wwPDB EM Validation Summary Report (i)

Nov 12, 2022 – 10:26 AM EST

PDB ID	:	6V05
EMDB ID	:	EMD-20969
Title	:	Cryo-EM structure of a substrate-engaged Bam complex
Authors	:	Tomasek, D.; Rawson, S.; Lee, J.; Wzorek, J.S.; Harrison, S.C.; Li, Z.; Kahne, D.
Deposited on	:	2019-11-18
Resolution	:	4.10 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

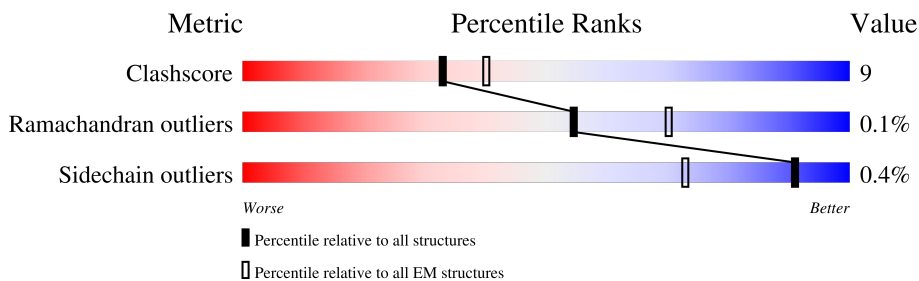|		
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		0.4%

Worse — Better

■ Percentile relative to all structures

▯ Percentile relative to all EM structures

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 <=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	810	19% / 82% / 12% / 6%
2	B	392	7% / 67% / 20% / 13%
3	C	344	36% / 45% / 7% / 47%
4	D	245	5% / 64% / 23% / 13%
5	E	123	57% / 11% / 33%
6	F	578	7% / 42% / 11% / 47%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 13705 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	758	Total 5429	C 3351	N 961	O 1104	S 13	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	690	SER	CYS	engineered mutation	UNP P0A940
A	700	SER	CYS	engineered mutation	UNP P0A940
A	804	CYS	PHE	engineered mutation	UNP P0A940

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	340	Total 2522	C 1588	N 436	O 492	S 6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	181	Total 919	C 516	N 197	O 205	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	213	Total 1722	C 1086	N 303	O 326	S 7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	83	Total 645	C 405	N 112	O 126	S 2	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	GLY	-	expression tag	UNP A0A3S5E0E0
E	115	GLY	-	expression tag	UNP A0A3S5E0E0
E	116	HIS	-	expression tag	UNP A0A3S5E0E0
E	117	HIS	-	expression tag	UNP A0A3S5E0E0
E	118	HIS	-	expression tag	UNP A0A3S5E0E0
E	119	HIS	-	expression tag	UNP A0A3S5E0E0
E	120	HIS	-	expression tag	UNP A0A3S5E0E0
E	121	HIS	-	expression tag	UNP A0A3S5E0E0
E	122	HIS	-	expression tag	UNP A0A3S5E0E0
E	123	HIS	-	expression tag	UNP A0A3S5E0E0

- Molecule 6 is a protein called Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	309	2468	1572	398	489	9	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	254	TRP	-	linker	UNP P0A940
F	255	SER	-	linker	UNP P0A940
F	256	HIS	-	linker	UNP P0A940
F	257	PRO	-	linker	UNP P0A940
F	258	GLN	-	linker	UNP P0A940
F	259	PHE	-	linker	UNP P0A940
F	260	GLU	-	linker	UNP P0A940
F	261	LYS	-	linker	UNP P0A940
F	262	GLY	-	linker	UNP P0A940
F	263	GLY	-	linker	UNP P0A940
F	264	GLY	-	linker	UNP P0A940
F	265	SER	-	linker	UNP P0A940
F	266	GLY	-	linker	UNP P0A940
F	267	GLY	-	linker	UNP P0A940
F	268	GLY	-	linker	UNP P0A940
F	269	SER	-	linker	UNP P0A940
F	270	GLY	-	linker	UNP P0A940
F	271	GLY	-	linker	UNP P0A940
F	272	SER	-	linker	UNP P0A940

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Chain	Residue	Modelled	Actual	Comment	Reference
F	273	ALA	-	linker	UNP P0A940
F	274	TRP	-	linker	UNP P0A940
F	275	SER	-	linker	UNP P0A940
F	276	HIS	-	linker	UNP P0A940
F	277	PRO	-	linker	UNP P0A940
F	278	GLN	-	linker	UNP P0A940
F	279	PHE	-	linker	UNP P0A940
F	280	GLU	-	linker	UNP P0A940
F	281	LYS	-	linker	UNP P0A940
F	467	CYS	THR	engineered mutation	UNP P0A940
F	690	SER	CYS	engineered mutation	UNP P0A940
F	700	SER	CYS	engineered mutation	UNP P0A940

