



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:36 AM UTC

PDB ID : 9NV3 / pdb_00009nv3
EMDB ID : EMD-49827
Title : Hybrid model of a complex of BREX proteins BrxB and PglZ from Salmonella typhimurium
Authors : Doyle, L.A.; Stoddard, B.; Blower, T.R.; Kaiser, B.
Deposited on : 2025-03-20
Resolution : 4.45 Å(reported)
Based on initial model : .

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:

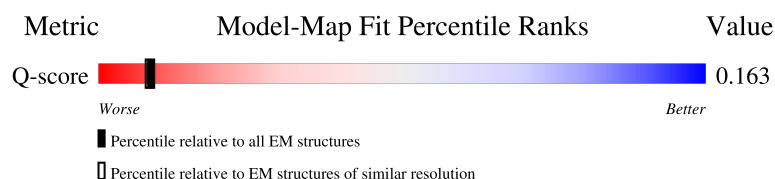
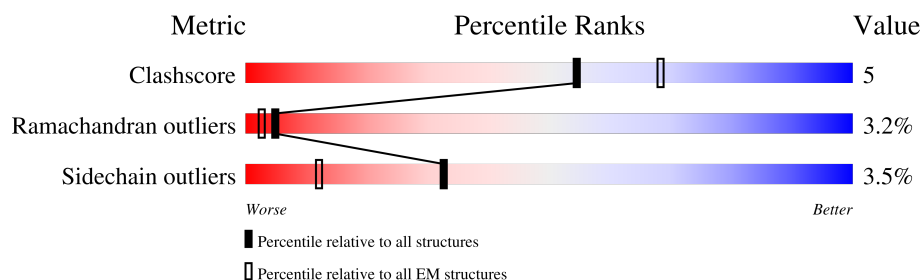
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.45 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	3027 (3.95 - 4.95)

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	199	 7% 94% 5%
2	C	887	 81% 13% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17287 atoms, of which 8603 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 DUF1788 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	199	Total	C	H	N	O	S	0	0
			3229	1033	1617	281	292	6		

- Molecule 2 is a protein called PglZ domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	866	Total	C	H	N	O	S	0	0
			14058	4490	6986	1230	1328	24		

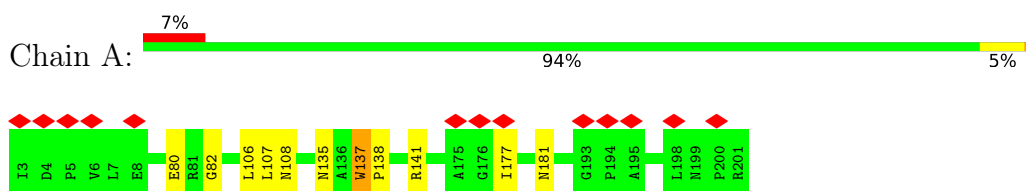
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	868	LYS	-	expression tag	UNP A0A6C7IK08
C	869	GLU	-	expression tag	UNP A0A6C7IK08
C	870	THR	-	expression tag	UNP A0A6C7IK08
C	871	ALA	-	expression tag	UNP A0A6C7IK08
C	872	ALA	-	expression tag	UNP A0A6C7IK08
C	873	ALA	-	expression tag	UNP A0A6C7IK08
C	874	LYS	-	expression tag	UNP A0A6C7IK08
C	875	PHE	-	expression tag	UNP A0A6C7IK08
C	876	GLU	-	expression tag	UNP A0A6C7IK08
C	877	ARG	-	expression tag	UNP A0A6C7IK08
C	878	GLN	-	expression tag	UNP A0A6C7IK08
C	879	HIS	-	expression tag	UNP A0A6C7IK08
C	880	MET	-	expression tag	UNP A0A6C7IK08
C	881	ASP	-	expression tag	UNP A0A6C7IK08
C	882	SER	-	expression tag	UNP A0A6C7IK08
C	883	SER	-	expression tag	UNP A0A6C7IK08
C	884	THR	-	expression tag	UNP A0A6C7IK08
C	885	SER	-	expression tag	UNP A0A6C7IK08
C	886	ALA	-	expression tag	UNP A0A6C7IK08
C	887	ALA	-	expression tag	UNP A0A6C7IK08

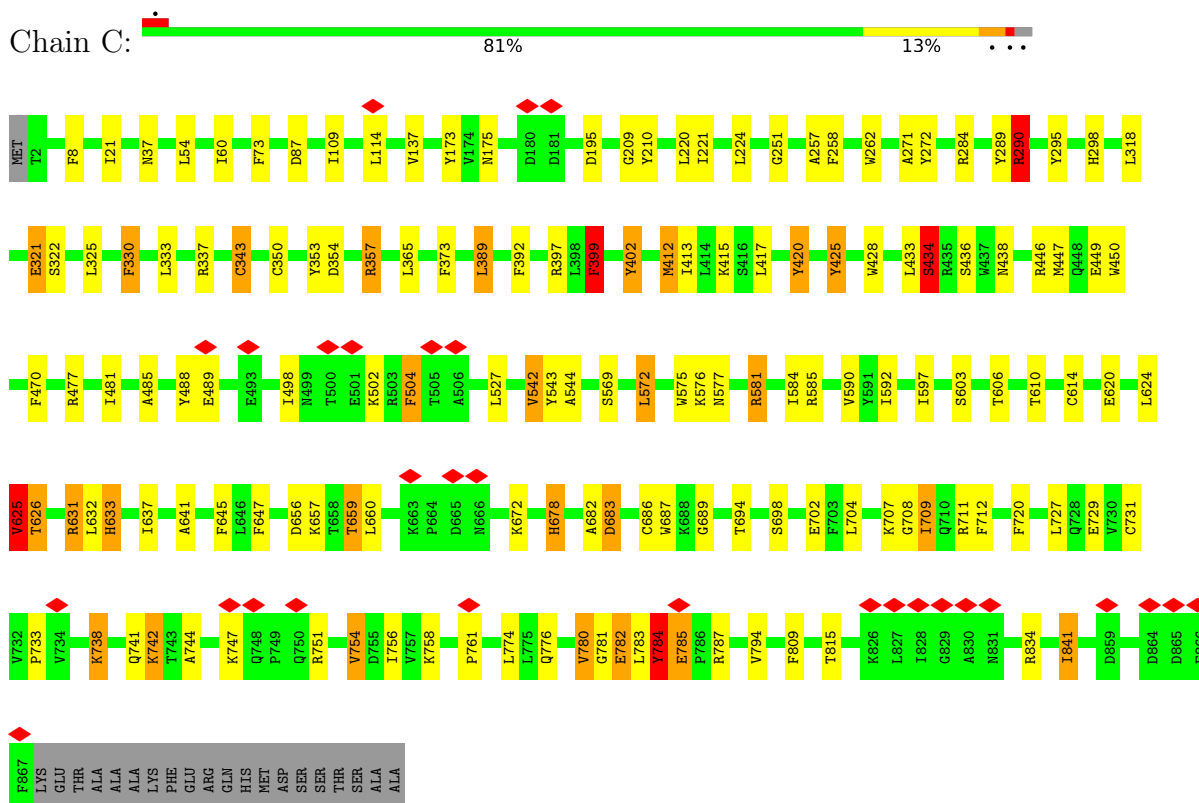
3 Residue-property plots [i](#)

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

- Molecule 1: DUF1788 domain-containing protein



- Molecule 2: PglZ domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123964	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.382	Depositor
Minimum map value	-1.959	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	336.6, 336.6, 336.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.122, 1.122, 1.122	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	A	0.82	0/1647	1.41	4/2224 (0.2%)
2	C	1.17	7/7222 (0.1%)	1.52	48/9778 (0.5%)
All	All	1.11	7/8869 (0.1%)	1.50	52/12002 (0.4%)

