:A:172:GLY:O	5:A:173:VAL:HB	2.19	0.41
5:A:395:PHE:O	5:A:395:PHE:CG	2.67	0.41
2:C:31:TYR:CG	2:C:31:TYR:O	2.73	0.41
2:C:56:MET:SD	3:D:237:ILE:HG13	2.61	0.41
1:B:63:LEU:HA	1:B:114:GLY:HA2	2.02	0.41
5:A:502:SER:HA	5:A:538:ASN:HB3	2.03	0.41
5:A:757:TYR:HB3	5:A:758:PRO:HD2	2.01	0.41
2:C:107:LEU:HG	2:C:173:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:146:LYS:O	5:A:147:TYR:HB2	2.21	0.40
5:A:475:ASN:OD1	5:A:475:ASN:C	2.62	0.40
5:A:686:TYR:O	5:A:687:ASP:HB2	2.21	0.40
1:B:77:ARG:O	1:B:110:LEU:N	2.52	0.40
4:E:96:ASN:OD1	4:E:96:ASN:C	2.64	0.40
5:A:85:LEU:C	5:A:85:LEU:HD12	2.46	0.40
5:A:690:CYS:O	5:A:691:ALA:HB3	2.21	0.40
2:C:152:ASP:OD1	2:C:152:ASP:C	2.64	0.40
5:A:126:ASP:C	5:A:126:ASP:OD1	2.64	0.40
5:A:401:ASP:OD1	5:A:401:ASP:C	2.62	0.40
5:A:568:ASP:OD1	5:A:568:ASP:C	2.63	0.40
5:A:234:GLY:O	5:A:266:TYR:N	2.53	0.40
5:A:250:ASP:OD1	5:A:250:ASP:C	2.64	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	B	369/371 (100%)	313 (85%)	39 (11%)	17 (5%)	2	16
2	C	163/165 (99%)	138 (85%)	19 (12%)	6 (4%)	2	19
3	D	216/218 (99%)	208 (96%)	5 (2%)	3 (1%)	9	39
4	E	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	1	13
5	A	781/783 (100%)	674 (86%)	76 (10%)	31 (4%)	2	18
All	All	1614/1624 (99%)	1401 (87%)	151 (9%)	62 (4%)	4	19

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	PRO

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Mol	Chain	Res	Type
1	B	247	VAL
1	B	386	THR
2	C	30	ARG
2	C	31	TYR
4	E	34	GLN
5	A	35	GLN
5	A	160	ARG
5	A	173	VAL
5	A	250	ASP
5	A	434	THR
5	A	500	ASP
5	A	582	ASP
5	A	586	PHE
5	A	682	TYR
5	A	698	ASP
5	A	705	ALA
1	B	37	THR
1	B	52	VAL
1	B	88	ASP
1	B	248	ASP
1	B	351	VAL
2	C	97	THR
4	E	67	PRO
4	E	82	GLY
5	A	147	TYR
5	A	161	ASN
5	A	264	ASP
5	A	651	ASN
5	A	676	PRO
5	A	687	ASP
5	A	790	PRO
1	B	105	SER
2	C	167	PRO
3	D	206	PRO
5	A	249	PRO
5	A	253	GLY
5	A	502	SER
5	A	504	TYR
5	A	686	TYR
1	B	86	ALA
1	B	107	GLU
1	B	300	ASP

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Mol	Chain	Res	Type
2	C	29	SER
2	C	187	PRO
4	E	81	PRO
4	E	108	PRO
5	A	202	GLU
5	A	320	PRO
5	A	350	ARG
5	A	499	ALA
5	A	585	TYR
1	B	238	SER
1	B	241	ILE
3	D	242	SER
5	A	425	SER
1	B	283	LEU
5	A	92	PRO
1	B	141	VAL
3	D	137	PRO
1	B	79	GLY
5	A	91	ARG

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	B	302/302 (100%)	302 (100%)	0	100	100
2	C	133/133 (100%)	133 (100%)	0	100	100
3	D	183/183 (100%)	183 (100%)	0	100	100
4	E	76/76 (100%)	76 (100%)	0	100	100
5	A	668/668 (100%)	666 (100%)	2 (0%)	86	84
All	All	1362/1362 (100%)	1360 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	546	TRP
5	A	586	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	87	GLN
2	C	128	ASN
3	D	139	HIS
4	E	89	GLN
5	A	196	HIS
5	A	259	ASN
5	A	555	HIS
5	A	594	ASN
5	A	678	GLN
5	A	789	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 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.