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 BamA

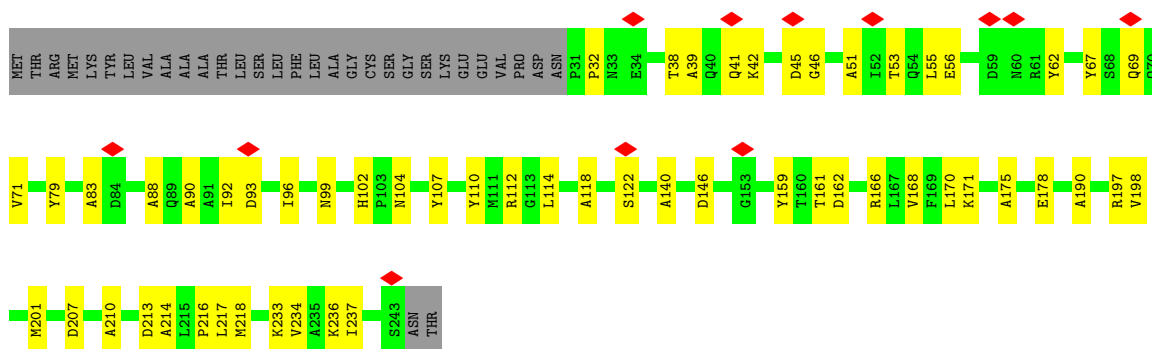• Molecule 2: Outer membrane protein assembly factor BamB

G89 K90 L97 A98 E99 LYS ASP GLY W103 F104 S105 K106 E107 L110 L111 S112 G119 L134 T140 E150 G160 N175 E176 G179 A180 V181 K182 M189 PRO SER LEU SER LEU R195 P200 A203 V209 R215 V219 L220 M221 G224 Q225 M226

Q229 Q230 R231 I232 S233 Q234 ALA THR GLY SER THR GLU ILE ASP ARG LEU SER D246 V247 D248 V253 L261 A262 G265 N266 L267 T268 D271 L272 G275 Q276 R281 GLU LEU GLY SER V286 N287 L298 V299 D300 Q301 N302 D303 R304 V314 W317 I318 Q319

L327 T328 S329 V339 G340 D341 S342 E343 G344 W348 E352 F356 V357 A358 Q359 G366 E370 P371 A374 K377 L378 L379 I380 I390 T391 R392

• Molecule 3: Outer membrane protein assembly factor BamC

Chain C:

36%
45%   7%   47%

MET ALA TYR SER VAL GLN LYS SER ARG LEU ALA LYS VAL ALA GLY VAL VAL SER LEU VAL LEU LEU LEU ALA ALA CYS SER SER ASP S29 R30 R33 Q34 E39 L42 L47 A48 E49 L50 P53 M56 I57 L58 P59 V60 T61 S62 G63 D64 V69 V70 N71 G72 S73

V76 G77 K78 A79 L80 D81 I82 R83 Q87 P88 L89 A90 L91 V92 S93 G94 A95 R96 T97 Q98 F99 T100 G101 D102 T103 A104 S105 L106 L107 V108 E109 N110 G111 R112 G113 N114 T115 L116 W117 P118 Q119 V120 V121 S122 V123 L124 Q125 A126 K127 N128 Y129 T130 I131 T132 Q133 R134 D135 D136

A137 G138 Q139 T140 L141 T142 T143 D144 W145 V146 Q147 W148 N149 R150 L151 D152 E153 D154 E155 Q156 Y157 R158 G159 R160 Y161 Q162 I163 S164 V165 K166 P167 Q168 G169 Y170 Q171 Q172 A173 V174 T175 V176 K177 L178 L179 N180 L181 E182 Q183 A184 G185 K186 P187 V188 A189 D190 A191 A192 S193 M194 Q195 R196

Y197 S198 T199 E200 M201 M202 N203 V204 I205 S206 A207 G208 L209 ASP LYS SER ALA THR ASP ALA ALA ASN ALA GLN ASN ARG ALA SER THR MET ASP VAL GLN SER ALA ASP ASP THR GLY ASP TYR LEU GLN VAL GLY ASP PHE ASN VAL TRP GLN LEU PRO

ALA ALA LEU GLU LYS VAL GLY MET LYS VAL THR ASP SER SER THR ARG GLN SER GLN GLY ASN MET ALA VAL THR TYR LYS PRO LEU SER ASP SER ASP TRP GLU GLU LEU GLY LEU ALA SER PRO GLY LEU ALA SER GLY ASP TYR LEU GLN LEU GLY VAL ARG GLY ASP LEU ASP ASN SER SER LEU

GLN PHE ILE ASP PRO LYS GLY HIS THR LEU THR GLN GLN SER GLN ASN ASP ALA LEU VAL ALA VAL PHE GLN ALA ALA PHE SER LYS

• Molecule 4: Outer membrane protein assembly factor BamD

Chain D:

5%
64%   23%   13%

MET THR ARG MET LYS TYR LEU VAL ALA ALA ALA THR LEU SER LEU PHE LEU ALA GLY CYS SER SER GLY LYS GLU GLU VAL PRO ASP ASN P31 P32 N33 E34 T38 A39 Q40 Q41 K42 D45 G46 A51 I52 T53 Q54 L55 E56 D59 N60 R61 Y62 Y67 S68 Q69 Q70