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
2	C	0	10

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	321	GLU	CG-CD	57.79	2.96	1.52
2	C	420	TYR	CG-CD2	17.06	1.75	1.39
2	C	420	TYR	CG-CD1	16.66	1.74	1.39
2	C	420	TYR	CE1-CZ	15.38	1.75	1.38
2	C	420	TYR	CE2-CZ	15.16	1.74	1.38
2	C	420	TYR	CD2-CE2	12.33	1.75	1.38
2	C	420	TYR	CD1-CE1	11.50	1.73	1.38

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	LEU	N-CA-C	11.05	125.12	110.53
2	C	321	GLU	CB-CG-CD	9.84	129.32	112.60
2	C	321	GLU	OE1-CD-OE2	-9.11	101.04	122.90
2	C	738	LYS	N-CA-C	8.16	123.71	113.43
2	C	785	GLU	N-CA-C	7.13	119.05	110.07
2	C	747	LYS	N-CA-C	7.07	118.88	111.03
2	C	446	ARG	NE-CZ-NH2	6.83	125.34	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASN	CA-CB-CG	6.56	119.16	112.60
2	C	470	PHE	CA-CB-CG	6.51	120.31	113.80
2	C	298	HIS	CA-C-N	6.44	129.23	120.54
2	C	298	HIS	C-N-CA	6.44	129.23	120.54
2	C	73	PHE	CA-CB-CG	6.39	120.19	113.80
2	C	8	PHE	CA-CB-CG	6.37	120.17	113.80
2	C	258	PHE	CA-CB-CG	6.33	120.14	113.80
2	C	175	ASN	CA-CB-CG	6.09	118.69	112.60
2	C	572	LEU	CA-C-N	6.09	128.76	120.54
2	C	572	LEU	C-N-CA	6.09	128.76	120.54
2	C	284	ARG	CB-CA-C	6.06	115.50	111.20
2	C	581	ARG	NE-CZ-NH2	5.97	124.57	119.20
2	C	257	ALA	CA-C-N	5.97	128.28	120.28
2	C	257	ALA	C-N-CA	5.97	128.28	120.28
2	C	333	LEU	N-CA-CB	-5.91	101.45	110.26
2	C	434	SER	CA-C-N	5.86	128.06	120.44
2	C	434	SER	C-N-CA	5.86	128.06	120.44
2	C	711	ARG	N-CA-C	5.67	117.40	108.96
2	C	682	ALA	N-CA-C	5.58	117.74	110.43
2	C	678	HIS	CB-CG-CD2	-5.51	124.04	131.20
2	C	659	THR	CA-CB-CG2	5.48	119.82	110.50
2	C	357	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	C	412	MET	CA-C-N	5.41	131.70	121.97
2	C	412	MET	C-N-CA	5.41	131.70	121.97
2	C	504	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	141	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	C	657	LYS	N-CA-C	5.26	117.98	109.83
2	C	625	VAL	CA-CB-CG1	5.21	119.27	110.40
2	C	290	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	137	TRP	N-CA-C	5.20	121.30	109.81
2	C	712	PHE	CA-CB-CG	5.20	119.00	113.80
2	C	784	TYR	N-CA-C	5.18	117.36	110.53
2	C	428	TRP	CA-C-N	5.18	127.48	120.65
2	C	428	TRP	C-N-CA	5.18	127.48	120.65
2	C	659	THR	CA-C-N	5.12	131.31	121.54
2	C	659	THR	C-N-CA	5.12	131.31	121.54
2	C	633	HIS	CA-CB-CG	5.11	118.91	113.80
2	C	625	VAL	N-CA-C	5.10	119.94	109.34
2	C	741	GLN	OE1-CD-NE2	-5.07	117.53	122.60
2	C	37	ASN	CA-C-N	5.06	128.53	121.24
2	C	37	ASN	C-N-CA	5.06	128.53	121.24
2	C	741	GLN	N-CA-C	5.06	116.93	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	585	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	C	776	GLN	OE1-CD-NE2	-5.05	117.55	122.60
2	C	834	ARG	NE-CZ-NH2	5.03	123.72	119.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	289	TYR	Sidechain
2	C	337	ARG	Sidechain
2	C	353	TYR	Sidechain
2	C	399	PHE	Sidechain
2	C	402	TYR	Sidechain
2	C	477	ARG	Sidechain
2	C	488	TYR	Sidechain
2	C	581	ARG	Sidechain
2	C	631	ARG	Sidechain
2	C	784	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1612	1617	1616	1	0
2	C	7072	6986	6985	88	0
All	All	8684	8603	8601	88	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 (88) 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)
2:C:420:TYR:CD2	2:C:420:TYR:CG	1.75	1.67
2:C:420:TYR:CE1	2:C:420:TYR:CZ	1.75	1.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:420:TYR:CZ	2:C:420:TYR:CE2	1.74	1.63
2:C:420:TYR:CD2	2:C:420:TYR:CE2	1.75	1.62
2:C:321:GLU:CG	2:C:420:TYR:CD2	2.29	1.16
2:C:321:GLU:CG	2:C:420:TYR:CG	2.29	1.15
2:C:321:GLU:CG	2:C:420:TYR:CD1	2.30	1.15
2:C:321:GLU:CD	2:C:420:TYR:CE2	2.25	1.14
2:C:321:GLU:CG	2:C:420:TYR:CZ	2.29	1.14
2:C:321:GLU:CG	2:C:420:TYR:CE2	2.31	1.13
2:C:321:GLU:CG	2:C:420:TYR:CE1	2.30	1.12
2:C:321:GLU:CD	2:C:420:TYR:CD1	2.27	1.12
2:C:321:GLU:CD	2:C:420:TYR:CZ	2.29	1.11
2:C:321:GLU:CD	2:C:420:TYR:CG	2.29	1.10
2:C:321:GLU:CD	2:C:420:TYR:CD2	2.27	1.10
2:C:321:GLU:CD	2:C:420:TYR:CE1	2.28	1.10
2:C:321:GLU:HG2	2:C:420:TYR:CE1	2.00	0.93
2:C:321:GLU:HG3	2:C:420:TYR:CG	2.04	0.91
2:C:321:GLU:HG3	2:C:420:TYR:CD1	2.02	0.91
2:C:321:GLU:HG2	2:C:420:TYR:CZ	2.05	0.89
2:C:321:GLU:CB	2:C:420:TYR:CD2	2.67	0.77
2:C:321:GLU:CB	2:C:420:TYR:CE2	2.68	0.77
2:C:321:GLU:HB3	2:C:420:TYR:CE2	2.22	0.73
2:C:572:LEU:HD22	2:C:592:ILE:CG2	2.24	0.68
2:C:321:GLU:OE2	2:C:420:TYR:CZ	2.46	0.67
2:C:321:GLU:OE1	2:C:420:TYR:CD2	2.50	0.65
2:C:321:GLU:OE1	2:C:420:TYR:CG	2.50	0.64
2:C:373:PHE:CE2	2:C:389:LEU:HD22	2.33	0.64
2:C:569:SER:HA	2:C:572:LEU:HD23	1.80	0.64
2:C:321:GLU:OE2	2:C:420:TYR:CE1	2.54	0.61
2:C:659:THR:HG22	2:C:660:LEU:H	1.65	0.60
2:C:262:TRP:CZ2	2:C:271:ALA:HB3	2.38	0.58
2:C:687:TRP:CH2	2:C:707:LYS:HE2	2.38	0.58
2:C:399:PHE:CD1	2:C:399:PHE:C	2.82	0.56
2:C:780:VAL:HG13	2:C:781:GLY:H	1.68	0.56
2:C:641:ALA:H	2:C:733:PRO:HD2	1.70	0.56
2:C:343:CYS:CB	2:C:350:CYS:HG	2.18	0.56
2:C:754:VAL:HG13	2:C:785:GLU:H	1.71	0.55
2:C:687:TRP:CZ3	2:C:707:LYS:HE2	2.41	0.55
2:C:597:ILE:HG21	2:C:645:PHE:CE2	2.43	0.54
2:C:433:LEU:HD12	2:C:436:SER:HB2	1.90	0.54
2:C:354:ASP:HB3	2:C:402:TYR:CE2	2.43	0.54
2:C:626:THR:HG22	2:C:784:TYR:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:450:TRP:CD2	2:C:694:THR:HG22	2.44	0.52
2:C:620:GLU:O	2:C:744:ALA:HB2	2.09	0.52
2:C:672:LYS:HE3	2:C:720:PHE:CE2	2.45	0.51
2:C:656:ASP:HA	2:C:709:ILE:HD12	1.91	0.51
2:C:572:LEU:HD22	2:C:592:ILE:HG23	1.92	0.51
2:C:659:THR:CG2	2:C:660:LEU:H	2.24	0.50
2:C:397:ARG:HG3	2:C:614:CYS:HB3	1.95	0.48
2:C:542:VAL:HG12	2:C:543:TYR:H	1.76	0.48
2:C:687:TRP:CD1	2:C:707:LYS:HA	2.48	0.48
1:A:80:GLU:H	2:C:54:LEU:HB3	1.79	0.48
2:C:626:THR:CG2	2:C:784:TYR:CD2	2.97	0.48
2:C:210:TYR:CE1	2:C:220:LEU:HA	2.49	0.47
2:C:637:ILE:H	2:C:738:LYS:HA	1.79	0.47
2:C:687:TRP:CE3	2:C:707:LYS:HE2	2.49	0.47
2:C:754:VAL:H	2:C:784:TYR:HB3	1.80	0.47
2:C:325:LEU:HD11	2:C:330:PHE:CE2	2.50	0.46
2:C:354:ASP:HB3	2:C:402:TYR:CD2	2.50	0.46
2:C:209:GLY:HA3	2:C:251:GLY:HA3	1.97	0.46
2:C:438:ASN:CG	2:C:707:LYS:HB3	2.41	0.45
2:C:610:THR:HB	2:C:647:PHE:CD1	2.51	0.45
2:C:625:VAL:O	2:C:742:LYS:HE2	2.17	0.45
2:C:527:LEU:HB2	2:C:544:ALA:HB3	1.99	0.45
2:C:209:GLY:HA3	2:C:251:GLY:CA	2.47	0.44
2:C:794:VAL:HG21	2:C:841:ILE:HG13	1.99	0.44
2:C:173:TYR:CD2	2:C:221:ILE:CD1	3.00	0.44
2:C:626:THR:CG2	2:C:784:TYR:H	2.31	0.44
2:C:632:LEU:CD2	2:C:809:PHE:CD1	3.02	0.43
2:C:481:ILE:HD12	2:C:481:ILE:N	2.34	0.43
2:C:686:CYS:HA	2:C:707:LYS:H	1.84	0.43
2:C:262:TRP:CZ2	2:C:271:ALA:CB	3.02	0.43
2:C:687:TRP:CZ2	2:C:707:LYS:HE2	2.53	0.43
2:C:318:LEU:HA	2:C:321:GLU:HA	2.01	0.42
2:C:597:ILE:HG21	2:C:645:PHE:CZ	2.54	0.42
2:C:295:TYR:CE1	2:C:330:PHE:HA	2.55	0.42
2:C:625:VAL:HG12	2:C:626:THR:N	2.35	0.41
2:C:659:THR:HG22	2:C:660:LEU:N	2.35	0.41
2:C:21:ILE:HG12	2:C:60:ILE:HG23	2.02	0.41
2:C:626:THR:H	2:C:782:GLU:CD	2.28	0.41
2:C:434:SER:HA	2:C:708:GLY:HA2	2.03	0.41
2:C:262:TRP:CD1	2:C:272:TYR:CE2	3.09	0.41
2:C:365:LEU:HD22	2:C:392:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:683:ASP:O	2:C:707:LYS:HE3	2.21	0.41
2:C:689:GLY:O	2:C:702:GLU:HA	2.21	0.40
2:C:727:LEU:C	2:C:729:GLU:H	2.29	0.40
2:C:354:ASP:HA	2:C:357:ARG:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/199 (99%)	172 (87%)	21 (11%)	4 (2%)	6	31
2	C	864/887 (97%)	706 (82%)	128 (15%)	30 (4%)	3	20
All	All	1061/1086 (98%)	878 (83%)	149 (14%)	34 (3%)	5	21