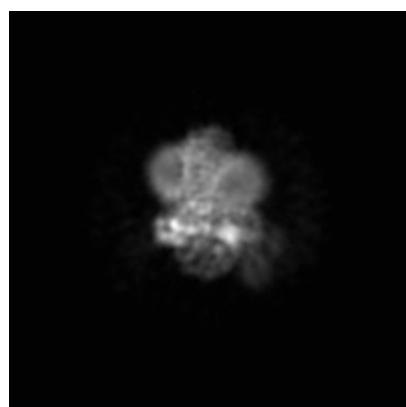
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4061. These allow visual inspection of the internal detail of the map and identification of artifacts.

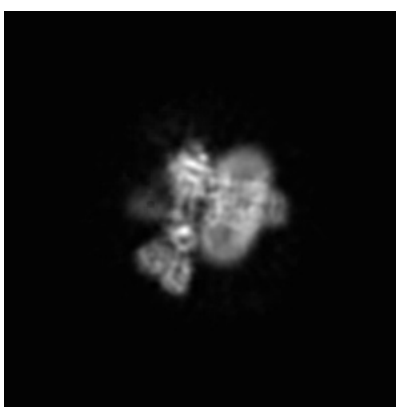
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

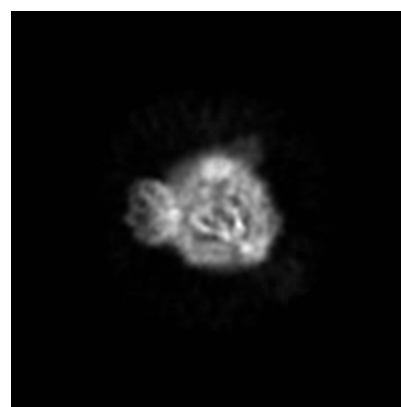
6.1.1 Primary map



X



Y

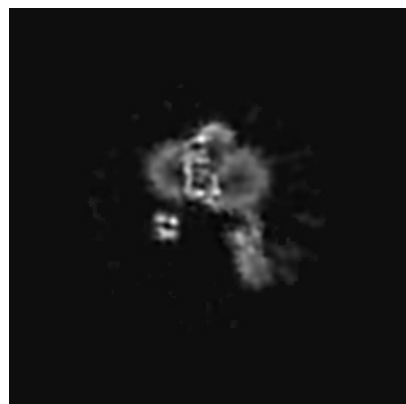


Z

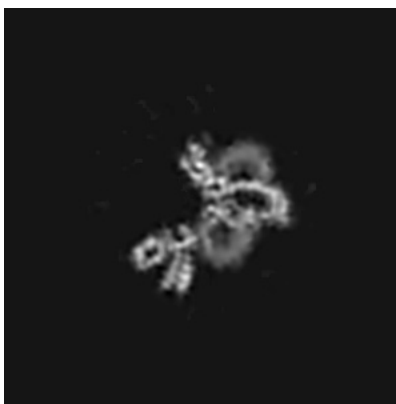
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

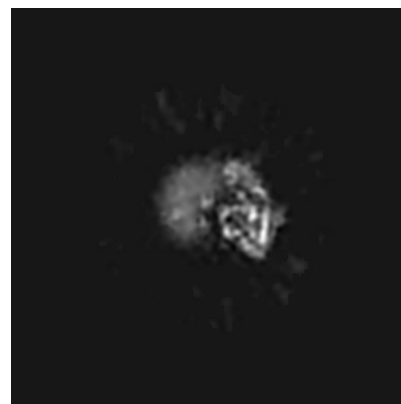
6.2.1 Primary map



X Index: 150



Y Index: 150

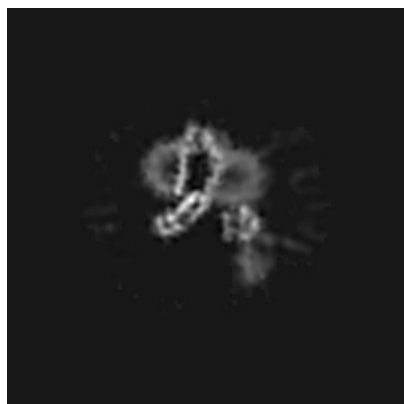


Z Index: 150

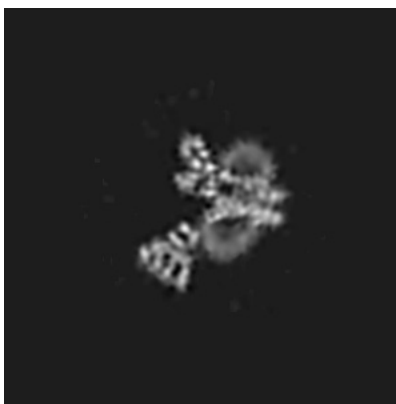
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