V71 Y79 A83 D84 A88 Q89 A90 A91 I92 D93 I96 N99 H102 P103 N104 Y107 Y110 M111 R112 G113 L114 A118 S122 A140 D146 G153 Y159 T160 T161 D162 R166 L167 V168 F169 L170 K171 A175 E178 A190 R197 V198

M201 D207 A210 D213 A214 L215 P216 L217 M218 K233 V234 A235 K236 I237 S243 ASN THR

• Molecule 5: Outer membrane protein assembly factor BamE

Chain E:

• Molecule 6: Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA,Outer membrane protein assembly factor BamA

Chain F:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	223353	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 $(e^-/Å^2)$	70	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	58717	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.482	Depositor
Minimum map value	-1.515	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	309.4, 309.4, 309.4	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84999996, 0.84999996, 0.84999996	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	0.26	0/5548	0.43	0/7462
2	B	0.24	0/2564	0.46	0/3495
3	C	0.29	0/929	0.54	0/1213
4	D	0.26	0/1761	0.44	0/2390
5	E	0.24	0/659	0.45	0/899
6	F	0.25	0/2543	0.47	0/3457
All	All	0.26	0/14004	0.45	0/18916

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
4	D	0	1
6	F	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	644	LYS	Peptide
1	A	645	GLU	Peptide
2	B	221	MET	Peptide
4	D	83	ALA	Peptide
6	F	466	GLN	Peptide

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	5429	0	4735	62	0
2	B	2522	0	2459	47	0
3	C	919	0	570	56	0
4	D	1722	0	1668	67	0
5	E	645	0	625	11	0
6	F	2468	0	2255	38	0
All	All	13705	0	12312	239	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 9.

The worst 5 of 239 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:PRO:HG3	4:D:237:ILE:HB	1.39	1.02
3:C:56:MET:SD	4:D:233:LYS:HB3	2.00	1.02
1:A:246:SER:HG	2:B:195:ARG:N	1.59	1.00
3:C:56:MET:HE1	4:D:236:LYS:HB2	1.52	0.92
4:D:45:ASP:OD1	4:D:46:GLY:N	2.05	0.89

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	752/810 (93%)	730 (97%)	22 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	330/392 (84%)	317 (96%)	13 (4%)	0	100	100
3	C	179/344 (52%)	166 (93%)	12 (7%)	1 (1%)	25	63
4	D	211/245 (86%)	202 (96%)	9 (4%)	0	100	100
5	E	81/123 (66%)	78 (96%)	3 (4%)	0	100	100
6	F	303/578 (52%)	295 (97%)	8 (3%)	0	100	100
All	All	1856/2492 (74%)	1788 (96%)	67 (4%)	1 (0%)	54	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	64	ASP

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	519/688 (75%)	519 (100%)	0	100	100
2	B	264/321 (82%)	263 (100%)	1 (0%)	91	94
3	C	44/276 (16%)	41 (93%)	3 (7%)	16	44
4	D	178/204 (87%)	178 (100%)	0	100	100
5	E	72/103 (70%)	72 (100%)	0	100	100
6	F	263/482 (55%)	261 (99%)	2 (1%)	81	88
All	All	1340/2074 (65%)	1334 (100%)	6 (0%)	91	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	87	GLN
6	F	639	ASP
6	F	767	ARG
3	C	50	LEU
2	B	189	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	72	GLN
6	F	459	ASN
5	E	33	ASN
6	F	523	ASN
1	A	731	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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-20969. 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 |
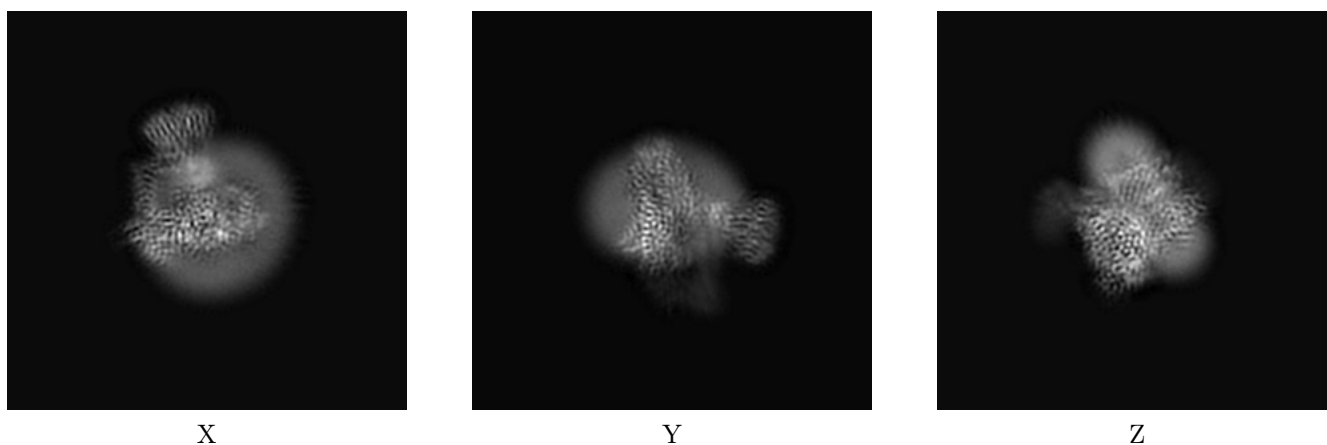
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