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	TRP
2	C	625	VAL
2	C	754	VAL
2	C	780	VAL
1	A	82	GLY
1	A	135	ASN
1	A	138	PRO
2	C	322	SER
2	C	434	SER
2	C	485	ALA
2	C	575	TRP
2	C	577	ASN
2	C	761	PRO
2	C	783	LEU

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Mol	Chain	Res	Type
2	C	290	ARG
2	C	412	MET
2	C	447	MET
2	C	502	LYS
2	C	576	LYS
2	C	603	SER
2	C	631	ARG
2	C	633	HIS
2	C	774	LEU
2	C	413	ILE
2	C	504	PHE
2	C	751	ARG
2	C	815	THR
2	C	624	LEU
2	C	698	SER
2	C	742	LYS
2	C	758	LYS
2	C	425	TYR
2	C	756	ILE
2	C	109	ILE

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	174/174 (100%)	171 (98%)	3 (2%)	53	67
2	C	767/783 (98%)	737 (96%)	30 (4%)	28	50
All	All	941/957 (98%)	908 (96%)	33 (4%)	32	53

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LEU
1	A	108	ASN
1	A	177	ILE

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Continued from previous page...

Mol	Chain	Res	Type
2	C	87	ASP
2	C	114	LEU
2	C	137	VAL
2	C	195	ASP
2	C	224	LEU
2	C	290	ARG
2	C	330	PHE
2	C	343	CYS
2	C	389	LEU
2	C	399	PHE
2	C	415	LYS
2	C	417	LEU
2	C	425	TYR
2	C	449	GLU
2	C	489	GLU
2	C	498	ILE
2	C	542	VAL
2	C	584	ILE
2	C	590	VAL
2	C	606	THR
2	C	626	THR
2	C	678	HIS
2	C	683	ASP
2	C	704	LEU
2	C	709	ILE
2	C	731	CYS
2	C	782	GLU
2	C	784	TYR
2	C	787	ARG
2	C	841	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	135	ASN
2	C	19	HIS
2	C	51	GLN
2	C	53	GLN
2	C	68	GLN
2	C	105	ASN
2	C	177	GLN

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Continued from previous page...

Mol	Chain	Res	Type
2	C	186	ASN
2	C	205	ASN
2	C	211	GLN
2	C	214	HIS
2	C	374	HIS
2	C	463	ASN
2	C	578	GLN
2	C	633	HIS
2	C	649	GLN
2	C	670	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.

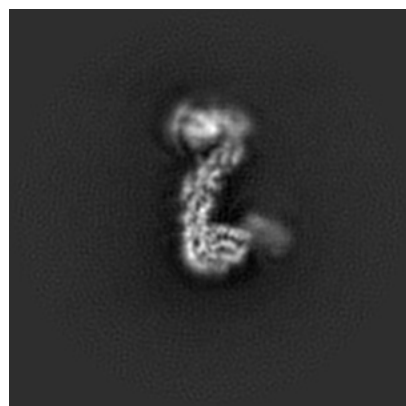
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49827. These allow visual inspection of the internal detail of the map and identification of artifacts.