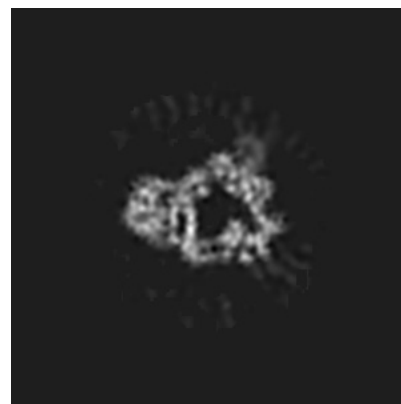
6.3.1 Primary map



X Index: 161



Y Index: 135

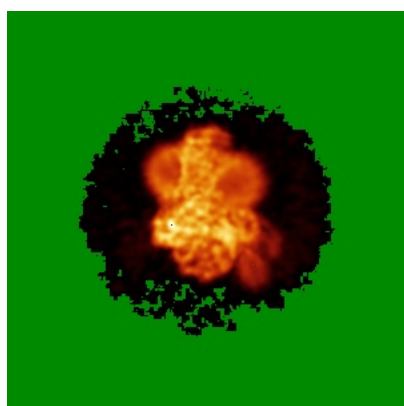


Z Index: 135

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

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

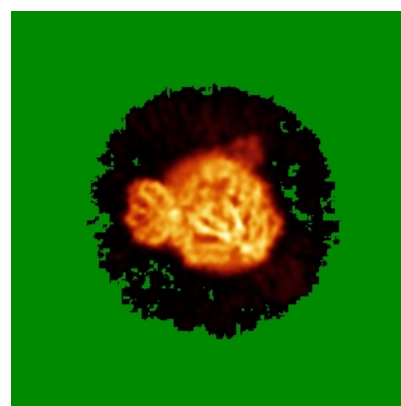
6.4.1 Primary map



X



Y

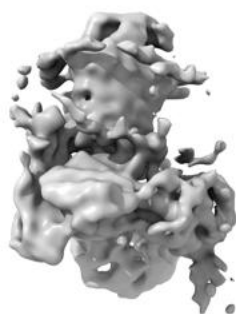


Z

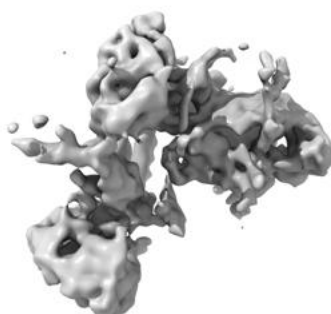
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

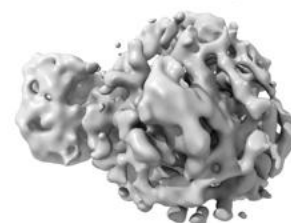
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

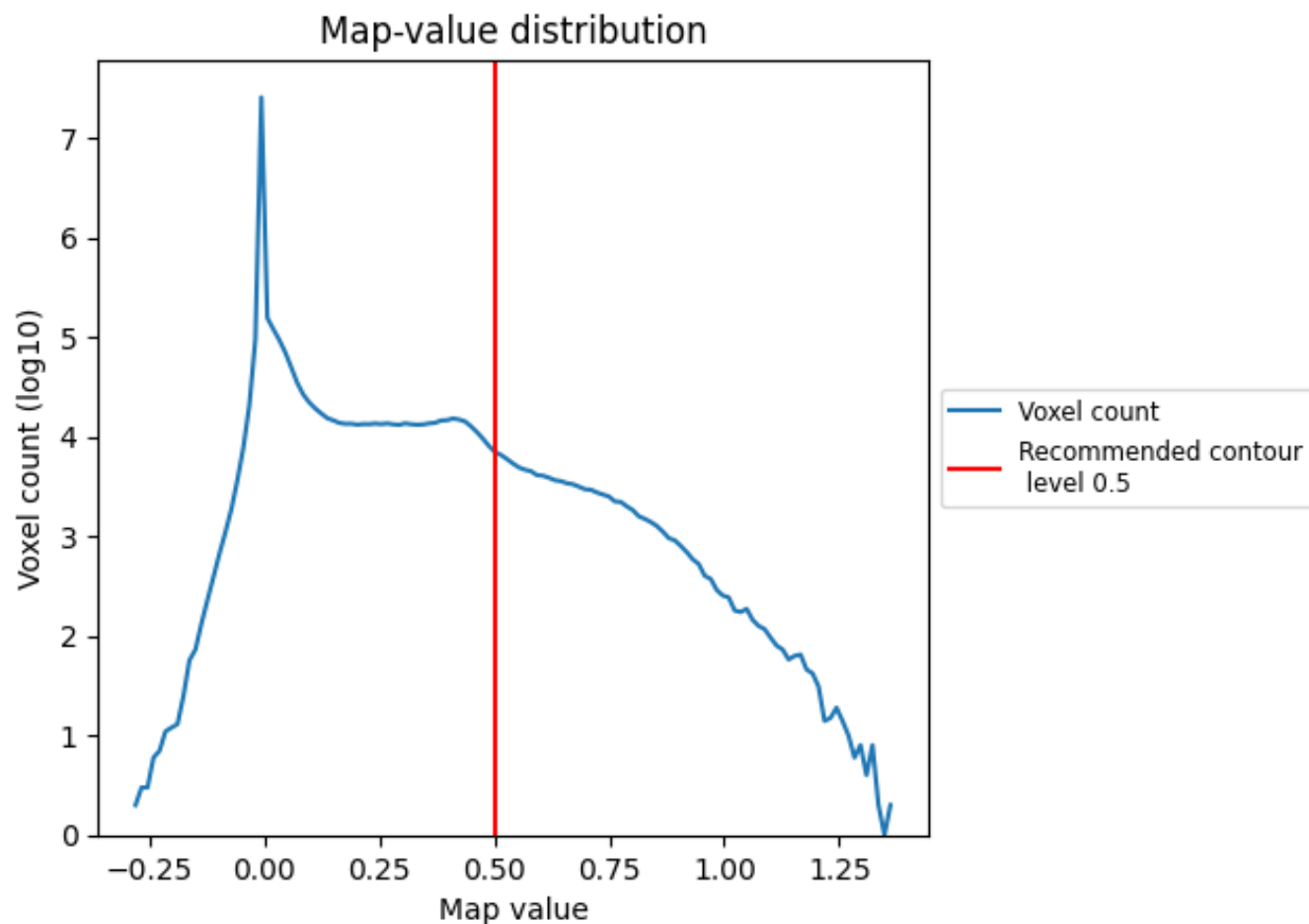
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