| X Index: 182 | Y Index: 182 | Z Index: 182 |
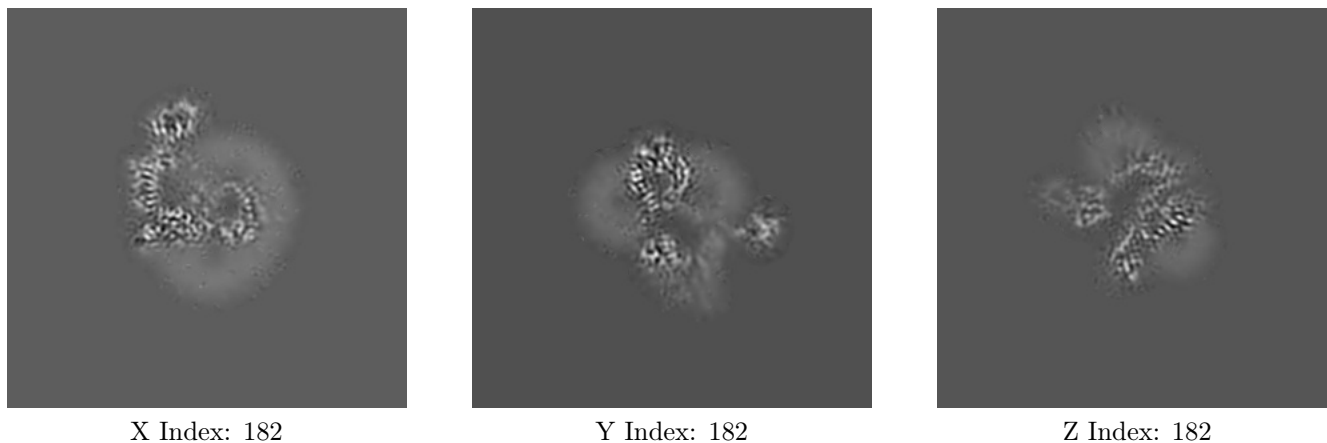
The images above show central slices of the map in three orthogonal directions.

6.3　Largest variance slices ⓘ
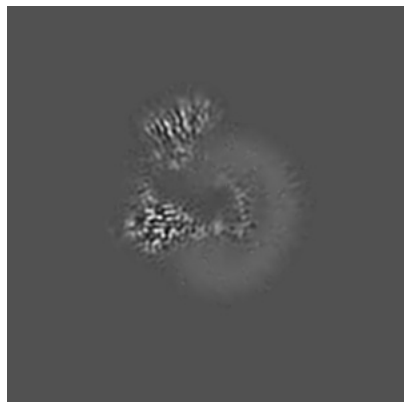
6.3.1　Primary map
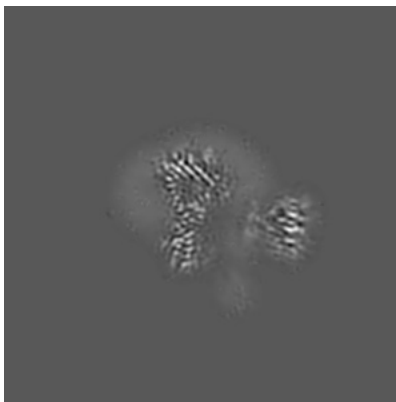
| X Index: 168 | Y Index: 164 | Z Index: 157 |
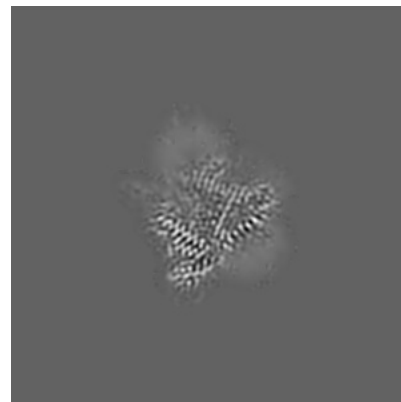
The images above show the largest variance slices of the map in three orthogonal directions.

6.4　Orthogonal surface views ⓘ

6.4.1　Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.35. 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 ⓘ