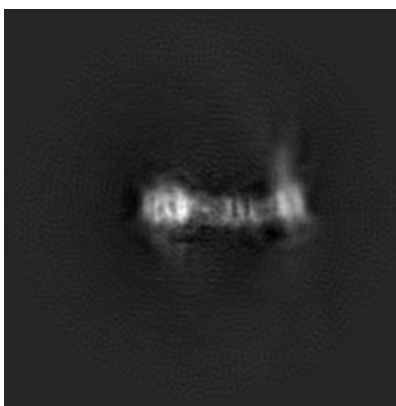
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

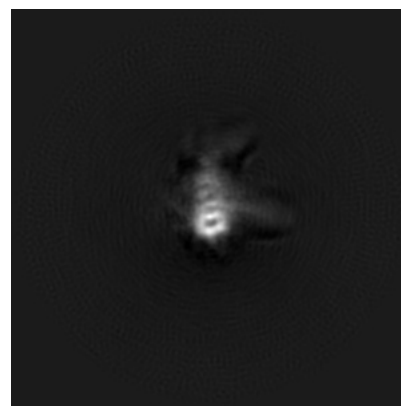
6.1.1 Primary map



X

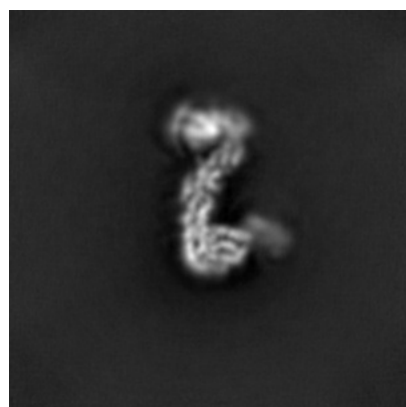


Y

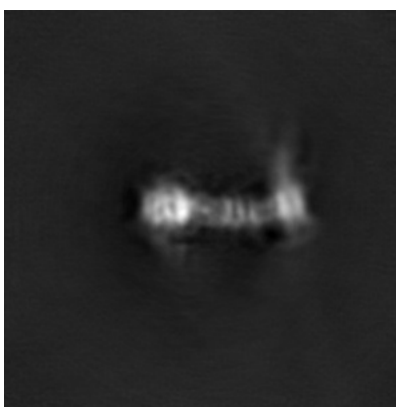


Z

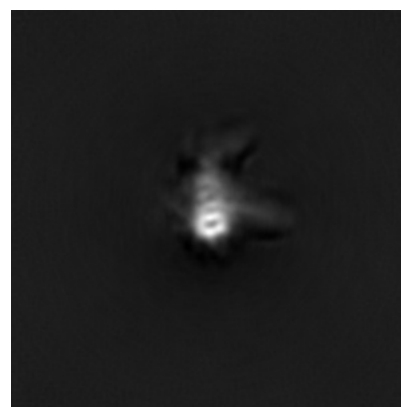
6.1.2 Raw map



X



Y

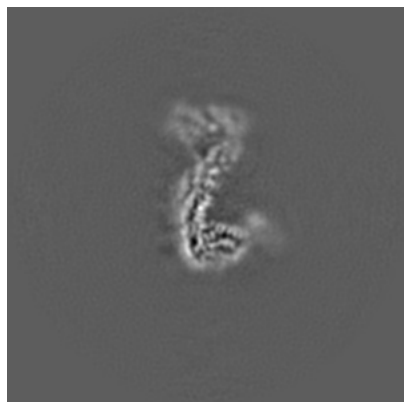


Z

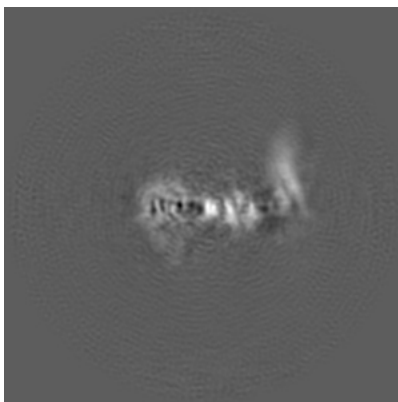
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

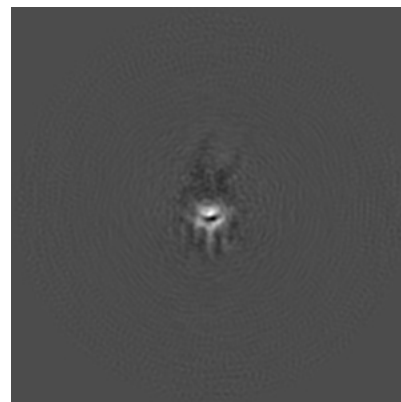
6.2.1 Primary map



X Index: 150

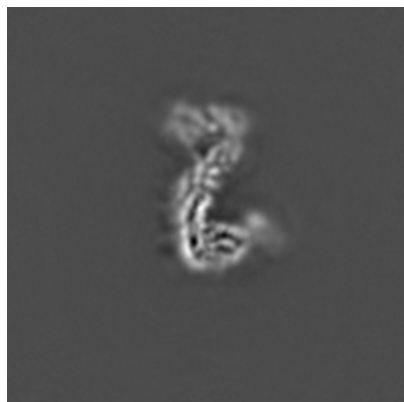


Y Index: 150

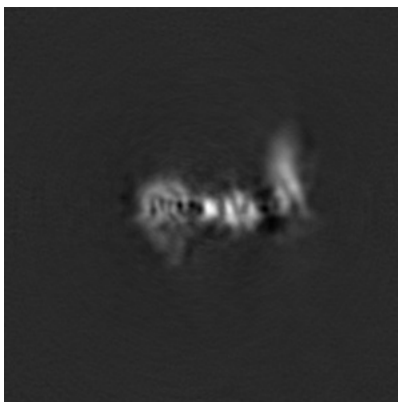


Z Index: 150

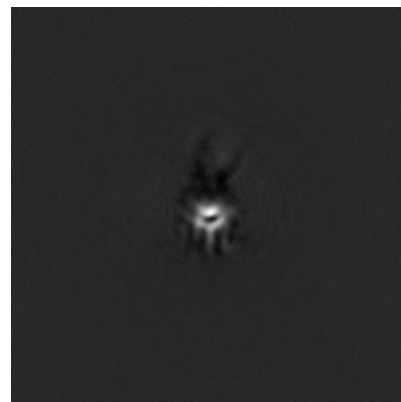
6.2.2 Raw map



X Index: 150



Y Index: 150

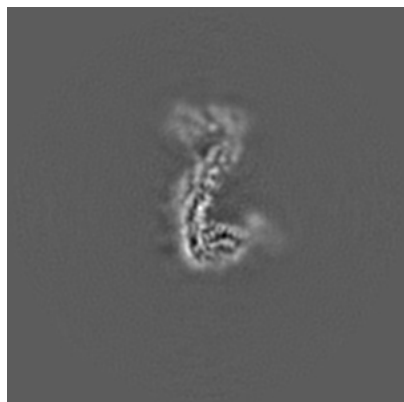


Z Index: 150

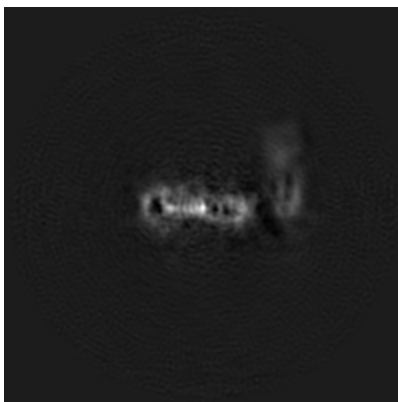
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