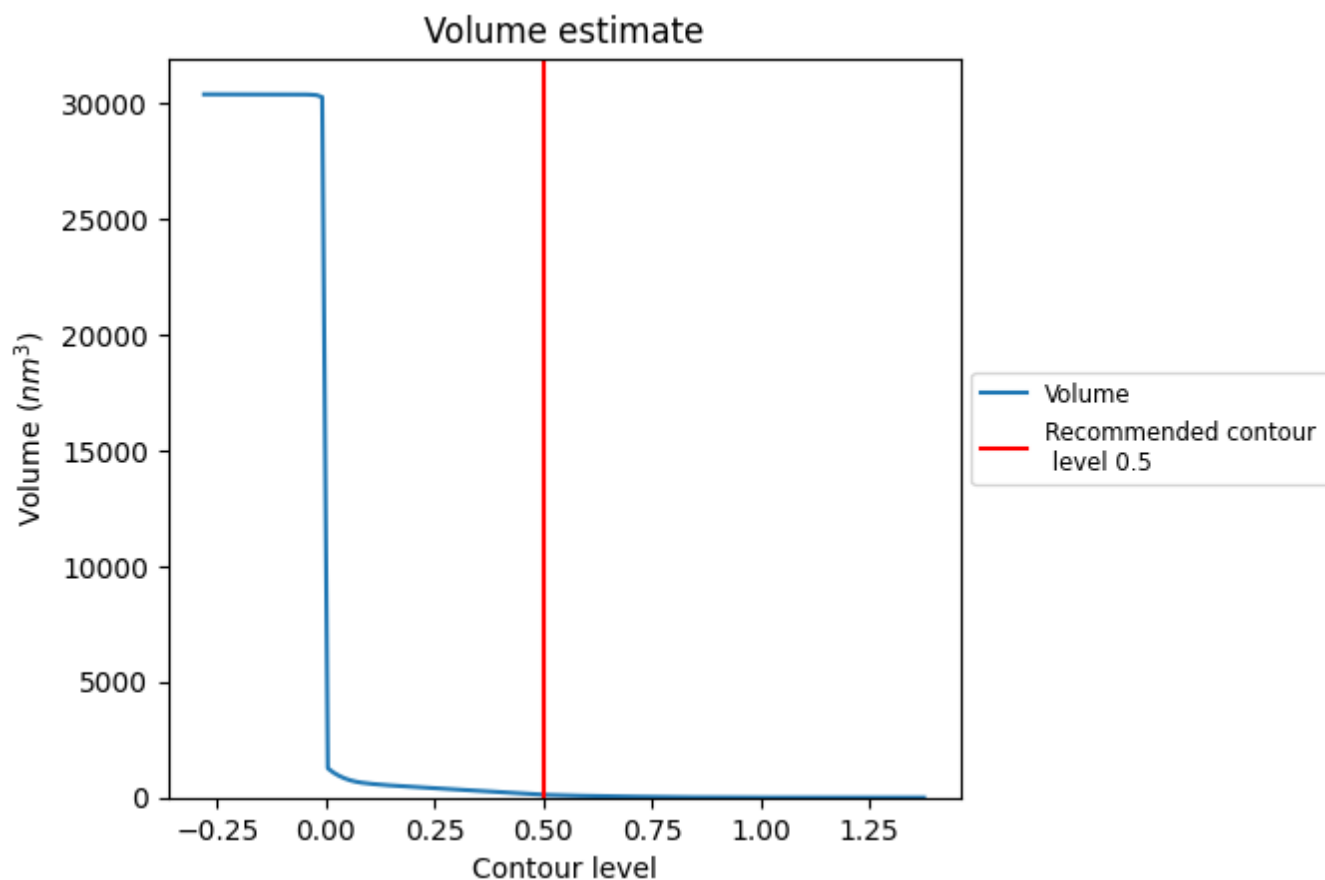
This section contains the results of statistical analysis of the map.