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

7.1 Map-value distribution ⓘ
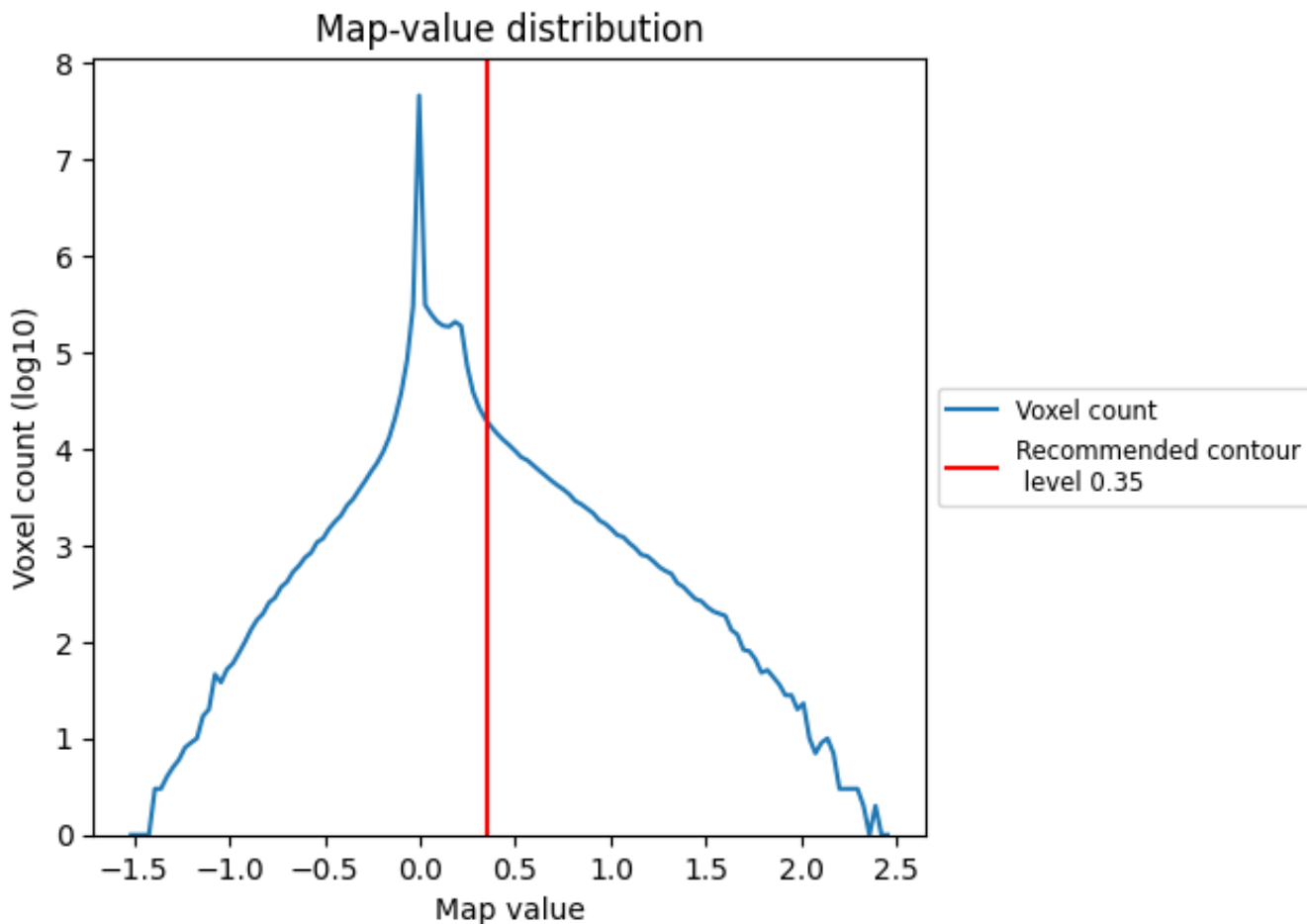
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
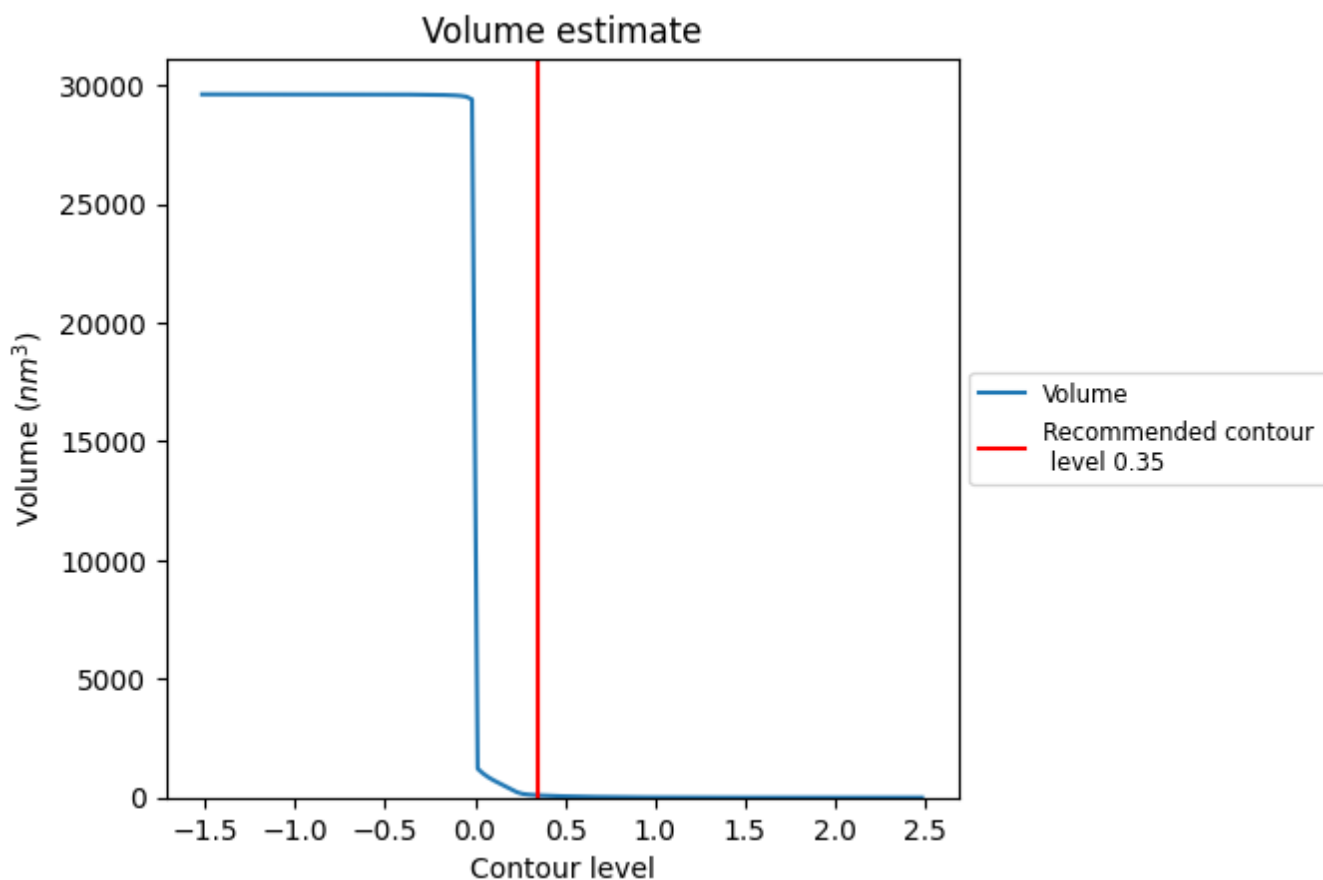
The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 kDa.