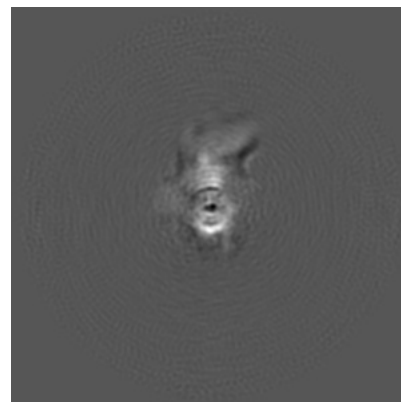
6.3.1 Primary map



X Index: 149

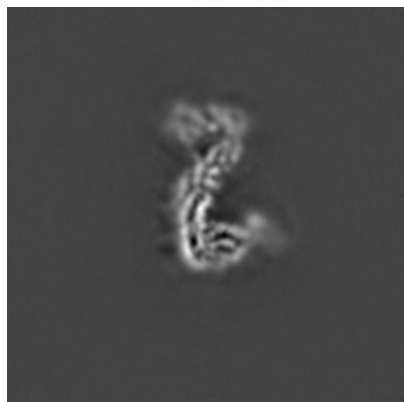


Y Index: 144

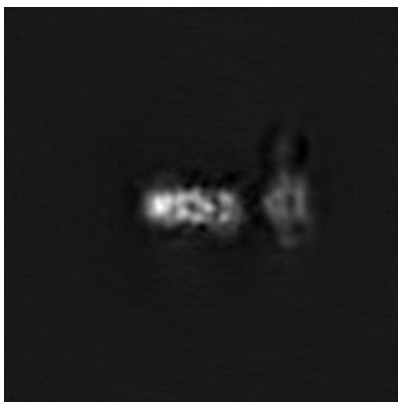


Z Index: 131

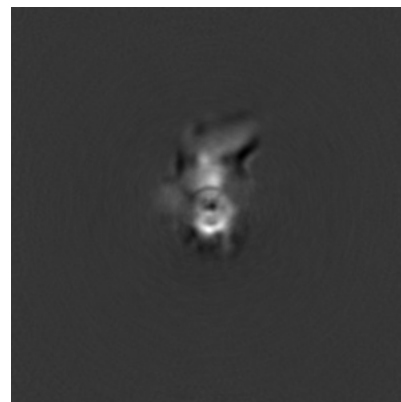
6.3.2 Raw map



X Index: 149



Y Index: 135



Z Index: 132

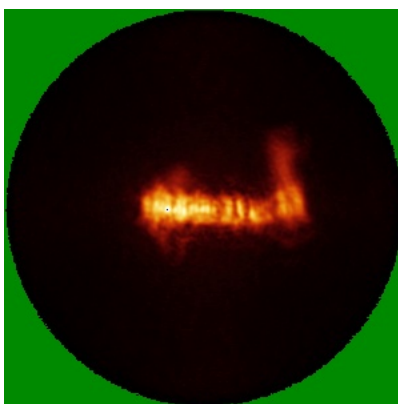
The images above show the largest variance slices of the map in three orthogonal directions.

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

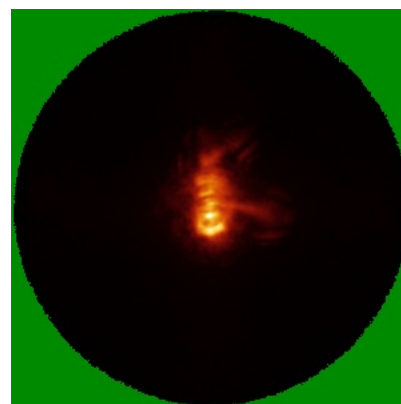
6.4.1 Primary map



X

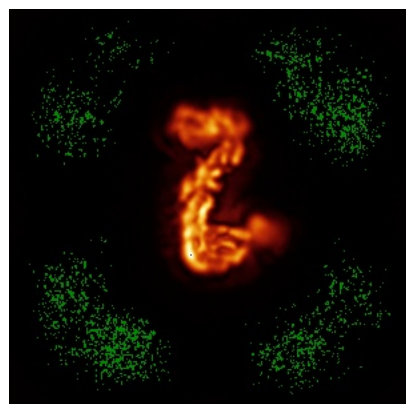


Y

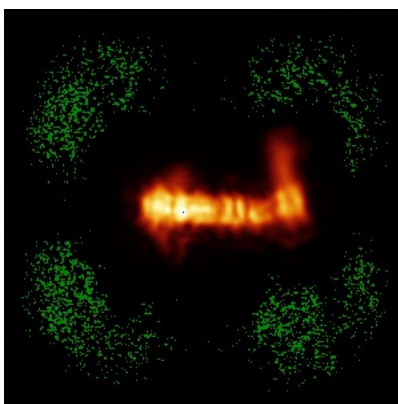


Z

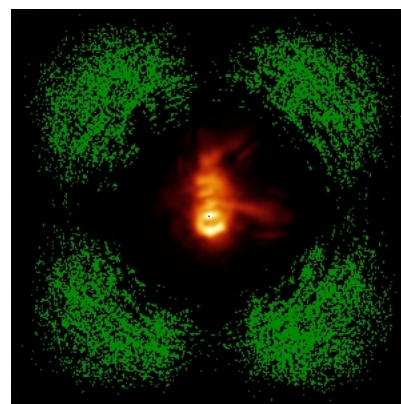
6.4.2 Raw map



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 0.27. 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.

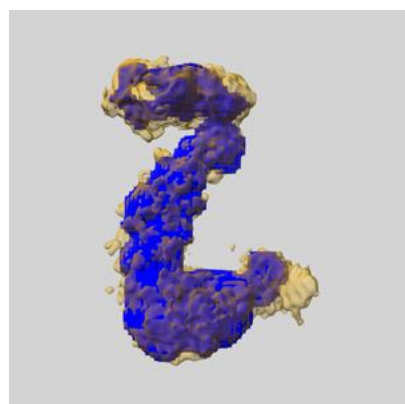
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

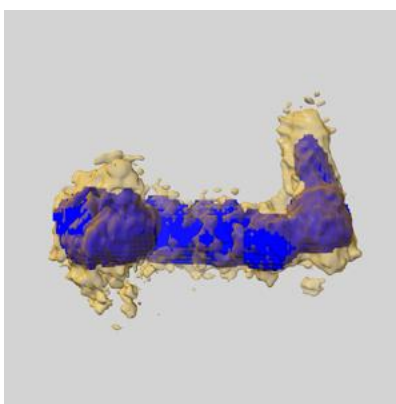
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

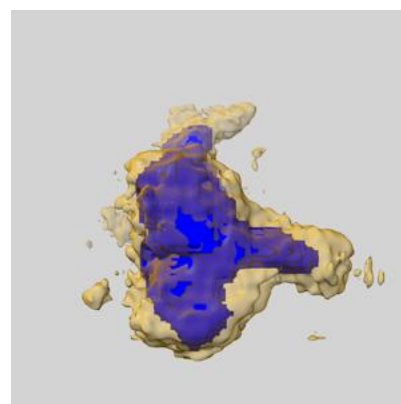
6.6.1 emd_49827_msk_1.map [i](#)