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.

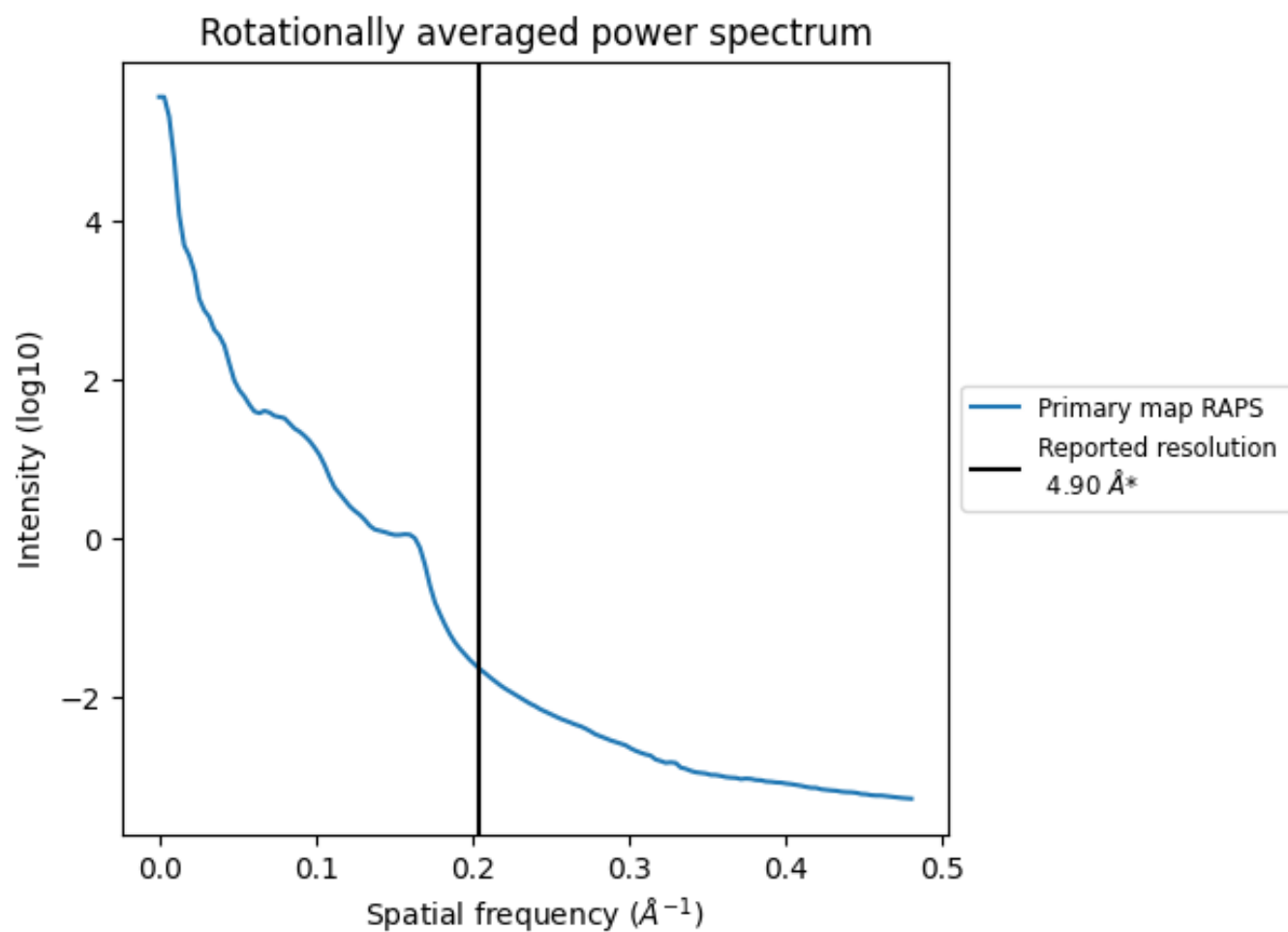
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 108 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 ⓘ