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   ⓘ
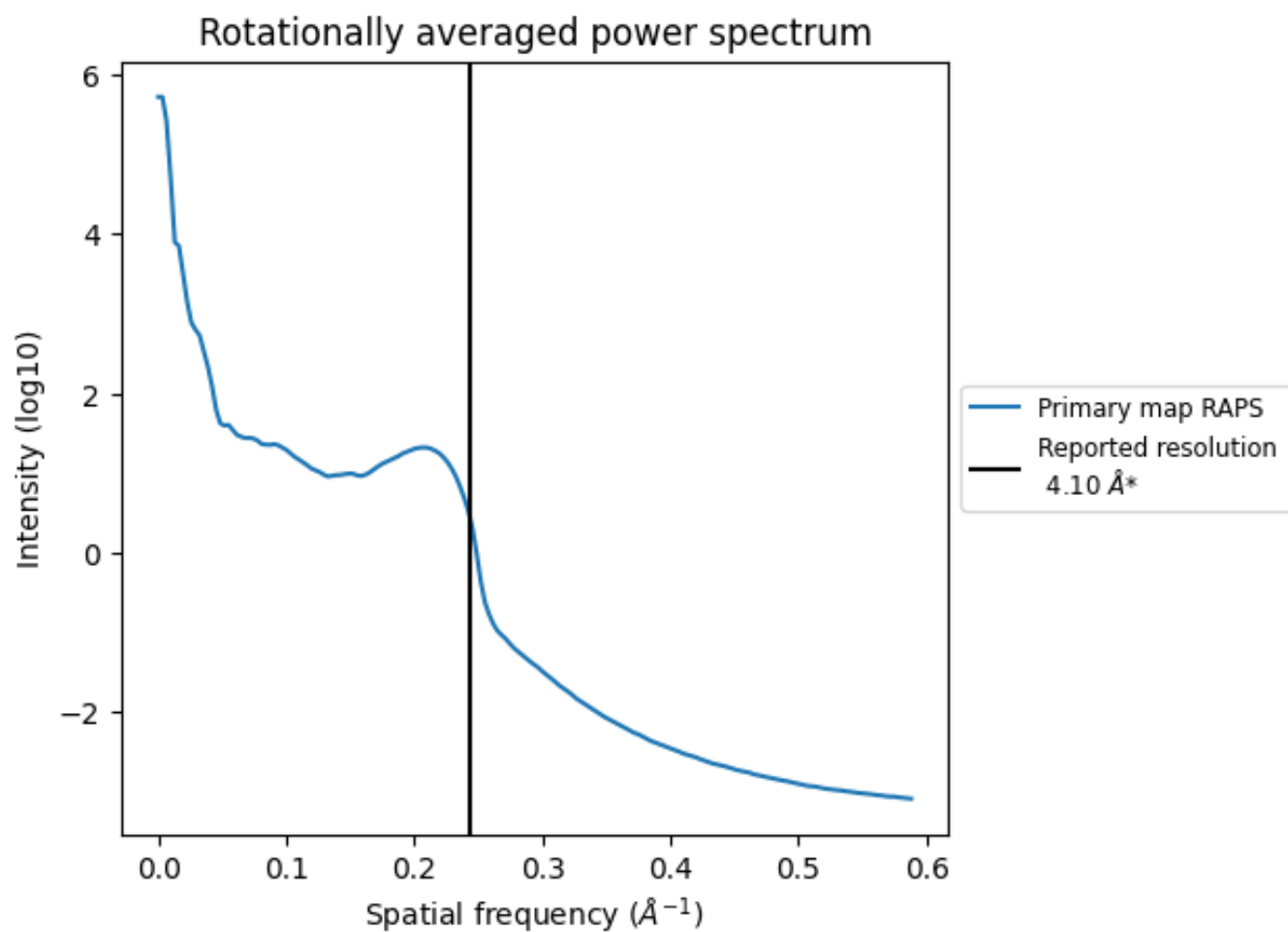
*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9　Map-model fit　ⓘ

This section contains information regarding the fit between EMDB map EMD-20969 and PDB model 6V05. Per-residue inclusion information can be found in section 3 on page 6.