X



Y

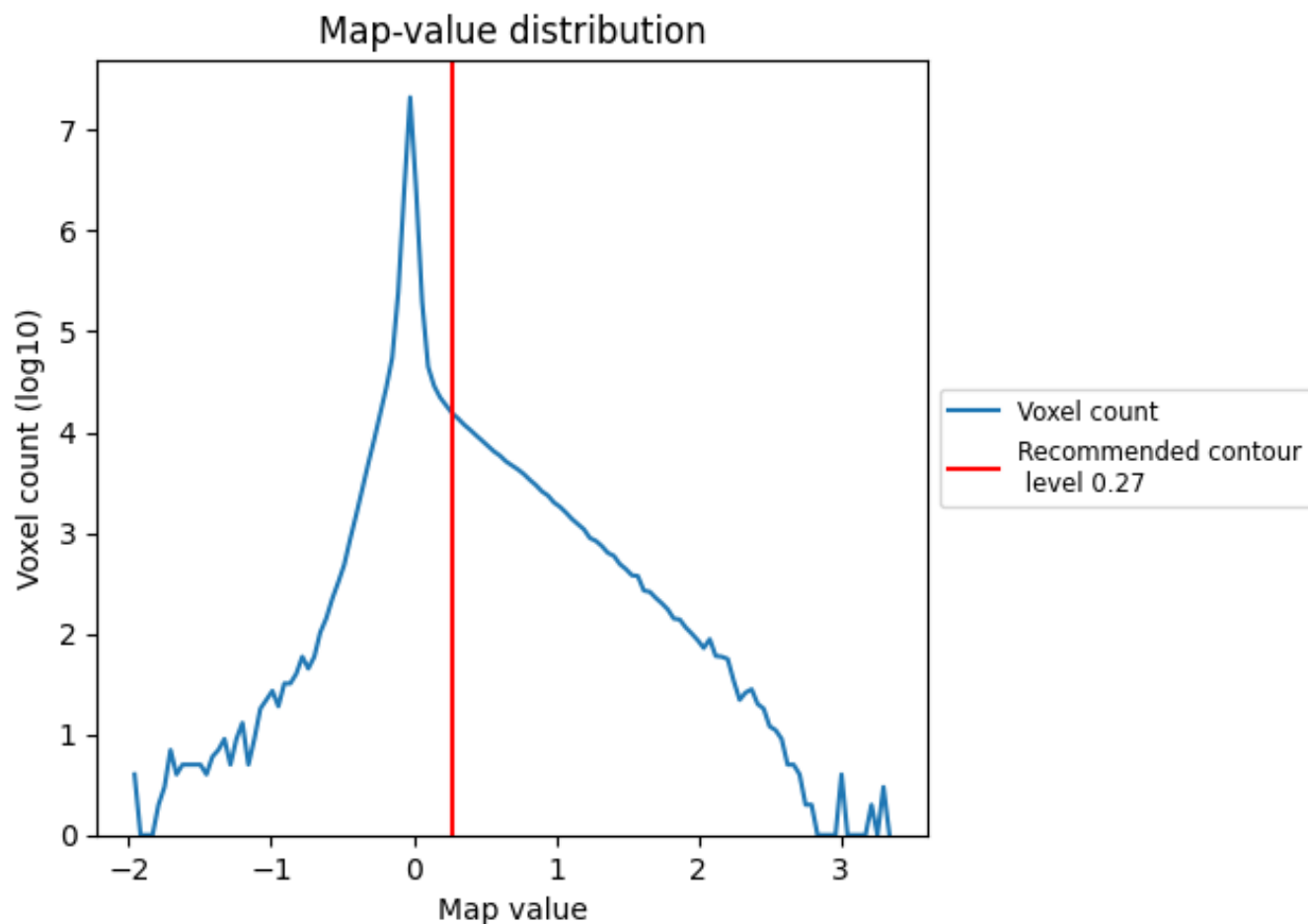


Z

7 Map analysis [i](#)

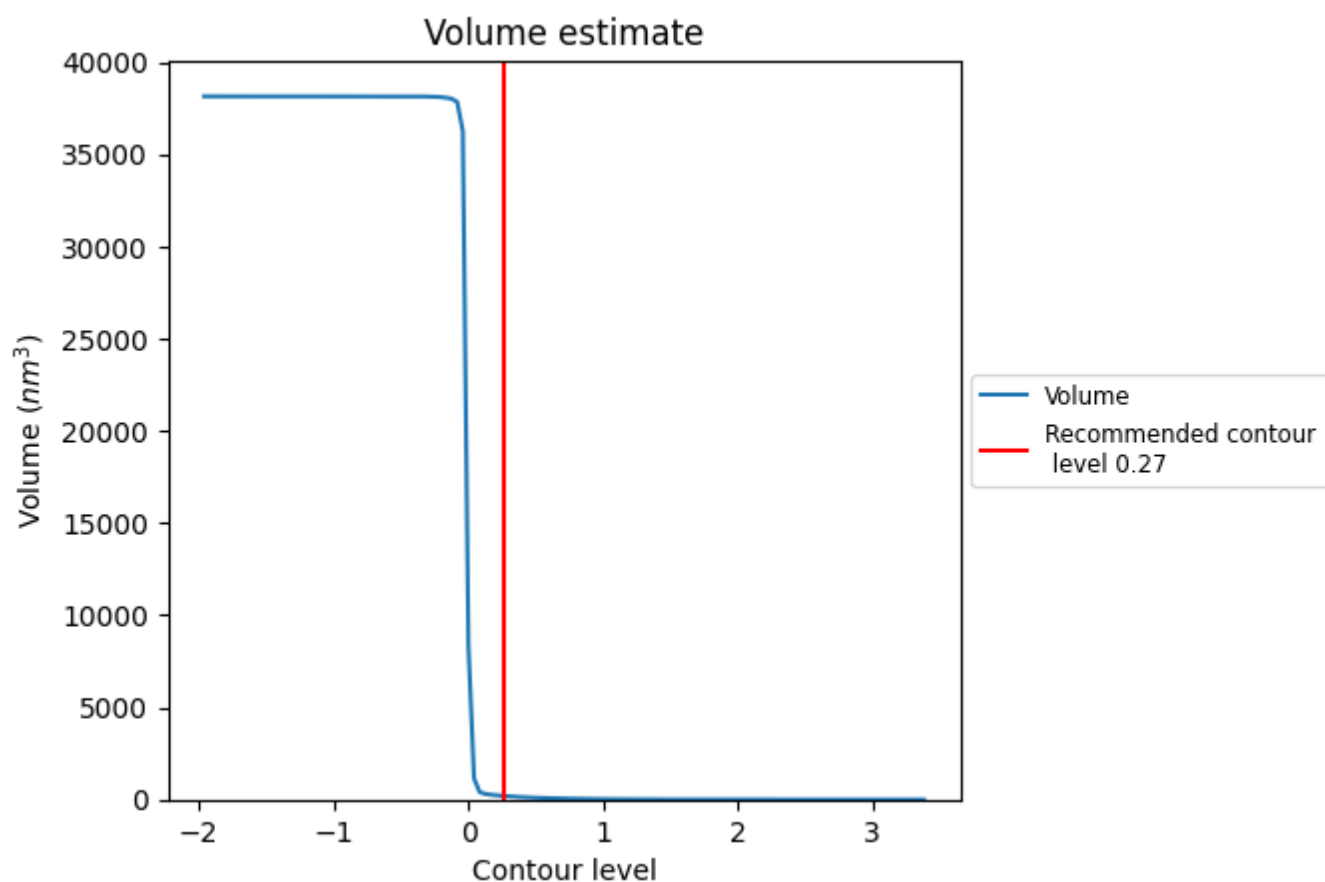
This section contains the results of statistical analysis of the map.

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.