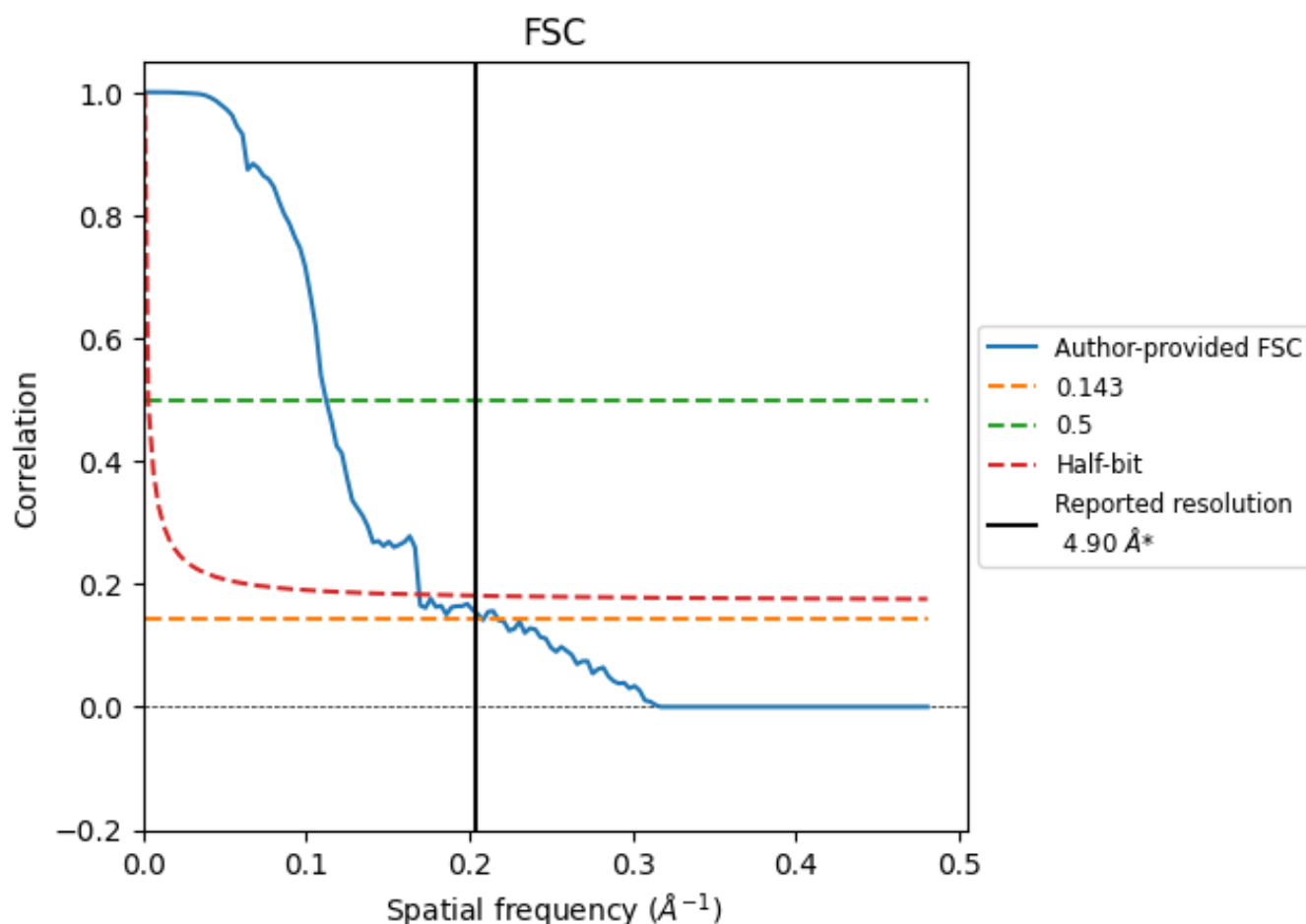


*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

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 0.204 Å⁻¹

8.2 Resolution estimates [i](#)

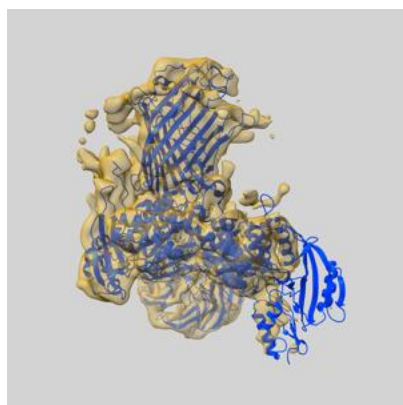
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.81	8.92	5.91
Unmasked-calculated*	-	-	-