9.1　Map-model overlay　ⓘ

| X | Y | Z |
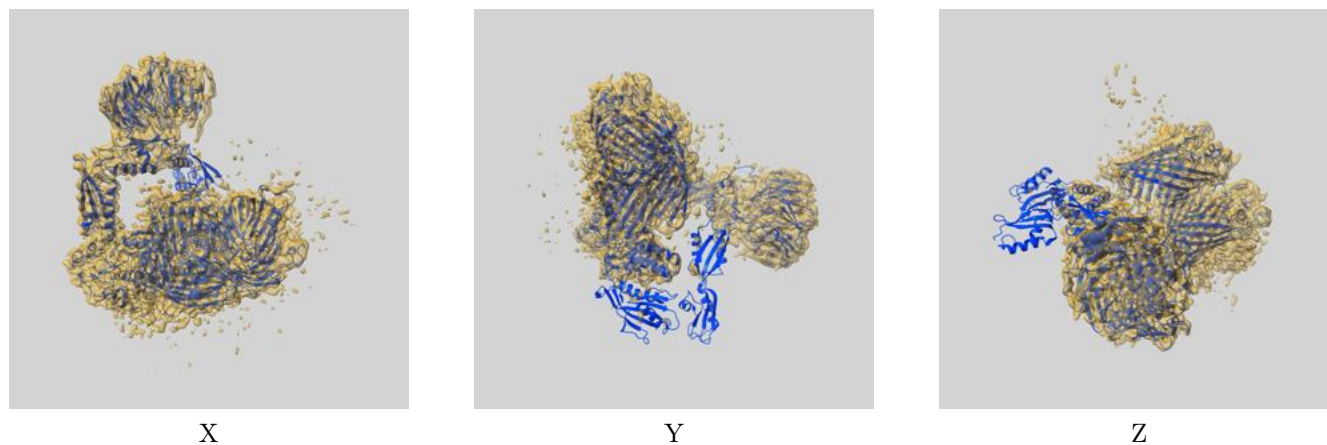
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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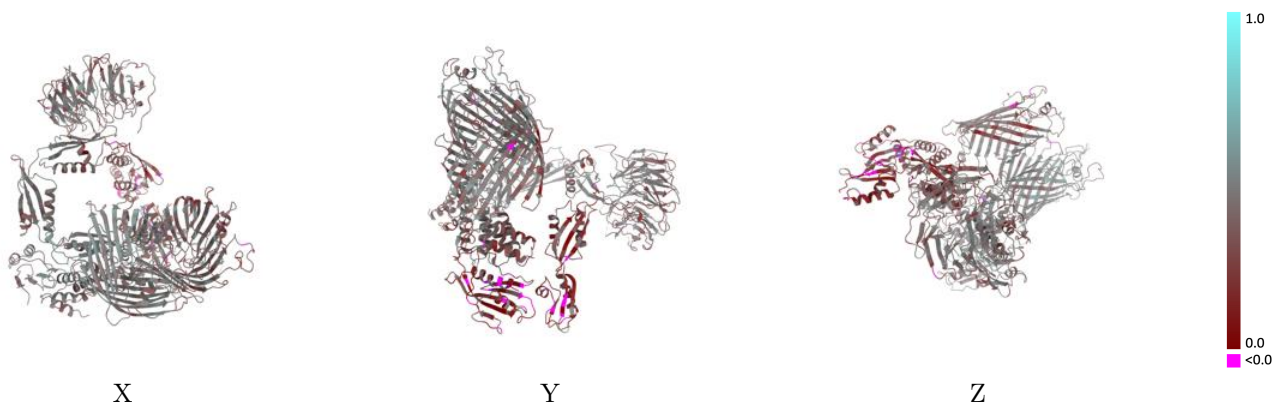
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)