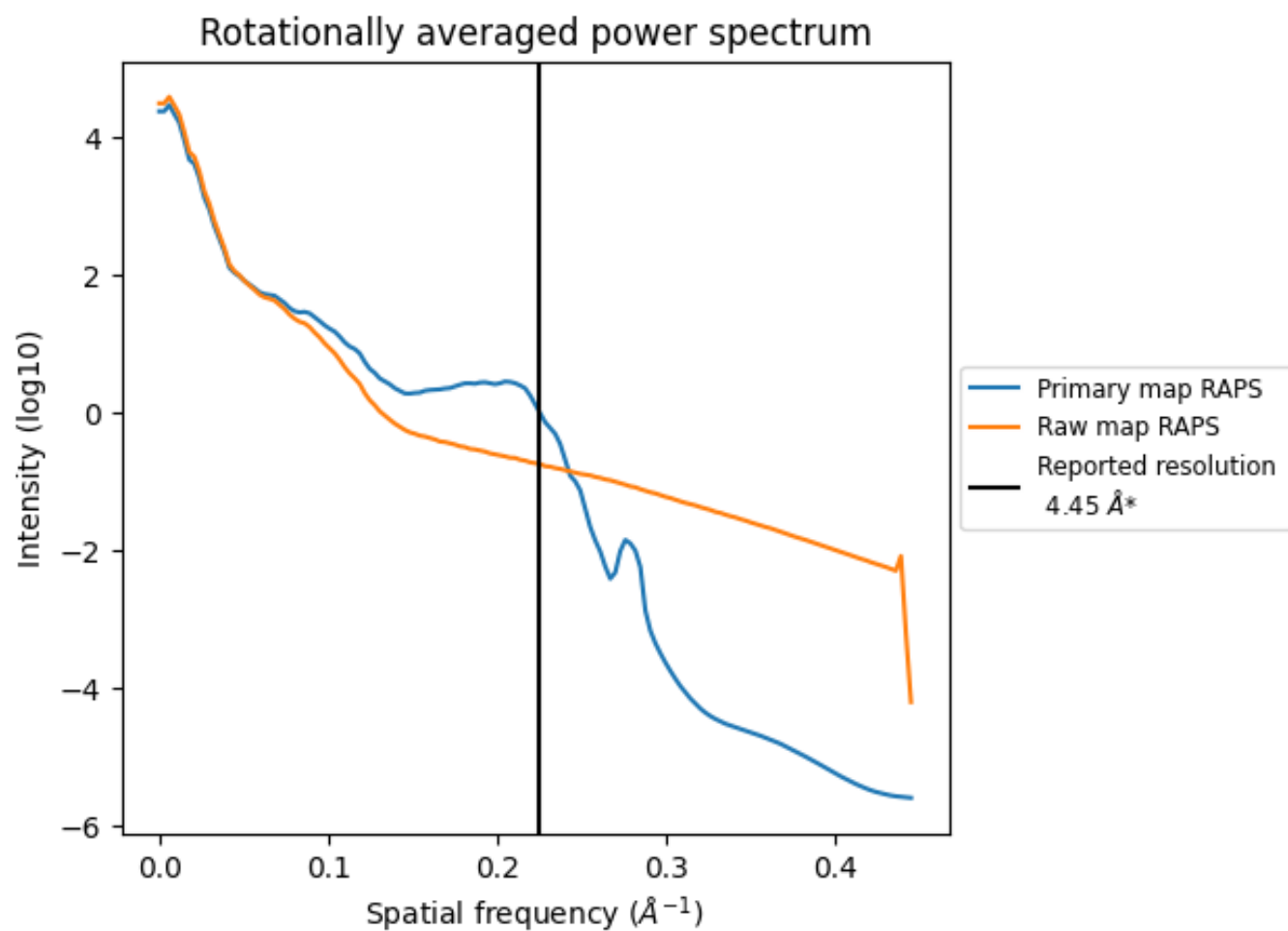
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 190 nm³; this corresponds to an approximate mass of 172 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 ⓘ

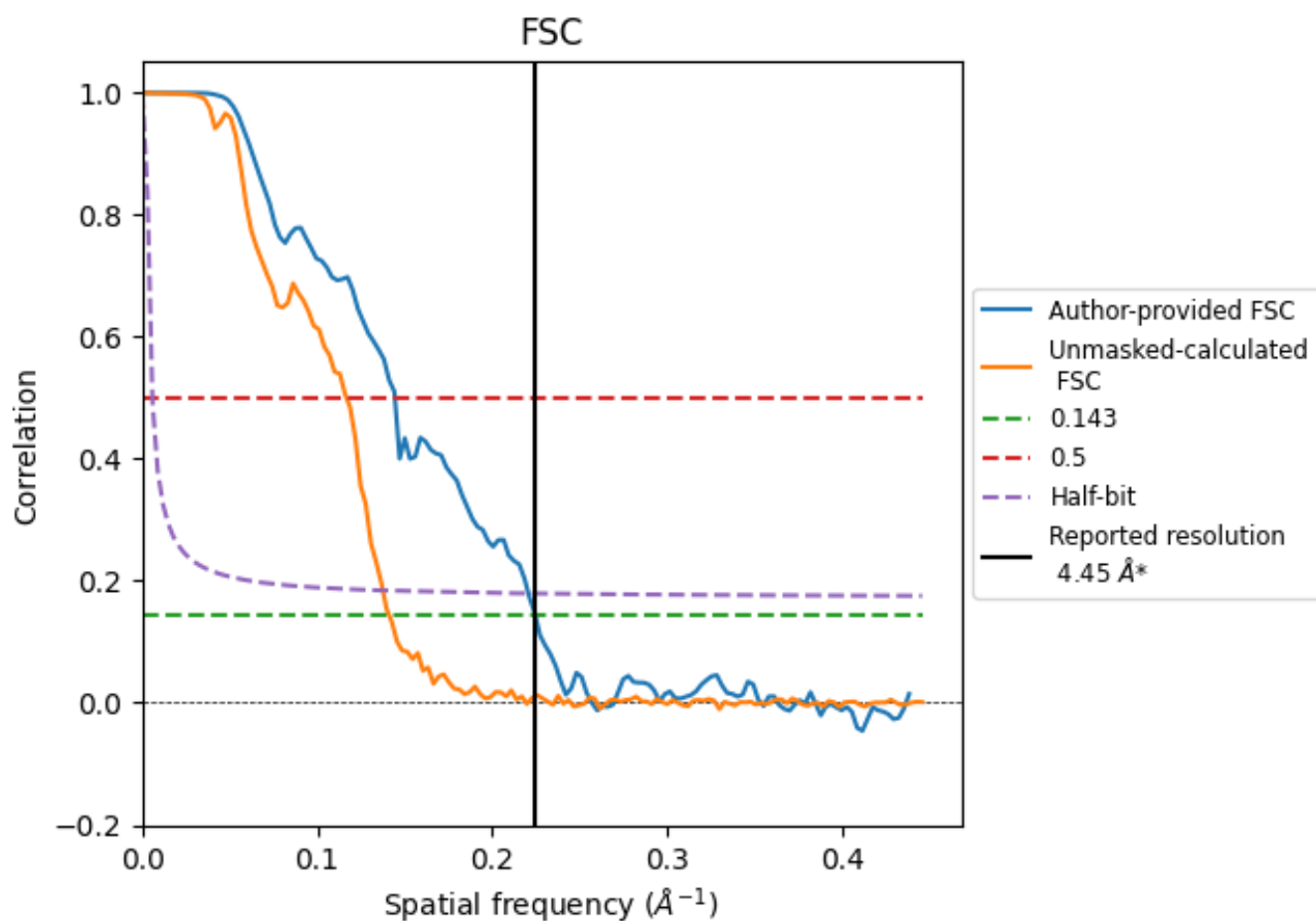


*Reported resolution corresponds to spatial frequency of $0.225 \text{ \AA}^{-1}$

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 0.225 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

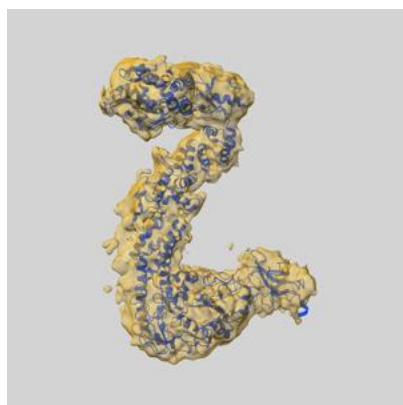
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.45	-	-
Author-provided FSC curve	4.45	6.93	4.53
Unmasked-calculated*	7.08	8.57	7.27

*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 7.08 differs from the reported value 4.45 by more than 10 %

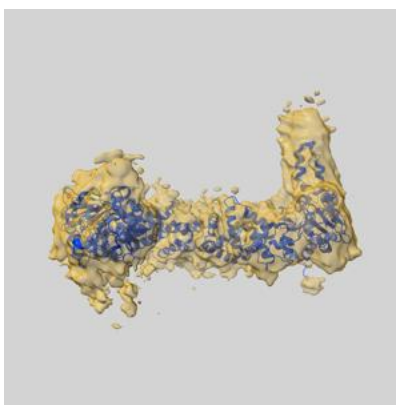
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49827 and PDB model 9NV3. Per-residue inclusion information can be found in section [3](#) on page [4](#).