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

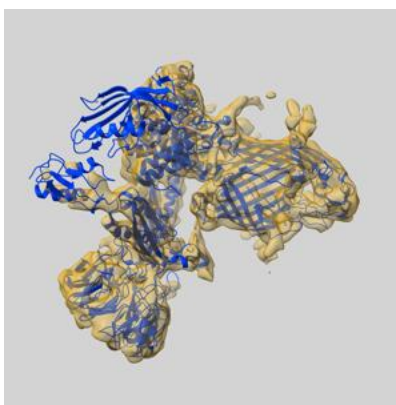
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4061 and PDB model 5LJO. Per-residue inclusion information can be found in section [3](#) on page [5](#).

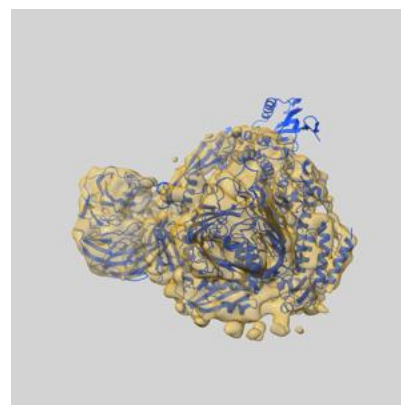
9.1 Map-model overlay [i](#)



X



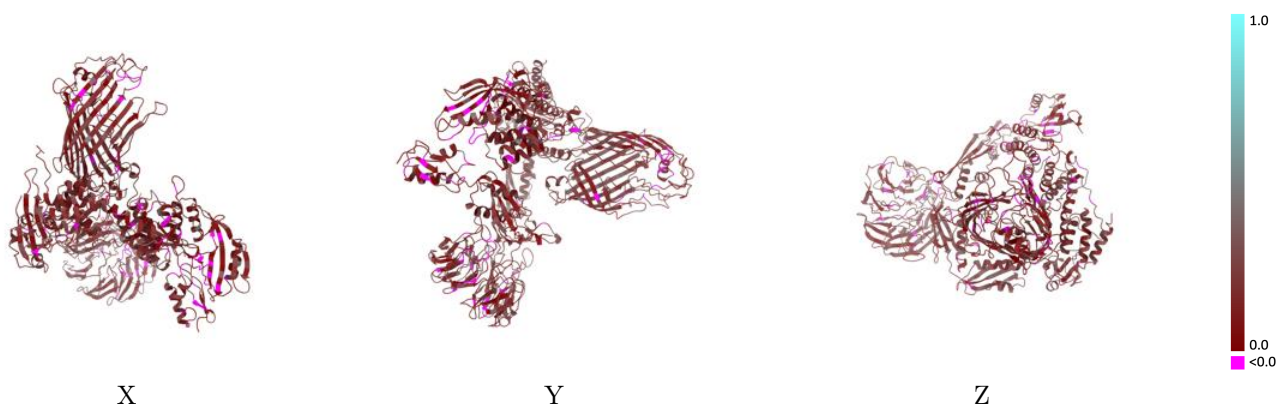
Y



Z

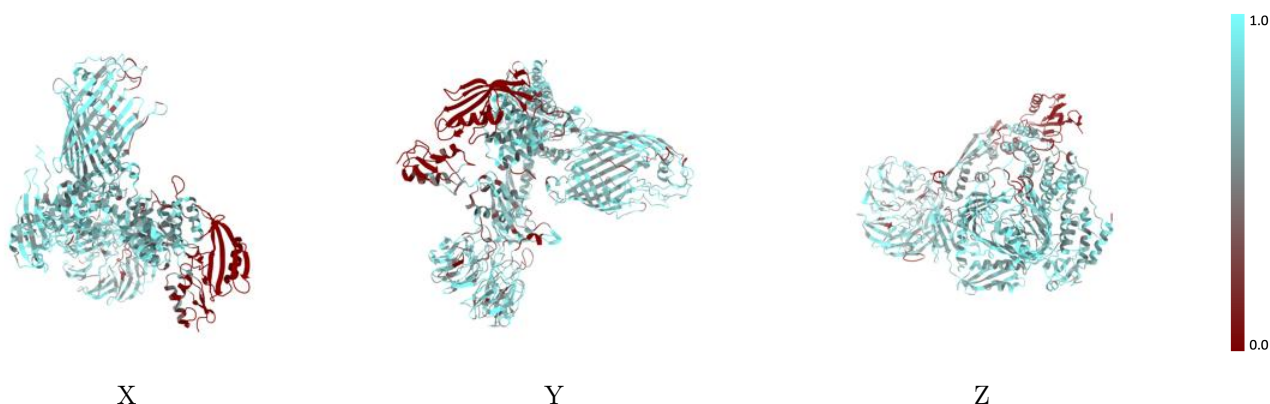
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