X Y Z
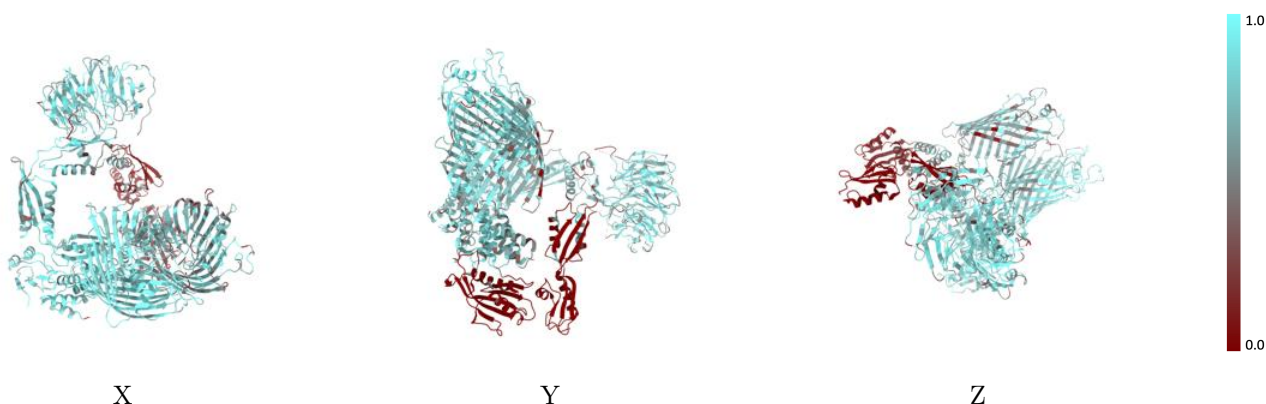
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4   Atom inclusion ⓘ
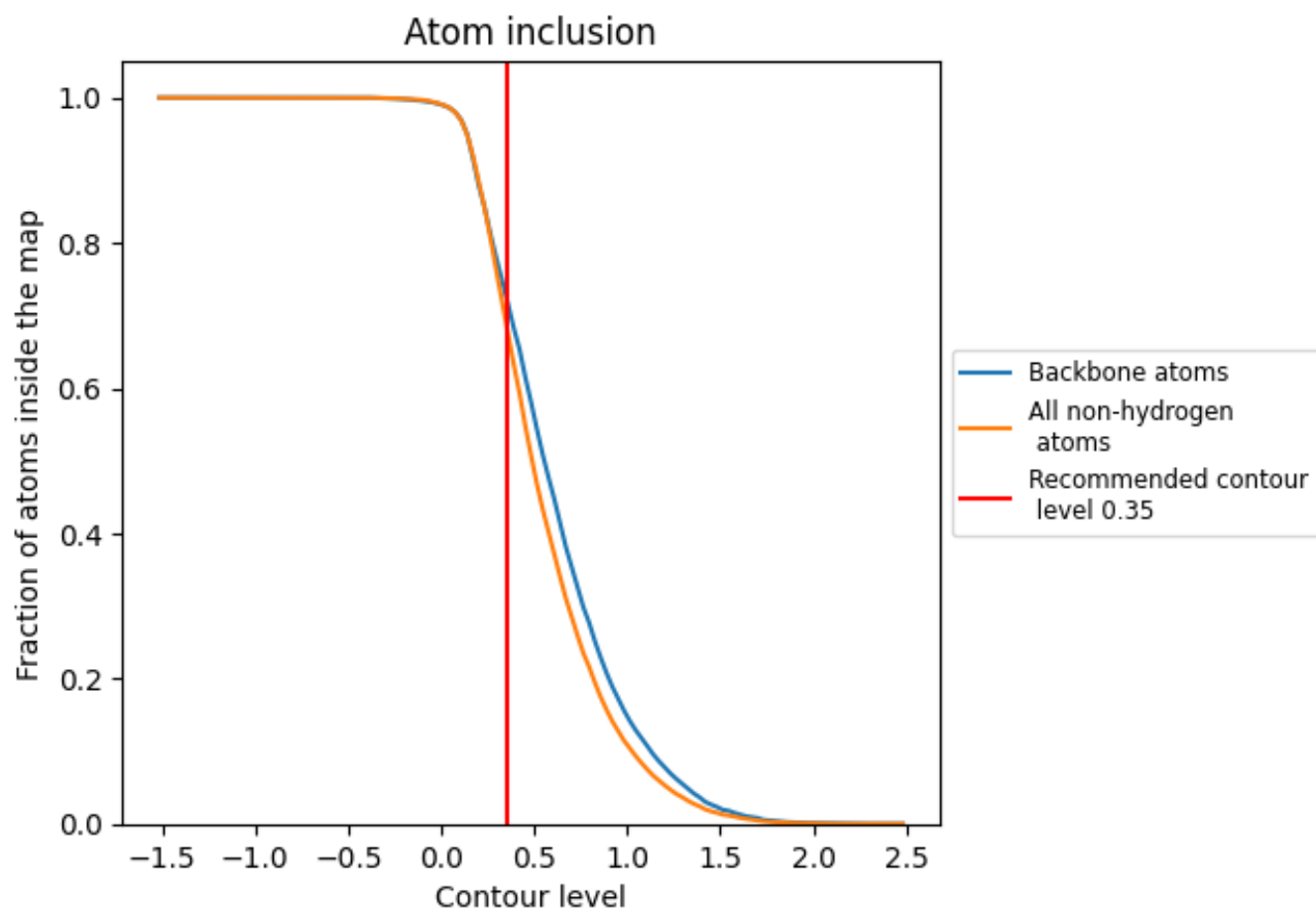
At the recommended contour level, 73% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6887	0.4010
A	0.7014	0.4290
B	0.7427	0.4020
C	0.3154	0.2270
D	0.7739	0.4010
E	0.8362	0.4620
F	0.6480	0.3870

1.0

0.0
<0.0