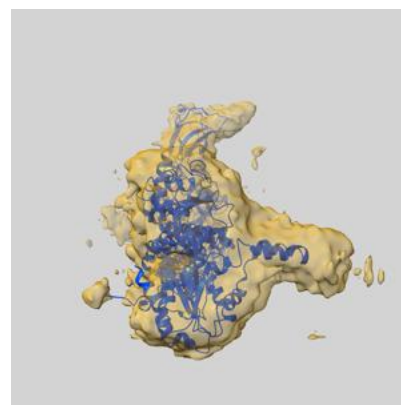
9.1 Map-model overlay [i](#)



X



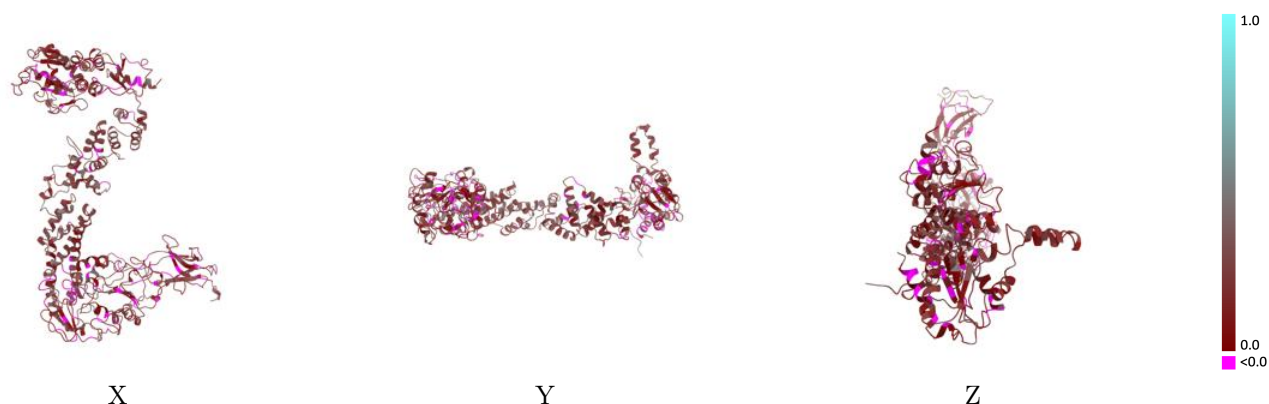
Y



Z

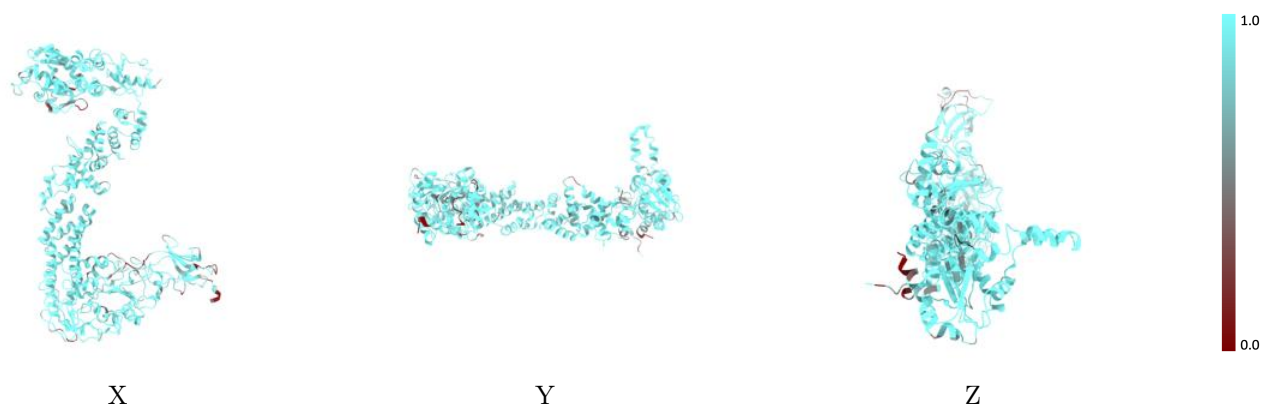
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



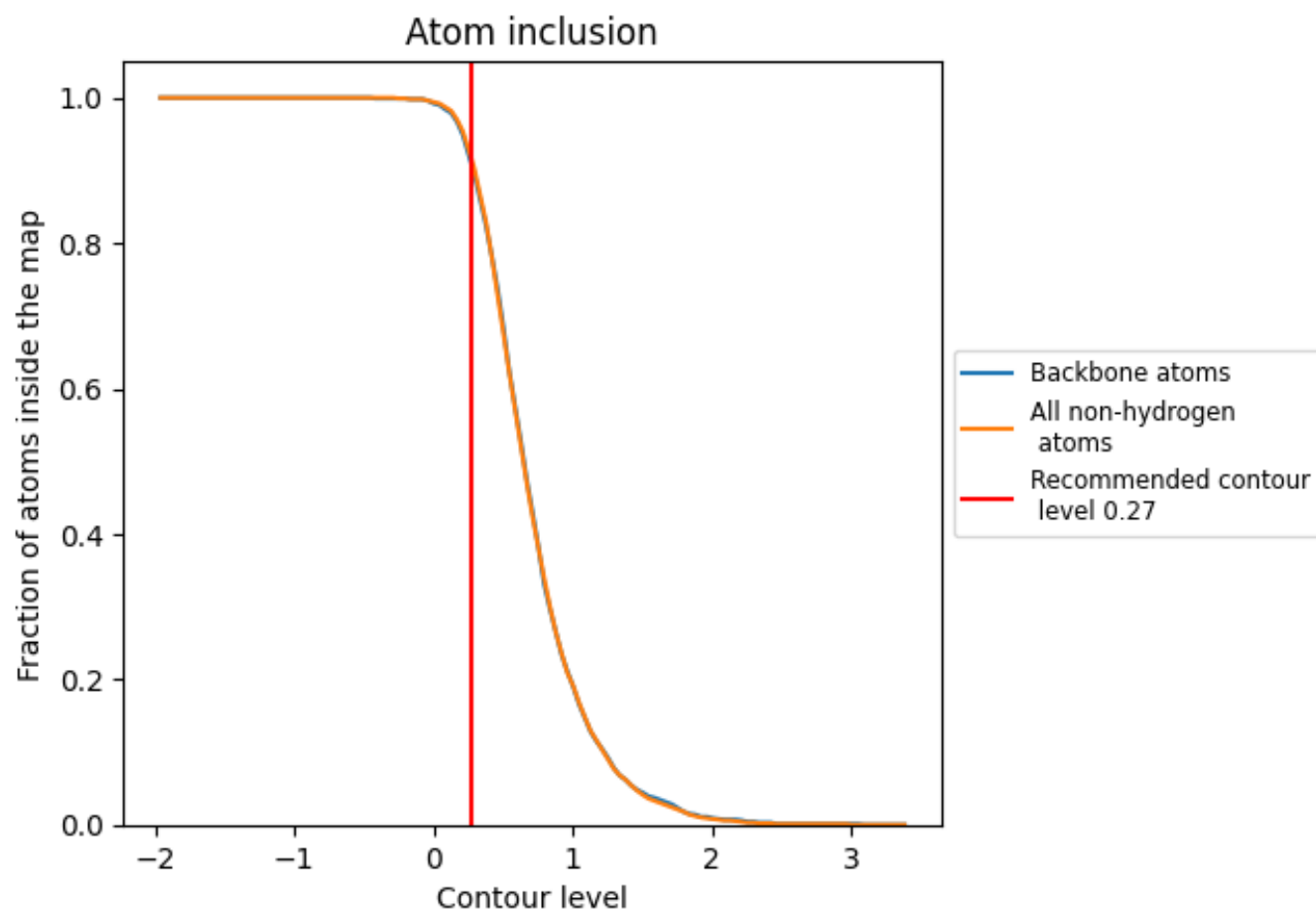
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 92% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.1630
A	0.9000	0.1470
C	0.9240	0.1660