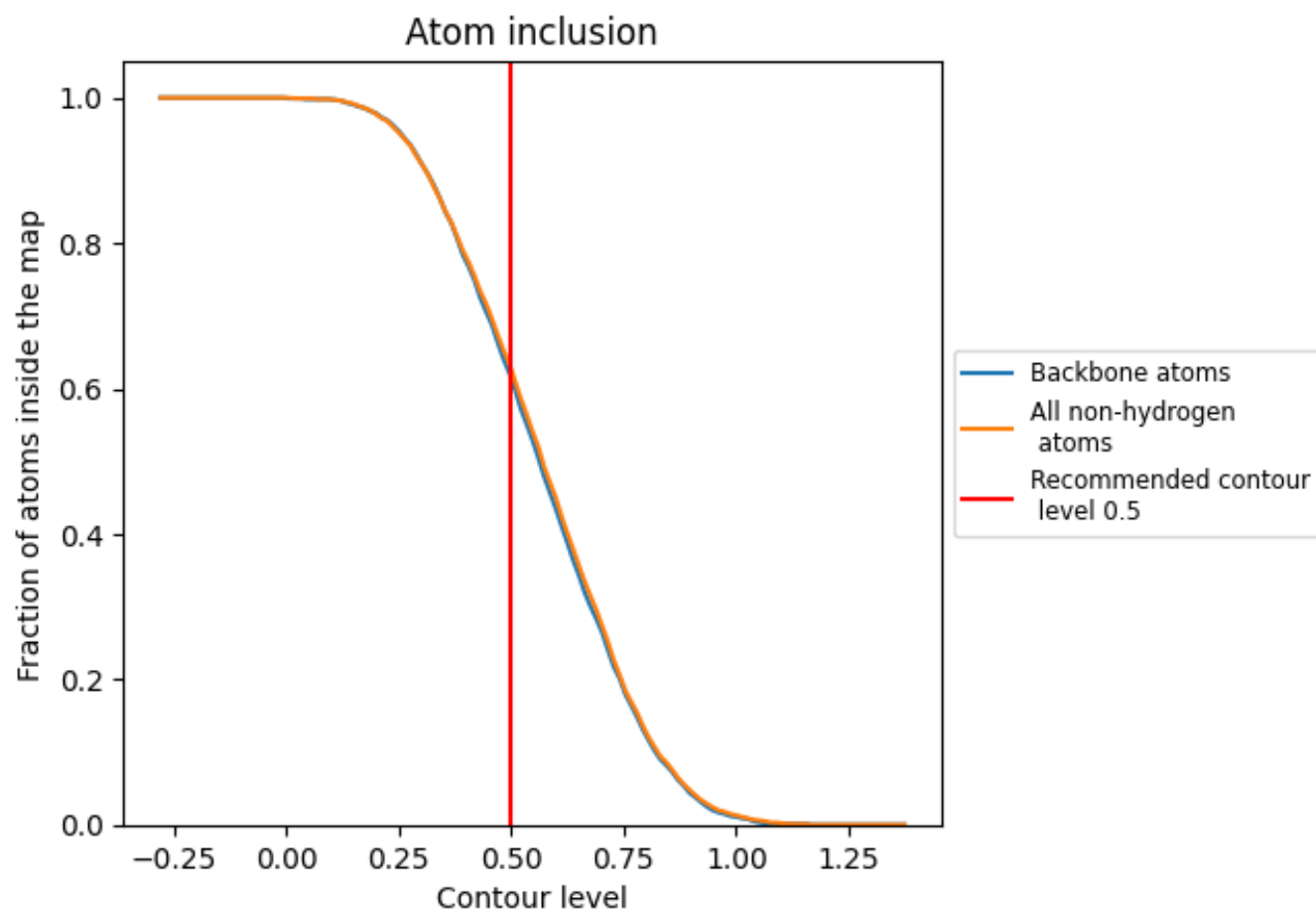
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 63% 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	0.6270	0.1790
A	0.6740	0.1820
B	0.6680	0.1760
C	0.2250	0.1530
D	0.7210	0.1820
E	0.8050	0.2060

